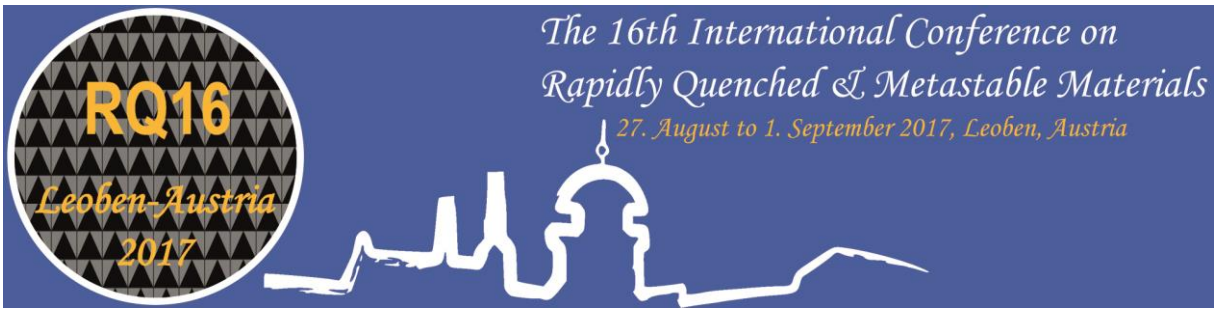
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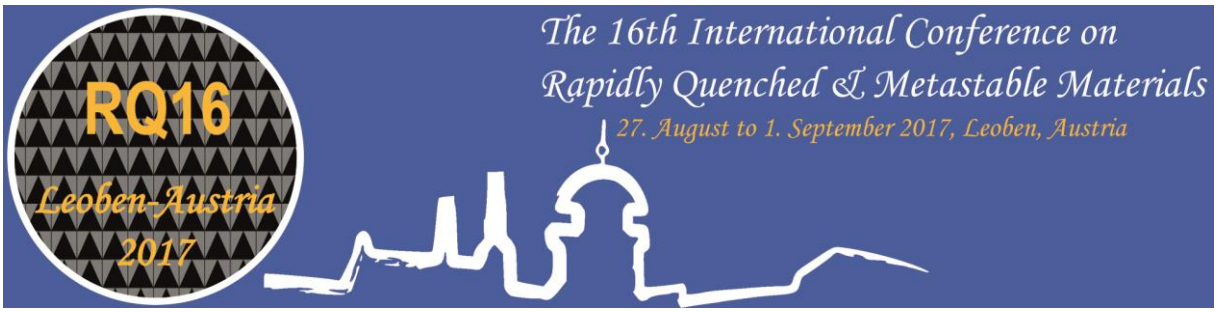
Abstract



Monday, 28th August

Multicomponent and high entropy alloys

Brian Cantor

University of Bradford

Conventional strategy for developing metallurgical alloys is to select the main component based on a primary property requirement, and to use alloying additions to confer secondary properties. This strategy has led to the development of many successful alloys based on a single main component with a mix of different alloying additions to provide a balance of required in-service properties. Typical examples include high temperature Ni superalloys, wrought Al alloys and corrosion resistant stainless steels. However, conventional alloy development strategy leads to an enormous amount of knowledge about alloys based on one component, but little or no knowledge about alloys containing several main components in approximately equal proportions. Theories for the occurrence, structure and properties of crystalline phases are similarly restricted to alloys based on one or two main components. Information and understanding is highly developed about alloys close to the corners and edges of a multicomponent phase diagram, with much less known about alloys in the centre of the diagram.

This talk describes a range of other multicomponent alloying strategies and gives a number of examples of high-entropy and other multicomponent alloys.

Presentation Method (Invited/Regular Oral/Poster): Plenary

An inside look at the deformation of a simple glass using colloids

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Tracking of micron-size particles with confocal microscopy makes it possible to study the dynamics of complex, dense colloidal systems on the particle level. Monodisperse colloidal glasses, formed e.g. by sedimentation, are simple, instructive models for glasses composed of atoms that interact by central potentials, like metallic glasses. They exhibit the classic dense-random-packed structure of hard spheres, as well as other glass properties such as crystallization and structural relaxation.

They can be deformed elastically and plastically, and some corresponding reversible and irreversible rearrangements on the particle scale can be identified. The local strains can be determined by fitting the changes in the nearest-neighbor vectors for each particle to a stress tensor. This makes it possible to identify the Eshelby-like strain fields associated with the shear-transformation zones that govern plastic deformation. At the same time, an analysis of the fluctuations in the strain energy density makes it possible to determine a local stiffness, which in turn is closely related to density. This technique makes it possible to observe the very small changes in density associated with shear dilatation and subsequent structural relaxation.

Most recently, we have developed a technique to measure the shear stress as well as the shear strain in these experiments. This is done by attaching the colloidal glass to a gel substrate with a calibrated stiffness that is slightly greater than that of the glass. By tracking the elastic deformation of the gel through embedded particles, it is possible to know the macroscopic shear stress, and hence to obtain a full stress-strain curve for these glasses (shear modulus, yield stress), as well as a more precise distinction between reversible and irreversible local rearrangements.

Presentation Method (Invited/Regular Oral/Poster): Plenary

Primary crystallization of Al nanocrystals in Al based metallic glasses: thermodynamic and kinetic analyses

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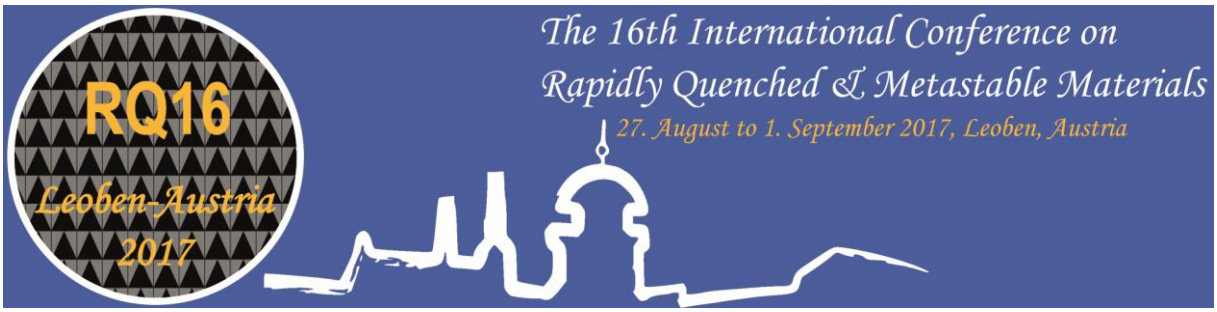
The high density of Al_{fcc} nanocrystals (>10^{21} m^{-3}) that develop during the primary crystallization in Al-rich metallic glasses indicates a high nucleation rate (~10^{18} $m^{-3}s^{-1}$) and relatively slow growth. The typical amorphous alloy compositions are hypereutectic and the thermodynamic driving free energy for crystallization favors the intermetallic phase nucleation by a significant margin. Thus, the selection of Al as the primary crystallization phase must be promoted by a nucleation catalyst to provide a significant kinetic advantage. Moreover, the character of the devitrification reaction has been demonstrated to be dependent upon the synthesis method employed to prepare the amorphous alloys. For an $Al_{92}Sm_8$ alloy, the amorphous phase induced by cold rolling exhibits a higher crystallization onset temperature than the one made by melt spinning and the fluctuation electron microscopy (FEM) analysis shows the amorphous phases made from melt spinning and cold rolling have different nanoscale MRO (medium range order). Several proposals have been advanced to account for the primary crystallization behavior, but none have been developed to completely describe the reaction kinetics or the underlying mechanism. The structural analysis by the fluctuation electron microscopy (FEM) has demonstrated the presence of the Al-like medium range order (MRO) regions as a spatial heterogeneity in the as-spun $Al_{88}Y_7Fe_5$ metallic glass that is representative for the class of Al-base amorphous alloys which develop Al nanocrystals during primary crystallization. From the structural characterization, a MRO seeded nucleation configuration is established whereby the Al nanocrystals are catalyzed by the MRO core to decrease the nucleation barrier. To complement the structural characterization a full set of nucleation product density measurements have been established along with a new method to determine directly the nucleation delay time. The MRO seeded nucleation model and the kinetic data from the delay time (τ) measurement, provide for a full accounting of the evolution of the Al nanocrystal density (N_v) during the primary crystallization under isothermal annealing treatments. Also, the theoretical values of steady state nucleation rates (J_{ss}) and the enthalpy ΔH at the onset crystallization temperature (T_x) predicted by the nucleation model agree with the experimental results. Moreover, the model satisfies all the constraints on the structural, thermodynamic and the kinetic parameters such as the critical nucleus size, the interface energy, the volume energy driving force and the activation energy for diffusion, that are essential for a fully self-consistent nucleation kinetics analysis. In general, the MRO catalyzed nucleation model reflects a generic scheme which may be applied more broadly to nucleation reactions in both amorphous and crystalline materials that are characterized by the presence of spatial heterogeneities that can act as a nucleation catalyst.

KEYWORDS: Metallic Glasses; Nucleation kinetics; Nanostructured materials; Crystallization

Presentation Method (Invited/Regular Oral/Poster): Plenary



A1-Metallic glass 1: Deformation

Metal-like ductile fracture of metallic glasses at room temperature

Y. Li

Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China

Plastic deformation of large-sized metallic glasses (MGs) is highly localized into shear band under uniaxial loading. Associated with this, the deformation behaviour of metallic glasses is characterized with 2% elastic limit and very little plastic strain. They usually fail in a catastrophical manner at room temperature. Much of the previous study of plastic deformation in BMGs was focused on the shear bands and shear banding. However, the deformation behaviour of metallic glasses would be quite different at room temperature if there are no shear bands present. In our talk, we will show the capability of plastic deformation and ductile fracture in BMGs if there is no shear banding involved. The mechanism for such a difference will also be discussed.

Key words: Bulk Metallic Glasses; Shear Bands, Plastic Deformation

Presentation Method (Invited/Regular Oral/Poster): Keynote

Rethinking atomic packing and cluster formation in metallic liquids and glasses

Mo Li[1,2]

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In traditional view, atomic packing is random in glasses made of metallic elements with non-directional interactions as the glass-forming liquid needs to be excited to remain in liquid state before being cooled sufficiently fast to a glass. Locally ordered packing however is possible if certain conditions are favorable, such as a strong bonding between elements, or low configuration energy of a cluster of atoms as suggested by Frank. In multicomponent alloy systems made of different metallic elements, we show that Frank's criterion alone does not necessarily lead to certain specific local ordered packing or cluster formation such as icosahedral packing. In this context, we revisit the issue of atomic packing and cluster formation, and show that an alloy system with fairly random liquid configuration could be sufficient to produce a variety of noticeable locally ordered packing with low energy, albeit largely statistical in nature. Therefore, we emphasize the importance of the system parameters such as the atomic size, alloy concentration, and interaction potential in their collective contribution to local atomic packing (Ref. 1).

KEYWORDS: Bulk metallic glass, multicomponent alloys, glass formability, clusters

1. Li, Qikai, Li Mo, *Rethinking atomic packing and cluster formation in metallic liquids and glasses*. Chinese Sci Bull, December (2011) Vol.56 No.36, doi: 10.1007/s11434-011-4833-0

Presentation Method (Invited/Regular Oral/Poster): Invited

Low-cost Fe-based bulk metallic glasses with good glass forming ability

Yaofeng Guo[1], Akihisa Inoue[2,3,4,5], André Costa e Silva[6], Claudio Shyint Kiminami[1], Claudemiro Bolfarini[1], Walter José Botta[1], Alberto Moreira Jorge Jr.[1]

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The development of Fe-based bulk metallic glasses (BMGs) has attracted much attention due to its low cost, good soft magnetic properties with high saturation magnetization, high permeability and low coercivity. Due to their excellent magnetic properties, commercialized Fe-based BMGs have found their application of magnetic devices, such as transformers and high efficiency sensors. However, researchers continue searching Fe-based glassy alloys with good glass forming ability and even better magnetic properties. In the present work, Fe(-Mo)-Cr-Nb-B BMGs with good glass forming ability are fabricated by melting spinning with low-cost industrial purity pre-alloys. The glassy ribbons are characterized by conventional X-ray diffraction (XRD) and scanning electron microscopy (SEM). The thermal properties are studied by differential scanning calorimetry (DSC). Moreover, the crystallization behavior of the Fe(-Mo)-Cr-Nb-B BMGs and the formation mechanism of the nanocrystals during annealing are investigated by transmission electron microscopy (TEM).

KEYWORDS: Fe-based bulk metallic glasses, GFA, Fe-Cr-Mo-Nb-B alloys

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Delocalized plastic flow in proton-irradiated monolithic metallic glasses

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[2]*Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea*

Creating new materials with novel properties through structural modification is the Holy Grail of materials science. The range of targetable structures for amplification of mechanical properties in metallic glasses would include types of atomic short range orders at the smallest scale through compositions or morphologies of phases in composites. Even though the usefulness of the latter approach has been successfully demonstrated in the past decades, the feasibility of the former has been incompletely proved with only marginal property improvements reported within experimentally-accessible atomic-level structural changes. Here, we report the significant enhancement of deformability in Zr-based monolithic metallic glass only through the atomic disordering by proton irradiation without altering any other structural traits. Metallic glass nanopillars that originally failed catastrophically without any notable plasticity become capable of attaining more than 30% uniaxial plastic strain accommodated by homogeneous deformation when irradiated to ~1 displacement per atom (DPA). We discuss the atomistic origin of this improved plasticity in terms of density and spatial distributions of icosahedral short range order influenced by irradiation.

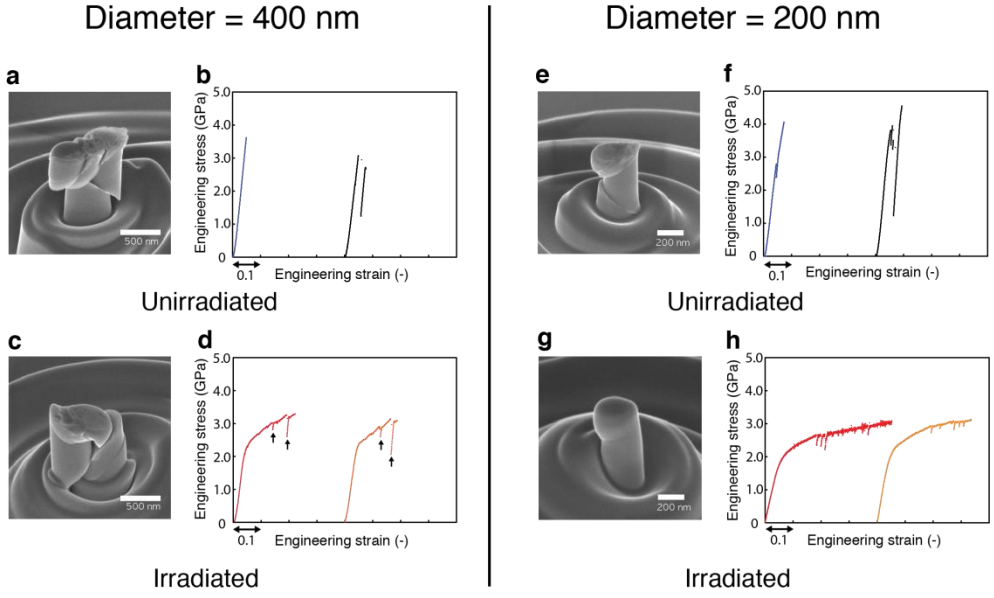

Fig1. Nano-compression results for proton-irradiated and unirradiated metallic glass specimens. (a,c) Representative SEM images for unirradiated (a) and proton-irradiaated (c) metallic glass specimens with 400 nm diameter. (b,d) Engineering stress and strain curves of nano-compression experiments on 400 nm specimens. (e,g) Representative SEM images for unirradiated (e) and proton-irradiaated (g) metallic glass specimens with 200 nm diameter. (f,h) Engineering stress and strain curves of nano-compression experiments on 200 nm specimens.

KEYWORDS: Plasticity, Deformation Modes, Proton Irradiation, Small-scale Mechanics.

1. J. Heo, S. Kim, S. Ryu and D. Jang, *Scientific Reports* **6**, 23224 (2016).

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Strain dependence of diffusion in Zr-based bulk amorphous alloy

Min-Ha Lee

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We evaluated the effect of strain on the diffusion process of metallic glass related to the strain mode in both as-cast and plastically deformed Zr-based bulk amorphous alloy. Experimental investigations of the diffusion process and the elemental distributions in the metallic glass were performed by secondary ion mass spectrometry (SIMS) after annealing at 523 K following 30% plastic deformation by multiple cold rolling. Mathematical modeling analysis clearly shows that an inhomogeneous sequence of the diffusion process by effective strain. The compressive strain near the surface of the deformed amorphous alloy retards the diffusion process compared to as-cast amorphous alloy. The combined experimental and mathematical analyses results reveal that the diffusion process of glass-forming alloys can be changed by strain variation and can be adjusted by controlling the effective strain during deformation.

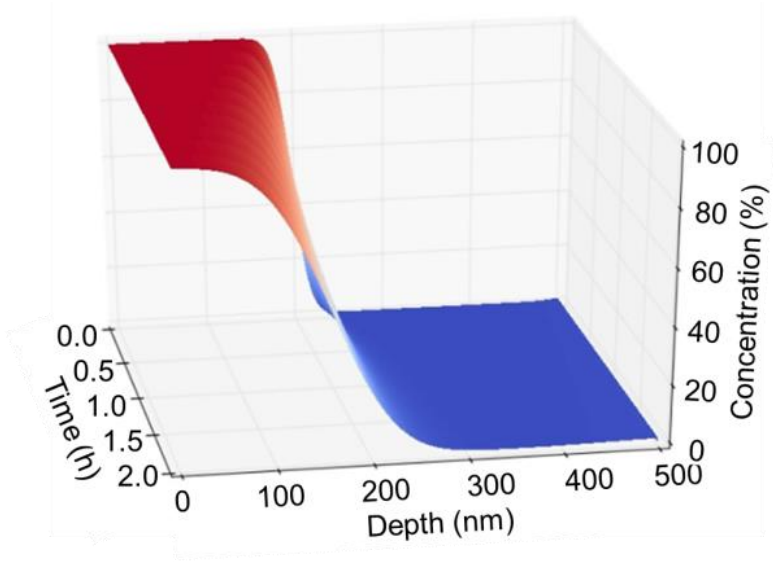
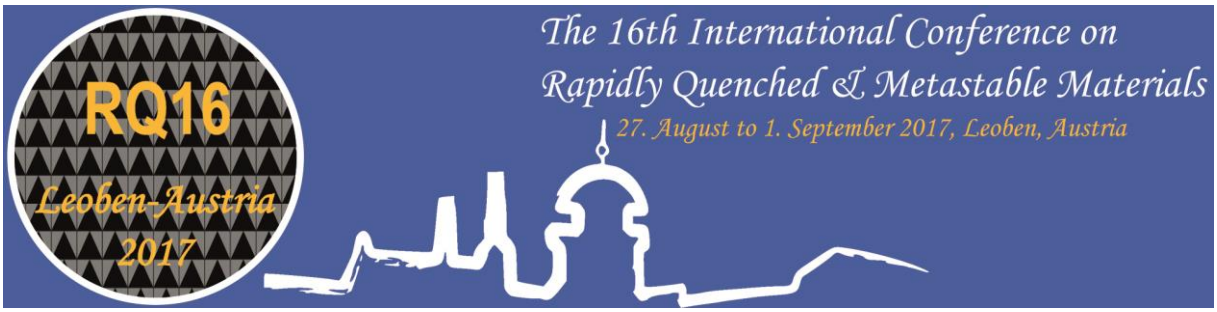


Fig1. Effect of strain on the variation of diffusion profile of Fe in cold-rolled Zr-based bulk metallic glass.

KEYWORDS: Bulk metallic glasses, Deformation

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



B1-Additive manufacturing & powder metallurgy

Rapid solidification of Al-Si alloys: a comparison with additive manufacturing (AM)

Silvia Marola[1], Diego Manfredi[2], Gianluca Fiore[1], Marco Gabriele Poletti[1], Mariangela Lombardi[3], Paolo Fino[3], Livio Battezzati[1],

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[2]*Istituto Italiano di Tecnologia, Center for Sustainable Future Technologies, Torino, Italy*
[3]*Dipartimento di Scienze Applicate e Tecnologie, Politecnico di Torino, Torino, Italy*

In Selective Laser Melting (SLM) layers of a metallic atomized powder are spread on a preheated building platform and melted locally by a high power laser. According to a CAD model, once the first layer is complete, the building platform drops one layer down, the material is recoated with new powder and the process is repeated until an entire build is additively manufactured. During this process the molten pool is quenched by the pre-solidified layers. Rapid solidification occurs whose microstructural features have consequences on the mechanical properties of the product [1].

In order to understand in detail the solidification mechanism in SLM, Al-Si eutectic samples were produced using other rapid solidification techniques, Copper Mould Casting (CMC) and Melt Spinning (MS), spanning a large range of cooling rates. The samples obtained through CMC, MS, and SLM were characterized using microscopy, XRD and DSC. From the results obtained in these experiments and from the literature available on rapidly solidified Al-Si alloys [2], a microstructural correlation between these three techniques is established. From data on supersaturation, calorimetric responses, and size of the microstructural features a mechanism for solidification is proposed and validated by dendrite growth modelling which enables interpreting the fine microstructures occurring in AM.

KEYWORDS: Additive Manufacturing, nanostructured materials.

W. Li, S. Li, J. Liu, A. Zhang, Y. Zhou, Q. Wei, C. Yan, Y. Shi, *Mater. Sci. Eng. A* 663 (2016) 116–125.
J. Wu, X.Q. Wang, W. Wang, M.M. Attallah, M.H. Loretto, *Acta Materialia*, 117 (2016) 311–320.

Presentation Method (Invited/Regular Oral/Poster): Keynote

Structure-property correlations in 3D printed metals

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[2]*Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, A-8700 Leoben, Austria, Email: kgprashanth@gmail.com*

For 3D printing of metallic components, selective laser melting (SLM) of powders is the most commonly used method, which offers a number of technological advantages such as near-net shape forming with zero material loss. Consequently, there is a considerable and recent interest in this new way of manufacturing components for advanced engineering applications. From the scientific perspective, this process offers a number of exciting opportunities, some of which I would like to discuss in this talk. The SLM process not only imparts a substantially finer microstructure but also distinct mesoscale features to them. A complex interplay between these micro- and meso-structural features can lead to property combinations that were hitherto thought not possible. For example, we demonstrated that in Al-Si alloy coupons manufactured using SLM, it is possible to enhance strength and toughness simultaneously. Some possible additional features that are specific to the SLM process are the presence of considerable residual stresses and microporosity. In this presentation, we will examine as to how all these features will affect the mechanical properties through a comprehensive microstructural and mechanical property characterization of several different alloy components made through SLM, with particular emphasis on understanding their quasi-static tensile, fracture, fatigue crack growth, and unnotched fatigue properties. We will demonstrate that while the SLM process offers new avenues for material design that can exploit the micro- and meso-structures generated by the process, their fatigue and corrosion resistances are a big concern due to the porosity.

KEYWORDS: Additive manufacturing, Mechanical Properties

Presentation Method (Invited/Regular Oral/Poster): Invited

Mechanically milled and spark plasma sintered pure copper

Masahiro Kubota

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Pure copper powder was mechanically milled (MMed) using a vibration type of ball milling, and the MMed powder was consolidated into bulk materials by the spark plasma sintering (SPS) process. Changes in hardness and solid-state reactions of the MMed powder and bulk materials have been examined by Vickers hardness measurements and X-ray diffraction (XRD), respectively.

The value of Vickers microhardness for the pure copper powders increased from 40 to 111 HV after the MM time from 0 to 8 h, respectively, and exhibited a broad hardness plateau at maximum hardness after MM time up to 32 h. The solid-state reaction between pure copper powder and stearic acid added as a process control agent (PCA) during the MM process was observed to form Cu_2O.

The Vickers hardness of the bulk materials fabricated from 0 h and 32 h MMed pure copper powders exhibited 40 HV and 230 HV, respectively. The solid-state reaction between pure copper powder and stearic acid added as a PCA during SPS process after MM process was observed to form Cu_2O. The MMed powders produced by 16 h and 32 h of MM process contained a little amount of Fe as a contamination, and the bulk materials fabricated from the powders containing Fe were generated to form Fe_3O_4. The MM-SPS process can be appreciable to produce the bulk copper materials exhibiting high hardness.

KEYWORDS : mechanical milling, pure copper, solid-state reaction, hardness, spark plasma sintering

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Effect of scan strategy and annealing on microstructure and properties of 316L stainless steel synthesized by selective laser melting

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Selective laser melting (SLM) is progressively becoming one of the prominent additive manufacturing routes for the synthesis of high-performance materials due to the ability to produce three-dimensional components of virtually any geometry and intricacy through an additive layer-by-layer strategy directly from powders/wires. Furthermore, due to the high cooling rate of the process, SLM offers the possibility to produce metastable phases and microstructures that are not accessible by conventional solidification techniques. Additional microstructural modifications can be achieved by properly varying the scan strategy and by annealing the SLM part at different temperatures. In this work, 316L stainless steel specimens have been produced by SLM using different scan strategies. Structural characterization followed by microstructural characterization as well as mechanical and wear properties have been investigated in detail and compared to the corresponding samples produced by conventional casting. Finally, the effect of annealing at different temperatures on the properties has been systematically studied by analyzing the microstructural changes as a function of annealing temperature.

Keywords: Additive manufacturing; metastable material; laser melting; AISI316L

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Heat-treatable Al alloys produced by selective laser melting

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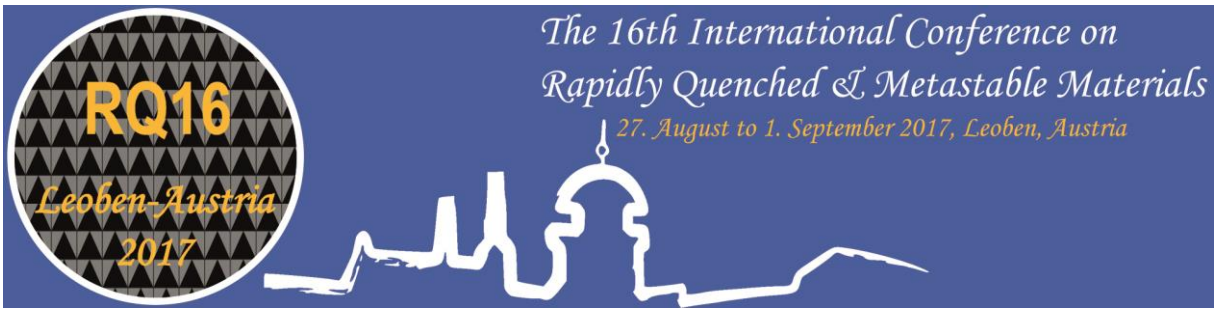
Selective laser melting (SLM) is one of the emerging layer-wise additive manufacturing techniques that allows generating complex 3D parts by selectively melting of successive layers through the use of a computer-controlled laser beam. Because of the high degree of freedom in the shape and geometry of the SLM parts, along with the non-equilibrium phases and fine microstructures resulting from rapid solidification during SLM processing, a progressively expanding spectrum of structural materials has been processed by SLM. The present work compares the microstructure and mechanical properties of heat-treatable Al alloys synthesized by SLM before and after conventional heat treatment. The results reveal that after heat treatment the yield strength under tensile loading is significantly improved due to the formation of secondary phase(s).

Keywords: Selective laser melting, rapid quenching, microstructure, mechanical properties

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



C1-Nanostructured materials 1

Towards thermally stable nanocrystalline alloys with exceptional strength: Cu-Cr as a case study

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Nanocrystalline metals reveal exceptional strength at room temperature. Unfortunately, they are prone to coarsening at elevated temperatures which leads to a rapid loss of strength. This drawback can be overcome if nanocrystalline alloys are used where grain growth is suppressed either by precipitates or grain boundary segregation. While the formation of precipitates at grain boundaries leads to a pinning mechanism, segregation can reduce the grain boundary energy at such an extent that a metastable condition is reached. In that case a thermodynamic stabilization of the nanocrystalline microstructure is accomplished.

Fabrication of nanocrystalline samples in bulk form requires either rapid quenching from the melt to get numerous nuclei during solidification, severe plastic deformation to reduce grain size or alternative techniques such as inert gas condensation. All these techniques are not well suited for rapid screening of different alloy compositions. In contrast, thin film deposition methods (e.g. evaporation, sputter deposition) are very versatile and lead to a nanocrystalline film microstructure due to rapid condensation of the supersaturated vapor phase on the substrate.

In this presentation the influence of chemical composition on the grain size evolution, thermal stability and mechanical properties is analyzed for the nearly immiscible system Cu-Cr. X-ray diffraction and transmission electron microscopy studies prove that a nanocrystalline body centred cubic (bcc) microstructure can be accomplished for Cu contents upto ~70at% - despite a Cu solubility limit of less than 1 at% in bcc Cr according to the equilibrium phase diagram. In contrast, the face centred cubic (fcc) Cu-Cr films can host only 4 at% Cr, which however also substantially exceeds the equilibrium solubility. Thermal annealing of fcc Cu96Cr4 (at.%) and bcc Cu67Cr33 (at.%) leads to completely different microstructures. The fcc system forms precipitates at the grain boundaries, while the bcc system spinodally decomposes inside the grains. In both cases grain growth is suppressed, however the Cu67Cr33 maintains a nanocrystalline structure up to ~ 0.5 of the absolute melting temperature of pure Cu. The kinetics of the decomposition processes of Cu96Cr4 and Cu67Cr33 are different as revealed by in-situ TEM experiments. This impacts both, the coarsening and the mechanical properties as discussed in the talk.

Presentation Method: Keynote

Abnormal Coarsening of a Nanoscale Microstructure Goes Fractal

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[2]*Institute of Micro and Nanomaterials, Ulm University, Ulm, Germany, Email: carl.krill@uni-ulm.de*

Despite the supposed rarity implicit in its name, abnormal grain growth appears to be a rather common mode of coarsening in nanocrystalline materials, regardless of composition or synthesis route. In inert-gas-condensed nanocrystalline $Pd_{90}Au_{10}$, thermally induced coarsening fulfills the criteria for abnormal grain growth, but with an unusual twist: the subpopulation of abnormally growing grains sends forth offshoots in many directions, first surrounding nearby matrix grains and then slowly consuming them, much like a tumor spreading into nearby tissue! The resulting growth fronts—*i.e.*, interfaces between abnormal and matrix grains—are quite tortuous in appearance, quite unlike the smooth morphologies characteristic of abnormal grains in conventional samples.

We have captured this phenomenon using channeling-contrast scanning electron microscopy (Fig. 1), electron backscatter diffraction (EBSD) and high-temperature x-ray diffraction. The direct imaging techniques reveal cross-sectional grain shapes that bear a striking resemblance to fractal objects—a rather unexpected finding, given the well-established curvature-driven mechanism for grain boundary migration, which would be expected to flatten out boundary fluctuations rather than accentuate them. By applying the box-counting method to micrographs of the abnormal grains, we find their perimeters to follow a simple scaling law over more than two orders of magnitude of box size, with a slope corresponding to a fractal dimension of about 1.2. Owing to these unusual findings, we suspect that a nonstandard mechanism is responsible for fractal grain boundary migration in nanocrystalline $Pd_{90}Au_{10}$—and potentially in other nanoscale systems, as well.

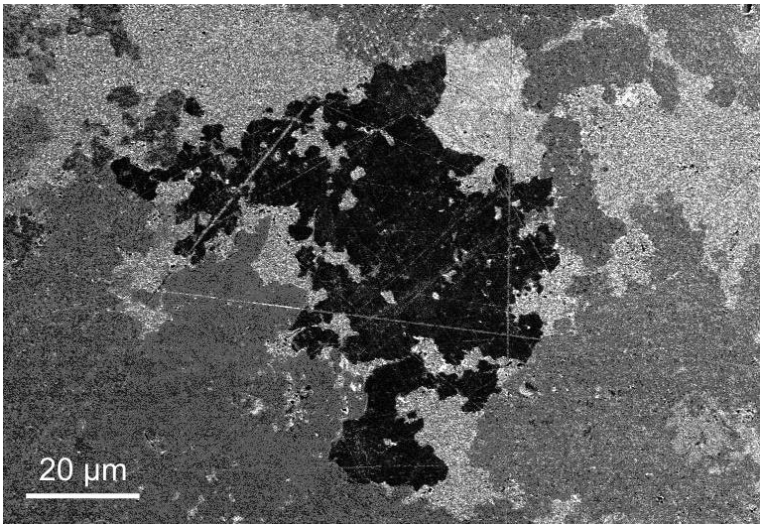

Fig. 1: Channeling-contrast SEM micrograph of fractal abnormal grain growth in nanocrystalline $Pd_{90}Au_{10}$, following a 5-min anneal at 270°C. The dark, fractal-shaped grain in the center is growing into a matrix of nanometer-sized grains (mottled white-gray). The darker-gray regions—traversed in places by polishing scratches—correspond to micrometer-sized grains having a crystal orientation different from that of the center grain.

KEYWORDS: abnormal grain growth; fractal microstructure; nanocrystalline material; inert gas condensation.

Presentation Method: Invited

Deformation mechanisms to ameliorate the mechanical properties of Co-Cr-Mo-(Cu) ultrafin eutectic alloys

Jeong Tae Kim[1], Jürgen Eckert[1, 2] Ki Buem Kim[3]
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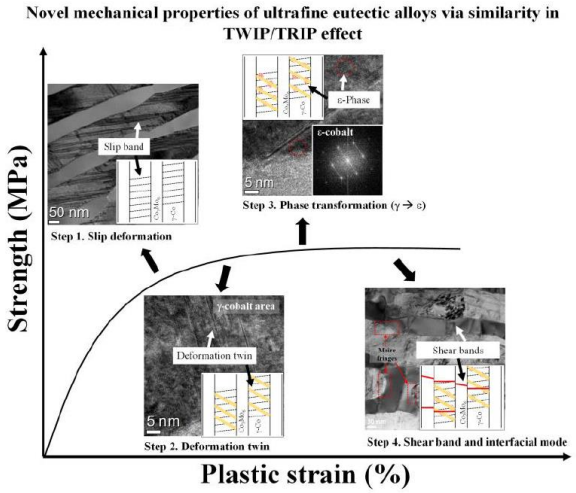
In the present study, the microstructural evolution and modulation of the mechanical properties have been investigated in Co-Cr-Mo (CCM) ternary eutectic alloy by addition of the small amount of copper content with 0, 0.5 and 1 at.%. The microstructures of the CCM and CCMCu alloys exhibit that the small addition of Cu does not bring the notable microstructural evolution and only formed Co dendrite phase slightly in eutectic colonies from the macro-scale analysis. However, the microstructural observation in the nano-scale analysis displays the distinct dissimilarity in the eutectic structure such as the broken lamellar structure and well-aligned lamellar structure. Moreover, these microstructural evolution leads to the improved plasticity from 1 % to 10 % without the typical tradeoff between the overall strength and compressive plasticity. Moreover, the investigation of the fractured samples indicated that the CCMCu alloy exhibits the higher plastic deformability and combinatorial mechanisms for higher plastic behaviors. Especially, the improved plasticity of CCMCu alloy can be originated from several deformation mechanisms; i) slip, ii) deformation twinning, iii) strain-induced transformation and iv) shear banding. These results reveal the mechanical properties of the Co-Cr-Mo system eutectic alloy can be ameliorated by the micro-alloying such as the Cu elements.



KEYWORDS: Metals and alloys, Ultrafine Eutectic alloys, Mechanical properties, Deformation mechanisms

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Delocalization of stress/strain partitioning between amorphous matrix and 2nd phase in a TRIP bulk metallic glass composite

Hyun Seok Oh[1], Wook ha Ryu[1], Jin Kyu Lee[2], Yeon Wook Kim[3],

Won Seok Ko[4], Cem Tasan[5], Dierk Raabe[6], Eun Soo Park[1]

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Several approaches have been proposed to improve the mechanical properties, such as work hardening and toughening of bulk metallic glasses (BMGs). Among proposed ones, introduction of dual phase - transformation induced plasticity (TRIP) effect by adding transformable 2nd phase in a BMG matrix has been shown as the successful method leading to work hardening and toughening even during tensile deformation. However, although TRIP effect has been well investigated in conventional materials, the TRIP mechanism of metastable 2nd phase in BMG composites has rarely been studied.

In the present study, we investigated the detailed deformation mechanism of TRIP behavior in Cu-based BMG composite with stress induced phase transformable NiTi phase as a 2nd phase using in-situ synchrotron radiation during compression test and ab-initio assisted molecular dynamic simulation. Martensitic transformation of 2nd phase results in relaxation of stress/strain partitioning between 2nd phase and the amorphous matrix. Consequently, delocalized shear banding with horizontal direction occurs at amorphous matrix, which can be a critical advantage of TRIP BMG composites for mechanical stability.

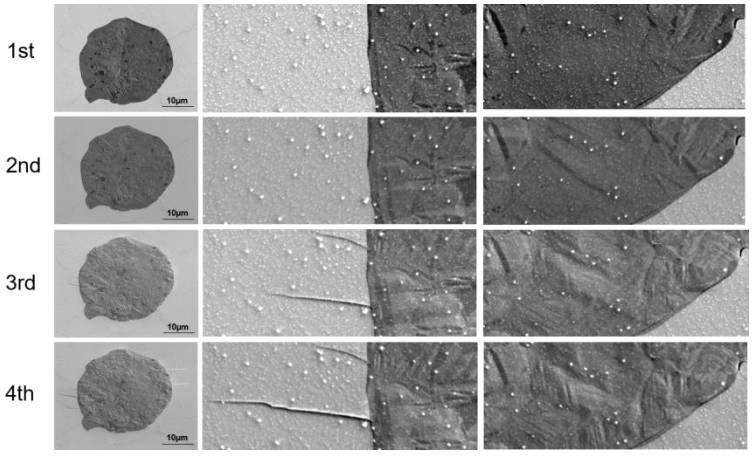

Fig1. Development of shear bands in a horizontal direction as a result of the delocalization of stress strain partitioning between amorphous matrix and transformable 2nd phase

KEYWORDS: Metallic glass composite, transformation induced plasticity

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Local investigation of superelastic behavior of titanium alloys during nanoindentation

Amélie Fillon[1], Hamza Jabir[1], Denis Laillé[1], Thierry Gloriant[1]

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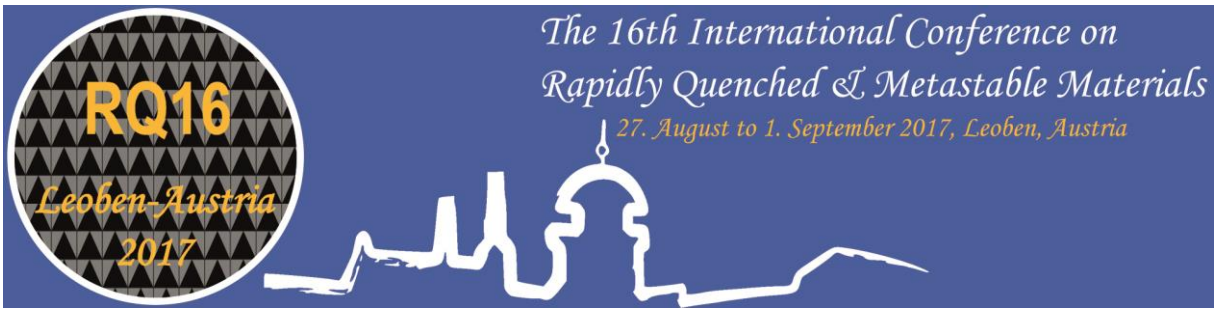
Titanium alloys are attractive metallic materials for applications in biomedical technologies, in aerospace and naval industries due to their high strength, low density, low elastic modulus, high strength/weight ratio (specific strength), good corrosion resistance and excellent biocompatibility. Depending on the nature and proportion of alloying elements and on the thermomechanical processing routes, a wide variety of possible microstructures and numerous combinations of mechanical behaviors have been observed. For example, β-type titanium alloys can display the same specific properties as superelastic Ti-Ni alloys which are assumed as contact allergens due to their high Ni content. Superelastic alloys are highly regarded in biomedical technologies for the fabrication of more flexible and durable guide wires for endoscopic and endodontic instruments. The development of new Ni-free superelastic β-Ti alloys composed of non-cytotoxic and biocompatible elements has been the subject of many researches over the last fifteen years. Metastable β-Ti alloys are obtained through the controlled addition of β-stabilizing elements (Mo, Nb, Ta, Zr…). The metastable β phase can be retained at room temperature either by direct quenching from the high temperature β phase field or by PVD process. The superelastic effect arises from the mechanical instability of the metastable β phase (BCC) that transforms into the non-equilibrium α'' phase (orthorhombic), also called martensite, to accommodate the increasing deformation. As the load is removed, the reverse transformation from α'' phase to β phase proceeds allowing a large recovery of the strain. This non-conventional and remarkable pseudo-elastic deformation is attributed to the reversible martensitic transformation.

While considerable attention has been paid to the superelasticity of metastable β-Ti alloys in their bulk form during macroscopic deformations, much less work exists on the occurrence of a superelastic response of these alloys in a confined geometry during nanoscale deformations. In the present work, nanoindentation technique is employed as a suitable tool to investigate the local mechanical properties of polycrystalline Ti alloys. We show that superelastic response still exists in metastable β-Ti alloys during local deformation under complex loading conditions. In another study, nanoindentation testing is conducted at the grain scale and reveals separate mechanical response depending on the crystallographic orientation of individual grains. Finally, we show that superelastic effect still exists in magnetron sputtered Ti-based coatings.

KEYWORDS: metastable β-titanium alloys, martensitic transformation, superelasticity, nanoindentation, local mechanical properties, nanograined coatings.

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



A2- Rapid Solidification & high undercooling

The structure-dynamics relationship in binary glass-forming alloy melts

Dirk Holland-Moritz[1], Benedikt Nowak[1], Fan Yang[1], Th. Voigtmann[1], T. Kordel[1], T. Hansen[2], Z. Evenson[3], T. Unruh[3], and Andreas Meyer[1]

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Despite considerable research effort, the mechanisms of glass-formation are not well understood on the atomic length and time scale. While the metallic alloys showing the best glass-forming ability are multi-component alloys, the less complex binary glass-forming systems are attractive for studies aiming to find a microscopic understanding of the glass-formation process.

In this work results of studies on the short-range order and on the atomic dynamics in different stable and undercooled binary glass-forming metallic melts are presented. In order to undercool the melts deeply below the melting temperature and to avoid chemical reactions of the melts with crucible materials, the samples are containerlessly processed utilizing the electromagnetic or the electrostatic levitation technique. The short-range structure of the containerlessly processed melts is studied by neutron diffraction at the high-flux diffractometer D20 of the ILL, and the atomic dynamics are investigated by quasielastic neutron scattering (QNS) at the time-of-flight spectrometer TOFTOF of the FRM-II.

For liquid $Zr_{64}Ni_{36}$ [1], $Zr_{50}Ni_{50}$, $Zr_{36}Ni_{64}$, $Nb_{40.5}Ni_{59.5}$ [2] and $Hf_{35}Ni_{65}$ the full sets of partial structure factors were determined by neutron diffraction combined with an isotopic substitution technique using samples prepared with natural Ni, ^{60}Ni and ^{58}Ni. Ni self-diffusion coefficients have been determined by QNS for the Zr-Ni melts as function of the temperature [1,3]. While for these alloys QNS gives only access to the Ni self-diffusion coefficients due to the vanishing incoherent scattering cross section of Zr, for Hf-Ni alloys the non-vanishing incoherent scattering cross section of Hf allows also to study the atomic dynamics of the early transition metal component. By using a $Hf_{35}Ni_{65}$ sample prepared with ^{60}Ni we have measured the Hf self-diffusion coefficient and using a sample prepared with natural Ni the mean Ni/Hf self-diffusion coefficient has been determined. Similar as recently reported from radio-tracer measurements in Ni-rich $Zr_{36}Ni_{64}$ alloys [4] a decoupling of the diffusion coefficients of the different alloy components has been observed for $Hf_{35}Ni_{65}$, showing a faster Ni diffusion as compared with the Hf-diffusion.

In order to analyze the structure-dynamics relationship, we have calculated the transport coefficients in the framework of the mode coupling theory (MCT) of the glass transition using the experimentally determined partial structure factors as an input. The MCT calculations are able to well reproduce the activation energies for self-diffusion inferred from QNS data as well as the decoupling of the diffusion coefficients of the different alloy components experimentally observed for Ni-rich Zr-Ni [4] and Hf-Ni alloys. This demonstrates that the space- and time-averaged structure of the melt, as described by partial static structure factors, is sufficient for an understanding of the atomic dynamics in metallic melts.

KEYWORDS: Melt structure and relaxation studies, metallic glasses

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Presentation Method (Invited/Regular Oral/Poster): Invited

Classical Nucleation Theory Analysis of Priming in Fast Crystallizing Chalcogenide Phase-Change Memory

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Chalcogenide phase-change (PC) materials, exemplified by $Ge_2Sb_2Te_5$ (GST) and (Ag,In)-doped Sb_2Te_3 (AIST), have been widely studied for their use in electrical (phase-change random-access memory, PC-RAM) and optical (DVD, Blu-ray™) data recording. More recently, display and data visualization, and synaptic switching, exploiting the high contrast in reflectance and resistance upon reversible glass-to-crystal transitions, have been gaining great momentum. In the case of PC-RAM, a *single* low-power electrical pulse heats the glass above its glass-transition temperature, crystallizing it (SET operation). Crystallization is a rate-limiting step of the memory operation taking < 100 ns. Glass is obtained by heating the crystal with short and high-power pulse above its melting temperature, and the consequent rapid quenching, 10^9–10^{11} K s^{-1}, of the liquid (RESET operation). For the memory to be commercially successful, several conflicting requirements must be met. Crystallization must be fast, but the glass should not crystallize spontaneously at elevated temperatures.

While there is on-going research to find the 'best-performance' composition, *priming* of the supercooled liquid, in other words inducing a pre-structural ordering by an auxiliary pulse ahead of the main crystallization voltage (SET), has been shown to be a promising alternative in reducing crystallization times to less than 10^{-9} s. There is some fading of the priming effect if there is a time interval between the priming pulse and the main heating pulse to achieve crystallization. This can be expected from thermodynamic parameters of PC chalcogenides. We provide a theoretical description of pre-bias priming in terms of classical nucleation theory (CNT). Two archetypical chalcogenide PC systems are considered, each with distinct input parameters for the temperature-dependent viscosity in the calculations of transient and steady-state nucleation rates. Firstly, GST is taken to exemplify a high-fragility liquid with crystal growth partly decoupled from viscosity. Secondly, the influence of a fragile-to-strong crossover on crystallization will be considered in liquid AIST.

Understanding and controlling the temperature dependence of atomic mobility, i.e. the kinetic term in nucleation and crystal-growth rates, can pave the way for trimming the PC-RAM switching times to less than 1 ns, ultimately leading to devices that are more power-efficient.

KEYWORDS: metastable materials, thin films and coatings, rapidly quenched materials.

Presentation Method (Invited/Regular Oral/Poster): Invited

PM2000: revitalization of Plansee's ODS-19YAT as well as ODS-20YAl (PM2017-AM) and NFA-14YWT (PM2018) - high-temp. & corrosion-resistant/irradiation-tolerant ODS/NFA-steels/powder from the shelf

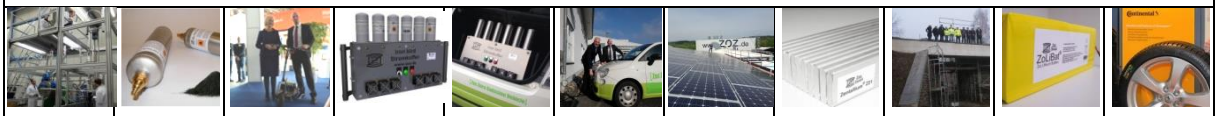
Prof. Dr. Henning Zoz

President & CEO, Zoz Group Germany

Any modern society considers sustainability, saving resources and increasing performance every day and our all future will be ruled by materials as never before. Based on general materials limitation, goal (a) is "making more with less" and since materials consumption contradicts with such limited resources, goal (b) is recycling. Both are leading to advanced materials processing with the utilization of larger surface and finer structures leading to nanostructures.

High Kinetic Processing (HKP) has been proven as a major route for reducing materials grainsize in large volume at economic manufacturing and cost capability where the "nanostructure-making-equipment", the Zoz-Simoloyer® is well-known including technology and key advantages.

Nanostructure and innovative solutions in green-/cleantech manufactured with Zoz Technology

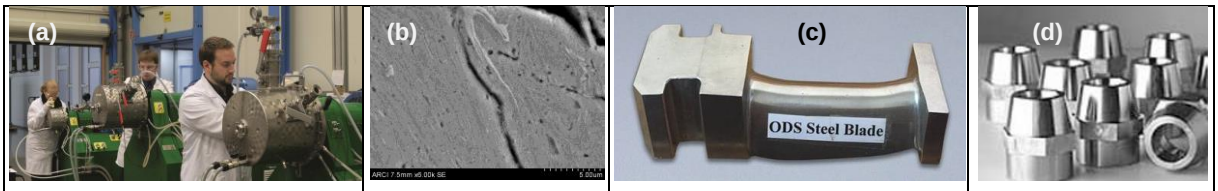


P2H® | P2G2F® | Hydrolium® | H2Tank2Go® | Zentallium® | ZoLiBat® | Simoloyer® are registered trademarks of Zoz Group, Taraxagum™ is so of Continental AG

oxide dispersion strengthening | ODS & Nanostructured Ferritic Alloys

One major focus at Zoz-customers is concentrated on the development and processing of Oxide Dispersion Strengthened Ferritic Steels (ODS). Due to their high temperature stability and strength along with a high irradiation tolerance, ODS-steels represent promising candidates for nuclear fusion and 4th gen. fission reactors likewise for components in gasturbines/aero- and combustion engines exposed to high temperature and high corroding environment [1-4].

This target does not at all contradict with the "green/cleantech-company" understanding of Zoz since the pure political German "no" to nuclear energy does not efficiently reflect global environmental responsibility.



Simoloyer® CM08 & CM20-ODS (a), Fe-0.03MOx after 4 h Zoz-HKP at Zoz-ARCI Center India (CM08), grainsize ~15nm (b), ARCI turbine blade (c) and PM-2000 burner nozzles [5] (d)

Particularly with the goal of achieving better resistance to radiation damage, Nanostructured Ferritic Alloys (NFA) with a dense dispersion of <10nm oxides occuring intra- and intergranulray as precipitates of complex oxides e. g. Y2Ti2O7 formed after a dissolution of

starting Y2O3 under the presence of Ti during intense/extended HKP (>20h, >8m/sMRV) and subsequent heat treatment (>1.000°C), were developed [6, 7].

Due to a general renaisseance of powder metallurgy (PM) by additive manufacturing processes (AM, ALM...) also conventional ODS-materials, where coarser "original" oxides >10nm located predominantly on grain boundaries or former particle boundaries [6] homogeniously dispersed by HKP (<4h, >8m/sMRV) opened another focus. The naturally irregular/equiaxial particles after HKP can be modified in morphology by so called spheriodization (SPH) to better meet flowability requirements for AM or MIM [8].

The difference in oxide character and location results in lower meachanical properties of the common ODS-material [6] where economics in processing cost do determine the proper material for the particular application.

Since Zoz has been providing not only the processing equipment but also most of the larger numbers of ODS/NFA-materials (powder, 2 t approx.) in recent years, in late 2016 it has been decided to invest into the semi-commercialization of 3 dispersion strengthened materials to on-shelf availability of powder and bulk (semi-finished). Under strict information and joint understanding/agreement policy towards all customers, partners, former manufacturer and future applicating industry, from whom Zoz has been and is learning a lot, a bilateral group USA/Germany has been formed [9]. A "geo-political" restriction appeared ultimate, since the Simoloyer® and its products as of 2016 are under full observation of BaFa (German Export Control) where e. g. military relevance of ODS and nuclear application of NFA are determining.

The goal of this joint undertaking between Zoz and core parters KIT in Germany and UCSB, ORNL as well as LANL in the USA is a commercial NFA from the shelf. Since this has never been done before, support from the US-DOE is on board and a joint submission within Euratom/INERI (International Nuclear Energy Research Initiative) based on DOE-NE's Advanced Fuels Program is planned for August 2017.

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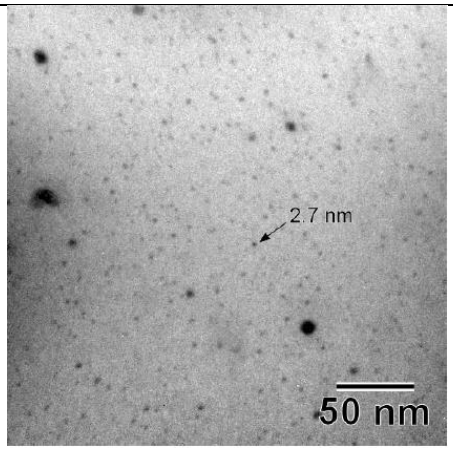
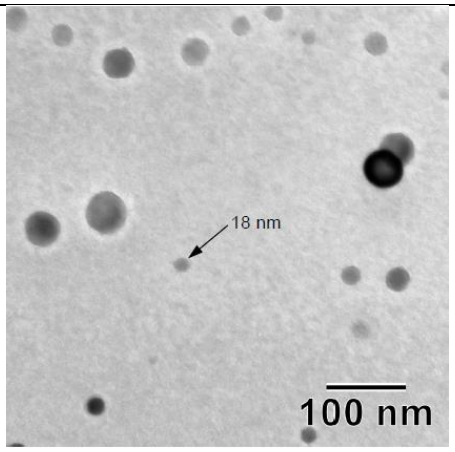
<tr><td> 
</td><td> 
</td></tr>
<tr><td>ORNL 14YWT EFTEM Fe M Jump Ratio Map</td><td>Plansee PM2000 TEM Bright Field Image</td></tr>
<tr><td colspan="2">14YWT contains significantly higher number density and smaller size of Ti-, Y-, and O-rich nanoclusters compared to YAG oxide particles in PM2000 (and other commercial ODS alloys) [4]</td></tr>
</table>

additive manufacturing ODS | nuclear fusion / 4th gen. fission NFA

For at most eonomic "fast/safe resulting", two milestones have been fixed. In 2017, the former Plansee PM2000 alloy (ODS-19YAT, manufacturing by Plansee until 2006 [10]) is going to be relaunched in powder and bulk (D40xL250mm) based on the simplier fine-grain/HIP-

consolidated type that e. g. the German car-manufacturer Porsche was utilizing for the injection nozzle of its GT4-engine [8] to serve under extremely high corrosive environment at high temperature. Under mutual understanding with Plansee [11], the name of PM2000 will survive. Also an immediate goal is a new material PM2017 (20YAl) with 1% more Cr and zero Ti (compared to PM2000) with a focus on AM consolidation routes including MIM.

brand	chem. composition (starting mat.)	ID	origin	t. b. on shelf
PM2000	Fe-19Cr-5.5Al-0.5Ti-0.5Y2O3	**19YAT**	ODS-PM	fine-grain/HIP only, D40xL250mm
PM2017	Fe-20Cr-5.5Al-0.5Y2O3	**20YAl**	ODS-RR	powder only (AM, ALM, MIM)
PM2018	Fe-14Cr-3W-0.4Ti-0.25Y2O3	**14YWT**	NFA-GE	t. b. d.
chemical (basic) compositions for on shelf (a) powder and bulk (b) bulk only (c) powder and bulk				

If the abitious schedule will be achieved, then the NFA-14YWT with the chemical starting composition Fe-14Cr-3W-0.4Ti-0.25Y2O3, demonstrated by GE with powder processing at Zoz [6] in large volume shall be available under the name PM2018 from that year in powder batches and small bulks.

ODS/NFA powder processing is done at the Zoz Technology Center (ZTC) in Germany, characterization of powder and bulk at core partners. For tolling HIP (PM2000) and starting materials supply, Zoz is searching for suppliers. For the upcoming (again after 10 years) availability of PM2000, Zoz is searching for the former and future customers and end user.

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[8] authors discussion with Prof. Gerhard Leichtfried, Innsbruck, 2017-03-02
[9] authors discussion with A. Moeslang (Karlsruhe Institute of Technology - KIT), G. R. Odette (University of California Santa Barbara), S. A. Maloy (Los Alamos National Laboratories), D. T. Hoelzer (Oak Ridge National Laboratory), 2016-11 through 2017-04
[10] Communication Plansee Nederland, 2017-04-05
[11] authors discussion and communications with Plansee Composite Materials GmbH Lechbruck am See, 2016-11 through 2017-04-11

Biography

Prof. Dr. Henning Zoz is the CEO & President of Zoz Group.

Inventions/Expertise:
CMB-materials, cycle operation, NdFeB-magnetic filter system, Zentallium®, Hydrolium®, H2Tank2Go®, High Performance Cement/Concrete and other. Numerous patents and trademarks, more than 50 papers, teaching at numerous universities and institutes all over the world. Due to his expertise in energy storage materials and energy storage, including integration and drives, Zoz became a prominent address, when it comes to cost-effective utilization of renewable energy sources for mobile and stationary applications (H2 Mobility, base-load capable CO2-free power plant).

Academia:
Doctoral Degree in Advanced Technology at summa cum laude;

Invited professor at CIITEC-IPN;

Chair Professor [2009-2014] and Assistant Professor [2015] at Ritsumeikan University;

Memberships:
KPMI, FPM, DKG, DEV, PMAI, MPIF and other.

Zoz is one of the founders and main organizers of the OZ-International|German-Japanese Symposium on Nanostructures and a member of a number of program/advisory committees all over the world.

Other Functions:
Deputy Chairman of M-E-NES [2010/12-2016];

Member of the Mobility Experts Group;

Implementation & Assessment Committee, Overseas Education Program at RITS [2008-2015];

Board member of "Nano in Germany" and NMWP (Nano-Micro-Materials-Photonic);

Member of the Innovation Arena of the German Federal Office for Street-affairs (BAST);

Awards:
Materialica-Award [2010], Germany;

Manager of The Year [2011], South Westphalia, Germany;
Ibero-American Silver-Award [2012], Mexico;
Innovation-Award-Sauerland [2012], Germany;
PMAI-Fellow-Award [2013], India;
Nomination for the German Environmental Award [2013] “Power to Gas to Fuel”

About Zoz Group

Zoz Group manufactures and supplies Mechanical Process Engineering Equipment and manufactures and supplies with insofar own equipment Nanostructured Materials from powders, layers and bulk parts to magnetic filters, batteries, hydrogen-drives with H2-solid-state-absorber tanks incl. vehicles.

Affiliated companies serve E- and E-H2-mobility, entertain a ZEV-Auto-Fleet, maintain buildings and operate a public technology center and student’s dormitories, solar energy-fuelcell- and electrolyzing plants, a tour operator as well as sailing and aircraft operations.

Presentation Method (Invited/Regular Oral/Poster): Invited

Extremely large undercooling during solidification of ternary Bi44In33Sn23 triphasic nanoparticles embedded in icosahedral matrix

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[2]*Institute of Micro and Nanomaterials, Albert-Einstein-Allee 47, Ulm University, Germany, D-89081 Ulm*

In the present investigation, bismuth-based eutectic alloy with a composition of 44.3%Bi-32.54%In-23.15%Sn (in atomic%) was prepared by induction melting. For matrix the alloy of composition Al65Cu20Fe15 (in atomic%) was prepared by melting in a vacuum electric arc furnace. Melt spinning (rapid solidification route) was used for synthesis of nanoscaled Bi-In-Sn alloy particle embedded in Al–Cu–Fe quasi-crystalline matrix. The phase transformation behavior of embedded alloy nanoparticle has been studied by a combination of Transmission electron microscopy, X – Ray diffraction techniques, Differential scanning calorimetry (DSC). In the study, it was found that nanoparticle consists of combination of three phases; (BiIn),(□Sn),(Bi). The thermal characteristics were monitored using DSC. Electron microscopic studies indicate that each phase bears specific orientation relationship (OR) with the quasicrystal having interfaces having low energy. The embedded alloy nanoparticles size ranges from 20 to 80 nm with average particle size being 48±12 nm. Every particles exhibits distinct three-phase contrast. The melting and cooling of embedded alloy nanoparticles has been carried by cyclic reheating and cooling experiment with different cooling temperature at a same heating and cooling rate. It is shown that bulk Bi-In-Sn alloy has low undercooling (~7 oC) and embedded alloy nanoparticle exhibit very large undercooling (~ 166oC) for solidification. The present study provides an insight into the mechanisms of phase transformation behavior of bulk alloy and embedded alloy nanoparticle.

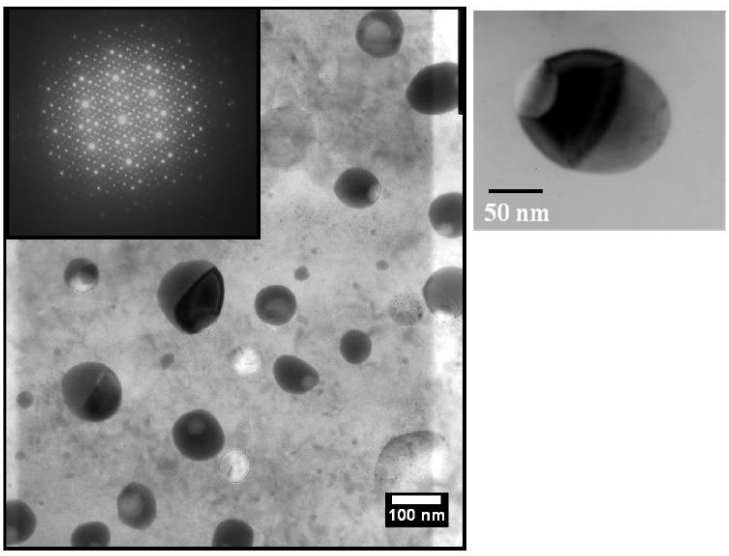

Figure1: Bright field micrograph showing nanoparticles embedded in QC matrix. The insets show the typical triphasic nanoparticle and 2-fold selected area diffraction patterns obtained from the matrix

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Microstructure and mechanical properties Al–Cu–Fe quasicrystalline reinforced AA 6082 Al matrix composite

Yagnesh Shadangi, Kausik Chattopadhyay, Joysurya Basu and N K Mukhopadhyay

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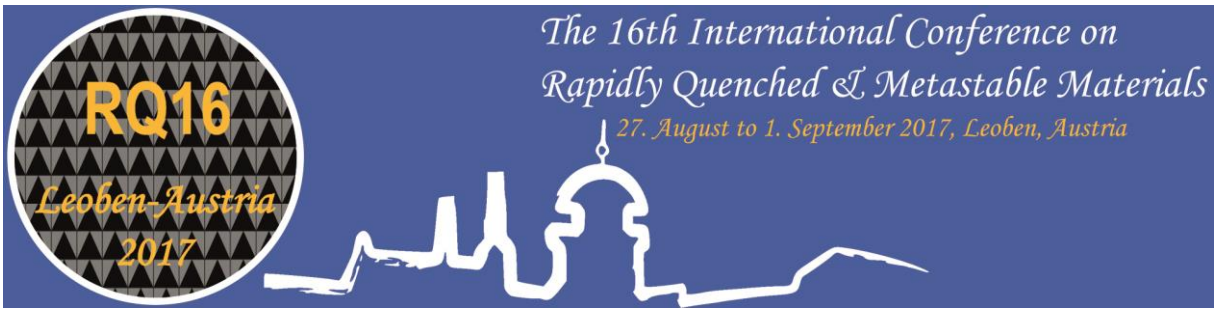
The 6XXX series, Al-Mg-Si based AA 6082 Al alloys are widely used for structural applications in automotive industry due to their excellent mechanical properties and good workability [1]. The properties of AA 6082 Al alloys may be improved for structural applications by reinforcing them with the quasicrystalline materials [2]. In the present investigation, the $Al_{62.5}Cu_{25}Fe_{12.5}$ (at%) quasicrystalline (IQC) powder was mechanically milled (MM) with 30 volume fraction of AA 6082 Al matrix in a high energy planetary ball mill at the rotation speed 200 rpm for 50 h using WC milling media. Efforts were made to study the microstructural and mechanical properties of IQC reinforced Aluminum matrix composites (AMC) powder as well as consolidated pellets (prepared by conventional and microwave sintering). The microstructure and phase composition of IQC reinforced AMC powder and consolidated samples were analyzed with x-Ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and differential electron microscopy (DSC). Increasing the duration of MM leads to broadening of the diffraction peaks, indicating a reduction of crystallite size.

The AMC powders were consolidated using conventional sintering and microwave sintering. The IQC reinforced AMC composite were sintered at 500, 550 and 600°C for 60 min (by conventional and microwave sintering). The mechanical properties of sintered samples were evaluated through micro-indentation and compressive testing techniques. The precipitation of Mg_2Si intermetallic phases were also evident during microwave sintering of AMC. With increasing the duration of milling, the grain refinement, hardness and yield strength were found to be increased. The increase in compressive strength is attributed to the strong interfacial bonding of Al matrix and reinforcement. The present study provides an insight into the microstructural evolutions and the interfacial strengthening of the $Al_{62.5}Cu_{25}Fe_{12.5}$ quasicrystal reinforced.

KEYWORDS: Mechanical milling, Al-Fe-Cu quasicrystal reinforcement, AA 6082 Al, microwave sintering.

M. R. Basariya, V.C. Srivastava and N K Mukhopadhyay, Mater. Des., 64, 542 – 549 (2014).
F. Ali *et al*., J. Alloys Comp., 607, 274 – 279 (2014).

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



B2- Metallic glass 2: Properties & application

Superelasticity of Ni-Ti-Cu-Zr alloy with high glass forming ability

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Although bulk metallic glass is known to have some exotic properties such as high strength, large elastic limit and good corrosion property, the application as structural materials has not been successful so far due to its limited plasticity. Recent development in BMG has introduced a new concept of composite which integrates shape memory alloy as the second phase in the glass matrix. The bulk metallic glass composites (BMGCs) based on reversible B2-type shape memory alloy are known to exhibit transformation induced plasticity which originates from deformation-induced martensitic transformation. Such BMGCs exhibit extensive work hardening behavior, which greatly enhances the potential for structural application.

B2-type CuZr shape memory alloy is a well-known example which is utilized for fabrication of high plasticity BMGCs due to high glass forming ability (GFA) of Cu-Zr alloy. Superelasticity is a reversible deformation motion which shows very large elastic strain limit by lattice shear and twinning at above austenite transformation finish temperature. Among the well-known superelastic alloys, NiTi alloy shows martensitic transformation from B2 to B19', accompanying high recovery strain under loading-unloading condition at room temperature. Although B2-type NiTi alloy is known to exhibit superior superelasticity, the obstacle to be used in BMGC is its inferior GFA.

One of the advantage of bulk metallic glass is to exhibit low viscosity when it is heated up to supercooled liquid region, enabling precise thermo-plastic forming of metallic parts down to nm scale. Therefore, to provide high strength and large superelastic strain in such thermos-plastic formed metallic parts, the Ni-Ti based amorphous alloy which exhibits high GFA and transforms into single B2 phase upon crystallization needs to be developed. The resulting B2-type Ni-Ti based alloy after partial or full crystallization should exhibit optimum combination of strength, superplastic strain and strain to failure.

In the present study, in order to find the alloy systems satisfying the requirement mentioned above, the Ni-Ti-Cu-Zr alloys with a wide range of composition, $Ni_{50-x}Ti_{50-y}Cu_xZr_y$ ($5 \leq x, y \leq 30$, at%), have been investigated. Addition of small amount of Si was found very effective in enhancing the GFA, resulting in casting fully amorphous sample with 300 ㎛ thickness. The corresponding B2-type alloy showed large recovery strain of ~ 7.5 % along with increased loading plateau stress at room temperature under compressive loading-unloading condition.

Presentation Method:Keynote

Multiple relaxation pathways and polyamorphism in a Au-based bulk metallic glass

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Bulk metallic glasses are formed from highly viscous, densely packed, multi-component liquids, in which the sluggish kinetics is the most important factor for impeding the nucleation and growth of crystals. This is also reflected in a reduced atomic mobility during annealing below the glass transition, T_g, that can hinder configurational changes at the atomic scale. Recent calorimetric investigations on the $Au_{49}Cu_{26.9}Si_{16.3}Ag_{5.5}Pd_{2.3}$ glass former showed the existence of multiple enthalpy relaxation pathways upon applying a wide range of annealing times, from less than one second up to several days, during annealing at temperatures of 50 to 20 Kelvin below T_g [1]. The distinct multiple decays in the enthalpy relaxation correspond to states of local and transient equilibrium with increasingly higher activation energies. The results are compared with detailed microscopic information on the collective atomic motion obtained using X-ray Photon Correlation Spectroscopy (XPCS). Different regimes of stationary dynamics are observed that are separated by intermittent temporary aging regimes, which facilitate the physical aging towards equilibrium [1]. Each explored dynamic stationary regime is viewed as corresponding to a thermodynamic local equilibrium with a distinct activation energy.

Additionally, during long-time annealing in the ultra-viscous state a thermodynamic signature of a liquid-liquid transition (LLT) is observed [1]. According to ref. [2], the LLT-temperature is slightly lower than the conventional T_g for this alloy system. The consequence is that the high-temperature kinetically *fragile* liquid freezes into the glass during conventional processing and the underlying LLT is thus accessed by the system during annealing below T_g. The process involves kinetics with relaxation times of the order of thousands of seconds. The transition is found to be reversible upon re-heating in DSC, marked by a small value of the ordering enthalpy as well as entropy change (2.4 % of the entropy of fusion). The weak ordering energy is the reason why the associated transition temperature is found at a very low temperature. These findings support the 'big-picture' proposed by Angell that liquids with different fragility occupy different flanks of an underlying order-disorder transition.

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2. S. Hechler, B. Ruta, M. Stolpe, E. Pineda, Z. Evenson, O. Gross, W. Hembree, A. Bernasconi, R. Busch, and I. Gallino, *Liquid-liquid transition revealed by quasi-static cooling of an ultra-viscous metallic liquid*, https://arxiv.org/abs/1704.0670 (2017).

KEYWORDS: Bulk Metallic Glasses, Relaxatio

Presentation Method: Invited

Rapidly Quenched Fe-based Glassy Alloys with Low Curie Temperature for Medical and Engineering Applications

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For a number of years, the only metallic material with a Curie temperature (T_C) around 300 K was Gd. However, the high cost and strong oxidation limited drastically its use in practical applications. More recently, it turned out that addition of Cr, Ba or Ni to some Fe or Co-based metallic glasses is shifting the ferromagnetic–paramagnetic transition of the amorphous phase below 400 K [1-3], which makes them interesting for high-sensitivity temperature sensors [3] or biomedical applications [4,5]. To overcome these issues, we developed new types of ferromagnetic materials, with nominal compositions $Fe_{79.7-x}ETM_xNb_{0.3}B_{20}$ (ETM = Cr, Ti, Mn; x = 12÷20 at.%), high saturation magnetization, reduced hysteresis losses, and low Curie temperature which can be tailored easily and precisely in the 30-50°C by modifying the ETM content, with an accuracy of less than 1°C, more suitable for self-regulating magnetic hyperthermia and other engineering applications.

$Fe_{79.7-x}Cr_xNb_{0.3}B_{20}$ glassy melt-spun ribbons and glass-coated microwires with T_C in the range 35-45°C (the lowest ever reported for metallic glasses) have been prepared by rapid solidification. Despite the fact that high resolution imaging and electron diffraction confirm that in the as-quenched state the samples are amorphous, independent of the Cr content, energy-dispersive X-ray spectroscopy mapping emphasizes clearly the presence of Fe and Cr clusters varying from approximately 1 to 2-3 nm in size with the increase of Cr content from 11 to 13 at. %. The Fe and Cr atoms segregate the atomic scale to form nanometer sized clusters, influencing strongly the macroscopic magnetic behavior. The Curie temperature of the system, T_C^{system}, confirmed by the magnetic susceptibility versus temperature measurements, gives the strength of the magnetic interactions between clusters. The inter-cluster interactions are much stronger for lower contents of Cr, the microstructure is less uniform, and T_C^{system} increases from 17°C for 13 at.% Cr to 57°C for 11.5 at.% Cr. The whole system transforms to a ferromagnetic state through interactions between the clusters. The observed stable behavior of low T_C glassy alloys up to very high frequencies (10 GHz) is another important feature for sensing and biomedical applications. The temperature sensor based on such glassy alloys has a very good sensitivity in a narrow temperature range (about 1°C).

Submicron powders with glassy structure and sizes between a few tens of nm and 1 μm have been prepared by high-energy ball milling from glassy melt-spun ribbons (MSRs) precursors. The glassy structure existing in the MSRs is preserved by milling the annealed MSRs in oleic acid and n-heptane. The glassy structure of the submicron powders confers the specific magnetic properties and allows tuning the Curie temperatures in the range of 15-50°C. The precipitation of α-Fe in excess shifts the Curie temperature to 780°C. The use of surfactants (oleic acid or heptane) avoids partially the agglomeration of powders, and their individual size goes down to 25-40 nm. The heating efficiency of the submicron powders in a. c. fields (H = 350 mT and f = 153 kHz) evidences a working regime in the range of 33-45°C, depending on ETM content, indicating the suitability of using such powders for self-regulation magnetic hyperthermia applications (compared with Fe-oxides (mainly Fe_3O_4) which work indeed up to moderate temperatures (below 47°C), but the capacity to retain the temperature in the range of 41-46°C requires a very rigorous control of the power of the high frequency generator.

We acknowledge the financial supported from UEFISCDI Grant #148/2012 (HYPERTHERMIA), EU FP7-REGPOT-2012-2013-1, Grant Agreement no. 316194 (NANOSENS) and NUCLEU Programme (PN 16 37 01 03 and PN 16 37 02 02).

KEYWORDS: glassy materials, powder and nanopowder synthesis, magnetic properties, applications.

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Presentation Method (Invited/Regular Oral/Poster): Invited

Oxidation behavior of Ti-Zr-Ni-Cu metallic glass alloys

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Thermoplastic forming (TPF) process can be applied to metallic glasses (MGs) showing supercooled liquid region to fabricate a part with complex shape and surface patterns. MG is heated rapidly into the supercooled liquid state and pressure is applied to induce deformation by viscous flow. For optimization the TPF process, it is important to understand the oxidation behavior of MG during rapid heating because oxidation can occur readily during the process and the resulting oxide scales bring negative effects on viscous flow. In the present study, we are reporting the oxidation behavior of $Ti_{50-x}Zr_xNi_{50-y}Cu_y$ MGs, which are transforming into single B2 crystalline phase exhibiting superelastic behavior. Oxidation behavior was monitored during continuous heating as well as isothermal holding the MGs by thermogravimetric analyzer (TGA) with a dry air. Cross sectional microstructure of heated samples was examined in detail using STEM and TEM and depth-profiles of composition was examined using X-ray photoelectron spectroscopy (XPS). The effects of alloy composition and matrix structure on the oxidation kinetics and resulting scale formation will be discussed.

KEYWORDS: Ti-Ni based metallic glass, oxidation behavior

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Microscopic evidence of a liquid-liquid transition below the conventional glass transition temperature

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Liquid-liquid transitions fascinate researchers for many years, since they occur in each class of glass-forming systems [1–4]. In most cases, the transition is observed for temperatures higher than the conventional glass transition temperature, suggesting large atomic mobility. Transitions involving lower diffusivity have also been proposed [2,5], although no microscopic evidence has been reported so far.

By combining advanced synchrotron techniques, we have followed the atomic motion and local structure while quasi-static cooling is applied to an $Au_{49}Cu_{26.9}Si_{16.3}$ $Ag_{5.5}Pd_{2.3}$ metallic glass-former from the supercooled liquid phase. With this thermal protocol, we could lower the glass transition temperature far enough to reveal a liquid-liquid fragile to strong transition between two kinetically distinct ultra-viscous states with relaxation times of thousands of seconds. This transition is usually hidden by the occurrence of the vitrification at standard cooling rates and is accompanied by structural changes distinct from those appearing at the glass transition. Our results provide new insight into polyamorphism, and challenge also the highly-debated topic on the divergence of the dynamics in ultra-viscous liquids.

KEYWORDS: Melt structure and relaxation studies, Thermodynamics and phase transformation studies, Bulk metallic glasses and composites, Chemical and physical properties.

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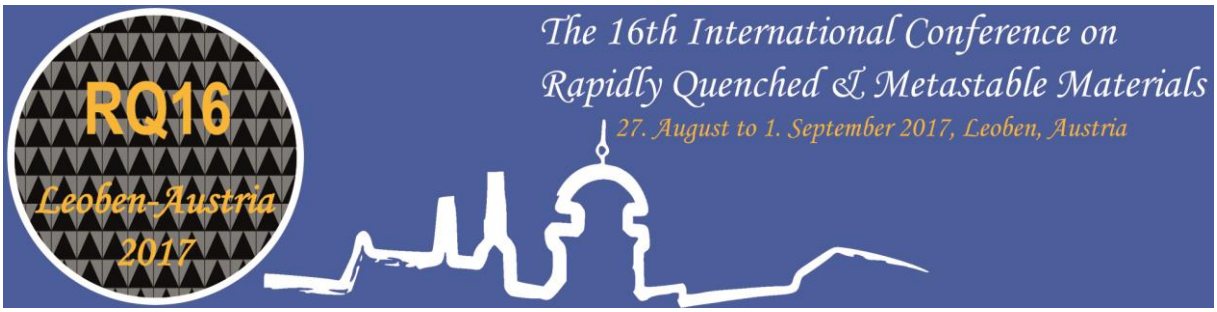
Presentation Method (Invited/Regular Oral/Poster): Regular Oral



C2- Severe plastic deformation 1

Excess volume and defect annealing in ultrafine-grained Ni studied by difference dilatometry and neutron diffraction

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The properties of ultrafine-grained metals prepared by severe plastic deformation are closely related to their high amount of excess volume localized in defects, such as grain boundaries, dislocations, and vacancies. A powerful tool to study free volume-type defects on an absolute concentration scale has turned out to be difference dilatometry [1]. This method allows for the precise measurement of the volume change associated with the annealing out of these defects upon time-linear heating.

The present work focuses on a comparative dilatometric defect study of the two processing techniques of high-pressure torsion (HPT) and equal-channel angular pressing (ECAP) using nickel as a model system. In the temperature regime below the onset of crystallite growth, both routes reveal characteristic orientation-dependent dilatometric length changes upon heating with an expansion in tangential (HPT) or extrusion direction (ECAP) and contraction perpendicular to these directions. Macroscopic residual stresses in the dilatometer samples can be ruled out as source of this anisotropy, as evidenced by dilatometry after plastic post-deformation of the HPT-samples and, in particular, by neutron diffraction measurements of the dilatometer samples. The anisotropic length change can be explained by the anisotropic annealing out of deformation-induced lattice vacancies owing to the anisotropic shape of the submicrometer-sized crystallites. This yields direct experimental access to the vacancy relaxation volume [2].

For both HPT- and ECAP-processed Ni pronounced recrystallization stages are monitored by dilatometry from which the amount of grain boundary excess volume can be deduced. Specific differences observed for HPT- and ECAP-Ni in the annealing behaviour with respect to amplitude and temperature are associated with the different degree of deformation and grain refinement achievable with both routes [3].

Financial support by the FWF Austrian Science Fund is appreciated (project P25628-N20).

KEYWORDS: metastable materials, ultrafine grained metals, defects, dilatometry, neutron diffraction

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Presentation Method (Invited/Regular Oral/Poster): Keynote

SPD as a tool to improve physical properties of functional materials

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During the last two decennia the various methods of "Severe Plastic Deformation – SPD" have revealed as highly successful to process bulk nanostructured materials with outstanding mechanical properties [1)]. At present the scientific community is increasingly concerned with the SPD processing of functional nanomaterials which mainly comprise thermoelectrics, materials for hydrogen storage, soft magnetic properties, and alloys used in biomedical applications [2)] . The most significant advancements were reached with the efficiency of thermoelectrics ("Figure of Merit"), by a factor >2 for Skutterudites, with the kinetics and storage stability of hydride forming metals, and with the strength and bio-corrosion rate of biodegradable alloys (orthopedics and prostheses techniques, Mg alloys). However, these improvements were made possible by optimization the densities and arrays of low-dimensional lattice defects such as dislocations and vacancy clusters, rather than those of high dimensional defects like grain- and phase boundaries. This optimization appears feasible by in-parallel application of different SPD methods and by combination of them with specific heat treatments.

Keywords: Functional Materials, Severe Plastic Deformation, Thermoelectricity, Hydrogen Storage, Biodegradable Alloys

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Presentation Method (Invited/Regular Oral/Poster): Invited

Partitioning and Segregation of Elements during Non-equilibrium Processing of an Al-Fe Alloy

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Atom probe tomography (APT) is a powerful technique for providing atomistic structural and chemical information of materials. The information unveiled by the technique is advancing our fundamental understanding about materials. Using advanced FIB technique, atom probe samples can be prepared successfully from a broad range of materials. Under laser-pulsing, APT is feasible for analyze brittle and poorly conductive material to reveal their unique structural and chemical information in three dimensions. In combination of other analysis techniques, we are able to develop comprehensive understanding about materials, which helps to guide optimization of material processing, and design and development of new advanced materials

In this contribution, I will present our work on understanding about partitioning and segregation of solute elements in an Al-Fe alloy during non-equilibrium processing using APT. Fe exhibits a negligible solubility in atomized Al-Fe alloy powders. Cryomilling can introduce significant amount of impurities and 2 at% Fe into the Al matrix of the Al-Fe alloy. Subsequent consolidation has led to the formation and growth of Fe-rich Al13Fe4 particles. The concentrations of Fe and impurities in the Al-matrix drop to extremely low levels after consolidation. In order to refine Fe-rich particles in the Al-Fe alloy by this non-equilibrium processing route, Fe content in the Al-Fe alloy should be no more than 2 at% to avoid the formation of coarse Fe-rich particles.

KEYWORDS: Atom probe tomography, FIB, partitioning, segregation, Fe-rich phase.

Presentation Method (Invited/Regular Oral/Poster): Invited

Microstructural evolution of Copper-(Chromium, Molybdenum, Tungsten) composites deformed by high-pressure-torsion

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A series of Cu-refractory composites containing either Cr, Mo or W were subjected to room-temperature severe plastic deformation using high-pressure torsion (HPT). Co-deformation of both components occurred, resulting in the formation of lamellar microstructures. This was despite the deformation temperature being significantly below the ductile-brittle transformation temperature of each of the refractory metals. Mo-containing composites formed finer microstructures than either Cr or W for equivalent levels of deformation. The lamellar spacing was quantified for various amounts of deformation using backscattered electron diffraction and scanning and transmission electron microscopy. The hardness of the composites initially followed a Hall-Petch type relationship in which the length scale was determined by the lamellar spacing. By applying a further, second step of HPT deformation to Cu-Mo and Cu-W composites it was found that in these composites the lamellar structure was stable up to equivalent strains of >30,000 and that the lamellar spacings could be reduced to ~50nm in Cu20W80(wt.%) and 10-20nm in Cu30Mo70(wt.%). For lamellar spacings below ~200nm the effect of microstructural refinement on the hardness was limited. This work shows that it is possible to form nanometer-scale layered composites of Cu-group V refractory metals via high-pressure torsion despite the inherent brittleness of the refractory component.

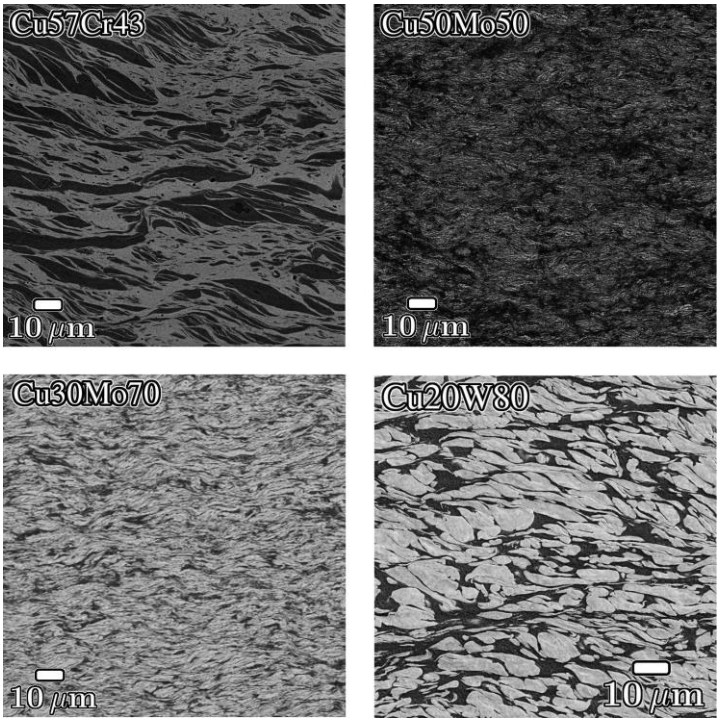

Figure 1: Backscattered electron micrographs of HPT-deformed Cu-refractory composites.

KEYWORDS: Nanostructured materials, Chemical and physical properties.

1. J. M. Rosalie, J. Guo, R Pippan, Z. Zhang Journal of Materials Science, Volume 52, 9872–9883 (2017).

Presentation Method (Regular Oral):

Growth of single quasicrystalline grains in Al-Cu-(Fe,Cr) mechanically alloyed powders at heating

V.V. Tcherdyntsev, A.I. Salimon, A.A. Stepashkin, L.K. Olifirov

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Almost single phase quasicrystalline powders consisting of icosahedral $Al_{65}Cu_{23}Fe_{12}$ and decagonal $Al_{73}Cu_{11}Cr_{16}$ phases were produced by mechanical alloying (MA) and subsequent heating at 700 ^{0}C. Heating up to 950 ^{0}C and and further cooling at the rate 30…40 K/min results in the formation of coarse agglomerate with the sponge-like sintered fraction and big massive particles. The likelihood to find bigger particles is higher for the outer layers of dilatometer specimens rather than in the core zone. It is believed that temperature and heating/cooling rate vary across the dilatometer specimen section providing temperature gradient and different thermal conditions for the melting and the grain growth – the structures of sponge-like fraction and big particles. It was possible to separate from the agglomerates bigger particles of two types. The first type of bigger particles – "the bunch of grape" - is characteristic for the Al-Cu-Fe system where its appearance has smooth shapes and surfaces. It is believed that these particles are formed in the rapidly cooled zones of the melt in the initially loose quasicrystalline powder. Provided the melting happened the non-melted single quasicrystalline grains may grow on account of liquid phase incorporating its material onto the surface that leads to smoothening of the surfaces – disappearing of the growth edges and dulling of the sharp edges and vertices. The second type – "the pile of logs" - is characteristic for the Al-Cu-Cr system where its appearance has perfect facets and edges. It is supposed that "log" particles are formed as a result of secondary recrystallization, i.e. due to the preferential growth of some grains in the initially loose quasicrystalline powder. It is important to notice that XRD reveals only slight traces of secondary phases (less than 5 vol. %) in big particles in the both systems, and further it is believed that these big particles are single phase quasicrystals.

This work was supported by the Ministry of education and science of Russia in the frame of the Federal targeted program "Research and development in priority directions of development of scientific-technological complex of Russia in 2014-2020 years", agreement 14.578.21.0108, unique identifier of the applied research RFMEFI57815X0108.

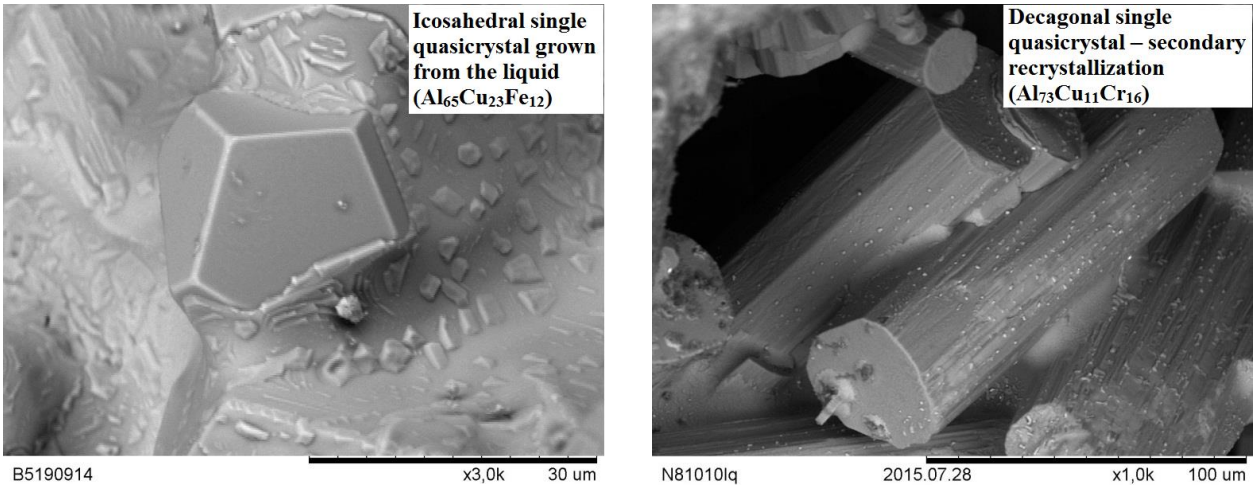
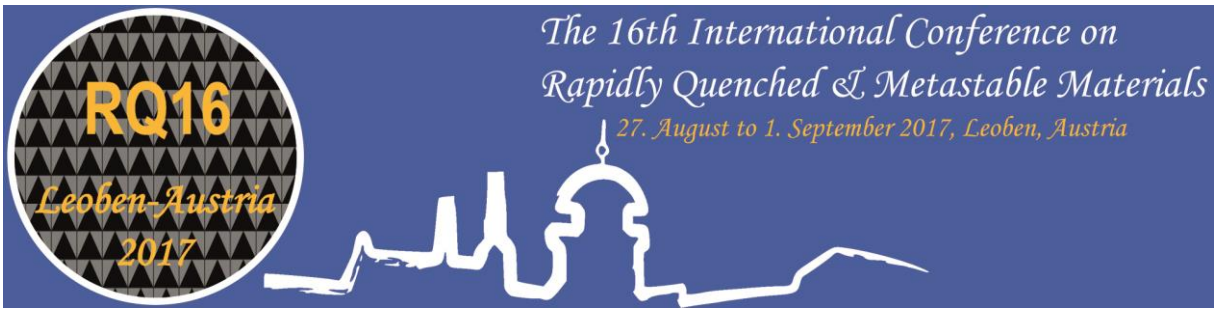


Fig. 1. Appearance of single quasicrystalline grains in the annealed Al-Cu-Fe and Al-Cu-Cr mechanically alloyed powders.

KEYWORDS: Mechanical alloying, quasicrystals

Presentation Method: Regular Oral



Tuesday, 29th August

Fast surface dynamics and unique related properties in metallic glasses

Wei-Hua WANG

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The surface viscosity and self-diffusion of a Pd-based metallic glass were measured. Strong surface dynamics and surface diffusion with the value of more than 10^5 times faster than bulk diffusion are found at below glass transition temperature. The high surface dynamic induces a fast crystallization below glass transition temperature at the free surface which is more than 100 times faster than that in bulk, self-lubrication, higher electrocatalytic activity and unique self-stabilizing catalytic performance over a long-cycling life than the commercial Pt/C catalysts in Pd-based MGs, and generation of the modulated superlattice-like nanostructure modulated nanostructure from the surface to interior. The observations have implications for understanding the glassy surface dynamics, and pave a way for controllable fabrication of unique and sophisticated nanostructure on glass surface to realize the properties modification.

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Presentation Method (Invited plenary)

Impact melting: rapid quenching and materials chemistry in small volumes and at extremely short timescales

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Mechanical impacts are at the heart of a variety of nonequilibrium processing techniques of great contemporary interest for both structural and functional materials, including, e.g., high-energy milling and cold spray forming. While these techniques all involve severe plastic deformation, it has generally been a domain of speculation whether impact-induced melting and rapid solidification can occur during such processes. This talk will review recent work aimed at quantitatively resolving the conditions under which impact melting occurs in metallic powder particles, through focused study of individual impacts at velocities up to ~km/s. Through direct observation of both the impact events (in real time) and sites (ex situ), we develop an understanding of the conditions needed to observe melting during metal-on-metal impacts. A number of counterintuitive results emerge. For example, we deduce that melting most likely does not happen for most materials under most processing conditions, which calls for renewed study on solid-state joining under impact conditions. In fact, when melting does occur at an impact site, the solidification time is often insufficiently rapid to permit joining/welding, so melting can counterintuitively hinder adhesion. These results point to a number of interesting future questions for research at the intersection of severe deformation and solidification science.

Presentation Method (Invited plenary)

Attractiveness and usefulness of multicomponent Fe-, Zr- and Al-based glassy alloys

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Very recently, Fe-based glassy alloys and Zr-Al-Ni-Cu base bulk metallic glasses (BMGs) have gained significant application fields as functional and structural material parts in personal computer and smartphone etc. and attracted further increasing interest as novel engineering materials. By synthesizing a new type of glass-based structure alloys and improving fundamental properties and engineering characteristics of glassy alloys including BMGs, their engineering importance is expected to increase further in the near future.

For the last several years, we have been searching for new Fe-, Zr- and Al-based nonequilibrium phase alloys with useful properties and found some unique structures and useful characteristics in conjunction with novel phenomena. In Fe-based glassy alloys, (1) the successes in forming Fe-Ni-P-C and Fe-P-C BMGs with high strength with unprecedented plasticity as well as good soft magnetic and magnetocaloric properties, (2) new Fe-based soft magnetic glassy alloys with very high saturation magnetization above 1.8 T, low coercivity below 3 A/m, high effective permeability above 2×10^4 at 1 kHz and high Curie temperature, (3) development of Fe-TM-P-B-Si (TM=transition metal) base soft magnetic glassy alloys with magnetic characteristics exceeding those for commercial magnetic glassy alloys “Liqualloy” and “SENNTIX”, (4) high entropy Fe-based glassy alloys containing sub-nanoscale clusters with high strength and good ductility which cannot be obtained for ordinary Fe-based glassy alloys, (5) high entropy Fe-based glassy alloys with distinct glass transition, high strength, good ductility and high corrosion resistance, (6) finding of ductilization phenomenon of nanostructure bcc-Fe + amorphous soft magnetic alloy ribbons by micro crack-induced softening mechanism, and (7) improvement effect of glass-forming ability of Fe-based bulk glassy alloys in air and the oxygen-containing atmosphere. In Zr-based glassy alloys, (1) synthesis of nanocluster-dispersed high entropy BMGs caused by easy nucleation and extremely low growth rate and their high thermal stability, (2) synthesis of new high entropy BMGs and the clarification of the role of high entropy component in the bulk glass-forming ability, (3) formation of granular glassy structure surrounded by immiscible element by copper mold casting process and its unique mechanical and crystallization behavior, (4) synthesis of BMGs coated with immiscible element by copper mold casting and their unique chemical properties, (5) significant changes in glass transition behavior and supercooled liquid region accompanying with the reversible changes in atomic configurations and fundamental properties only by controlling the ejection temperature of alloy liquid, and (6) development of a new type of biomedical engineering bulk glassy alloys. In Al-based glassy alloys, (1) clarification of the preparation condition to extend Al + glassy phase field by choosing suitable multicomponent alloy systems, (2) finding of a novel reverse transformation phenomenon from metastable multicomponent intermetallic compound to Al + amorphous phase upon heating, (3) finding of the proportional relation between the solute content in amorphous phase and hardness in a wide hardness range, and (4) synthesis of Al + amorphous phase alloys with extremely high hardness exceeding the previous data etc. This paper aims to review our recent results on various new glass-based structure alloys with novel phenomenon and useful properties for Fe-, Zr- and Al-based multicomponent alloys prepared by melt spinning and copper mold casting processes in association with recent practical application states.

KEYWORDS: Bulk glassy alloys, High entropy BMGs, Soft magnetic properties

Presentation Method (Invited/Regular Oral/Poster): Invited plenary

Universal Parameter to Quantitatively Predict Metallic Glass Properties

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Quantitatively calculating and predicting the physical properties of metallic glasses (MGs) has been a long-sought goal. Here we introduce "flexibility volume" as a universal indicator of the glassy state, to correlate with properties on both atomic and macroscopic levels. The flexibility volume is assessed via atomic vibrations that probe local configurational space and interaction between neighboring atoms, and as such combines information from static structure and local dynamics. The parameter is defined in a simple form to be measurable both computationally and experimentally. We show that this indicator deterministically predicts the shear modulus [1], which is at the heart of key properties of metallic glasses. The flexibility volume correlates strongly on the one hand with atomic packing topology, and on the other hand with the activation energy for thermally activated relaxation and the propensity for stress-driven shear transformations [1]. As such, the flexibility provides a tractable underpinning of the mechanical heterogeneities. The concrete correlations discovered are robust and prognostic for all metallic glass compositions, processing conditions and length scales. All these advantages advocate flexibility volume as a powerful single-parameter indicator, in lieu of the widely cited but ambiguous "free volume", in characterizing the structural state of metallic glasses and understanding their properties.

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Presentation Method (Invited/Regular Oral/Poster): Invited plenary

Evolution of the Glassy State in the Potential Energy Landscape

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The concept of the potential energy landscape (PEL) is an attractive one. However, in reality it is so difficult to imagine or describe it that it is usually given as a one-dimensional hand-written diagram, $V(x)$, where x is the reaction coordinate which nobody knows what is. Whereas we have some knowledge of the static state through the distribution of the energy minima, little is known about the dynamics and the excited states. We examined the nature of the process of excitation from a local minimum to the saddle point, and the following relaxation to the next minimum, using molecular dynamics (MD) simulation and the activation-relaxation-technique (ART) [1]. To our surprise we found that the processes of excitation and relaxation are fundamentally decoupled. The excitation process depends strongly on the thermodynamic state of the system, such as cooling history. But the relaxation process does not. Memory is lost when the system gets to the saddle point of the PEL. This result implies that the conventional picture is profoundly wrong, or at least misleading. Everybody knows that PEL is highly multi-dimensional, but its implication has not been widely understood. We found that the saddle point does not just connect two adjacent energy minima, but is connected to a very large number of minima. PEL is extremely densely connected, and the saddle point is a communal assembly point where people come and go (Fig. 1). Based upon this assumption a master equation to describe the evolution of the state was derived, and was shown to predict the results of the MD simulation accurately (Fig. 2). We will discuss the implications of the results to various properties, including the relaxation and rejuvenation phenomena, the glass transition, mechanical deformation and failure, the nature of the shear-transformation-zone (STZ), and the Kauzmann paradox.

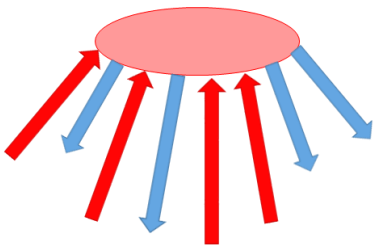

Fig1. The saddle point of the PEL is a plaza where people come and go.

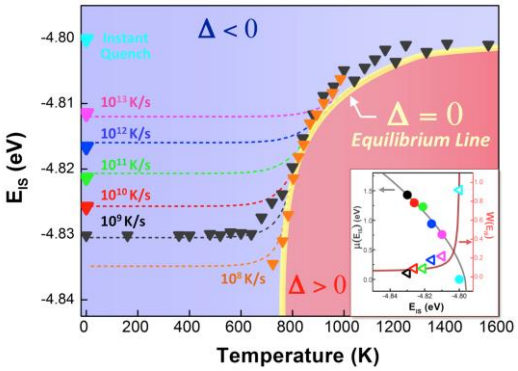

Fig. 2. The energy of the inherent structure, E_{IS}, as a function of temperature. The yellow line is an equilibrium line which separates domains of relaxation (above) and rejuvenation (below).

KEYWORDS: Chemical and physical properties, melt structure and relaxation studies, thermodynamics.

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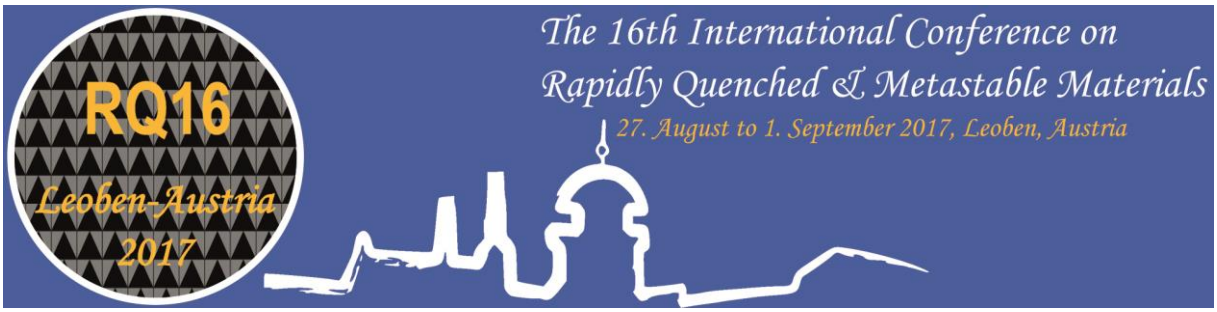
Presentation Method: Invited plenary



A3-Metallic glass 3: Deformation

Bulk Metallic Glasses: A High, but Narrow Path to Success

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Bulk metallic glasses combine plastic like processing with superb high-strength metal properties. Their processing opportunities originate from their high thermal stability which has been explored for exciting novel metal processing methods such as fused filament fabrication to 3D print, stretch blowmolding to fabricate previously unachievable shapes for metals, and micro and nanofabrication.

As BMGs are metastable, processing has to avoid crystallization, structural relaxation, and reduction of fictive temperature. We show here that drastic embrittlement can occur during processing or can be entirely avoided. Specifically, we reveal a flaw tolerance behavior of metallic glasses, a critical volume fraction of crystallinity for embrittlement, and a mechanical glass transition behavior, which all have to be understood to process BMGs such that embrittlement is avoided throughout the processing and complex BMG parts can be net-shaped which exhibit high fracture toughness.

KEYWORDS: Metallic Glasses, Mechanical Properties, Processing

Presentation Method (Invited/Regular Oral/Poster): Keynote

$Zr_{61}Ti_2Cu_{25}Al_{12}$ bulk metallic glass: Failure under torsional loading and Mode III fracture toughness

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From torsional tests of cylindrical samples, we have determined the torsional properties of high-toughness $Zr_{61}Ti_2Cu_{25}Al_{12}$ (ZT1) bulk metallic glass (BMG), including its shear yield strength, τ_y=950 MPa, its shear elastic strain limits, γ_C=3.0%, and its shear modulus, G=31.5 GPa. Under torsional loading, the BMG fails via a major shear band, without obvious macroscopic plasticity on the specimen surface. The shear band maintained stable propagation by a distance of ~300 μm (~20% of cylinder radius) before final catastrophic failure, owing to the constraint of stress gradient along the radial direction.

The intrinsic mode III fracture initiation toughness is measured for the $Zr_{61}Ti_2Cu_{25}Al_{12}$ BMG, which is known to have a high mode I fracture toughness (K_{IC}). The plastic strain intensity factor Γ_{III} was used as a measure of the fracture resistance under elastic-plastic conditions. The intrinsic mode III fracture initiation toughness of ZT1 BMG, Γ_{IIIC}, is found to be 29 μm, equivalent to a K_{IIIC} of 51 MPa√m. The corresponding fracture energy release rate is similar to or higher than that of conventional engineering metals such as high-strength aluminum alloys and some steels. The subcritical crack growth in ZT1 prior to catastrophic fracture is characterized by an extension of a microscopically zig-zag crack front. ZT1 exhibits a relatively low ratio of K_{IIIC}/K_{IC} of ~0.39, indicating that the material is more susceptible to mode III fracture. In engineering design with BMGs, the mode III fracture toughness is thus a useful baseline to ensure the reliability of structural components.

Presentation Method (Invited/Regular Oral/Poster): Invited

Quantifying the Commonalities in Structure and Plastic Deformation in Disordered Materials

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The nonequilibrium nature of kinetically frozen solids such as metallic glasses (MGs) is at once responsible for their unusual properties, complex and cooperative deformation mechanisms, and their ability to explore various metastable states in the rugged potential energy landscape. These features coupled with the presence of a glass transition temperature, above which the solid flows like a supercooled liquid, open the door to thermoplastic forming operations at low thermal budget as well as thermomechanical treatments that can either age (structurally relax) or rejuvenate the glass. Thus, glasses can exist in various structural states depending on their synthesis method and thermomechanical history. Nanocrystalline (NC) metals, also considered to be far-from-equilibrium materials owing to the large fraction of atoms residing near grain boundaries (GBs), share many commonalities with MGs both in terms of plastic deformation and its dependence on processing history. Despite these similarities, the disorder intrinsic to both classes of materials has precluded the development of structure-property relationships that can capture the multiplicity of energetic states that glasses and GBs may possess.

Here, we report on experimental studies of MG and NC materials and novel synthesis and processing routes for controlling the structural state – and as a consequence, the mechanical properties. A particular focus will be on strategies for rejuvenation of disorder with the goal of suppressing shear localization and endowing damage tolerance. We also describe a microscopic structural quantity designed by machine learning to be maximally predictive of plastic rearrangements and further demonstrate a causal link between this measure and both the size of rearrangements and the macroscopic yield strain. We find remarkable commonality in all of these quantities in disordered materials with vastly different inter-particle interactions and spanning a large range of elastic modulus and particle size.

KEYWORDS: Metallic Glasses, Nanocrystalline Metals

Presentation Method (Invited/Regular Oral/Poster): Invited

Research on the thermoplastic formability of lightweight Ti-based bulk metallic glasses

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In order to extend the application scope of bulk metallic glasses (BMGs), much attention has been paid to the processing of BMGs in recent years. Taking advantage of the superplasticity in supercooled liquid region, thermoplastic forming is a particularly well adapted technique for processing BMGs as near-net-shape products on length scales ranging from nanometer-order to several centimeters. Ti-based BMGs are very attractive for engineering applications because of their outstanding properties such as high specific strength, good corrosion resistance, etc. However, the relatively poor thermoplastic formability greatly restrain the wide application of Ti-based BMGs. In this study, a series of novel lightweight Ti-based BMGs with enhanced thermoplastic formability have been developed by alloying method based on a $Ti_{41}Zr_{25}Be_{34}$ alloy. The improvement mechanisms of thermoplastic formability induced by different alloying elements have also been systematically studied. The representative $Ti_{41}Zr_{25}Be_{28}Fe_6$ alloy exhibits a wide supercooled liquid region of ~123 K and low viscosity of ~10^6 Pa s in its supercooled liquid region, resulting in the best thermoplastic formability among all the developed Ti-based BMGs. This alloy can be molded into 200 nm-diameter pores in air with the help of wetting layer. Moreover, the good GFA and excellent mechanical properties of $Ti_{41}Zr_{25}Be_{28}Fe_6$ alloy also make it applicable as engineering materials. This work will greatly promote the development and application of Ti-based BMGs.

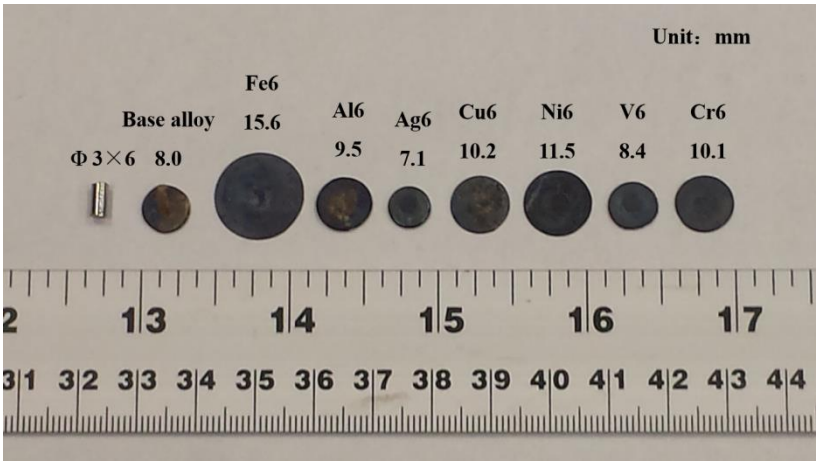

Fig1. Top view of the $Ti_{41}Zr_{25}Be_{34}$ and $Ti_{41}Zr_{25}Be_{28}M_6$ (M: Fe, Al, Ag, Cu, Ni, V and Cr) glassy alloy samples after thermoplastic formability characterization evaluation

KEYWORDS: Bulk metallic glasses; Thermoplastic forming; Thermal stability; Formability

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Development of a novel family of Bulk Metallic Glasses

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Bulk glass formation is observed in many alloy systems when quenching them from the equilibrium liquid. However, the best glass forming compositions show high concentrations of rare, expensive and/or toxic elements like zirconium [1], phosphorous [2,3], or beryllium [1,4], limiting their commercial application. Thus, new glass forming compositions are desirable for the commercialization of metallic glasses on an industrial scale.

Here we report on a completely novel family of bulk metallic glasses (BMGs). We observed bulk glass formation in a variety of multicomponent systems, including Pd-, Ni-, Cu-, Zr- and Ti-based bulk glass forming systems. The compositions differ significantly from the glass forming compositions known so far, making them very interesting for characterization and application.

Among these novel systems, especially the Ti-based alloys are of great interest for many fields of application, since they show casting thicknesses of up to 1 mm in combination with record Ti-contents of 70 at%, resulting in densities comparable to crystalline Ti-alloys. Such a high Ti-content has not been reported for a bulk glass forming alloy so far. By reduction of the Ti-content through specific substitution and addition of alloying elements, the glass forming ability (GFA) can be increased even further up to a diameter of 3 mm. Our results allow designing a new class of low cost Ti-based alloys with good processability and superior properties.

The results of this study are discussed regarding the glass forming process in terms of kinetics and thermodynamics. Due to the compositional differences to the BMG forming liquids known so far, these novel systems may lead to an extended understanding of the thermophysical properties of metallic glasses in general. In summary, this study reveals new strategies for alloy development, leading to a wider application of BMGs.

KEYWORDS: Bulk Metallic Glasses; Synthesis and Processing; Alloy Development;

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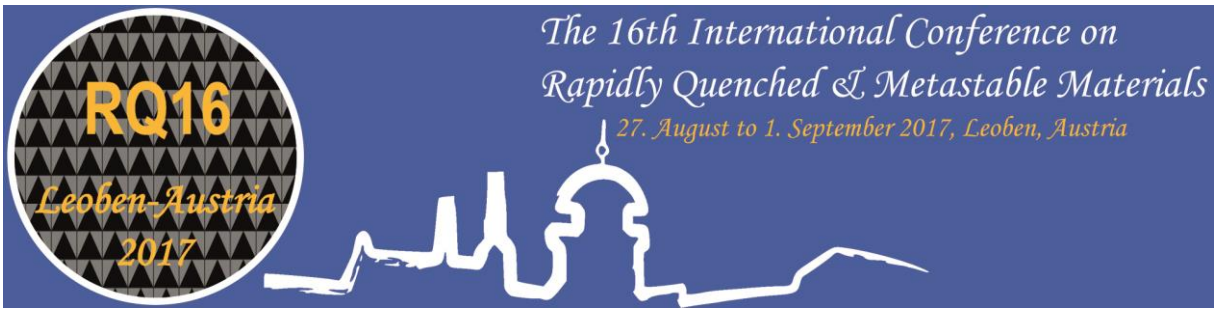
Presentation Method (Invited/Regular Oral/Poster): Regular Oral



B3-Nanostructured materials 2

Fundamental compositional limitations in the thin film growth of metastable alloys

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Epitaxial thin film growth allows synthesizing crystallographic phases and chemical compositions with a high crystalline quality that are unstable under thermodynamically equilibrium conditions. Thus, this technique provides a much wider compositional space for the design of novel materials then what would be possible based on thermodynamic phase diagrams only. Utilization of such non-equilibrium alloys is crucial for many technological applications. Prominent examples are ultra-hard coatings or bandgap engineering for electronic and optoelectronic applications. While the composition range under non-equilibrium growth conditions is significantly larger than the one realizable by equilibrium conditions, compositional limitations still exist. However, the fundamental mechanisms that cause these limitations are often unknown. This makes it hard to predict them or to identify strategies to overcome them.

For ternary $In_xGa_{1-x}N$ group-III-nitride semiconductors, which are the backbone of all modern energy efficient lighting devices, a severe limitation is the efficiency drop in the green part of the optical spectrum. This drop is largely related to the lack of $In_xGa_{1-x}N$ alloys with more than 30% In. Combining efficient thermodynamic sampling strategies with density functional theory we identified the fundamental mechanism that limits the maximum amount of In in epitaxial layers to 25% under experimental growth conditions. A detailed analysis shows that this barrier is related to a hitherto undiscovered surface mechanism – elastically frustrated hybridization. It will be shown that the newly discovered mechanisms link so far contradicting experimental results, lead to chemical ordering and provide a new route to quantitatively predict stoichiometric limitations in alloys synthesized with non-equilibrium growth techniques.

KEYWORDS: thin film growth, metastable alloys, modelling

Presentation Method (Invited/Regular Oral/Poster): Invited

Recent Development on the Processing, Microstructure, and Properties of Nano-eutectic Composites

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Nanostructured alloys exhibit high strength and large elastic strain limit. Unfortunately, the plasticity of these alloys is disappointingly low at room temperature than that of the coarse grain counterparts. In this work, a series of nanostructured-matrix reinforced with second phase dispersions have been developed in Ti-Fe and Ni-Zr based eutectic alloys. These composites exhibit high strength (~ 2 GPa), like bulk metallic glasses and large plasticity (~ 15%) at room temperature, showing superior deformability than that of monolithic nanostructured metallic alloys with uniform grain size distribution, which exhibit <1% plastic strain. Systematic investigations have revealed that the ternary alloy addition produce micrometer-sized proeutectic bcc/fcc solid solution phase(s) with dendritic morphology. Whereas, the residual melt solidifies into a binary nanoeutectic, containing alternating soft bcc/fcc phase together with hard intermetallic phase. It has been observed that the presence of micrometer-size phases are essential in order to avoid catastrophic failure by their interaction with shear bands during deformation. Furthermore, electron microscopic studies of differently deformed specimens have been performed to reveal the role of alternating nanolamellar phases during the transfer of slip across their mutual interface and the origin of plasticity in nanoeutectic composites for possible applications. The effect of alloy additions on the microstructure formation, volume fraction as well as the length scale of the constituent phases and mechanical properties will be been discussed using an analytical model.

KEYWORDS: Bulk Metallic Glasses, Metastable Materials.

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Presentation Method (Invited/Regular Oral/Poster): Invited

In-situ transmission electron microscopy study of freestanding amorphous thin films under stress

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The mechanical behavior of amorphous materials and its connection to the structure are of high technological and scientific interest. But due to the lack of long-range order in amorphous structures this interrelation is not easily amendable even for the case of elastic deformation. Nevertheless, it has been shown that atomic-level elastic strain can be measured by the use of X-ray scattering and the quantification of distortions of diffraction images from circular symmetry [1-2]. Recently, we demonstrated the applicability of this experimental approach to electron scattering of micro/nanoscaled thin films in the transmission electron microscope (TEM) by analyzing distorted selected area electron diffraction (SAD) images that can be acquired down to submicron scale [3]. We applied this method to study the structural and mechanical response of amorphous TiAl thin films deformed within the elastic regime. Hitherto, we focused (i) on the elastic stress-strain response to calculate Young's modulus and Poisson's ratio, (ii) on the local atomic-level elastic strain as a function of sample position (strain mapping), (iii) on uncoupling anelastic and elastic strain [4] and (iv) on the time dependent viscoelastic strain response. In order to obtain the 2D atomic level strain tensor from the geometric changes of the first diffuse ring with sub-pixel accuracy an automatic evaluation procedure was developed.

In-situ tensile deformation was carried out in a standard TEM (Philips CM200) on freestanding amorphous TiAl thin films deposited by magnetron sputtering on a MEMS device. SAD patterns were acquired as function of stress, time and sample position. The distortion of the SAD pattern occurring under stress can be visualized by an image overlay of the pattern with its rotated and inverted counterpart (cf. Fig. 1a). By applying our evaluation procedure the change of the intensity maxima position of the ring with increasing stress can be tracked (cf. Fig. 1b) and the corresponding 2D strain tensor can be calculated.

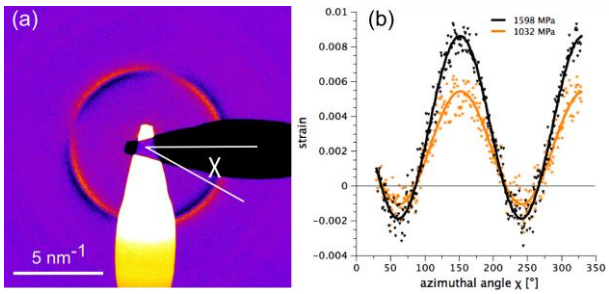

Fig1. Amorphous TiAl thin film under stress. (a) Color coded image overlay of a distorted SAD pattern and its by 90° rotated and inverted counterpart. (b) Atomic level elastic strain (as a function of azimuthal angle χ) measured at two different stress states of the same sample position.

KEYWORDS: Metallic glasses, thin films, mechanical properties.

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5. Financial support by the Austrian Science Fund (FWF): [I1309] and the National Science Foundation (NSF) Grants CMMI 1400505 and DMR 1454109 is acknowledged.

Presentation Method (Invited/Regular Oral/Poster): Invited

Hierarchically Structured Porous Ceramics by Rapidly Freezing Process

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Taking advantage of the principle of unidirectional solidification of a liquid vehicle such as water, ice-templating was developed as a simple and novel method for the preparation of porous structures. The pore characteristics, i.e. the porosity, the lamellar thickness, the pore width and the orientation, have shown a strong correlation with the processing conditions, including the suspension parameters and the freezing conditions. In our study, bioceramics and piezoceramics, i.e. hydroxyapatite (HA) [1], hydroxyapatite-barium titanate (HA/BT) [2], ceramics (alumina) [3] and Lead zirconate titanate (PZT) [4], were used as the raw materials. Results showed that by controlling the rheological properties of the suspensions and the freezing temperatures, the lamellar-type architectures and the properties of ice-templated ceramics can be readily adjusted, as shown in Fig.1(A) and (B). Aligned pores in the surface parallel to the macroscopic ice growth direction and the coexistence of aligned cylindrical and lamellar pore morphologies were obtained by freeze gelcasting, as shown in Fig. 1(C). Both types of pyroelectric harvesting figures-of-merit (F_E and F_E^o) of the PZT ceramics with a porosity level of 25-45 vol.% increased in all porous ceramics, for example, from 11.41 to 12.43 pJ/m^3/ K^2 and 1.94 to 6.57 pm^3/J, respectively, which were higher than the dense PZT counterpart.

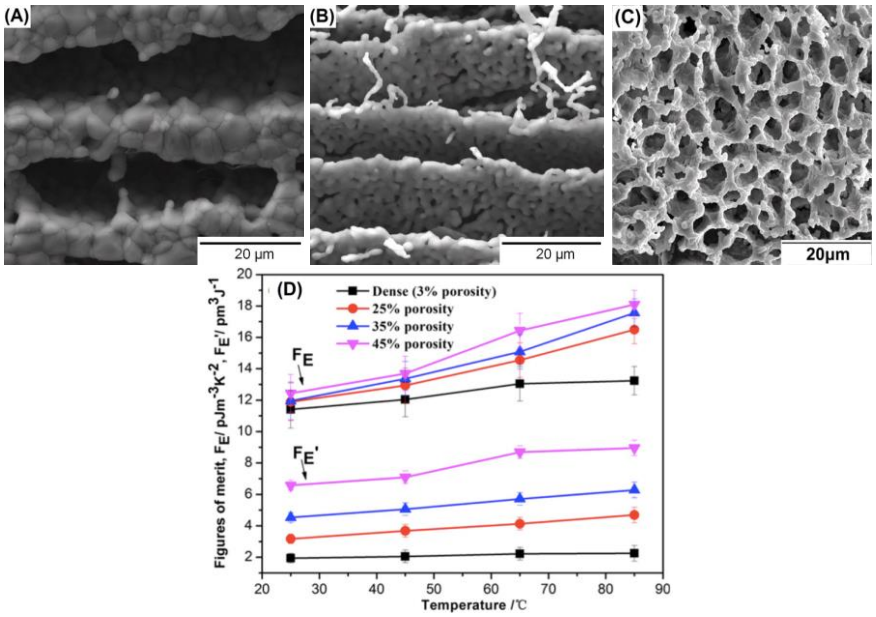

Figure 1 SEM micrographs of (A) and (B) sintered hydroxyapatite porous ceramics obtained from the suspension incorporating different particle sizes[1]; (C) sintered alumina porous ceramics prepared using freeze gelcasting[3]; (D) Pyroelectric figure of merit of the porous PZT[4].

KEYWORDS: Rapidly freezing; Ice-templating; Aligned pores; Bioceramics; Piezoceramics

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Presentation Method (Invited/Regular Oral/Poster): Regular oral

Effects of minor elements on transition energy and color change of Cu-M alloys

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Until now, the color of solid materials is limited to dielectrics, colourimetric sensors, nitrogen coating materials and some novel metal. [1-3]. In case of metal, it is hard to expect another color of metal without gold, silver and copper. They have been used as coloring materials since ancient times because of the change in color of the alloy as the additive elements are added. In the case of gold, from the 14k, 18k and 24k to the rose gold color in recent years, there has been a widespread use of color metals based on gold. In addition, it is used as a dental material and recent research on gold base amorphous [4,5] has attracted much interest as well. However, while it has beautiful color and good mechanical properties, it is being applied at very limited field in small quantities with very expensive electronics or watch of luxury cars. Unlike gold and silver, copper is abundant resources and has been used to focus on mechanical properties and application, such as bronze and brass, rather than being used as precious metals. Copper was easily oxidized compared to gold, which never changes color, and therefore its value as a precious metal was not recognized, so it was not used as a coloring materials. Recently, however, the demand for copper as a coloring material is increasing. As people's attention has shifted from plastic to real metal textures, there has been a growing interest in the optical properties of copper in the interior of luxury automobiles and some parts of electronics. Copper is colored due to the interband transition in the d-band.[6,7] Also, in common with gold alloys the color and transition energy of alloys is changed depend on the kind and component of the added elements.[6,7]

In this study, the influences of additive elements on the transition energy and color difference[8,9] of Cu-X alloy were studied. The elements are divided into three groups which are transition metal zinc, post-transition metal gallium and metalloid silicon. Changes in the transition energy and the color difference of the alloys were analyzed when the elements with the broad solubility in copper were added at the same content of 1,3at%. The transition energy and difference of color are obtained by reflectivity spectrum which is measured by photospectrometer. Measured reflectivity is transformed into tristimulus XYZ value [10] and retransformed to CIE L*a*b* value. The CIE L*a*b* color space [8,9,10] is used to determine the color difference of the material, and furthermore, it is expressed as a chromaticity diagram to determine in which direction the color of the alloy moves. Ultimately, the study aim to find the correlation between color change and transition energy in the color coordinate system.

KEYWORDS: Metals and alloys, interband transition, color metal, Cu alloys, Optical properties

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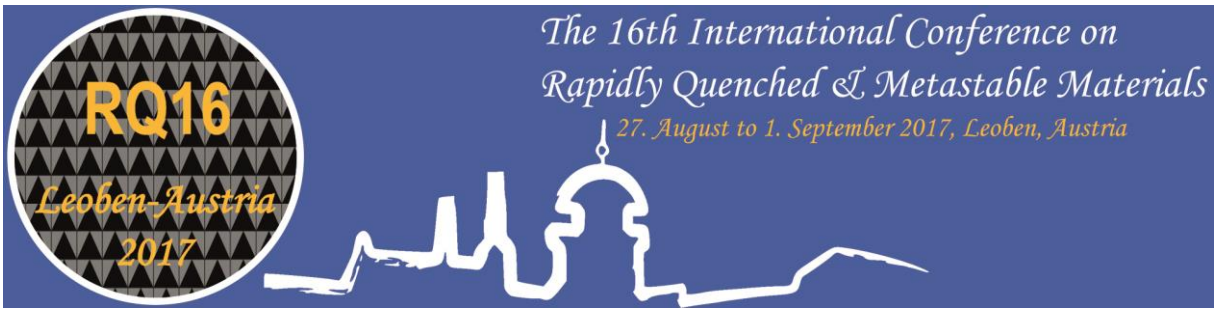

C3-Metallic glass 4: Properties

Liquid-liquid transitions in metallic melts

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Polymorphic transitions are very common in crystalline metals and can be first order transitions like e.g. from austenite to ferrite or second order like in the case of the ordering transition from BCC to B2. Recently polymorphic transitions within the liquid state termed polyamorphisms or liquid-liquid transitions (LLT) have been observed or proposed. This contribution focuses on LLT in bulk metallic glass (BMG) forming melts and gives an overview of recent developments.

The LLT in metallic melts is associated with a crossover from a relatively fragile kinetic behavior at high temperatures to a stronger behavior at low temperatures [1-3]. If the transition is not obscured by crystallization, one observes a latent heat [Fig.1 (b)] of about 10% of the heat of fusion associated with the LLT [3-4]. Recent synchrotron X-ray investigations show that the kinetic fragility is linked to structural changes. [5]. In-situ electrostatic levitation (ESL) undercooling experiments under synchrotron X-ray radiation [Fig.1 (a)] reveal in the $Zr_{58.5}Cu_{15.6}Ni_{12.8}Al_{10.3}Nb_{2.8}$ (Vit106a) alloy system that the transition is associated with structural changes on a length scale of about 1 nm indicating the establishment of medium range order upon transformation [4]. The magnitude of entropy change in conjunction with the ordering energy determines the critical temperature for the transition, which in most BMG forming liquids is located between T_m and T_g. For some systems like Au-based BMG with a weak ordering energy, the LLT may be hidden under the glass transition. In those systems the LLT can be revealed, if the alloy is observed on a long time scale shifting T_g to lower temperatures. The picture emerges, that in multicomponent BMG a LLT is rather the norm than an exception. In these systems the fragility parameter changes from about D*=8-12 in the fragile high temperature liquid to about D*=20-25 in the strong low temperature liquid.

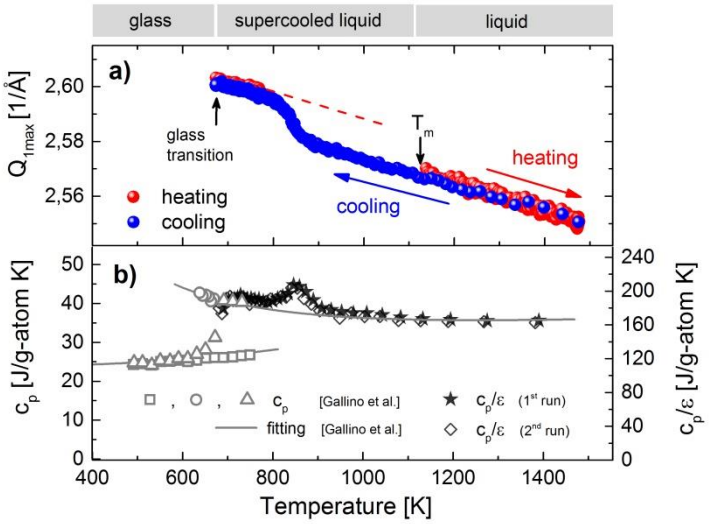

Fig.1. [ref.4] (a) Position of the first maximum of S∗(Q), Q1max, during heating of an initially glassy sample and subsequent cooling down to the glassy state. (b) Ratio of specific heat capacity to total hemispherical emissivity cp/ε calculated from ESL during cooling to the glassy state in comparison with the measured calorimetric cp data of Gallino et al., Acta Materialia 56 (2007) 1367. The LLT is located at about 850 K.

KEYWORDS: Bulk metallic glasses, Chemical and physical properties

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Presentation Method: Invited (Keynote)

Exploiting the elastic properties of metallic glasses

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[2]*Department of Physics, University of Ioannina, Greece*

[3]*Laboratoire de Mécanique de Sousse LMS, ENISo, Université de Sousse, Tunisia*

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Unlike crystalline metals, metallic glasses do not have a periodic lattice with glide planes on which mobile dislocation can cause plastic flow. Consequently, they show a wide elastic strain range on the order of 2% before the onset of plastic deformation which occurs in a highly localized manner on planes of maximum shear stress. Their exceptional mechanical properties lead to a unique and reversible sinusoidal mechanical response of metallic glass foils that are elastically shaped to form an arc. Under a normal load applied on the top of the sinusoidal arc, the foil deforms elastically leading to the successive formation of sinusoidal wavy patterns of higher order. The non-linear load versus displacement response allows metallic glass foils to act as a non-conventional spring with variable equivalent spring constants at different ranges of applied load [1]. This recently discovered mechanically induced undulatory behaviour of metallic glasses [2], resulting from their exceptional buckling response, offers new opportunities for exploring novel functionalities of metallic glasses in a wide range of applications including micro-springs, sensors and actuators, shock absorbance and energy harvesting.

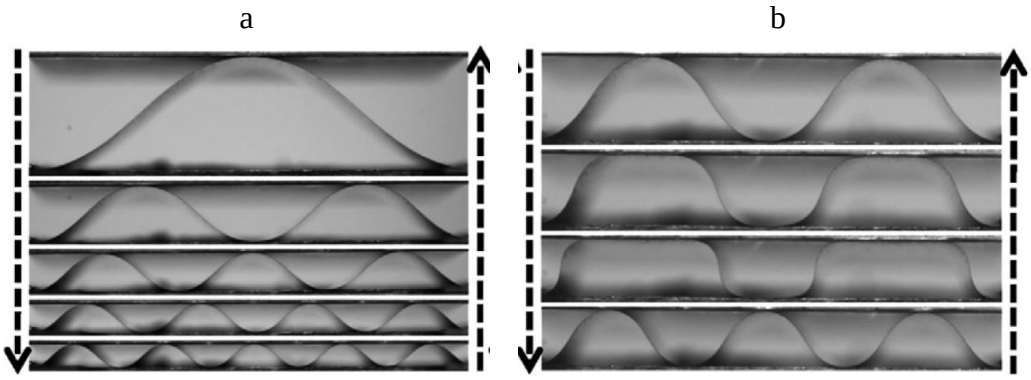

Fig1. Formation of successive sinusoidal wavy patterns of a metallic glass foil under loading applied on the top of an elastically shaped sinusoidal arc and b) elastic deformation between the formation of two (top picture) and three sinusoidal arcs (bottom picture) [1].

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Presentation Method (Invited/Regular Oral/Poster): Invited

Rapidly quenched and amorphous magnetocaloric alloys

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Worldwide, more than 15% of total electric energy consumption is spent on cooling applications. Magnetocaloric cooling is a new cooling technology expected to offer significant energy savings while at the same time the use of harmful, ozone-depleting gases is eliminated [1]. Currently, the most promising candidates for this application, like e.g. La-Fe-Si or NiMn-based compounds, exhibit first-order magnetostructuraltransitions,. Rapid quenching methods can help to refine the microstructure of these materials. For the case of La-Fe-Si, it furthermore reduces the duration of the heat treatment that is needed for the main phase to evolve in a peritectoid reaction [2].

Some magnetic amorphous alloys have magnetocaloric properties that might not be competitive in magnitude with first-order materials [3], but they offer negligible hysteresis and comparatively good mechanical and corrosion-resistant properties in comparison to the crystalline materials mentioned above. Furthermore, amorphous alloys like Pd-based glasses have proven to be suitable matrix materials for making magnetocaloric composites, due to their good thermal conductivity and excellent shapability at the glass transition temperature [4]. We will hence show the potential and limitations of amorphous alloys for magnetocaloric cooling and outline the role of rapid quenching for the production of first-order magnetocaloric alloys.

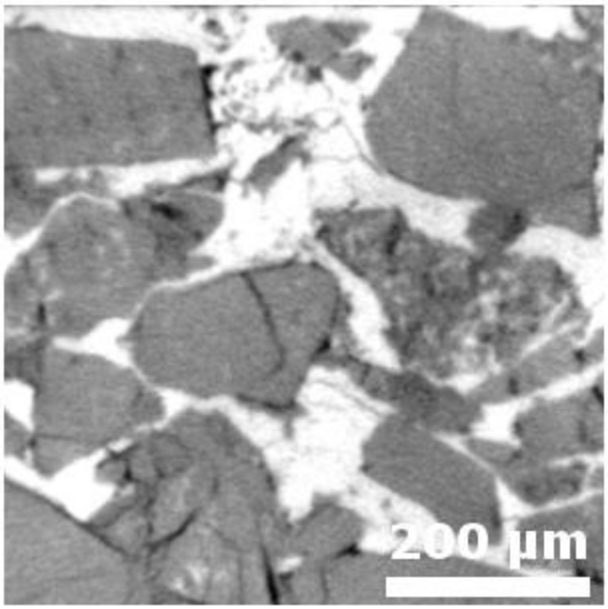

Fig1. Magnetocaloric composite with Pd-based amorphous matrix.

KEYWORDS: magnetocaloric materials, functional amorphous alloys

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Presentation Method (Invited/Regular Oral/Poster): Invited

Characterisation of Corrosion Products of a Ti-Based Metallic Glass in Artificial Pits by In Situ Synchrotron X-ray Diffraction

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Current standard corrosion tests of metallic biomaterials are carried out in vitro in simulated body conditions on bulk components or specimens. These test conditions may not be sufficient to predict the actual behaviour of an implant in vivo. Indeed, it was demonstrated recently that titanium implants can corrode in the absence of wear, generating pro-inflammatory corrosion products leading to revision surgery [1]. The observed corrosion products may have been produced through a localized form of corrosion called mechanically assisted crevice corrosion. Conventional corrosion testing on passive surfaces is not able to predict those corrosion products. More aggressive tests like artificial pit methods, provide more realistic conditions leading to corrosion products similar to the ones found in vivo. Synchrotron X-ray methods can be employed to identify and characterise in situ such corrosion products [2].

Titanium-based metallic glasses hold promise for use in small implants due to their high yield strength. So far, their corrosion behaviour has been characterised using standard polarisation methods on passive bulk specimens. Most of them are passive and have a relatively high pitting corrosion resistance in simulated body conditions.

In this work, we use in situ synchrotron X-ray diffraction to characterise corrosion products generated by a Ti-based bulk metallic glass, i.e. $Ti_{40}Zr_{10}Cu_{34}Pd_{14}Sn_2$ (at.%) [3], inside artificial pits formed in 0.9% NaCl (+ 4% albumin; + 0.1% H_2O_2; + 4% albumin + 0.1% H_2O_2). In all electrolytes, the pit cavity contains a black layer, predominantly Pd, with $PdCl_2$ in some cases, and closer to the interface CuCl typically within ≤100 μm. This suggests Pd nanoparticles may be generated by the glassy $Ti_{40}Zr_{10}Cu_{34}Pd_{14}Sn_2$ alloy during service. The effect of Pd nanoparticles on cell behaviour will be determined in future work.

KEYWORDS: bulk metallic glasses and composites, biomedical and energy materials, chemical and physical properties.

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Effect of yttrium on surface chemistry and passivation stability in Al-based metallic glasses

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Metallic glasses (MGs) possess vastly improved mechanical properties and advanced resistance to corrosion over their crystalline counterparts owing to chemical and structural homogeneity. Also, they are an appropriate reservoir containing active species beyond solid solubility, making them as an ideal model material to elucidate readily the intrinsic feature against corrosion of addition elements.

We note that the formation and stability of passive film for MGs are susceptible to RE addition, but such a correlation has been drawn based on multicomponent alloy systems. In these glassy systems, transition metals as key constituent elements obscure inevitably the RE effect on corrosion itself. To clarify the intrinsic effect of RE on corrosion, excluding the effect of transition metal elements in MGs by proper selection of model alloy system becomes premier. Al-Y binary alloys are useful candidates as an ideal model alloy system due to several considerations. Firstly, aluminum owns a reasonable pitting potential easily to amplify the variation caused by yttrium doping. Secondly, pure aluminum has a better isoelectronic with yttrium, which favors avoiding diffusion and distribution of yttrium ions in passive film being disturbed. Third, Al-Y is a base system for forming best Al-rich BMGs, holding a wide range for yttrium to form fully amorphous structure.

Our aims are to make an attempt to understand how yttrium element influences the corrosion behavior in MGs, especially the formation and stability of passive film. We have examined the polarization behavior of three Al-Y binary glassy samples with different yttrium contents (9-11 at.%), as well as the semiconducting property and composition distribution of passive films. Interestingly, electron work functions (EWF) associated with yttrium effect on electronic transfer and stability of passive film are characterized. This work provides a useful insight into the effect of yttrium on corrosion from the perspective of the structure and energy band of passive film.

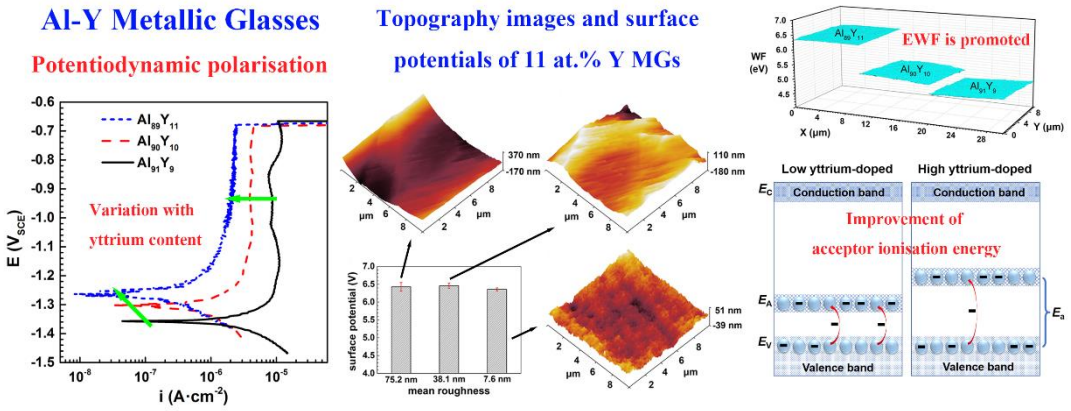
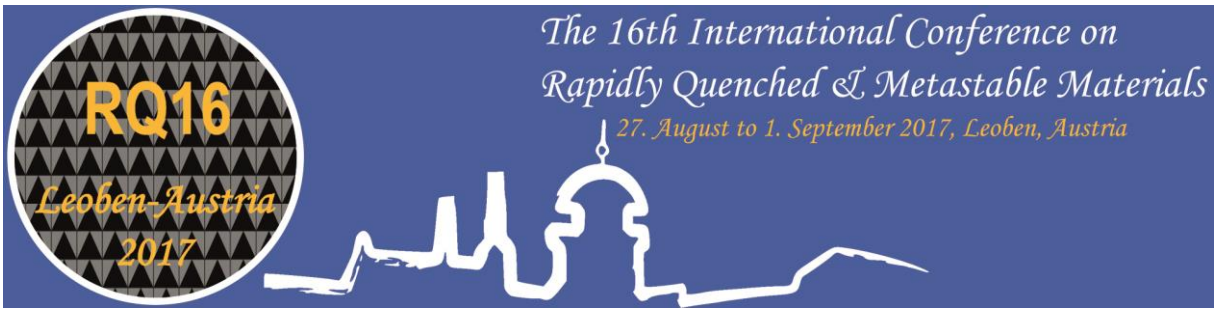


Fig1. Effect of yttrium on corrosion resistance and stability of passive film in Al-rich MGs.

KEYWORDS: High performance materials; Chemical and physical properties

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



A4-Metallic glass 5:

Kinetics

Phase transformations under rapid heating and cooling in metallic nanolaminates

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Heating and cooling rate effects on phase transformations in metallic materials are of importance in many applications. Here, reactive materials in metallic systems, such as metallic nanolaminates, are considered. They produce large amounts of energy when their formation reaction is locally initiated. During initiation and the subsequent self-propagating reaction, reactive nanolaminates transform to intermetallic compounds under heating rates up to 107 K/s. In addition, the characteristic length scales in these materials, e.g. bilayer thickness and grain sizes, can be precisely controlled during deposition. This also enables one to explore correlations between the phase transformations and the initial microstructure. Several in-situ and ex-situ experimental approaches using metallic nanolaminates as model materials will be presented where various heating and cooling rate effects on the nucleation and growth of the intermetallics can be identified and analyzed. Finally, it is shown how these effects serve as a prerequisite for the development of "pulsed metallurgy" as a novel microstructure design tool, e.g. to fabricate nanocomposites with tailored mechanical properties.

Presentation Method: Invited (Keynote)

Phase evolution and kinetics in undercooled $FeCoNiCuX_{0.5}$ alloys

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Recently there has been a surge in the synthesis and evaluation of properties of equi-atomic multi-component alloys that are referred to as "high entropy alloys" and "complex concentrated alloys". These are multi-component alloys and have shown promise in structural and functional application, particularly due to their microstructure stability at high temperatures. Microstructures of these alloys processed through melt route have shown multiple phases which challenges their designation as high entropy alloys. Nevertheless, understanding phase selection as a function of undercooling is crucial to development of these alloys for any significant manufacturing process. Undercooling is an important process parameter that controls the phase selection during solidification. We have chosen equiatomic mixture of Fe, Co, Ni and Cu as the base alloy to which different transition elements have been added to obtain a series of $FeCoNiCuX_{0.5}$ alloys. The fifth element has been varied from the explored list of elements namely Al, Nb, Mo, Ti, W and Zr. Undercooling experiments are carried out on these alloys reaching more than 200 K undercooling in all the alloys. The solidification pathways at different undercooled samples have been determined. Recalescence speeds were measured using a high speed camera. The speeds were sluggish (around 0.5 m/s at deep undercoolings of about 200 K) compared to dilute alloys of Nickel for which reliable experimental data is available in the open literature. We have also studied the segregation behavior using both phase-field approach as well as experimentally characterizing the microstructure. Phase evolution in these alloys includes dendrite phase with eutectic reactions at inter-dendritic region as well as nearly phase-pure microstructure at high undercoolings. Magnetic property measurements and high temperature deformation studies on some of these alloys show promise. A summary of these studies will be presented along with discussion using existing dendrite theories and comparison to the current experimental data. Good agreement between calculations and experimetnal data show that current models of solidification can be extended to these novel alloys too.

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Martensitic transformation behavior related with work-hardening on initial deformation stage of Ti-based bulk metallic glass composite

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Bulk metallic glass composites (BMGCs) have been spotlighted as a highly accessible engineering materials for structural application due to their greatly improved ductility compared with monolith bulk metallic glasses. For example, the Ti- and Zr-based BMGCs with ductile BCC phases have exhibited large plasticity through a severe interaction of deformation mechanism including the dislocation in the crystalline phase and the shear bands in the metallic glass matrix [1-3]. However, the BMGCs containing ductile BCC phases commonly undergo a work-softening during plastic deformation due to the absence of work-hardening mechanism.

Recently, CuZr- and TiCu-based BMGCs containing intermetallic B2 phase represent obvious plastic deformation and exceptionally pronounced work-hardening behavior under compression as well as tension [4, 5]. They asserted that improved mechanical properties are mainly attributed to a stress-induced martensitic transformation behavior of austenite B2 phase to martensite B19' phase, as shape memory alloys (SMAs). The plasticity of these BMGCs depends on the volume fraction and length scale of the B2 phases distributed in metallic glass matrix. Especially, the work-hardening behavior is strongly related with the martensitic transformation and deformation twinning of B2 phase during deformation. These phenomenon of B2 phases have been widely studied in crystalline shape memory alloys. However, most studies about stress-induced martensitic transformation behavior on SMAs are related with deformation mechanism of B2 phase itself. On the other hand, in the BMGCs, B2 phases are surrounded by metallic glass matrix with different mechanical characteristics such as higher modulus, elastic limit and hardness. This implies that stress-induced martensitic transformation progress of B2 phase maybe different with that of SMAs. Therefore it is noteworthy to study detailed martensitic transformation progress of B2 phase at the initial stage of deformation to understand the work-hardening phenomenon of B2 phase-reinforced BMGCs.

In this study, we investigate the progress of stress-induced martensitic transformation depending on the stress state on Ti-based bulk metallic glass composite via systematical transmission electron microscopy analysis. On the stage of elastic deformation (before yielding), the martensitic transformation from austenite B2 phase to martensite B19' phase occurred from interface between B2 particle and amorphous matrix with ~50 nm region. Just after yielding, the martensitic transformed region was extended toward B2 particle with distance of ~130 nm from the interface. Moreover, the deformation twinning of martensite B19' phase in martensitic transformed region was also observed. When 1% plastic deformation occurred, the martensitic transformed region reached up to ~600 nm. Based on these results, it is believed that the high level of stress can be concentrated around the interface due to the elastic mismatch of B2 and metallic glass matrix. As a result, structural gradient morphology originated from phase transition was formed into the B2 particle during early stage of deformation.

KEYWORDS: Bulk metallic glasses; Composite; Mechanical properties; Martensitic transformation behavior; Work-hardening

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

The kinetics behavior of Au-based metallic glass upon ultrafast heatling and cooling

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The crystallization behavior of $Au_{50}Cu_{25.5}Ag_{7.5}Si_{17}$ metallic glass during continuous heating/cooling and isothermal treatment is investigated by ultrafast calorimetry. The relationship between the transformation and the time/temperature scales of the alloy is established experimentally in a wide temperature range from glass transition temperature to the melting point. The compatibility of additivity rule with the crystallization behavior of the glass for both isothermal and isochronal transformations is investigated. The compatibility of additivity rule is verified in a solidification process for the first time; it is proved to be effective in predicting the beginning and the end of isochronal crystallizations during continuous heating and cooling from the kinetic analysis of corresponding experimental isothermal transformation [1]. The predicted isochronal curves are fairly in accordance with the experimental results, especially for the incubation and crystallization processes during rapid solidification of the glass forming liquid. Temperature-dependent viscosity in the expanded supercooled liquid region is derived from the thermodynamic and kinetic analysis of the crystallization behavior of the metallic glass. The nucleation rate and growth velocity for crystallization of the supercooled liquid are analyzed by applying classical nucleation theory and diffusion-controlled growth theory [2].

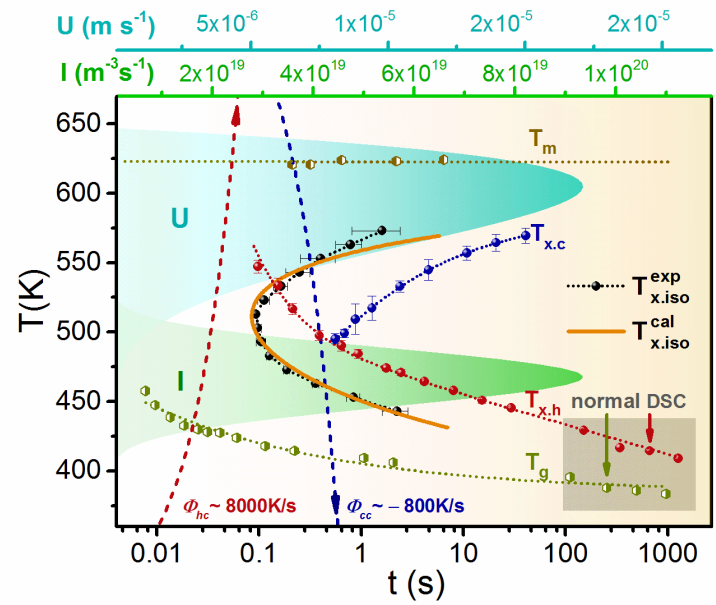

Fig. 1 Summary of isochronal CHT ($T_{x,h}$), CCT ($T_{x,c}$), and the isothermal TTT ($T^{exp}_{x,iso}$ and $T^{cal}_{x,iso}$) curves of $Au_{50}Cu_{25.5}Ag_{7.5}Si_{17}$ MG. The peak shaped shadows in the background show the temperature dependent nucleation rate and growth velocity [2].

KEYWORDS: metallic glass, supercooled liquid, kinetics, crystallization.

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

The kinetic fragility of Pt-P based bulk glass-forming liquids and its thermodynamic and structural signature

Oliver Gross, Benedikt Bochtler, Moritz Stolpe, Simon Hechler, William Hembree, Ralf Busch,

and Isabella Gallino

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Phosphorous containing bulk metallic glass forming alloys (BMGs) are among the best metallic glass formers known to date [1,2]. Pt-P-based BMGs feature a large supercooled liquid region and an attractive color, which makes them highly promising for jewelry applications [3].
In this comparative study, the thermophysical properties of different Pt-P based alloys are investigated using differential-scanning calorimetry and thermal mechanical analysis for the determination of the specific heat capacity and equilibrium viscosity, respectively. The specific heat capacity data was used to calculate the enthalpy and entropy difference between the liquid and the crystalline mixture. The observed compositional dependence of the kinetic fragility in the Pt-P alloy family is attributed to the more pronounced medium range order in the strongest liquid, supported by X-ray scattering experiments, which reveal a pre-peak in the total structure factor with increasing fragility. Adapting a previously reported empirical correlation [4], we show that the more fragile liquid alloys are characterized by a more pronounced dilatation of atomic pair correlations on the length scale of 1 nm. Moreover, the isothermal time-temperature-transformation (TTT) diagram of the $Pt_{42.5}Cu_{27}Ni_{9.5}P_{21}$ composition is presented. In connection with the viscosity data, these measurements are a useful tool for determining process parameters for thermoplastic forming.

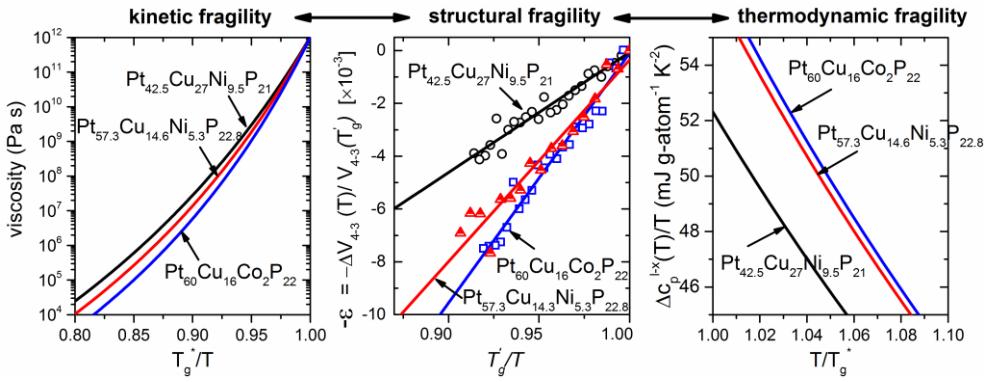

Fig.1: Kinetic (temperature dependence of viscosity), structural (volume dilatation on a length scale of about 1 nm) and thermodynamic (rate of excess entropy change) fragility of three different Pt-P-based bulk metallic glasses [5].

KEYWORDS: Bulk metallic glasses, thermodynamics, kinetic fragility

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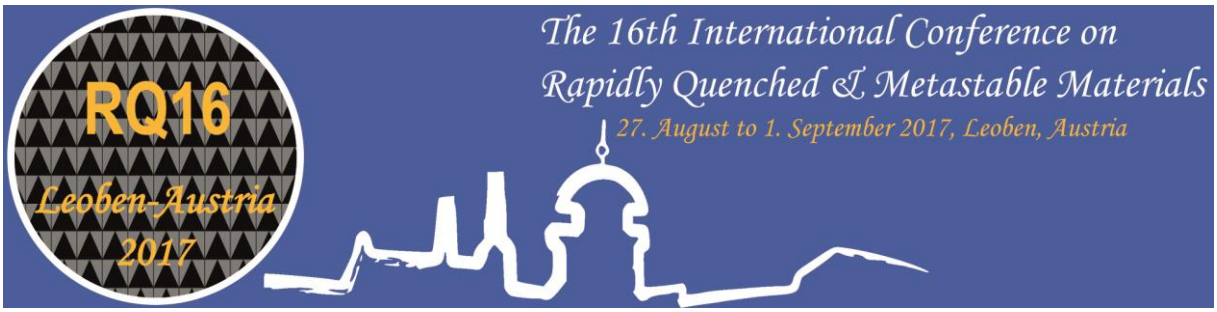
Presentation Method (Invited/Regular Oral/Poster):	**Regular Oral**



B4- Undercooled melts & rapid solidification

Atomic structure changes in disordered materials under hydrostatic pressure

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In last ten years, we have been working on the subject of pressure-induced atomic structure changes in disordered materials, La-based [1], Ce-based [2-4,8], Ca-based [5,9], Pr-based [6], Pd-based [7], As-Se amorphous materials [10,11] at the International Center for New-Structured Materials, Zhejiang University, P. R. China. In this talk, we will summary all results and address two issues: (1) amorphous-to-amorphous phase transformations and (2) amorphous-to-crystalline phase transformations.

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Presentation Method (Invited/Regular Oral/Poster): Invited keynote

Metastable Solidification and Melting in Indium-Tin System

Keiichi N. Ishihara[1], Takayuki Uchima[1], Hideyuki Okumura[1] and Eiji Yamasue[2]

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[2]*Colledge of Science and Engineering, Ritsumeikan University, Shiga, Japan*

The small particles embedded in non-crystalline substance [1] or metallic matrix [2] achieve very high undercooling when they solidify. An added interest is due to reports in the literature [2, 3] of the melting behavior of metastable phases which solidified from a high undercooled liquid. Especially, authors found metastable phase in the undercooled Sn-Bi system using an organic solvent (small droplet method) [2]. In this study, the solidification and melting behaviors of the indium-tin system in silicone oil by the small droplet method were investigated using DSC and X-ray diffractometry. The observed metastable phases can be the supersaturated indium, β' as shown in Fig.1. Considering the published equilibrium phase diagram and thermodynamic data, we will discuss the origin of phase boundary (See Fig.1).

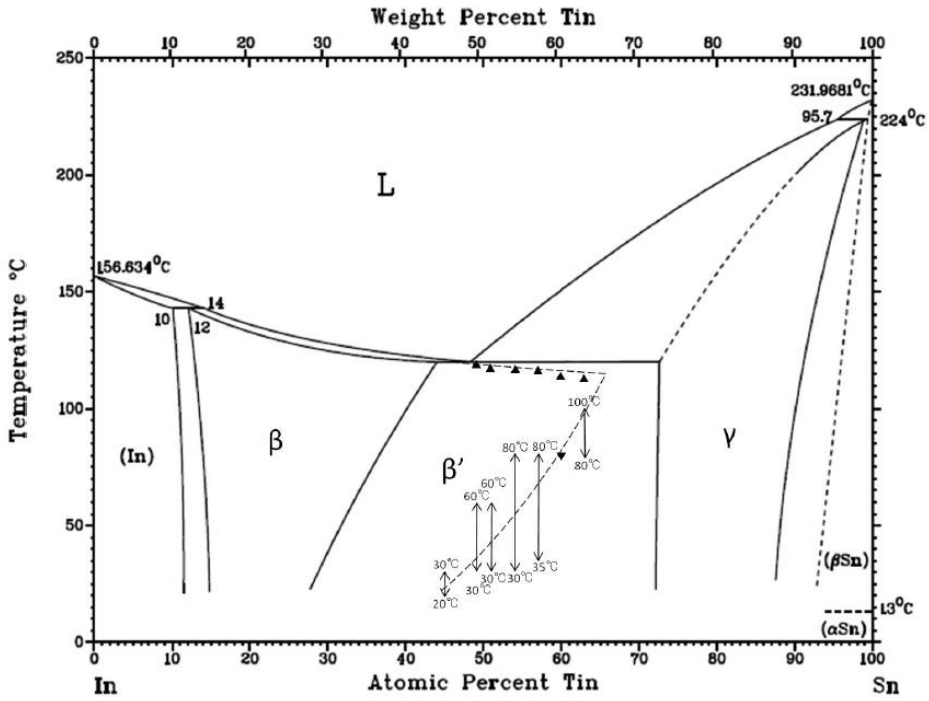

Fig1. Observed metastable melting and decomposition temperatures in the In-Sn equilibrium phase diagram.

KEYWORDS: Nanostructured materials, Chemical and physical properties, In-Sn system, Metastable phase

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Presentation Method: (Invited)

Anomalous sudden drop of temperature-dependent Young's modulus arisen from ferrite-austenite phase transition

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This work reports an anomalous sudden drop of Young's modulus associated with the spike of loss rate during heating a rapidly quenched and severely cold-rolled (CR) duplex stainless steel (DSS) – a phenomenon does not occur in the as-cast (AC) material, as shown in Fig. 1. To understand this phenomenon, the theoretical model for describing both phase transition and mechanical vibration was established. The analytical results indicate that if only the transition between ferrite and austenite phase is considered, the sudden drop of Young's modulus cannot be explained. Considering that the severe plastic deformation induces significant crystalline defects and that these defects serve as nucleation sites of new phases, the recent finding that the nucleation of an ordered phase may involve the intermediate metastable phase [1, 2] is involved in the theoretical model, which can finally well describe both the sudden drop of elastic modulus and the spike of loss rate.

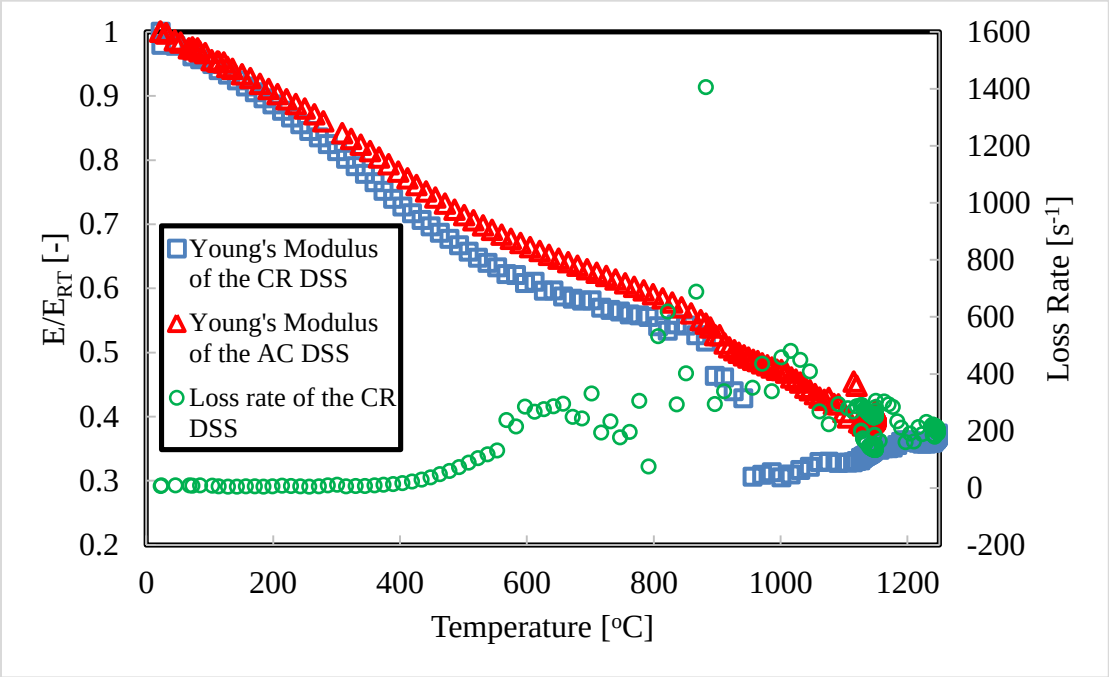

Fig 1. The change of Young's Modulus and loss rate with the temperature.

KEYWORDS: Duplex Stainless Steel, Young's Elastic, Metastable, Phase Transformation

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Combination of the variational method with the random phase approximation for calculation the Helmholtz free energy of simple liquid metals

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The thermodynamic perturbation theory (TPT) is widely used for investigating the structure and thermodynamics of liquid and amorphous metals and their alloys [1]. There are two groups of the TPT methods: methods of the high temperature approximation (HTA) proposed by Zwanzig [2] and methods of the field theory (FT). Within the HTA the entropy and structure functions of the whole system are respectively equal to those of the reference system. The FT approximations allow to avoid these equivalences and give the correction to the HTA Helmholtz free energy obtained in a general form by Itoh [3].

In the present work, the HTA+FT formalism is developed for liquid metals described by the nearly-free-electron approximation for the case when the HTA method is the variational one [4] and the FT method is the random phase approximation (RPA) [5]. The hard-spheres (HS) reference system is used. The different ways of the HS diameter defining are studied.

The work is supported by the Russian Government assignment № 0396-2015-0076.

KEYWORDS: Thermodynamics and phase transformation studies; Chemical and physical properties.

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Relation between self-diffusion and viscosity in liquid $Ni_{66,7}B_{33,3}$

Sarah Zimmermann[1], Fan Yang[1], Zach Evenson[2] and Andreas Meyer[1]

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[2]*Technische Universität München, Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany*

The self-diffusion D describes a single-particle diffusive transport, whereas the viscosity η describes the macroscopic transport of momentum by the collective motion of the particles in a liquid. In liquids, usually both are linked by the phenomenological Stokes-Einstein relation [1]. This relation is based on a model of a large sphere immersed in a fluid, but has been widely applied to derive D from η in liquids or vice versa. However, in $Zr_{64}Ni_{36}$ it has been observed that $D\eta$ = const. in contrast to the Stokes-Einstein relation.
This is on the other hand in line with Mode-Coupling-Theory (MCT) predictions [2] for dense liquids. In order to study whether other metallic melts also exhibit similar behavior we investigated the viscosity and the self-diffusion coefficient of nickel D_{Ni} in $Ni_{66,7}B_{33,3}$. This alloy is of great interest due to its lower packing fraction compared to $Zr_{64}Ni_{36}$.
We measured D_{Ni} and η of the melt using quasielastic neutron scattering (QNS) experiments on the time-of-flight spectrometer TOFTOF at FRM II and oscillating drop technique, respectively. Combined with electrostatic levitation (ESL) technique, this allows precise data being obtained over large temperature range even for the undercooled state of the liquid. It is found that both the Ni selfdiffusion coefficient and the viscosity of the $Ni_{66,7}B_{33,3}$ melt are similar to that of liquid $Zr_{64}Ni_{36}$ within the experimental uncertainties. Furthermore, the product of $D\eta$ exhibits a similar trend for $Ni_{66,7}B_{33,3}$ like $Zr_{64}Ni_{36}$.

KEYWORDS: Melt structure and relaxation studies, Bulk metallic glasses and composites

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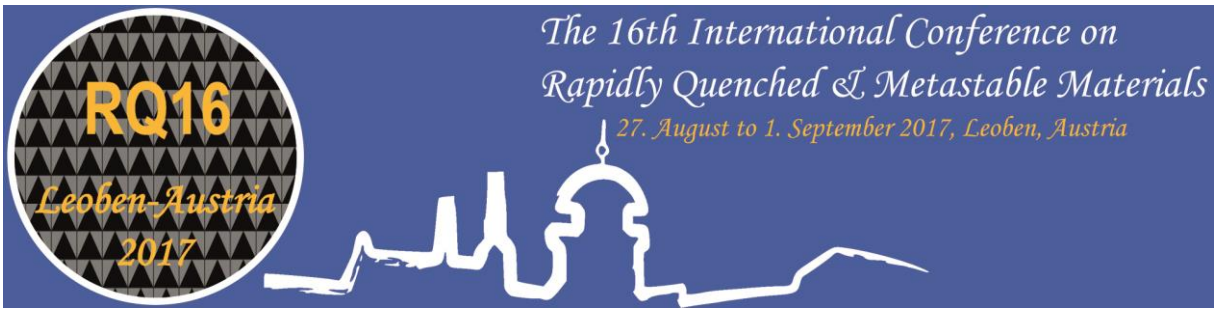
Presentation Method (Invited/Regular Oral/Poster): Regular Oral



C4-High-Entropy Alloys 1

Stability of Solid Solution Phases in High Entropy Alloys

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High entropy alloys (HEAs) are a new class of multi-component equiatomic (or near equiatomic) alloys, which are expected to form simple solid solutions due to their high configurational entropy. However, there are a number of cases where these HEAs show the formation of intermetallics or phase separation. Prediction of the phase formation in HEAs is a major challenge in this field. Phase diagram calculations using Calphad approach indicate that many of the HEAs show the presence of intermetallics at low temperatures. Understanding the stability the phases in these systems is also a major challenge due to possible sluggish diffusivity in these alloys making it difficult to understand whether the phases obtained are thermodynamically stable or kinetically stabilized. The present paper highlights such Calphad calculations in a number of HEA systems and experimental efforts in validating these phase diagrams. Efforts were also made in the present work to measure the diffusivities in some of the HEA compositions both through interdiffusion studies and tracer diffusion studies to get a better understanding on the stability of the phases in the HEA systems. The present talk brings out the excitement in this field and addresses some of the above challenging issues based on the ongoing work in the research group of the speaker.

KEYWORDS: High entropy alloys, Phase stability, Diffusion

Presentation Method (Invited/Regular Oral/Poster): Keynote

Cooling-Rate Effect on the Phase-Formation of High-Entropy Alloys

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High-entropy alloys were developed based on the conception of chemical disorder by mixing 3 ~ 5 major elements. According to the Boltzmann equation: S = k Ln W, (W is the number of real microstates corresponding to the macrostate, k is the Boltzmann constant), high-entropy alloys should be the alloys with many major components and/or the components with high concentrations. Thus, high-entropy alloys also have other names like, complex multicomponent-alloys, multiprincipal elements-alloys, complex-concentrated alloys, compositionally complex-alloys, and concentrated solid-solution alloys.

The phase formation rule for the high-entropy alloys are usually summarized by using the parameters, such as enthalpy of mixing, entropy of mixing, atomic size misfits, electronic negativity, and valence-electron concentration. A parameter like $\Omega=T\Delta S_m/\Delta H_m$, has been proposed to evaluate the balance between the entropy of mixing, ΔS_m, and enthalpy of mixing, ΔH_m, at temperature T. The parameter Ω can also play a role of high-entropy effect for an open system at temperature T.

However，the cooling rate also has a strong influence on the phase formation and microstructure of HEAs. Higher cooling rate may promote the generation of amorphous phase, reducing the micro and macro segregations, and even suppress the formation of intermetallic compounds. The paper will compare the phase formations for the high-entropy alloys with several typical techniques, [1] copper mold casting; [2] melt spinning; [3] sputtering film; [4] Bridgman solidification; [5] electric-magnetic levitation melting. The cooling rate effect on the phase formation and microstructure will be discussed in detail.

KEYWORDS: High-entropy Alloys; Thin films and coatings; Bulk metallic glasses and composites

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5. W. Sheng, *et al., Entropy 18, (2016).*

Presentation Method (Invited/Regular Oral/Poster): Invited

Optimization of Soft Magnetic Properties of High-entropy Alloys by Tailoring Saturation Magnetostriction

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Soft magnetic materials are widely used in many fields, e.g., silicon steel and amorphous alloys for transformers, sensors, and motors. It was reported that, high-entropy $FeCoNi(AlSi)_{0.2}$ alloy has excellent soft magnetic properties, e.g., high saturation magnetization, and low coercive force (H_c), and high resistance. As the soft magnetic material were usually made into thin plates, fibers, films, or complex shapes, the shape-forming ability, such as plastic forming, is also very important. High-entropy soft magnetic alloys may play a balance role between the silicon steels and the amorphous alloys.

It is well known, the H_c is related to the grain size, which shows a maximum curve, that is when the grain size is very close to the domain size, the H_c is the largest, and it will decreasing with the grain size increasing or decreasing. That means the nanocrystalline or amorphous or with single crystal alloys, H_c will be greatly decreased. Our previous work reported two different techniques, e.g., copper mold casting and Bridgman directional-solidification, respectively, to regulate the grain sizes, and then reduce the H_c of the materials.

On this basis, the purpose of this study is to tailor the saturation magnetostriction of the alloys from the idea of changing the alloy composition so as to reduce the H_c. A series alloys with formula of $(Fe_{0.3}Co_{0.5}Ni_{0.2})_{100-X}(Al_{1/3}Si_{2/3})_X$ (X=0、5、10、15、25) were selected, the magnetic and mechanical properties were studied. The alloy samples were prepared by non-consumable arc melting furnace, suction casting, Bridgman directional solidification, and melt-spinning.

KEYWORDS: High-entropy Alloys; Soft magnetic alloys; Saturation magnetostriction; Coercive force; Plasticity

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Nano-scale structural transformations in NiCoFeCrGa high entropy alloy as a function of heat treatments

Ádám Vida[1,5,6], Dávid Molnár[2,4], János L. Lábár[3], Shuo Huang[4], Levente Vitos[4], Nguyen Q. Chinh[1], Jozef Kovac[7], Z. Dankhazi[1], Eva Fazakas[5,6] and Lajos K. Varga[6]

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[2]*Materials Science Group, Dalarna University, Falun, Sweden*
[3]*Research Institute for Technical Physics and Materials Science, Budapest, Hungary*
[4]*Applied Materials Physics, Department of Materials Science and Engineering, Royal institute of Technology, Stockholm, Sweden*
[5]*Bay Zoltán Nonprofit Ltd for Applied Research, Engineering Division, Budapest, Hungary*
[6]*Wigner Research Centre for Physics, Institute of Solid State Physics and Optics, Hungarian Academy of Sciences, Budapest, Hungary*
[7]*Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia*

The non-equilibrium nature of the as-cast NiCoFeCrGa High Entropy Alloy (HEA) is studied as a function of applied heat treatments. Adding *sp* elements to the well known paramagnetic, single-phase (FCC) NiCoFeCr HEA, a multiphase (FCC+BCC) structure will appear, in accordance with the VEC rule [2], where BCC phase is ferromagnetic [1]. With varying cooling speeds, one can tune the ratio of FCC and BCC phases in the alloy. Our SEM, TEM, EELS, AES, MFM and EBSD studies suggest that chromium is the leading element in stabilization of the ferromagnetic BCC phase. In the case of annealing ending with slow cooling speeds, the ferromagnetic BCC phase disintegrates into chromium rich, nano-sized BCC precipitates distributed in FCC matrix. In addition, the correlation of these transformations with the change in mechanical and physical properties will be presented.

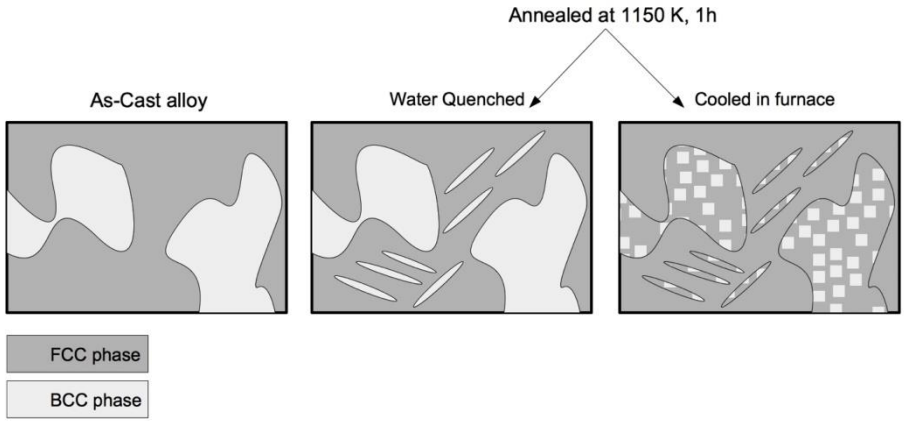

Fig1. Schematics of phase transformations regarded to different cooling speeds.

KEYWORDS: High Entropy Alloys, Non-Equilibrium Alloys.

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Thermomechanical processing of FeCoCrNi(Mn, Al) high entropy alloys

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[2]*OCAS & Material Engineering and Applications, TU Delft, Delft, The Netherlands, Email: mpoluru.tud@gmail.com*

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Conventional alloys consist typically of one main base element and minor additions of other elements, e.g. steel where the base element is Fe. High entropy alloys are a new class of multicomponent metallic alloys, typically built up of 5 elements or more, all present in more or less equimolar amounts. Although the microstructure is rather simple, being either single-phase bcc or fcc or a two-phase mixture of these, very interesting properties have been reported [1,2].

The properties of high entropy alloys are mostly studied in as-cast condition. However, for practical applications, it is reasonable to suppose that further processing (mechanical and/or thermal) might be required to reach the desired shape. It is well known from conventional metal processing that such further processing can alter the properties significantly, via grain refinement, texture development, precipitation.

Recent publications started to highlight the influence of severe plastic deformation (high pressure torsion, severe cold rolling) on the mechanical properties of FeCoCrNiMn [3,4]. In this paper, the feasibility of (hot) rolling and its influence on the mechanical properties is studied. Four compositions from the FeCoCr(Ni, Mn, Al)-family, extensively characterized in literature in the as-cast state [5,6], were lab cast and rolled further to 3mm thickness. After rolling, several heat treatments were applied in the range of 300-1200°C for times of 10 minutes up to 72 hrs. Mechanical properties were assessed in a first step via macro-hardness (HV10). The microstructure was studied by optical and electron microscopy, as well as by X-Ray Diffraction.

Hot rolling was found to induce an increase in hardness in all compositions. Recrystallization kinetics was typically very sluggish, although strongly dependent on the actual composition. Heat treatment after rolling can induce further strengthening. The correlation with the microstructure will be discussed.

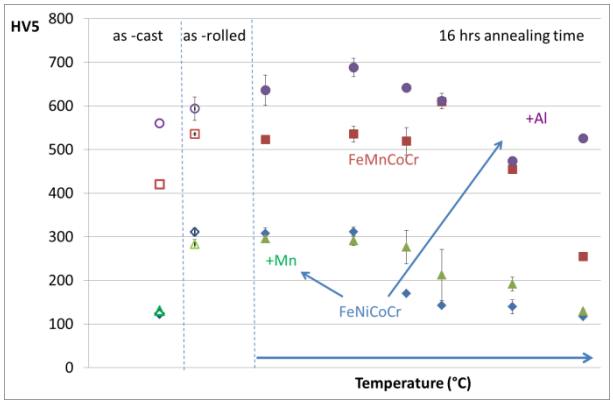

Fig 1: Evolution of hardness after rolling and heat treatments

KEYWORDS: High entropy alloys, Thermodynamics and phase transformation studies

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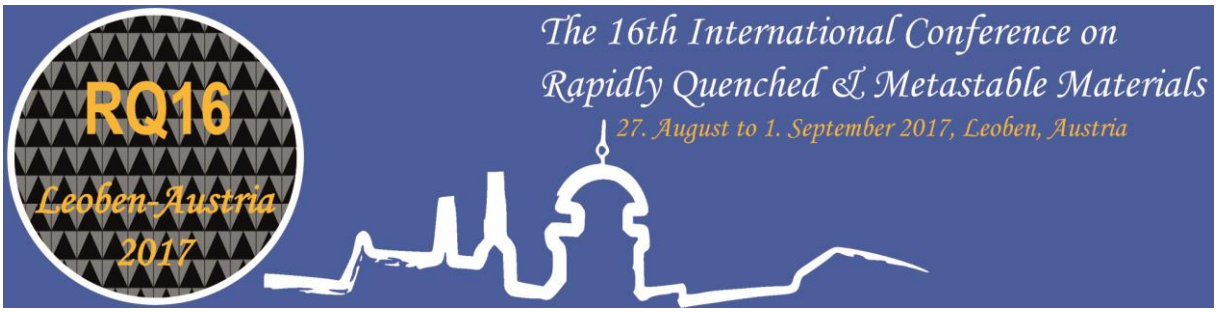
Presentation Method (Invited/Regular Oral/Poster): Oral



Wednesday, 30th August

Homogeneous deformation of metallic glasses at room temperature

A. L. Greer

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What are the prospects for bulk metallic glasses with tensile ductility? There is increasing interest in how thermomechanical processing can change the structure and properties of metallic glasses, giving access to a wider range of glassy states [1]. It is well known that when metallic glasses are plastically deformed at room temperature, the flow is sharply concentrated in *shear bands*. This instability arises from work softening, leads to effectively zero ductility, and is the main impediment to wider exploitation of the otherwise highly attractive mechanical properties of metallic glasses.

Microscopical observations and atomistic simulation provide strong evidence that the shear-band thickness is only 10-20 nm [2]. Yet it has become ever more clear in recent years that the effects of plastic deformation at room temperature must extend far beyond the ultra-thin central plane of the shear bands. Affected zones more than 100 mm thick are suggested by mechanical [3-5], calorimetric [3], and microstructural observations [6,7]. Indeed, thicker affected zones are necessary to explain the effects of deformation on overall properties such as enthalpy and volume of metallic-glass samples [1]. The shear-band instability can be suppressed in small samples and when the flow is constrained [8,9].

We review recent findings on the remarkable structural and property changes that can be induced in small samples of metallic glass, and assess the prospects for realising these changes in bulk samples.

KEYWORDS: Metallic glasses, mechanical properties

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Presentation Method (Invited/Regular Oral/Poster): Plenary

Structure and dynamics of hyper-quenched metallic glasses

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The cooling rate dependence of structure and properties of metallic glasses has been an important topic of intense discussion because of the metastable nature of glassy state. However, despite great efforts devoted to this subject for decades, many fundamental questions remain to be poorly known. We developed a hyper-quenched Zr-based metallic glass with a cooling rate as high as ~3.6×10^9 K/sec, which is ~3-6 orders of magnitude higher than that of conventional metallic glasses fabricated by melt spinning. The ultrahigh cooling rate effectively freezes the glass at a high energy state with a high fictive temperature (T_f) approaching to the melting point T_m (T_f=0.83T_m) of the alloy.[1] The hyper-quenched metallic glasses show significant structure heterogeneity, originating from local structure variation from icosahedral to tetragonal crystal-like order, together with amplified sub-Tg relaxation. By controlling the excess enthalpy release of the hyper-quenched glasses, the coupling between successive degeneration of spatial heterogeneity and the evolution of dynamic properties provides compelling evidence on the structural origins of sub-T_g relaxation and thereby mechanical properties of metallic glasses.[2]

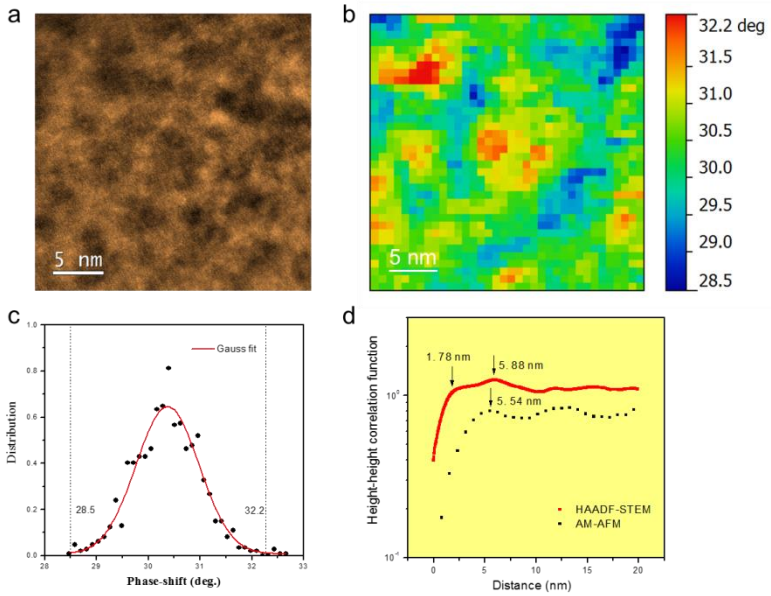

Fig1. Spatial heterogeneity of a hyper-quenched metallic glass characterized by HAADF-STEM and AM-AFM. (a) HAADF-STEM image and (b) a magnified AM-AFM phase shift mapping. (c) The phase shift distribution. (d) Correlation function curves derived from the HAADF-STEM image and the AM-AFM mapping.

KEYWORDS: Metallic Glass, Dynamics, Structure.

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Presentation Method (Invited/Regular Oral/Poster): Plenary

Alloy nanoparticle ink for printing obtained through non-equilibrium processing

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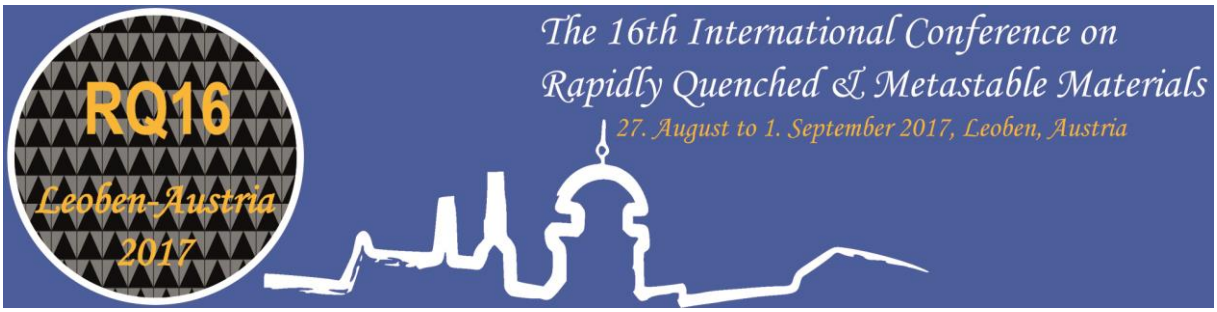
Printing represents a powerful tool for manufacturing lower dimension architectures for functional, chemical and biological applications. This is a thin film counterpart of the additive manufacturing and has immense potential. However, the success depends on understanding and synthesising nano metals and alloys that can be converted to ink with all the consequent effects of nano-dimensions on the phase formation and their stability. For several years we are exploring ways of producing inks of metals and alloys without resorting to chemical reactions that often modify or contaminate the particles by the reaction products. The two most successful non-equilibrium techniques for preparation of inks of metals and alloys that we have adopted are laser ablation under a liquid (PLAL) and cryomilling. Both of these represent powerful techniques for developing colloidal ink and are capable of controlling both the chemistry, phase morphology and sizes. We shall discuss through examples from pure iron, silicon, intermetallics as well as nanoparticles of immiscible alloys, the scientific and technological challenges that we have faced and new results that we have obtained on structures, morphologies and the properties of these nanoparticles and their inks.

Presentation Method (Invited/Regular Oral/Poster): Plenary



A5-Metallic glass 6: Structure

Phase transitions in Au based metallic glasses studied via chip calorimetry

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The glass formation, crystallization and phase transition behavior of Au based metallic glasses is studied via chip calorimetry, which provides heating and cooling rates of several 10^4 Ks^{-1} and 10^3 Ks^{-1}, respectively. It is shown that critical cooling and heating rates can be determined. Moreover, complete time-temperature-transformation maps for Au based metallic glasses on cooling and on heating can be measured and insights into the temperature dependence of crystal growth can be gained [1]. Suitable conditions and influences of FDSC measurement parameters like sample mass and sensor surface material are shown [2]. Finally, experimental evidence for an exotic solid-solid transition in an Au based metallic glass occurring via metastable melting under strong non-equilibrium conditions, is given. The transformation path starting from the glassy state and evolving to the supercooled liquid, a metastable crystalline state, a metastable liquid, a more stable crystalline state and finally the equilibrium liquid is discussed under its thermodynamic and kinetic prerequisites [3]. Such behavior is not usual in metallic systems, but has recently been confirmed via the pressure path for pure bismuth [4]. We also shown that the detection of the solid-liquid-solid transformation in chip calorimetry depends on the thermal history, which is explained via a thermal route effect on the nucleation of the stable condition. Moreover, the microstructure evolution is discussed using scanning electron and transmission electron microscopy and X-ray diffraction results.

KEYWORDS: Bulk metallic glasses, Thermodynamics and phase transformation studies

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Presentation Method (Invited/Regular Oral/Poster): Invited

On the universality of cryothermal cycling as a method for structural changes in metallic glasses

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Plasticity of metallic glasses highly depends on their atomic composition and energy state. It appeared that, more relaxed glasses exhibit less plastic strain, therefore, to increase the glass plasticity the energy level of the glass should be increased. There are many different ways to store the energy in the glass. It can be done from top down approach (fast quenching) or from bottom up (plastic deformation, static loading *etc*.) Recently another method for metallic glass rejuvenation was found [1]. Cryothermal cycling of metallic glass found to induce an increase of plastic strain by several percents. However, the applicability boundaries of the method for metallic glasses are still unknown.

The influence of cryothermal treatment on the mechanical properties of metallic glasses with different compositions ($Zr_{60}Cu_{20}Fe_{10}Al_{10}$, $Zr_{60}Cu_{20}Co_{10}Al_{10}$, and $Zr_{60}Cu_{20}Ni_{10}Al_{10}$) was investigated in the present work. It was found that cryothermal cycling can induce rejuvenation as well as relaxation of metallic glasses. The increase of the local Young's modulus and its spatial distribution width on the surface of metallic glass after cryothermal cycling was found. It was evaluated by quantitative nanomechanical measurements using an atomic force microscope (AFM) with a diamond tip cantilever. However, this increase was temporary and disappeared after some time. This effect was connected with the large distribution of relaxation times in metallic glasses due to their heterogeneous structure and formation of native oxide on the outer surfaces of the glass. It was established that cryothermal cycling treatment can improve or deteriorate the plasticity of metallic glasses and the atomic bond structure appears to be very important to determine the outcome of the treatment.

KEYWORDS: Bulk metallic glasses and composites, Chemical and physical properties

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Characterization of the $Fe_{67}Mo_6Ni_{3.5}Cr_{3.5}P_{12}C_{5.5}B_{2.5}$ bulk metallic glass forming alloy

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Fe-based metallic glasses gained considerable interest as they show extraordinary material properties, like high strength and high hardness even compared to other metallic glasses [1]. A further crucial advantage is the low price and good availability of iron, thus making Fe-based glasses interesting for industrial applications. Of special interest is the production of small and/or complicated structures, like precision gears or micro actuators, where the high hardness and wear resistance of Fe-based BMGs come into effect.

In the present work, the bulk metallic glass steel $Fe_{67}Mo_6Ni_{3.5}Cr_{3.5}P_{12}C_{5.5}B_{2.5}$ (0.52 wt% C) is characterized in detail to evaluate its general applicability [2]. This alloy was designed by Johnson and co-workers [3] and provides a high critical casting thickness of 13 mm, thus allowing for the casting of amorphous parts with a considerable size and a high yield strength of 3.1 GPa. For the casting of amorphous parts, as well as the processing via thermoplastic forming, thermodynamics and viscosity of an alloy are crucial.

The thermophysical properties including the specific heat capacity were measured using calorimetric methods. The crystallization behavior of amorphous samples upon heating was characterized by differential scanning calorimetry and X-ray diffraction and a time-temperature-transformation diagram was constructed. The equilibrium viscosity below the glass transition as well as volume relaxation behavior were measured by three-point beam bending and dilatometry, to assess the kinetic fragility. Viscosity in the liquid state was determined, using electromagnetic levitation in microgravity on a reduced gravity aircraft during the TEMPUS campaign of the German Aerospace Center (DLR). The alloy displays a strong liquid behavior at low temperatures (three-point beam bending) and a fragile behavior at high temperatures (electromagnetic levitation), as shown in Fig 1. These results are analog to the ones observed in several Zr-based bulk metallic glass forming liquids [4], indicating a strong to fragile liquid-liquid transition.

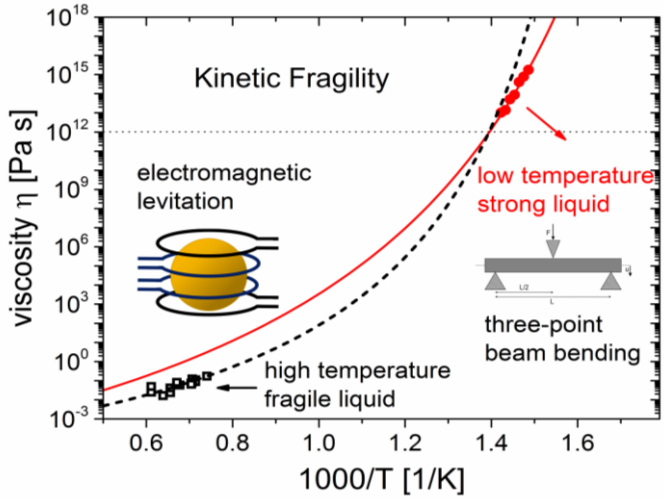

Figure 1: Viscosity over inverse temperature, measured at high and low temperatures by the oscillating drop method in electromagnetic levitation and by three-point beam bending respectively.

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2. B. Bochtler, O. Gross, I. Gallino, and R. Busch, Acta Mater. **118**, 129 (2016).

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4. S. Wei, F. Yang, J. Bednarcik, I. Kaban, O. Shuleshova, A. Meyer, and R. Busch, Nat. Commun. **4**, 2083 (2013).

KEYWORDS: Bulk metallic glasses, Thermophysical properties, Rheology, Kinetic fragility

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Microstructural characterization of brazed Ti joint using $Ti_{20}Zr_{20}Cu_{10}Ni_{50}$ metallic glass ribbon as filler

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In the present investigation, we present our results on characterization of Ti joints, brazed with metallic glass ribbons of $Ti_{20}Zr_{20}Cu_{10}Ni_{50}$ alloy. Initially, metallic glass ribbons were produced using a vacuum melt spinner. These ribbons were then used as filler materials for vacuum brazing of two Ti alloy plates at 1000°C. The thermal stability of the as-spun ribbon was determined using Differential Scanning Calorimetry (DSC) in the non-isothermal mode. Both as-spun and brazed joints were characterized using X-ray Diffractometry (XRD), Field-Emission Scanning Electron Microscopy (FESEM), Transmission Electron Microscopy (TEM) and the energy dispersive X-ray spectroscopy (EDX) attached to both TEM and FESEM. The as-spun ribbons showed fully amorphous when examined on both surfaces by XRD and also verified by TEM investigation. The detailed DSC results revealed that the amorphous phase crystallized at approximately 512°C. The brazing joint of two Ti-plates using the metallic glass ribbon was found to be very sound. FESEM characterization of the cross-sectioned brazing joint shows sub-micron size grains uniformly distributed in the matrix with brighter appearance. EDX analysis revealed that the sub-micron grains are rich in Ti while the matrix phase has Zr-enrichment. BSE image also suggests substantial reaction of the brazing ribbon with Ti plates, whose typical lath microstructure is modified to nanostructured lamellar eutectic microstructure comprising of Ti-rich and Zr-enriched phases.

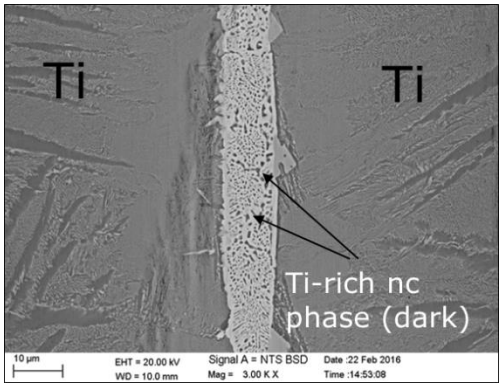

Fig.1.Interfacial microstructure of Ti joints brazed with Ti–Zr–Ni–Cu filler metal at 1000°C for 10 min.

KEYWORDS: Metallic glass, Brazing, Scanning electron microscopy, Energy dispersive spectroscopy, Transmission Electron Microscopy.

Presentation Method (Invited/Regular Oral/Poster): Oral

Metallic Glass Composites with Shape Memory Alloys

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Bulk metallic glass composites (BMGC) reinforced with a crystalline phase, which shows stress-induced martensitic transformation exhibit both enhanced ductility and work hardening as compared to the conventional BMGC. By using molecular dynamics simulations we investigate the deformation mechanism of BMGC with B2 CuZr inclusions and provide an effective strategy to control the strain localization by systematically varying the fraction of the martensitic phase and its spatial distribution. [1] We show that the shear band nucleation and localization is strongly influenced by the martensitic transformation of the B2 phase. We seek to understand the competing deformation mechanism in martensitic nanoparticles and glassy matrix, especially, the shear band nucleation induced by the martensitic transformation in crystalline precipitates and the intersection of a shear band with a shape memory inclusions. The interaction between shear bands and B2 nanoparticles can be witnessed from the shear band morphology changes with the evolution of the phase transformation in the martnesite. The width increase of a shear band reduces the elastic shear stress in the vicinity of the nanoparticles, and thereby impedes the further propagation and formation of critical shear bands. Due to their unique and complex deformation behaviour the BMGC with shape memory alloys represent a promising route for controlling the properties of glassy materials.

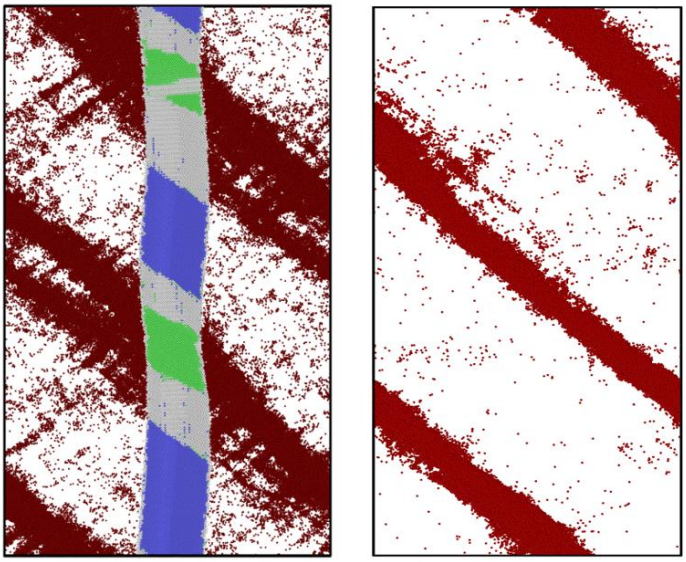
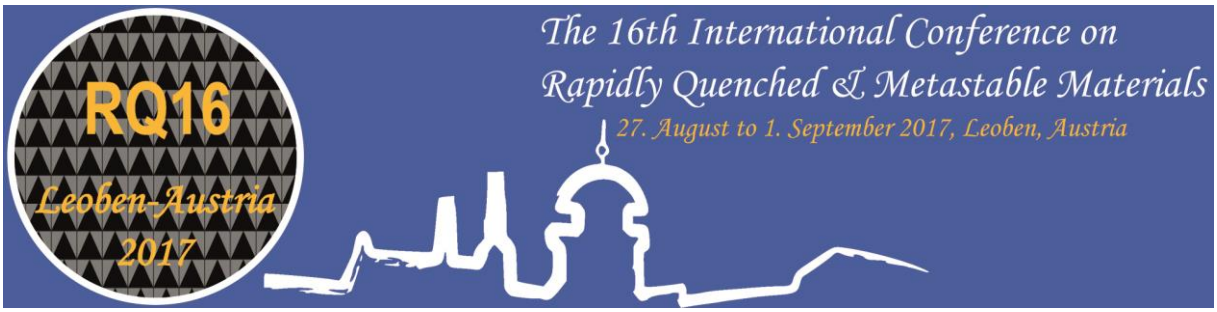


Fig1. Local atomic shear strain from MD simulations in a composite BMG with a B2 CuZr nanowire in comparison to a monolithic BMG deformed in uniaxial tension. Only those atoms with a local atomic strain higher than 0.2 are plotted.

KEYWORDS: bulk metallic glasses and composites, nanostructured materials

1. D. Sopu, M. Stoica and J. Eckert, *Appl. Phys. Lett.* **106**, 211902 (2015).

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



B5-Metallic glass 7: Deformation

On the Fracture Behavior of Bulk Metallic Glasses

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High strength in combination with low stiffness, high hardness, large elastic strain limits and near net-shape castability make bulk-metallic glasses (BMGs) candidate materials for many structural applications. Major drawbacks for their use in engineering service, however, are highly variable fracture toughness values (ranging from less than 10 to more than 200 MPa.m$^{1/2}$) and ductilities which can be entirely different for loading in tension, compression or bending. Specifically, whereas ductility is rather limited in ten-sion/compression, BMGs can be quite ductile in bending. Due to the often limited dimensions of cast BMGs, standard fracture-toughness tests are generally performed on smaller-sized samples with dimensions often comparable to the critical bending thickness of a glass. This critical bending thickness is defined as the dimension below which a glass can achieve the relevant number of shear bands to demonstrate significant bending ductility [1] (Fig. 1a). To date, however, it is not clear how BMGs would behave in such fracture toughness tests evaluated on samples with dimensions that are either below, above, or comparable to a glass's critical bending thickness. Furthermore, while fracture toughness tests are often performed with "bending" geometries (three-point bending, compact-tension specimens), it has yet to be determined how the behavior in BMGs under these constrained stress-states relates to that in tension; as such, the extent of validity of nonlinear-elastic fracture mechanics to characterize their toughness may be brought into question. Here, we report on a systematic study on Zr and Pd-based glasses to investigate the influence of sample size and loading condition on the fracture toughness of BMGs. Results show that with decreasing sample size the fracture behavior changes from brittle failure with low fracture toughness, via a semi-brittle failure regime, to fully ductile fracture and non-catastrophic failure with sub-critical crack growth, *i.e.*, *R*-curve behavior [2] (Fig. 1b). Our tests on samples subjected to different stress-states (three-point bending vs. tension loading) result in highly variable data which brings into question the extent of validity of nonlinear elastic fracture mechanics to characterize the toughness of BMGs.

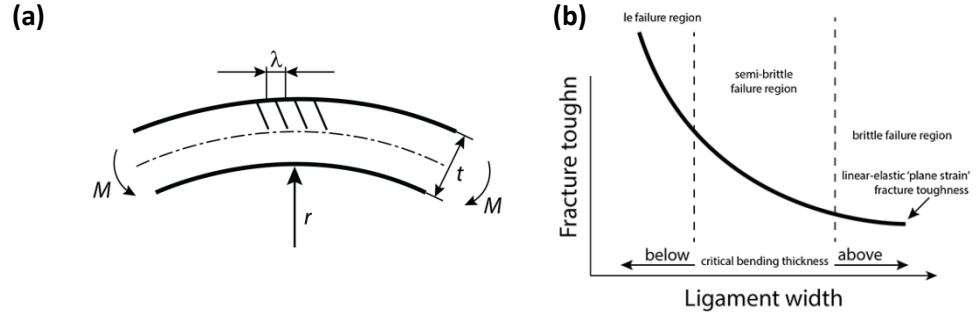

Fig1. (a) Below a certain critical thickness, *t*, the spacing of shear bands, λ, in BMG samples decreases with increasing bending moment, *M*, and decreasing radius, *r*, thereby enabling glasses to prevent catastrophic failure through the formation of multiple shear bands resulting in increasing ductility in bending with decreasing thickness [1]. (b) BMGs show a strong dependence of their fracture toughness on the size, particularly the ligament width, *b*, of the tested samples. (Figure taken from [2].).

KEYWORDS: bulk metallic glasses, fracture toughness, sample size, strain softening, bending ductility.

R.D. Conner, W.L. Johnson, N.E. Paton, W.D. Nix, *J. Appl. Phys.* **94**, 904 (2003).
B. Gludovatz, D. Granata, K.V.S. Thurston, J.F. Löffler, R.O. Ritchie, *Acta Mater.* **126**, 494 (2017).

Presentation Method (Invited/Regular Oral/Poster): Invited Oral

Case study on $Ti_{40}Zr_{10}Cu_{36}Pd_{14}$ bulk metallic glass: from lab-scale samples to real-size machined dental implants

A. Liens[1, 2], A. Etiemble[1], P. Rivory[1], S. Balvay[1], J. M. Pelletier[1], S. Cardinal[1], D. Fabrègue[1], H. Kato[3], N. Courtois[2], D. J. Hartmann[1], J. Chevalier[1]

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Titanium Ti-64 alloy (Ti-6Al-4V) has been traditionally used for many years to design implants and other medical devices. However, this alloy has reached a *plateau* in terms of mechanical properties, which can be a concern as down-sizing of implants has become one of the major issues in modern medicine. For these reasons, Bulk Metallic Glasses (BMGs) have gained increasing attention during the past decades, as they exhibit an excellent combination of properties and processing capabilities desired for biomedical applications. However, for a long time and despite their promises, the use of amorphous metallic alloys has been restrained due to the small dimensions achievable. Nevertheless, in the case considered here, this is not an issue regarding the small dimensions of dental implants pieces.

In this study, focus was set on the well-known Ti-based $Ti_{40}Zr_{10}Cu_{36}Pd_{14}$ BMG developed and extensively studied in the last ten years by Inoue's team [1, 2]. This BMG appears very attractive for future biomedical applications thanks to its high glass forming ability, the absence of toxic elements such as Ni and Be and its good mechanical properties.

Machining of mini-invasive dental implants and standard mechanical testing of implant-abutment assemblies made of metallic glasses have never been done before, which is a crucial step to ensure that they can be used as dental materials. For the first time, in this study, a complete and exhaustive characterization on a unique batch of this glassy alloy was performed, including electrochemical measurements, analysis of the effect of medical sterilizations and cytocompatibility tests, together with ISO standard mechanical tests on implant-abutment assemblies prototypes machined in real conditions. The results were compared to the benchmark Ti-6Al-4V (ISO5832-3) to assess its potential in dental implantology and its easy and feasible machinability.

BMG rods with diameter of 5 mm were prepared by copper mold-tilt casting. Real-sized narrow diameter dental implants (Ø 2.8 mm) and abutments assemblies prototypes were machined following the same machining conditions as real medical grade Ti-6Al-4V implants, including a turning step on Computer Numerical Control lathe and a sandblasting with a resorbable blasting media (HAP/TCP mixture) followed by acid washing in HNO_3. Mechanical characterization and evaluation of the load to failure of the implant-abutment assemblies were evaluated following the geometrical specifications of ISO 14801. Fatigue was performed in 0.9% NaCl solution. Resistance to sterilization was checked after 20h of heating at 134°C or submission to 4 doses of 40 kGy of gamma rays. Electrochemical measurements were conducted in a three electrode cell in saline solution (0.9% NaCl, pH: 7.4, following the ISO 10271 standard), at 37 °C open to air. Direct cytotoxicity tests were carried out using MG63 osteoblasts and Human Dermal Fibroblasts (HDFa) cells to evaluate the cells' proliferation and adherence after 3, 6 and 10 days of culture.

The results show that the $Ti_{40}Zr_{10}Cu_{36}Pd_{14}$ can be as easily machined as Ti-6Al-4V alloy. Tests on dental implants reveal a load to failure 1.5 times higher than that of Ti-6Al-4V alloy and a comparable fatigue limit (despite the presence of quite large casting defects). Moreover, the alloy exhibits excellent mechanical properties (compressive strength of 2 GPa, hardness of 5.5 GPa and a toughness of 56 MPa$\sqrt{m}$) with good corrosion resistance and satisfactory biocompatibility. The alloy is perfectly resistant to sterilization.

These properties make this metallic glass the most promising class of materials for mechanically challenging applications and $Ti_{40}Zr_{10}Cu_{36}Pd_{14}$ appears as a viable alternative to Ti-6Al-4V alloy for the manufacturing of implants and abutments assemblies for future dental applications.

KEYWORDS: Ti-based bulk metallic glass; biomaterials; dental application; mechanical properties; machining; biocompatibility.

S.L. Zhu, X.M. Wang, F.X. Qin, A. Inoue, *Mater. Sci. Eng.* A 459 (2007) 233-237.

F.X. Qin, M. Yoshimura, X. Wang, S. Zhu, A. Kawashima, K. Asami, A. Inoue, *Mater. Trans.* Vol. 48, No.7 (2007) 1855-1858.

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Different ways to improve plasticity in bulk metallic glasses

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Metallic glasses are easily deformable at high temperatures. On the other hand, at room temperature the majority of them are brittle and do not show any noticeable plasticity. This constitutes a major handicap for applications in the mechanical or biomedical field. To overcome this disadvantage, various methods can be envisaged: (i) by modifying the chemical composition, for example by adding a small percentage of rare earths. (Ii) By formation of in-situ composites. Indeed some alloys decompose during the quenching and a ductile crystalline phase is observed. (Iii) By making ex-situ composites by adding a second ductile phase, generally in the form of powders, followed by a sintering operation.

These three solutions are illustrated by way of examples, for metallic glasses based on titanium and zirconium. Large plastic deformations (up to several tens of %) are measured. The observation of the rupture facies reveals the mechanisms of rupture.

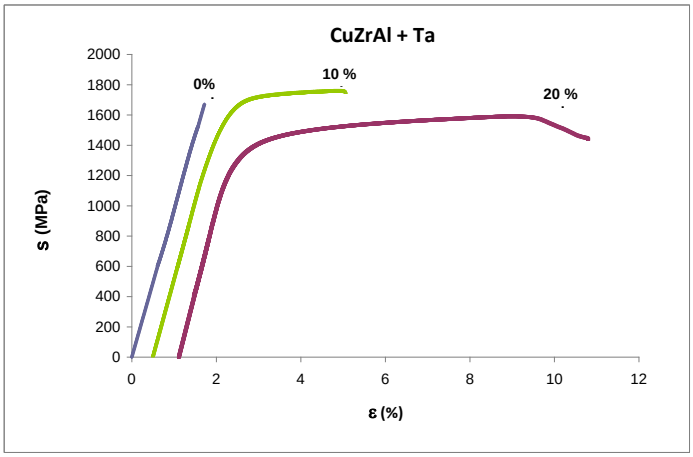

Figure: Compressive strain-stress curves of CuZrAl bulk metallic glass containing various volume fraction of Ta crystalline powder. The composite has been manufactured using spark plasma sintering.

KEYWORDS: bulk metallic glasses, composites, plasticity, fracture mechanisms.

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Presentation Method: Regular Oral

Effect of Hydrogen on the Pop-in Behavior in a Metallic Glass

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Hydrogen is a detrimental element in structural materials since it usually causes obvious reduction in fracture toughness. For example, hydrogen embrittlement is a well-known reason for the failure of steels. In contrast, hydrogen can play a beneficial roll for enhancing plasticity of metallic glasses which are always considered as brittle materials. This research focuses on the hydrogen induced plasticity in a metallic glass. Specifically, the effect of H content on the early plasticity of a Vit 105 alloy is studied by spherical nanoindentation. Samples are charged to different H content (H/M) with electrochemical hydrogen loading and then pop-in loads and sizes are recorded during nanoindentation. While the load of the first pop-in increases with increasing H content, the occurrence of pop-ins decreases dramatically. Investigations of the deformation morphologies confirm that a transition from shear band dominant to homogeneous deformation has occurred. We propose that the suppression of shear band initiation by H is caused by changes in local environment, including changes in local strain.

KEYWORDS: Metallic glass, Hydrogen, Nanoindentation, Pop-in

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Ultrasonic Hammering Reveals Serrated Energy Storage Ability of Metallic Glasses

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Thermomechanical processing [1] of metallic glasses is one of the most investigated strategies for promoting the mechanical functionality in these type of metallic materials. During mechanical treatments, metallic glasses can store energy of imposed mechanical [2] or thermal strains [3] and rejuvenate to a higher energy state; inversely, they can very occasionally cut their initial frozen-in energy back to a more relaxed state and age [4]. To date, signaling monotonic changes in the level of stored energy towards a possibly steady state of either rejuvenation or aging has been recognized as the essential nature of dynamics in glassy metals during thermomechanical treatments [1, 2, 5].

By utilizing the ultrasonic hammering technique and striking a variety of bulk metallic glass compositions (La-based, Pd-based, and various Zr-based glasses) at different processing conditions (varying the preset force and the hammering time), we found that enthalpy relaxation values (taken from DSC thermograms) evolves non-monotonically into both directions of aging and rejuvenation. Measurements of mechanical properties (hardness, plasticity, and shear modulus) shows a good correlation between enthalpy and property variations in treated glasses. This serrated-like behavior in storing energy of deformation might emanate from a complicated coupling of mechanically driven and thermally driven atomic rearrangements, which would further launch a fierce competition between aging and rejuvenation.

KEYWORDS: *Bulk metallic glasses and composites, Chemical and physical properties*

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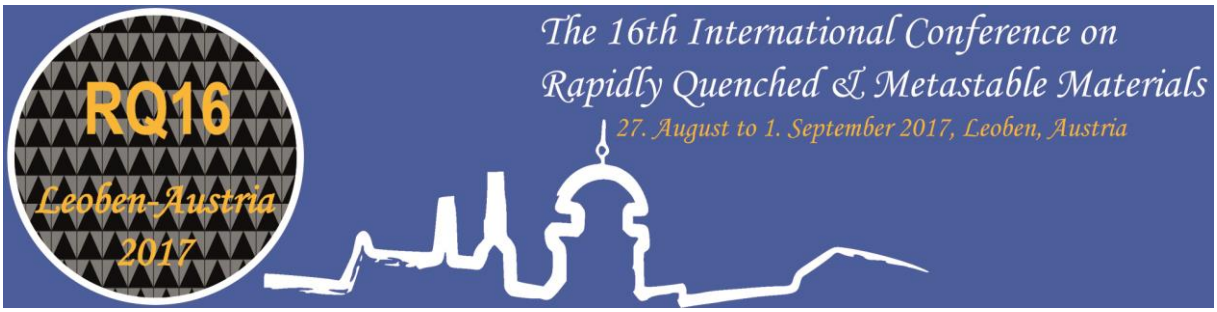
Presentation Method (Invited/Regular Oral/Poster): Regular Oral



C5-Additive manufacturing & powder metallurgy

Manufacturing of large components for the aviation using Laser additive manufacturing

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Through laser solid forming additive manufacturing (LAM), the parts with complicated geometry can be free-form near-net shaped rapidly without using the mold, meantime, the mechanical properties of the LAMed parts is equivalent to those of the wrought. These features make LAM be a viable and promising manufacturing technology for aviation industries, especially for the manufacturing of large components. In present work, the current applications of LAM technology on the aviation field are reviewed.The typical technical characteristics of LAM technology, the microstructure and mechanical properties of typical LAMed parts are analyzed, the effect of scanning pattern on the thermal/stress field during LAM of large components is introduced. Finally, the problems for the applications of LAM technology on the aviation field are discussed.

Fig. 1 The upper and lower margins of central wing of the the C919 large passenger aircraft manufactured by Northwestern Polytechnical University

KEYWORDS: Laser solid forming; Additive manufacturing; Microstructure; Mechanical properties

Presentation Method (Invited/Regular Oral/Poster): Invited Oral

Joining of Selective Laser Melted parts

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Additive manufacturing like selective laser melting (SLM) is of the rapid prototyping processes that are used to produce metallic components directly from a 3D CAD model [1]. The processes like SLM offers variety of advantages like: theoretically any shape, improved properties, processing of almost any kind of materials, etc. [2]. However a big disadvantage over this process is the limitation with the size of the components that can be fabricated. In theory, the size of the component cannot exceed the size of the building chamber. Also, increasing the size of the building chamber will have the following disadvantage of flushing the whole chamber with huge quantities of inert gas (which becomes expensive), in order to avoid the oxidation of parts during the fabrication process and may not be a viable option. Hence, there is a need to look for alternative secondary process like the additional/conventional metal joining techniques that may at a later stage can join these SLM components. Conventional fusion welding processes are not suitable for joining the SLM parts, since it may lead to coarse microstructure at the weld zone, which loses fine microstructures observed in the SLM parts and may lead to deterioration of mechanical properties. Hence, solid state welding process like friction welding is used to join the SLM parts. The structural and microstructural characterization along with the mechanical properties of the parts will be analyzed in detail.

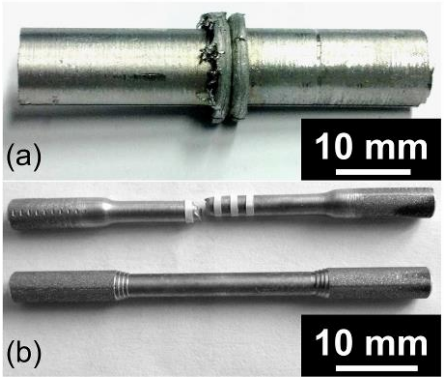

Fig 1. (a) Typical image of a friction welded Al–12Si joint with symmetrical and smooth flash at the joint. (b) Examples of tensile specimens machined from the welded samples.

KEYWORDS: Additive Manufacturing, Nanostructured Materials.

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2. E.O. Olakanmi et al., *Progress in Materials Science* **74**, 401 (2015).

Presentation Method (Invited/Regular Oral/Poster): Invited

Effect of heat treatment on morphology evolution of γ′ phase of laser additive manufactured K465 nickel-based superalloy

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K465 nickel-based superalloys possessing the excellent elevated temperature strength and the superior hot corrosion, which could be applied for a long time in the severe operation environment such as high temperature and high pressure, are thus widely used in the manufacturing of turbine blades and turning vanes of aeroengines. Recently, the requirement for rapid manufacturing of this kind of components in the advanced aero engines with more complex structure and high performance is urgent, and laser additive manufacturing technique has become the ideal way to solve this key demand. In the present work, K465 superalloy deposits are fabricated on 316L stainless steel substrate by laser additive manufacturing technique. The effects of the heat treatment on the morphology evolution of γ′ phase, the chemical composition homogeneity and the hardness of laser additive manufactured K465 superalloy are investigated. It is found that both the morphology and size of γ′ phase show obvious changes at different temperature of the deposit specimen. When solution treatment temperature ranges between 1050℃ and 1100℃, the size of γ′ precipitations is about 200 nm and morphology of rafting shape, and the size of γ′ phase show unimodal distribution. However, when the solution treatment temperature increases to 1150℃ and 1200℃, the size of γ′ phase shows the bimodal distribution. The grain boundaries become much clearer with the rising of the solution treatment temperature. When the solution treatment temperature is 1250℃, during the different solution treatment time like 1h, 2h, 3h, 4h, 5h, 6h and 7h, the morphology of γ′ particles appear different shapes. The chemical homogeneity can be observed through the solution treatment at 1250℃ for 6 h. With the increasing of the solution treatment temperature, the hardness decreases rapidly firstly, and then become slowly when the solution treatment temperature is about 1250℃, which can be explained by the morphological evolution of γ′ phases during the different solution treatment regime.

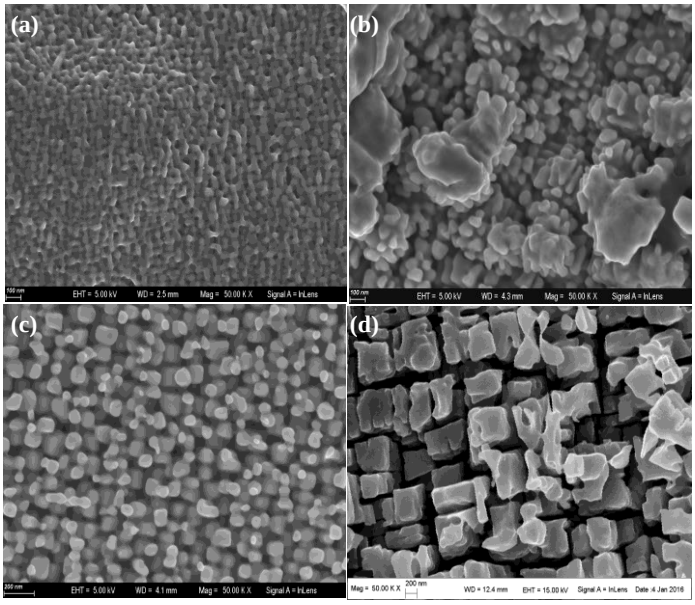

Fig. 1. Morphologhy of γ′ phase after different solution temperature treatment: (a) Laser additive repaired; (b) , (c) corresponding to 1150℃ and 1280℃,4h/AC; (d) As-cast state

KEYWORDS: Laser additive manufacturing; K465 superalloy; γ′ phase; Heat treatment

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Strong and ductile Inconel 718 superalloy fabricated by additive manufacturing

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Email: pkhqchenchao@126.com

Selective laser melting (SLM) is one of the most promising additive manufacturing (AM) technique in that components are built by controlled melting of subsequent powder layers with a focused laser beam. In this work, we investigate the microstructure and mechanical properties of Inconel 718 processed by SLM via in situ precipitation strengthening. It is demonstrated that the densification of Inconel 718 fabricated by SLM can be controlled by adjusting the energy density of the laser beam. The highest density achieved in the work is 99.52% corresponding to the energy density of 123.46 J/mm^3 and power of 400 W. Inconel 718 fabricated by SLM leads to the evolution of a columnar grained microstructure. The dispersion distribution of precipitated particles makes the strength of Inconel 718 fabricated by SLM increase higher than that produced by casting. The results of the electronic probe tests signify that the phase γ" (Ni_3Nb) and the phase γ' ($Ni_3(Al,Ti)$) distributes evenly over the grain. The second phases via in situ precipitation strengthening lead to the high strength and ductility of the as-fabricated alloy. Columnar grains tend to align along the build direction (Z-axis) of all Inconel 718 samples, which results in the anisotropy of mechanical properties between horizontally and vertically oriented test samples. It is found that the building orientation of In718 samples during SLM plays a significant role on their eventual mechanical properties. Horizontal In718 samples show higher tensile strength but a lower elongation than vertical samples. The high strength and excellent ductility of the materials were ascribed to the refined microstructure resulting from the high cooling rate imposed by laser processing.

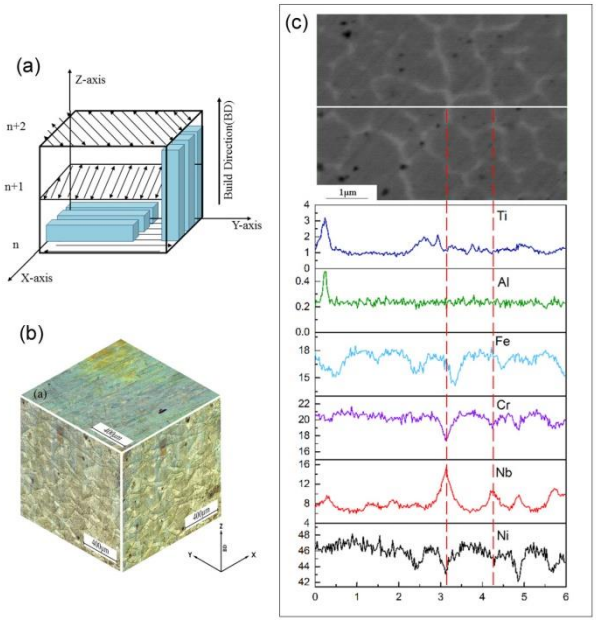

Fig.1. Additive manufacturing of In 718. (a) Laser scanning strategy, (b) Microstructure, (c) Element distribution.

KEYWORDS: Additive manufacturing; selective laser melting; Inconel 718; precipitation strengthening

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Presentation Method (Invited/Regular Oral/Poster): Regular oral

Evolution of reverted γ-Fe and precipitation in 18Ni300 manufactured by Selective Laser Melting

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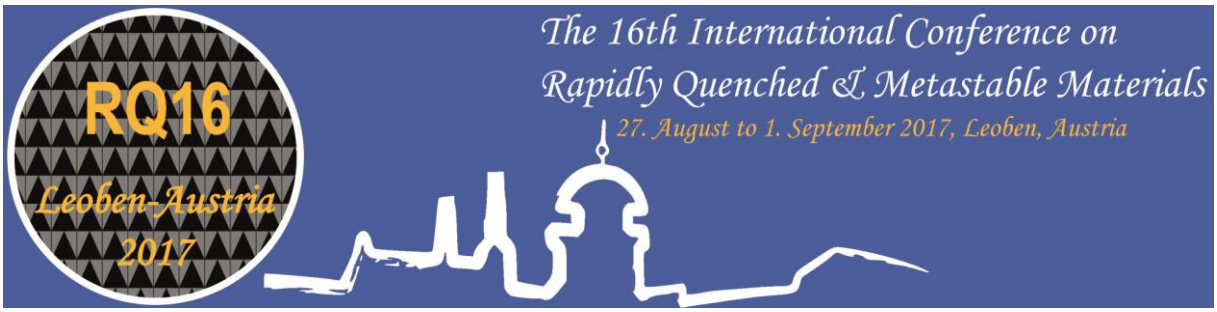
Materials produced by Selective Laser Melting (SLM) experience a thermal history that is markedly different from that encountered by conventionally cast materials. Finer solidification microstructure is obtained under steep temperature gradient and rapid cooling conditions. The steel 18Ni300 is studied in this work to evaluate and improve its microstructure and properties for manufacturing injection die. Evolution of microstructure and mechanical properties with aging process is investigated by X-ray diffraction and transmission electron microscopy. The combined effects of age hardening induced by precipitation and softening by formation of reverted austenite (γ-Fe) are discussed. Based on the experimental results, optimal heat treatment procedure for SLMed 18Ni300 is proposed.

KEYWORDS: Selective Laser Melting, 18Ni300steel, Reverted austenite, Precipitation

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



Thursday, 31st August

Metastability Alloy Design

Dierk Raabe

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Efficient bulk alloy design for high strain hardening and damage tolerance can be achieved by designing matrix metastability in such a way that with increasing mechanical loading athermal transformation mechanisms are activated, providing additional strain hardening reserves at higher deformation.

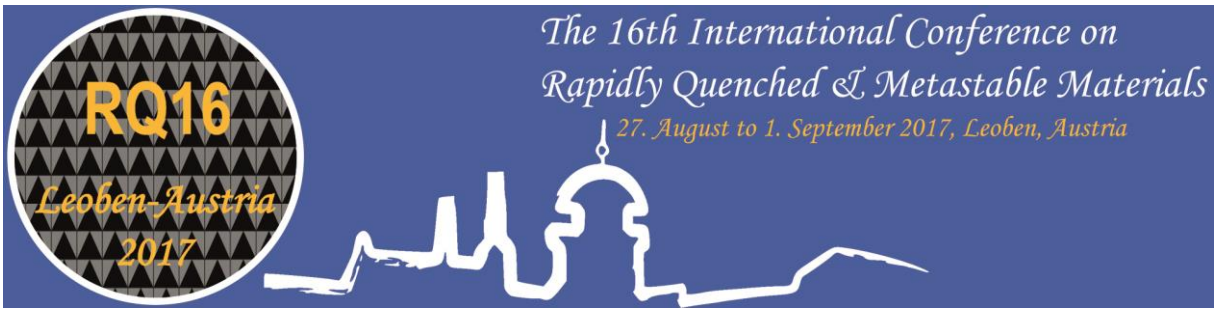
Ideally, these additional deformation mechanisms, such as formation of stacking faults, mechanical twinning and martensitic transformations, are not activated at the same load but subsequently when the preceding hardening effects are getting exhausted.

When applied to metallic alloys with face centered cubic structure this approach enables the design of a number of ultrahigh strength steels based on mechanical twinning (TWIP steels) and on martensitic transformations (TRIP steels). In these materials matrix metastability is carefully adjusted through adequate alloying to tune the desired stacking energy.

Recently this metastability design concept has in steels, high entropy alloys and beta titanium also been applied to the activation of athermal transformation effects occurring primarily in confined microstructure regions such as at interfaces and dislocations.

In such cases local transformation and the associated confined strain hardening equip metallic alloys with enhanced damage tolerance.

Presentation Method (Invited/Regular Oral/Poster): Plenary



A6-Metallic glass 8: Structure

$Fe_{36}Co_{36}B_{19.2}Si_{4.8}Nb_4$ bulk metallic glasses with small Cu addition

Mihai Stoica[1], Parthiban Ramasamy[2], Robin Schäublin[1], Jürgen Eckert[3,4], Jörg F. Löffler[1]

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[2] *Institute for Complex Materials, Leibniz Institute for Solid State and Materials Research, Dresden, Germany*

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Fe-based BMGs are well known for their attractive combination of structural and magnetic properties. Moreover, these alloys are widely studied and considered for potential applications because of low price and good glass forming ability (GFA). Fe-Co-B-Si-Nb system was first introduced by Inoue et al. in 2004 [1]; among this class of BMGs the $[(Fe_{0.5}Co_{0.5})_{0.75}Si_{0.05}B_{0.20}]_{96}Nb_4$ shows the highest GFA, high mechanical strength and excellent soft magnetic properties. A drawback, which may limit the possible industrial applications, is the brittleness of the monolithic BMGs, as well as their relatively low saturation magnetization. It was demonstrated that in the case of Fe-based glassy ribbons with small contents of Nb, minor addition of Cu might be a good way to trigger nanocrystallization of Fe(Si), averaging out the magnetic anisotropy and therefore increasing the soft magnetic properties, as in case of FINEMET alloys [2]. However, the nanocrystallization provokes a serious embrittlement of the amorphous ribbons, which makes their handling difficult. In contrast, small Cu additions to bulk amorphous alloys with similar composition may support the plastic deformation, by promoting the formation of bcc-Fe-type clusters in the monolithic BMGs.

Very recently [3] we have shown that fully amorphous rods with diameters of up to 2 mm can be obtained upon 0.5 at.% Cu addition to the base $[(Fe_{0.5}Co_{0.5})_{0.75}Si_{0.05}B_{0.20}]_{96}Nb_4$ alloy. The new Cu-added glass shows very good thermal stability and a drastically changed crystallization behavior compared to the Cu-free base alloy. On heating, the $(Fe_{36}Co_{36}B_{19.2}Si_{4.8}Nb_4)_{99.5}Cu_{0.5}$ BMG samples show two glass transition-like events separated by an interval of more than 100 K, with a bcc-(Fe,Co) solid solution forming in-between. Further [4], we have shown that the primary precipitation of bcc-(Fe,Co) is promoted by the formation of medium-range order clusters. The addition of Cu also improves the plastic deformability of the BMG samples, and the combination of a high fracture strength of 3913 MPa and 2.45% fracture strain make these glasses attractive for applications.

The Cu-added glassy samples remain magnetically very soft, with 1.1 T saturation, less than 2 A/m coercivity, and 712 K Curie temperature. By controlling the annealing temperatures one can also tailor the magnetic properties, and the precipitation of bcc-(Fe,Co) grains changes continuously the composition of the remaining amorphous matrix. The variation of the saturation magnetization and the coercivity with temperature is in very good agreement with the crystallization behavior as observed by calorimetric studies. Time-resolved synchrotron X-ray diffraction in transmission mode also allowed us to fully investigate the mechanism of phase formation upon heating. The variation of the lattice parameter revealed that the precipitated phase contains mostly Fe, while the matrix is continuously enriched in Co upon heating. The soft-magnetic properties are also changed by the precipitation of the cubic ferromagnetic crystals. The present work will show and discuss the crystallization behavior and kinetics in detail, in context with the variations of the soft-magnetic properties.

KEYWORDS: Bulk metallic glasses and composites, Materials

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Presentation Method (Invited/Regular Oral/Poster): Invited

Surface patterning of Ni-free Ti- and Zr-based bulk metallic glasses via thermoplastic forming

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[2]*Erich Schmid Institute of Materials Science, Austrian Academy of Sciences (ÖAW), Leoben, Austria*

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Ti- and Zr-based bulk metallic glasses (BMGs) are attracting increasing interest as potential biomaterials due to their unique combination of properties: high fracture strengths, large elastic limit, excellent wear and corrosion performances and good biocompatibility [1]. Many BMGs exhibit excellent thermoplastic properties at super cooled liquid temperatures where they undergo drastic softening. Thermoplastic forming of BMGs is uniquely suited to generate micro- and nano-scale surface topographies leading to a stronger cell-material interaction necessary for an optimal osseointegration [2]. Thermoplastic forming is strongly dependent of the specific metallic glass properties such as glass-forming ability, thermal stability in the supercooled liquid region, wettability, and oxidation behavior.

In this work, the thermoplastic forming ability for micro-scale surface patterning of two Ni-free Ti- and Zr-based BMGs ($Ti_{40}Zr_{10}Cu_{34}Pd_{14}Ga_2$ and $Zr_{48}Cu_{36}Al_8Ag_8$) was studied [3]. The alloys were obtained in bulk form by copper mold casting. The surface patterning of the BMGs is achieved by thermoplastic net-shaping (TPN) into anisotropically etched cavities of silicon chips. Parameters such as temperature and time for optimized pressing conditions while retaining the fully glassy state are determined by thermos-physical and thermo-mechanical measurements. The correlation between the filling depths of the investigated Zr- and Ti-BMG alloys is best described by the formability criterion, which is defined by the ratio of the width of the supercooled to the undercooled liquid region. The highest material flow occurs when the temperatures for the Zr- and Ti-BMGs are selected as 748 K and 693 K, respectively, while retaining a pressure of 40 kN and a time of ~3 min constant. An order of magnitude difference between the viscosities of these alloys and the variation of the maximum applied load during TPN are reflected in the final feature height and geometry. The practicality of the TPN process with high-resolution surface patterning capability, together with their intrinsic properties make the studied BMGs potential candidates for implant applications.

Financial support through the EC (FP7 VitriMetTech-ITN) and ERC-Advanced Grant 'INTELHIB' is gratefully acknowledged.

KEYWORDS: Bulk metallic glass, thermoplastic net-shaping, biomedical applications.

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Presentation Method (Invited/Regular Oral/Poster): Invited

Electronic structure of $Zr_{45}Cu_{45}Ag_{10}$ bulk metallic glass

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[4]*Institute for Materials Research, Tohoku University, Sendai, Japan*

Atomic structure of $Zr_{45}Cu_{45}Ag_{10}$ bulk metallic glass (BMG) was discussed in [1], and the three-dimensional atomic configurations were clearly determined using a combination of anomalous x-ray scattering, neutron diffraction, and reverse Monte Carlo modeling. To clarify the relation between the glass-forming ability and electronic structure of this BMG, we measured the incident-photon energy, $h\nu$, dependence of the electronic structure of the valence band by photoemission spectroscopy (PES) using synchrotron radiation, from which the Zr, Cu, and Ag partial densities of states (DOS) could be estimated. Figure 1 shows The PES spectra normalized with the corresponding maximum intensities as a function of electron energy, E, with respect to the Fermi energy, E_F. The $h\nu$ values are indicated upper-left of each spectrum. As clearly seen in the figure, PES spectra highly depend on the $h\nu$ value. Since the photo-ionization cross-sections, σ_p, of Zr, Cu, and Ag electrons has a large $h\nu$ dependences in this region, in particular the existences of Cooper minima, it is possible to obtain partial DOS using the $h\nu$ dependence of σ_p, as was performed in the $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ [2] and $Pd_{30}Pt_{17.5}Cu_{32.5}P_{20}$ [3] BMGs, and the results will be presented in detail at the conference.

The PES experiments were performed at BL7 in the HiSOR with the approval of the Hiroshima Synchrotron Radiation Center (Proposal Nos. 13-B-22 and 13-B-23). This work was performed under the inter-university cooperative research program of the Institute for Materials Research, Tohoku University (Project Nos. 14K0033, 15K0003, and 16K0076).

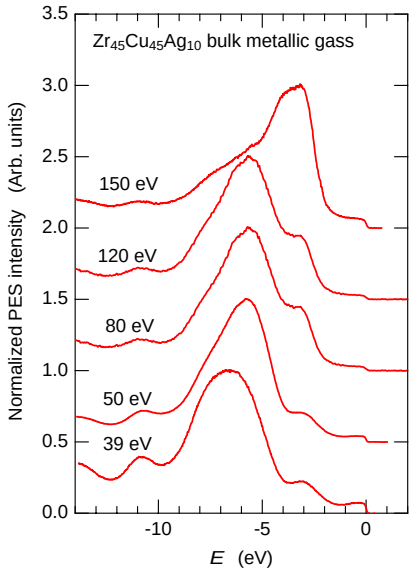

Fig1. $h\nu$ dependence of valence-band PES spectra for $Zr_{45}Cu_{45}Ag_{10}$ bulk metallic glass..

KEYWORDS: Bulk metallic glasses and composites; Chemical and physical properties

1. S. Hosokawa et al., *JPS Conf. Proc.* **8**, 031002 (2015).
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3. S. Hosokawa et al., *Phys. Status Solidi B* **253**, 676 (2016).

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Investigation of amorphous Fe-based alloy ribbons

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Development of new metallic materials is a considerable scientific research worldwide. Metallic materials with amorphous and nanocrystalline structure play an increasingly important role in modern industries as an essential part of electric devices, transformers and sensors. Amorphous and nanocrystalline Fe-based alloys are the main materials for dust-core application due to their excellent soft magnetic properties, high saturation magnetization and low core losses [1]. These properties strongly depend on alloy composition, production technique and thermal treatment. Nowadays, many studies explore influence of alloying transition metals or metalloids, heat treatment to the structure and soft magnetic properties of Fe-based amorphous alloys [2-5]. Han et al. [2] showed positive effect of minor alloying of Mo and Cr in Fe-Si-B-P-(C) alloy system on thermal stability, oxidation resistance and corrosion resistance and enhanced soft magnetic properties, such as saturation magnetization is above 1.5 T and coercivity is below 10 A/m. Dan et al. [3] examined effect of substitution of Cu by Au and Ag to Fe-Si-B-P-Cu alloy. They reported that Cu seed element plays an optimal role in controlling the microstructure and soft magnetic properties of NANOMET® alloys. And Sharma et al. [4] defined the mechanism of nanocrystallization in Fe–Si–B–P–Cu alloys: the grain size is controlled by the cooperation of growth of the pre-existing and newly formed nuclei. This study aims to present the structure, thermal stability and soft magnetic properties of Fe-based amorphous and to investigate the influence of annealing process on structure for the Fe-rich amorphous alloys.

Metallic ribbons of Fe-based alloy with minor alloying of Mo (2 at.%) and Cu (0.5, 1 at.%) were synthesized by the melt spinning technique. The structure was examined by X-ray diffraction (XRD) with Cu-Kα radiation; in as-spun state ribbons have fully amorphous structure. Thermal stability was studied by differential scanning calorimetry (DSC) at a heating rate of 0.67 K/s under argon flow; DSC curves show two exothermic peaks corresponding to the two-stage crystallization behavior. The temperature interval between the two exothermic peaks was about 150 K. The addition of Cu reduces the onset temperature of the first exothermic peak (T_{x1}) due to the precipitation of the primary bcc-Fe phase. Annealing at the temperature lower by 100 K than T_{x1} is effective to release internal stress. Although the amorphous structure remains unchanged after the annealing treatment and the Hc decreases by about 30 % as compared with the as-spun state. Increasing of annealing temperature causes precipitation and further growing of bcc-Fe phase till 45 nm (by Scherrer equation). Thus, the structure evolution and thermal properties of Fe-rich amorphous alloys were clarified and further detailed investigation of soft magnetic properties for the amorphous and nanocrystalline alloys is expected to cause much valuable characteristics for application of Fe-based soft-magnetic amorphous and nanocrystalline materials.

This work was supported by the Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST «MISiS» (№ K2-2017-002).

KEYWORDS: Amorphous Fe-based alloy, Soft magnetic alloy, Nanocrystallization

G. Herzer, *Acta Mater.* **61**, 718 (2013).

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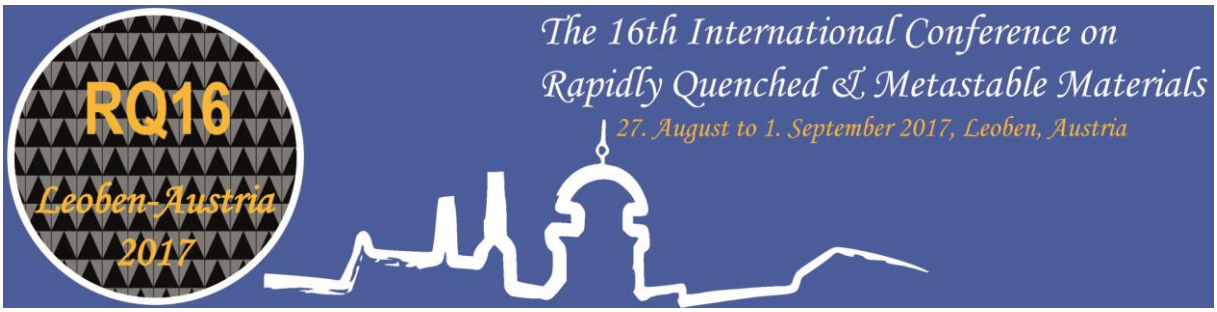
H.R. Lashgari, D. Chu, Sh. Xie, H. Sun, M. Ferry, S. Li, *J. Non-Cryst. Solids* **391**, 61 (2014).

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



B6-Metallic glass 9: Deformation

Tuning for the deformation mode in nanoscale metallic glasses

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The extrinsic size reduction of metallic glass into the nanoscale is a unique route for enhancing plasticity of metallic glasses with avoiding the general propensity of strength-ductility trade-off. Despite the accumulated researches on mechanical behaviors of nanoscale metallic glass, however, the homogeneous deformation of a nanoscale metallic glass with the increased strength compared to its bulk yield strength is still controversial due to its veiled origin and a lack of understandings on its characteristics. Here, we elucidate the origin and flow characteristics of homogeneous deformation of nanoscale metallic glasses from the viewpoint of viscous flow, based on nanocompression tests of metallic glass nanoparticles (MG-NPs) and a deformation map for the metallic glass. The quantitative viscosity analysis of homogeneously deformable nanoscale metallic glasses reveals that the non-Newtonian homogeneous flow occurs under a sufficiently low viscosity state through a whole sample volume as supercooled liquid state. Motivated by this finding, we construct a deformation map reflecting the stress-induced viscosity variation (or "mechanically-induced" glass transition) and the sample size effect enabling the detectable homogeneous flow without shear banding at room temperature. We also investigate the effect of alloy composition and electron beam irradiation on the components of the deformation map, which reflect the difference of sample conditions for deformation mode transition depending on the factors. This systematical approach provides fruitful interpretations from a novel perspective on the homogeneous deformation of metallic glass at room temperature, and also be very useful for manipulating deformation mode transition of nano-architected metallic glasses, and eventually bulk forms.

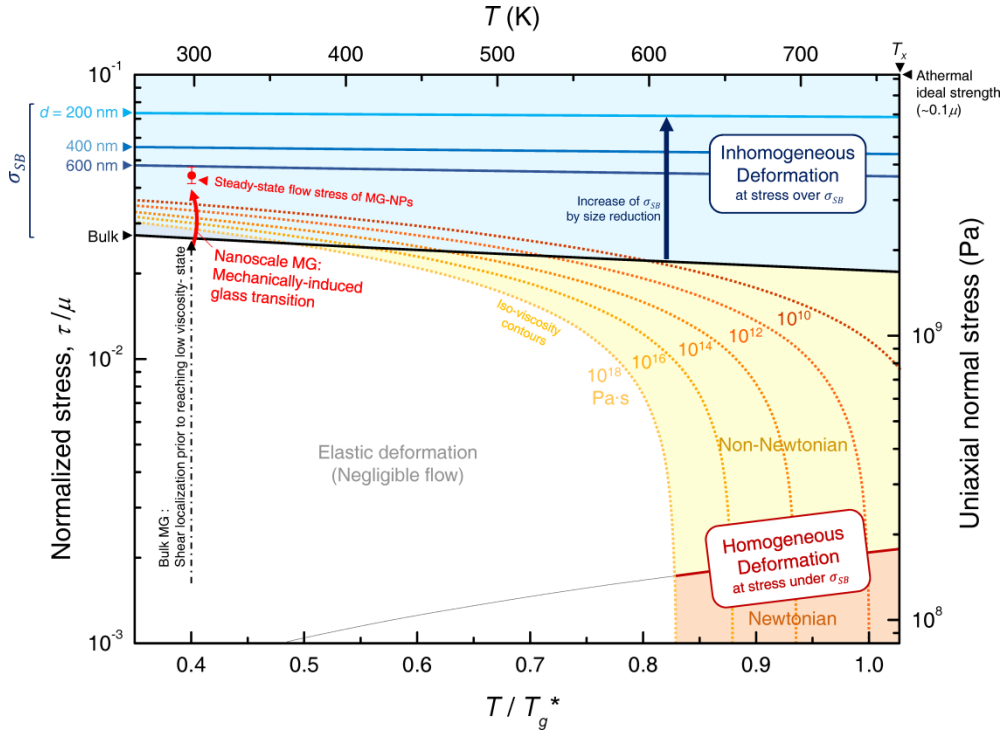

Fig1. Deformation map of metallic glass

KEYWORDS: Metallic glass, Deformation map, Deformation mode transition, alloy composition, Irradiation

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Presentation Method (Invited/Regular Oral/Poster): Invited

A universal deformation mechanism for metallic glasses

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It is commonly believed that shear banding in metallic glasses originates from individual stress concentrators having quadrupolar symmetry. In this contribution we show experimental evidence of a characteristic signature present in shear bands manifested in the form of sinusoidal density variations elucidating the underlying mechanisms of shear band formation. We present an analytical solution for the observed post-deformation state derived from continuum mechanics using an alignment of quadrupolar stress field perturbations for the plastic events. It crucially provides the non-trivial connections between the different magnitudes for dilated and densified regions, on one hand, and the bulk modulus and sample's density, on the other. Since qualitatively similar features were observed for different types of metallic glasses having different compositions and vastly different characteristics, the conclusion is drawn that periodic density variations in shear bands, resulting from the alignment of Eshelby-like quadrupoles, are fundamental for the plastic deformation of all metallic glasses, and, possibly, for all amorphous materials in general [1].

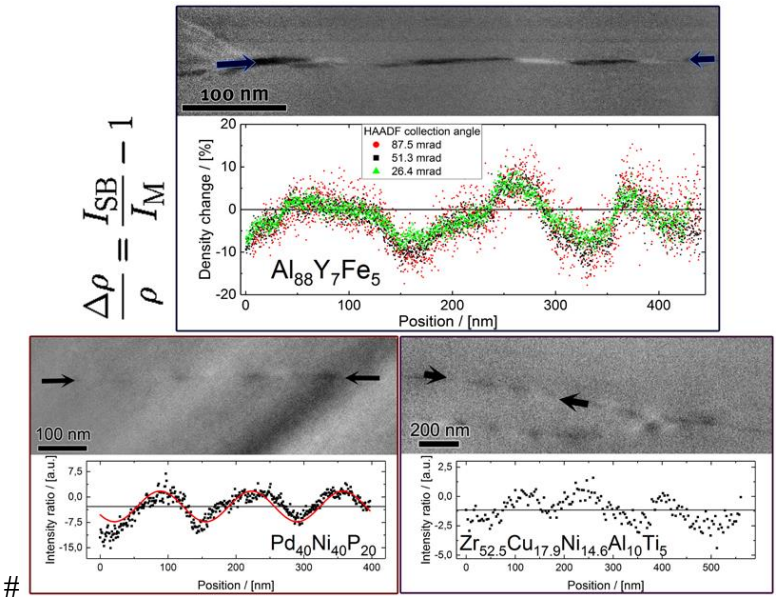

Fig1. Alternating (periodic) density switches in shear bands observed for three different metallic glasses.

KEYWORDS: Bulk metallic glasses and composites, chemical and physical properties, shear banding.

1. V. Hieronymus-Schmidt et al., *Physical Review B* in print.

Presentation Method (Invited/Regular Oral/Poster): Invited

Mechanical and thermal properties of Palladium based bulk metallic glasses regarding relaxation and rejuvenation

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Most bulk metallic glasses (BMGs) deformed at low temperatures and high stresses suffer from a lack of ductility thus making the material unsuitable for many applications. To describe the deformation in BMGs the concept of 'free volume' in the frame work of the critical fictive temperature concept (see Fig.1) is applied here [1]. This implies that an increment or redistribution of the present free volume, which can be achieved in different ways: i) cryogenic rejuvenation [2] or ii) micro-alloying [3]), may lead to enhanced ductility.

In our study we investigated PdNiP based bulk metallic glasses in detail: Effects of different degrees of cryogenic rejuvenation on the amount of free volume and mechanical properties due to changes in cycle numbers and resting times at different temperatures of the same metallic glass were investigated. Moreover, the effects on the mechanical properties by micro-alloying were monitored [3]. Adding Iron or Cobalt to the PdNiP BMG leads to a huge change in ductility. To calculate the critical fictive temperature the BMGs were annealed at different temperatures in the undercooled liquid region to reduce the fictive temperature and subsequently deformed by three point bending. Finally, the Poisson's ratios of cold-rolled samples having different degrees of deformation were measured showing no changes upon deformation.

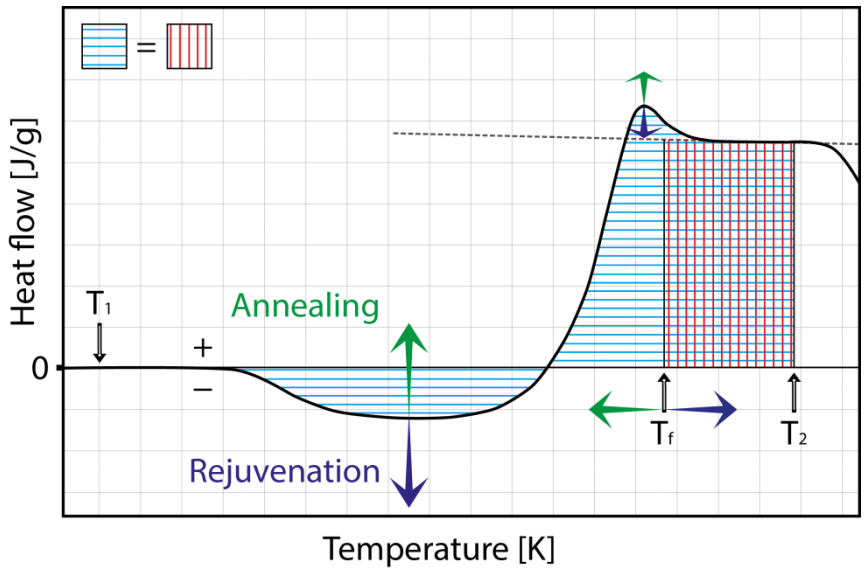

Fig1. Concept of the fictive temperature shown in a DSC measurement of the glass transition.

KEYWORDS: BMGs, metallic glasses, fictive temperature, rejuvenation, micro alloying.

G. Kumar, P. Neibecker, Y. H. Liu and J. Schroers, Nature communications 4, 1536 (2013).
S. V. Ketov et al. Nature 524, (2015).
N. Nollmann, I. Binkowski, V. Schmidt, H. Rösner and G. Wilde, Scripta Materialia 111, 119-122 (2016).

Presentation Method: Regular Oral

In situ TEM deformation of a bulk metallic glass

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[2]*NCEM, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, USA*
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Bulk metallic glasses are an exciting new class of materials due to their unique mechanical properties, such as high strength and good wear resistance. However, potential applications are hindered by their low ductility caused by the formation of shear bands leading to catastrophic failure. Still, the origin of these shear bands remains unknown. In order to investigate the structural mechanisms of shear band formation, *in situ* deformation was carried out inside a transmission electron microscope (TEM) using a Hysitron PI-95 picoindenter. Samples were made from a bulk CuZrAlAg rod produced by vacuum casting. In addition to compression tests, tension tests of the metallic glass were carried out. Figure 1 shows the result from an *in situ* tensile test acquired in bright-field mode. The corresponding load displacement curve shows elastic deformation followed by an abrupt fracture with no indication of plasticity. In addition, digital image correlation from decorated samples was used to examine the origin of shear band formation and measure the local plastic strain during deformation. Finally, we will demonstrate that the local elastic strain can be measured during *in situ* deformation with nanometer resolution. Our method is based on diffraction mapping [1]. During scanning TEM (STEM) imaging, the beam rasters over the sample and on top of the image, a full diffraction pattern is recorded for every probe position. A Gatan K2 IS direct electron detector is used to acquire the diffraction patterns at a rate of 400 frames/s and a strain map is calculated from the diffraction maps.

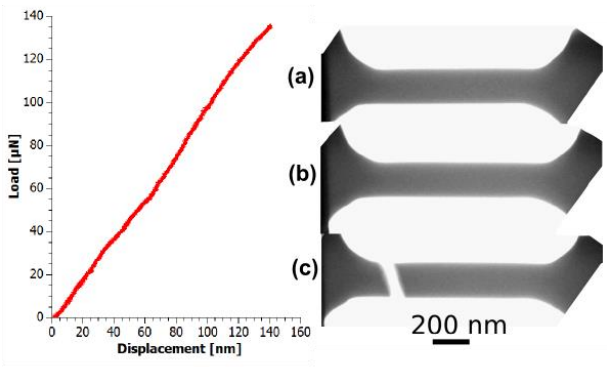
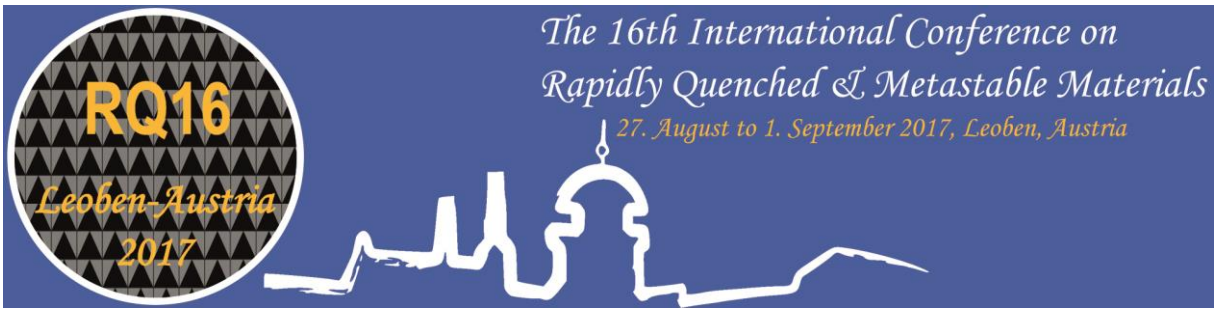


Fig1. Load displacement curve recorded during an *in situ* tensile test. The video acquired in TEM bright-field mode shows an elastic elongation of the tensile specimen. Two frames corresponding to the initial state and the elongated state are shown in (a) and (b). After elongation the sample fractures abruptly and shows no ductility. An image of the sample after fracture is shown in (c).

KEYWORDS: bulk metallic glasses, in situ deformation

1. C. Gammer, J. Kacher, C. Czarnik, O.L. Warren, J. Ciston and A.M. Minor. *Applied Physics Letters* **109** 081906 (2016).

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



C6-Severe plastic deformation 2

Nanocrystalline steels produced by ball milling, high pressure torsion and wire drawing

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[2] *International Institute for Carbon Neutral Energy Research (I2CNER), Fukuoka, Japan*

[3] *Institute for Materials Ruhr-Universität Bochum, Germany*

[4] *Max-Planck-Institute for Iron Research GmbH, Düsseldorf, Germany*

A review based on the extended work of the authors [1-7] is presented on the fundamentals of stabilizing nanocrystalline solids by solute segregation at grain boundaries as well as its application in producing nanocrystalline steels by severe plastic deformation. Preparation methods include ball milling of Fe-B, Fe-C and Fe-O alloys, their subsequent compaction by high pressure torsion (HPT), and wire drawing of pearlitic steels. Samples were characterized by X-Ray Diffraction, Electron Microscopy and Atom Probe Tomography. At concentrations of up to 10 at.-% of B, C or O most of the interstitial solute atoms segregate to grain boundaries with an average excess solute of about $1x10^{-5}$ mole/m^2 (about half a monolayer) leading to grain sizes of 5 to 10 nm. For Fe-C alloys it could be shown that the grain boundary energy was reduced to zero leading to a metatstable thermodynamic equilibrium of the nanocrystalline structure. Annealing leads to grain coarsening accelerated at temperatures above 700 K by precipitation of a corresponding boride, carbide or oxide. Thermal stability of the nanocrystalline alloys increases in the order Fe-O, Fe-C and Fe-B. Powders obtained by ball milling were compacted by HPT at room temperature and at about 500 ^{o}C. In the latter case some grain coarsening was observed at the sample periphery of the disc shaped samples being subjected to the largest total strain. The Vickers hardness of HPT samples reached values of up to 1000. By wire drawing of pearlitic steels and very large strains the carbide phase dissolves via mechanical alloying, rendering the initially two-phase pearlite structure into a carbon-supersaturated iron phase. This carbon-rich iron phase evolves into a columnar nanoscaled subgrain structure which topologically prevents grain boundary sliding which leads to a material with an extreme tensile strength of 7 GPa, making this alloy the strongest ductile bulk material known.

KEYWORDS: Nanocrystalline alloys, ball milling

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4. Y.Z. Chen, A. Herz, Y.J. Li, C. Borchers, P. Choi, D. Raabe, R. Kirchheim, *Acta Mater.* **61,** 3172 (2013)
5. Y. Li, D. Raabe, M. Herbig, P. Choi, S. Goto, A. Kostka, H. Yarita, C. Borchers, and R. Kirchheim, PRL 113, 106104 (2014)
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Acta Mater. **97,** 207 (2015)
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Presentation Method: Invited

Grain refinement in powder metallurgical FeCoCrNi high entropy alloy during room temperature severe plastic deformation

Yong Liu[1], Min Song[1], Wenqian Wu[1], Bin Liu[1], Jingshi Wang[1], Xiaozhou Liao[2]

1. State Key Laboratory of Powder Metallurgy, Central South University, Changsha 410083, P.R.China, Email:yonliu@csu.edu.cn

2. School of Aerospace, Mechanical and Mechatronic Engineering, The University of Sydney, Sydney, NSW 2006, Australia

High entropy alloys (HEAs) are composed of several alloy elements with nearly equiatomic propotions. The HEAs have drawn more and more attention due their unique properties, for example, good combination of strength and plasticity, high corrosion and irradiation resistance. In this work, a metastable FeCoCrNi high-entropy alloy with a face-centered cubic structure was fabricated by a powder metallurgical route, and then processed by high-pressure torsion (HPT). The Microstructural evolution was studied by using transmission electron microscopy. After HPT, the grain size can be refined to below 100 nm, and the microstructures contain numerous nanotwinning, nanobanding and other substructures. It was found that the grain refinement was induced by concurrent nanoband (NB) subdivision and deformation twinning. There were strong interactions between the sub-structures, resulting in severe lattice distortion and accumulation of high densities of dislocations. Interestingly, some amorphous phase nucleated and grew at twin-twin interacted regions. The mechanism of the grain refinement with regard to the interactions of various sub-structures was discussed in details. Finally, the formation of amorphous phase ahead of crack tips can be successfully predicted by MD simulation on HEAs.

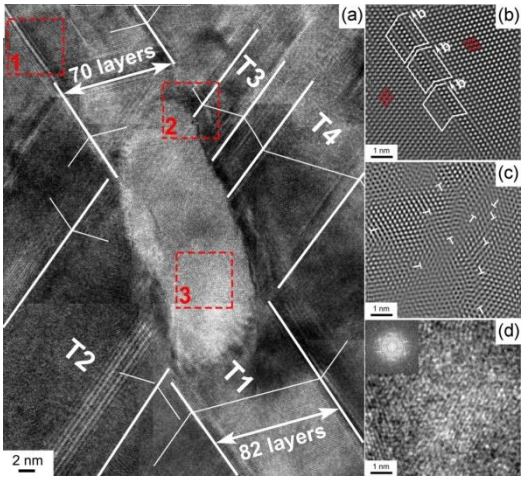

Fig1. The amorphous phase nucleated and grew at twin-twin interacted regions, while its expansion was restricted by the intersected twin boundaries. (a) An HRTEM image of the twin-twin interaction, (b,c) Fourier filtered images of the square parts 1 and 2 in (a), respectively, and (d) the enlarged HRTEM image and the corresponding FFT pattern of the square part 3 in (a).

KEYWORDS: High entropy alloy; powder metallurgy; severe plastic deformation

Presentation Method (Invited/Regular Oral/Poster): Invited

Comparative investigation of oxygen effects in Cu-Fe nanocrystalline alloys deformed by high pressure torsion

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Normally immiscible Cu-Fe system was mechanically alloyed directly from blended powders and vacuum arc-melted bulk, which contain different levels of content of oxygen impurity, with a series of compositions (1-*x*) at.%Cu - *x* at.%Fe (*x* = 0, 5, 15, 25, 35), by means of high pressure torsion. Finally, all investigated compositions were deformed to reach a strain-saturated state forming single face-centered cubic structure after large straining, 100 rotations, i. e., effective strain of 1360. It is found that lattices expand for the powders-deformed samples compared to bulk-deformed samples, which implies oxygen atoms facilitate the lattice expansion of supersaturated single-phase nanocrystalline alloys as interstitials. Our theoretical calculations confirmed the lattice expansion effect caused by oxygen atoms. However, the grain size change shows a different trend against lattice parameters, Fe solutes can significantly refine the grains, i. e., higher Fe concentration causes finer grains. Simultaneously powders-deformed sample has a much smaller grain size compared to the same composition sample deformed from arc-melted bulk, which induces large differences in mechanical properties between powders- and bulk-deformed samples, for example, the hardness value is 350 – 370 HV for 75Cu-25Fe deformed from powders while 280 – 300 HV for the same composition deformed from arc-melted bulk. The oxygen-mediated grain refinement process was captured on samples deformed with different amount of strains with recording transmission electron microscopy dark-field images. A phenomenological model was proposed to interpret the oxygen effect on the deformation and grain refinement process. The current work systematically investigated the oxygen contamination effects for the first time, which may be helpful for nanocrystalline alloys designing and manufacturing.

KEYWORDS: nanostructured materials, mechanical alloying, high pressure torsion, oxygen effects

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2. J. Guo, J. Rosalie, R. Pippan, Z. Zhang, Mater. Sci. Eng. A 695 (2017) 350–359.
3. We acknowledge Andrea Bachmaier, Timo Müller and Pradipta Ghosh at Erich Schmid Institute for their kind assistance. Our collaborators of Dr. Georg Haberfehlner, Prof. Gerald Kothleitner at TU Graz and Prof. Yunbin He, Mr. Lei Li at Hubei University, China are gratefully acknowledged.

Presentation Method (Invited/Regular Oral/Poster): Invited

Cryomilling: The synthesis of free standing ultra-pure metal nanoparticles in large quantity

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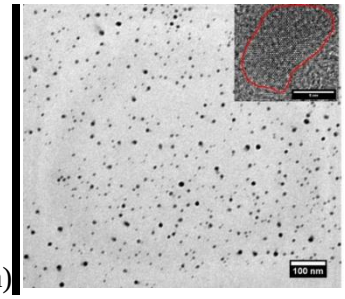
In the modern era, research groups are devoted to synthesize large amount nanomaterials by top-down and bottom-up routes. However, the definite shapes and narrow size distribution could be required to achieve with higher yield. The purity of nanoparticles and protection from oxidation of pure metal nanoparticles is also a challenging issue.

The cryo-ball milling (top-down approach) is cost effective powerful tool to prepare nanomaterials in large quantity[1] in which, the extreme low temperature accelerate the fracture phenomenon of metals and suppress the cold welding phenomenon. Consequently, the metal particles get ultra refined with narrow size distribution[2]. The low temperature also helps to reduce the rate of oxidation during preparation (milling), where pure metal nanoparticles are highly prone to oxidized. The present study reports the large quantity preparation of free standing metal nanoparticles of FCC metals (Al, Ag, Cu). Therefore, the metal nanoparticles characterized in order to investigate the size, shape, purity, thermal stability and dispersion stability in the polar solvents utilizing TEM, EPMA, ICP-MS and zeta potentials. The metal nanoparticles are average size <10 nm with high purity and the particles capable to remain dispersed in the polar solvent (methanol, ethanol, and glycol) for more than 10 days. The oxygen concentration has been estimated and compared with precursor powder using surface sensitive (depth of information few atomic layers) X-ray photoelectron spectroscopy. The cold welding phenomenon has been studied for different temperature (ice, room, LN_2 temp) at different percent deformation and compared for different metals. The mechanism of free standing nanoparticles formation has been discussed with available literature and cold welding strength of metal at different temperature.

The cryomilling technique is capable to prepare large quantity free standing pure metal nanoparticles and suitable for thermonanofluids, antibacterial agents and conducting ink formation.

(a) 

(b) 

Fig. 1**(a)** Silver metal nanoparticles **(b)** Free standing metal nanoparticles in ethanol

KEYWORDS: Mechanical milling, cryomilling, nanomaterials, ultra pure metal nanoparticles

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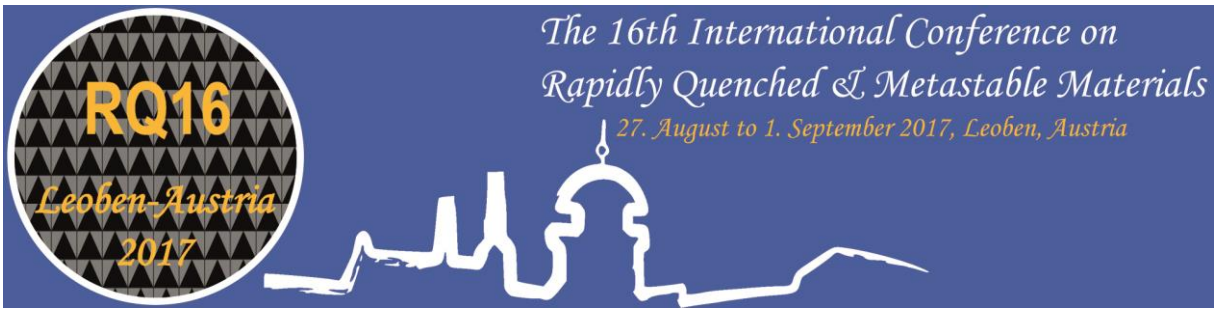
Presentation Method (Invited/Regular Oral/Poster): Regular oral



A7-Metallic glass 10: Properties

Nanostructured metallic glasses: insights from MD simulations

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TU Darmstadt, Fachbereich Material -und Geowissenschaften, FG Materialmodellierung, Jovanka-Bontschits-Str. 2, D-64287 Darmstadt

The mechanical properties of metallic glasses can not only be influenced by their chemical composition, but also by their nanostructure [1]: Secondary phases in the form of precipitates, as well as a glass-glass interfaces are possible means to enhance the plasticity of the material. In this contribution results from molecular dynamics simulations of nanostructured Cu-Zr based metallic glasses under mechanical load will be discussed and compared with experimental findings, especially with results from transmission electron microscopy. The influence of crystalline nanoprecipitates on shear band nucleation and propagation is investigated, and also the effect of grain size and composition on the deformation behavior of nanoglasses and nanoglass composites.

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Presentation Method (Invited/Regular Oral/Poster): Invited

Using strains in the elastic regime to enhance the properties of metallic glasses

C. M. Meylan and A. L. Greer

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The structure and properties of a metallic glass (MG) depend not only on its composition, but also on its thermal history. Depending on the cooling rate when forming a MG, a higher or lower energy state is reached, and the resulting sample's properties may differ to a large extent. By forming the MG at a lower cooling rate, a lower energy state is reached; the glass is more relaxed, with a more dense structure and higher hardness. But in this state, the glass is typically also more brittle. In contrast, a higher cooling rate leads to a less relaxed glass with higher structural disorder, which often has better plastic deformability.

Many studies have shown that less relaxed states can also be reached through mechanical treatments, such as cold-rolling [1], high-pressure torsion [2] or shot-peening [3]. These processes heavily deform the glass's structure. Interestingly, even when the macroscopic strain of a MG sample is relatively small, i.e. within the elastic regime, permanent change to the structure can be induced [4, 5]. Elastic deformation is by definition recoverable; however, it has been found that the flow units of MGs, i.e. shear transformation zones, can be activated even below the macroscopic yield stress.

In the present work, we explore the effects of thermomechanical treatments using strains in the elastic regime. Lee et al. [4] found that the structure of a MG was modified after applying a static compressive load below the yield load for several hours. We investigate the effects of elastostatic loading on a CuZr-based bulk MG. In contrast to earlier work, we examine the effects of not only uniaxial compression, but also uniaxial tension and torsion. While we know that elastostatic loading gives rejuvenation (i.e. introduces free volume), we do not know whether this is aided or hindered by hydrostatic compression or tension. The experiments in compression, tension and torsion are designed to address this question. Changes in the MG are monitored through property changes: nanoindentation and resonant ultrasound spectroscopy are used to measure the variation in mechanical properties, and differential scanning calorimetry is used to determine the heat of relaxation. We conclude that using strains in the elastic regime provides many opportunities for modification and improvement of MG properties.

KEYWORDS: Bulk metallic glasses, mechanical properties and behavior

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

High Pressure Quenched Glasses – Unique Structures and Properties

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Through high-energy x-ray diffraction and atomic pair density function analysis we find that Zr-based metallic alloy, heated to the supercooled liquid state under hydrostatic pressure and then quenched to room temperature, exhibits a distinct glassy structure. High pressure quenched (HPQ) glasses are stable in ambient condition i.e. at RT and ambient pressure. The HPQ samples have a different structure and mirror the pressure induced structure in the liquid state. In this contribution we clearly show that: HPQ samples are stable at ambient condition and they have a different structure than glasses quenched without applied pressure (Fig 1); the change in the HPQ structure is not due to structural relaxation, which is a standard aging process for glasses; HPQ sample transforms back to the structure, quenched without pressure, which proves that pressure induced change is not caused by nano-crystallization.

The data suggest that pressure induces a phase transition in the supercooled liquid. The pair distribution function shows that without pressure the Zr neighbor shell of Zr is distorted, whereas such distortion is removed by applying pressure in the liquid state and the structure becomes better packed. The results indicate that Zr-based alloy liquid has two distinct structures, a low-density more distorted structure at ambient pressure, and a high-density better packed structure under pressure. The Zr-shell distortion in metallic glasses formed under ambient pressure reflects covalency of Zr-Zr bonding. Quenching under pressure suppresses such distortion and HPQ glasses have more densely packed structure. The HPQ glasses exhibit distinct relaxation spectra near T_g, and have higher physical density.

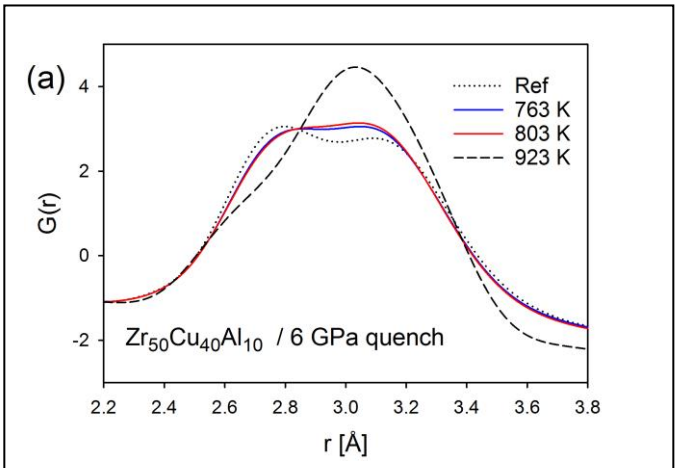

Fig1. Reduced Pair Density Functions of glasses quenched under pressure from different temperatures in the

KEYWORDS: Bulk metallic glasses and composites; Melt structure and relaxation studies.

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Role of amorphous 2nd phase on electric property and magnetic property in Cu-Zr-Al-Gd phase separating metallic glasses

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It is widely accepted that metallic glasses generally consist of elements with large negative mixing enthalpies. However, an addition of alloying elements having repulsive interaction (positive mixing enthalpies) can induce liquid-liquid phase separation and result unique microstructure with two different amorphous phases during rapid solidification. [1] In particular, the minor addition induces the heterogeneity, which can enhance plasticity of metallic glass by resulting nucleation of multiple shear bands and interruption of their propagation. [2] Thus, it can be predicted that the unique microstructure of phase separating metallic glass also affect the electric and magnetic properties of the alloy, but the effects of 2nd amorphous phase on electric and magnetic properties of metallic glass has not been widely investigated. In the present study, the $Cu_{46}Zr_{47-x}Al_7Gd_x$ (x=0-47 at.%) phase separating metallic glasses were fabricated and the effect of replacement of Zr with Gd in $Cu_{46}Zr_{47}Al_7$ metallic glass on electric and magnetic properties has been investigated. First, phase separation into Cu–Gd-rich and Cu–Zr-rich amorphous phases occurs during rapid cooling when the Gd content x is above 15 at.% in $Cu_{46}Zr_{47-x}Al_7Gd_x$ system. Phase separation behavior during solidification of $Cu_{46}Zr_{47-x}Al_7Gd_x$ metallic glass was analyzed by CALPHAD method via calculation of phase diagram. Secondly, electrical resistivity of $Cu_{46}Zr_{47-x}Al_7Gd_x$ metallic glass at room temperature was measured by 4-point probe method. Indeed, saturation M-T curves from 300 K to 5 K under the magnetic field of 0.01 T and M-H loops at 5 K for $Cu_{46}Zr_{47-x}Al_7Gd_x$ metallic glass was measured by MPMS (magnetic property measurement system). And magnetization (Ms) of $Cu_{46}Zr_{47-x}Al_7Gd_x$ metallic glasses was systematically determined by Gd content of the alloy. We show that the coercivity was significantly affected by microstructure of Gd-rich amorphous phase and electrical resistivity was affected by microstructure and volume fraction of 2nd amorphous phase. Our results could provide an effective guideline for tailoring electric and magnetic properties by amorphous 2nd phase in phase separated metallic glasses.

KEYWORDS: metallic glass, phase separation, amorphous 2nd phase, electrical property, magnetic property.

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Melt fluxing to elevate the forming ability of Al-based bulk metallic glasses

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Salt-fluxing treatment is an effective technique to improve the glass-forming ability (GFA) of bulk metallic glass (BMG)-forming melts, as demonstrated before in Pd- and Fe-based systems. However, the mechanisms as to how the oxide inclusions are removed are not fully clarified. More importantly, it has been challenging to develop similar fluxing protocol for more reactive melts, such as Al-rich BMG-forming systems. Here we design new fluxing agents from the thermodynamics perspective, taking into account combined effects of physical absorption and chemical absorption (reaction) between the fluxing agents and oxide inclusions. MgCl2-CaCl2 composite salts were selected based on this guideline, and their fluxing effects were systematically studied on an Al86Ni6.75Co2.25Y3.25La1.75 alloy, the best BMG-forming composition reported thus far for Al-rich systems. The oxygen content was found to continuously decrease in the master alloy with increasing cycles of salt-fluxing treatment. The appearance of chlorate products on the surface of the master alloys provides the evidence of concurrent physical absorption and chemical reaction. The fluxing treatment developed has enabled a record critical size (diameter) of 2.5 mm for Al-based BMGs. Our finding not only is an advance in developing highly desirable Al-based BMGs, but also provides guidance for designing processing protocol to produce larger-sized BMGs in other reactive systems.

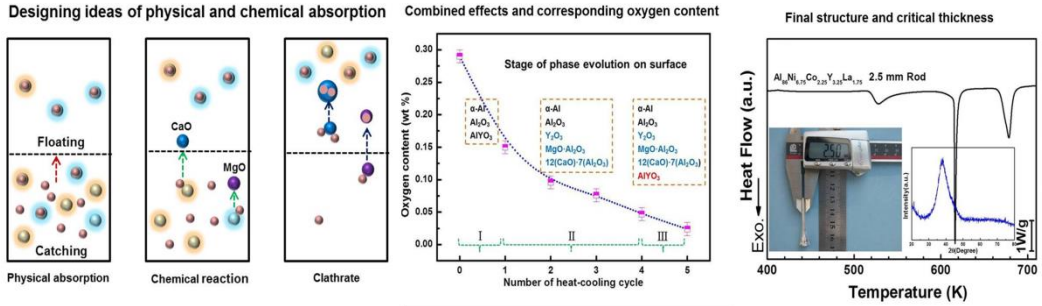
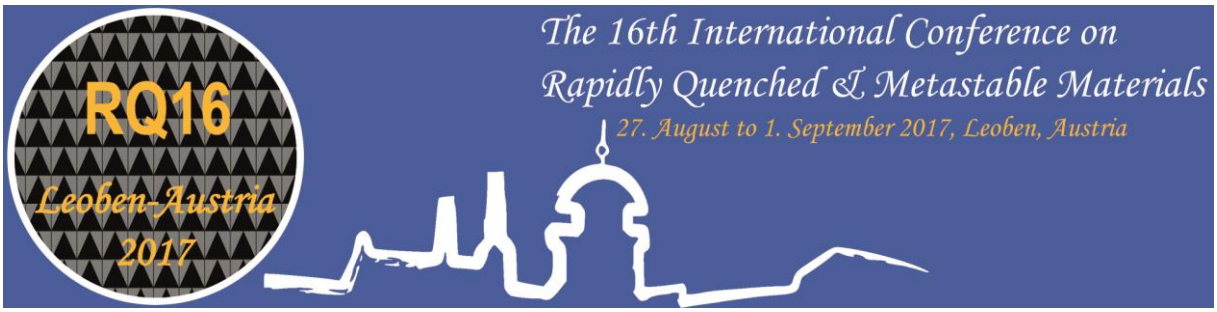


Fig1. Schematic illustration of salt-fluxing to remove oxide inclusions and critical thickness in an Al-TM-RE alloy melt.

KEYWORDS: Fluxing; Glass forming ability; Al alloys.

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



B7-Metallic glass 11: Structure

The role of structural heterogeneities in bulk metallic glass

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Based on recent theoretical predictions and experimental evidence it is found that the inherent limitation of metallic glasses, such as lack of toughness and hardening ability can be overcome by introducing structural heterogeneities in the amorphous state. As such, a glassy material can be designed which exhibits a pronounced and controlled free volume dispersity. Experimentally, this can be achieved by a number of different methods, such as thin film deposition, severe plastic deformation, spinodal decomposition, and inert gas condensation among others. Here, we report on thin film sputtering experiments from Au- and Zr-based BMG targets and high pressure torsion of Pt-based BMG samples. By variation of the argon back pressure the resulting nanostructures in x-ray amorphous films can intentionally be varied from fully amorphous, to a nanoglobular structure / nanoglass and to a glassy columnar structure with varying volume dispersity as shown in Fig. 1. While in general glassy structures lack ductility (Fig. 1 left), the nanoglass state (Fig. 1 middle) exhibits superior mechanical properties due to the interaction of the interfaces with shear bands initiated under strained conditions, as well as pronounced differences of the de-alloying characteristics. Further experimental results including high pressure torsion methods will be discussed (Ref. 1).

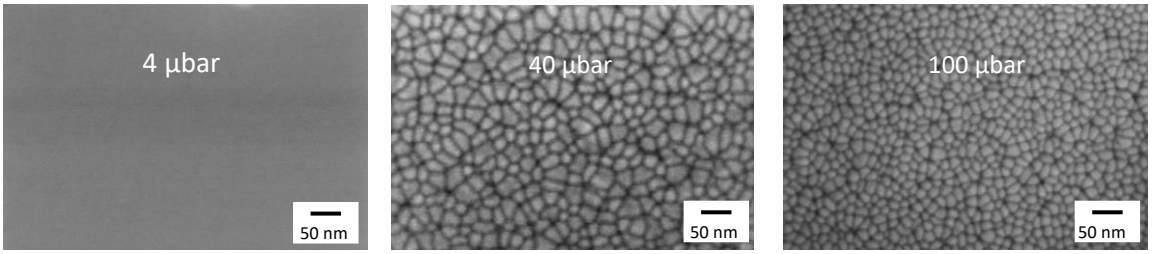

Fig 1: $Au_{40}Cu_{28}Pd_5Ag_7Si_{20}$ fully amorphous thin films prepared by magnetron sputtering from BMG targets at varying argon gas back pressure exhibiting different levels of volume dispersity.

KEYWORDS: Bulk metallic glass, glass / glass composites, amorphous thin films, free volume dispersity

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Presentation Method (Invited/Regular Oral/Poster): Invited

Correlation between structural and mechanical heterogeneities of a CuZr based bulk metallic glass

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Bulk metallic glasses (BMGs) have exceptional properties such as high strength and a high elastic limit, which makes them promising materials for structural application. Unfortunately, these favorable properties come with the major drawback of almost non existing ductility. A promising treatment to improve ductility is severe plastic deformation by high pressure torsion (HPT) [1].

In this work $Cu_{45}Zr_{45}Al_5Ag_5$ specimens produced by copper mold suction casting are deformed by HPT using several different deformation parameters. Post deformation cross-sections of the 8 mm diameter discs are analyzed by means of nanoindentation, synchrotron diffraction and differential scanning calorimetry (DSC). Statistical analysis of the creep and the discontinuities during nanoindentation (popins) is performed. Figure 1-1 shows the relative hardness maps of the HPT disc cross-sections for specimens deformed at (a) 8GPa 20 turns @ LNT, (b) 8GPa 80 turns @ RT and (c) 4GPa 80 turns @ RT. A strongly inhomogeneous deformation is observed for all the specimen, leading to a strong structural gradient over the specimen height. This is especially pronounced for the specimens deformed to higher strain. Both, hardness and Young's modulus are reduced within the deformed volume, that increases with increasing distance from the center. The strongly deformed regions show also a distinct difference in creep depth as compared to the harder regions and a shift of the mean number of popins as compared to the as-cast state. Further structural analysis is carried out by synchrotron diffraction. The cross-section mapping shown in Figure 1-2 reveals a shift of the first diffraction maximum q_1 to lower q-values, matching with positions of reduced hardness in the nanoindentation maps. This is consistent with a local increase in free volume in the severely deformed regions. DSC heat flow curves of all the deformation states show distinct relaxation enthalpies below the glass transition temperature. The enthalpies correlate well with the volume fraction of the deformed regions in the specimen.

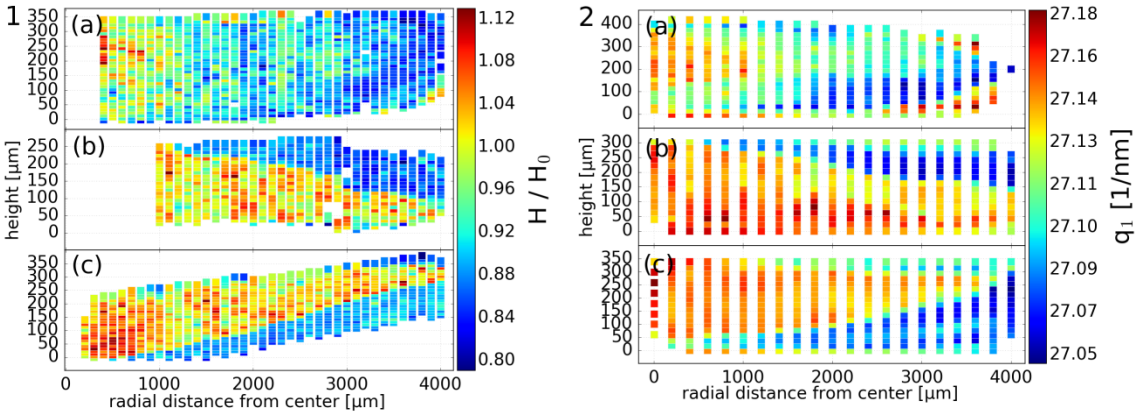

Figure 1: **1: Hardness maps of HPT disc cross-sections**: The mapping of hardness variations relative to the average hardness of the as cast state for specimens deformed at (a) 8GPa 20 turns @ LNT, (b) 8GPa 80 turns @ RT and (c) 4GPa 80 turns @ RT shows strong structural inhomogeneities in the post deformed specimen. **2: Synchrotron diffraction maps**: Mapping of the first maximum peak position q_1 reveals a shift to lower q-values for the severely deformed regions.

KEYWORDS: bulk metallic glasses, microstructure

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Radial distribution function imaging: a TEM method in resolving the multiphase amorphous materials

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Interpreting the atomic structure of amorphous materials has attracted attention for a century and, in recent years, especially heterogeneous nanoglasses have fueled the interest because of their unusual structure and properties [1]. However, only few experimental means offer a way to characterize the disordered structures. Radial distribution function (RDF) is one of the important tools which describes the probability to find certain pairs of atoms as a function of the atom separation and consequently, provides short- and medium-range structural information [2-3]. However, traditional diffraction experiments only provide an average over large sample areas and lack spatial resolution especially at the nanometer scale. Critical information is therefore hidden in the averaged signal.

In this work, we demonstrate a newly developed scanning transmission electron microscopy (STEM) method, RDF-imaging [4], to achieve structural mapping of multiphase amorphous materials with nanometer resolution. As illustrated in figure 1, this method acquires a 4-dimensional (4D) diffraction map [5] in STEM with quasi parallel nano-beam configuration and ~1 nm spot size, and converts the diffraction patterns to a 3D data cube of RDFs. The data cube of RDFs can then be analyzed by hyperspectral analysis, such as multivariate statistic analysis, to obtain the phase map of the multiphase amorphous materials. The structure of each phase can be analyzed according to the corresponding RDFs in terms of bond distance, bonding angle and coordination number. We apply RDF imaging to a variety of different materials and will illustrate the technique and the information that can be obtained by looking at multilayered metallic glasses, shear bands in metallic glasses as well as the structure of nano glasses.

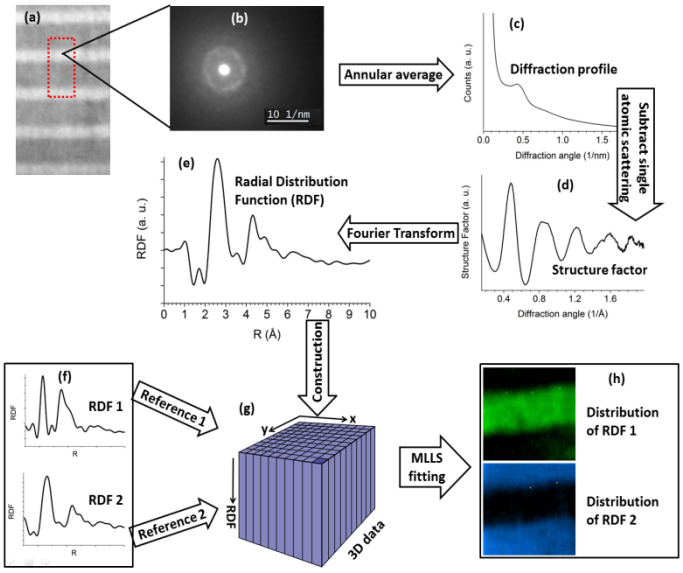

Figure 1. Sketch of procedures to calculate the RDF-cube from experimental STEM-diffraction data and MLLS analysis of the RDF-cube. (a) HAADF image. (b) A typical diffraction pattern in STEM-diffraction. (c) Annular averaged diffraction profile. (d) Structure factor. (e) RDF obtained by Fourier transform of structure factor. (f) Reference RDFs. (g) Sketch of the constructed RDF data cube (RDF-Cube). (h) Imaging results: structural maps.

KEYWORDS: Electron diffraction, Radial distribution function, multiphase amorphous materials

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Alloy Development of 18-karat premium-white gold bulk metallic glasses with improved tarnishing resistance

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In the last decade, 18-karat gold Au–Ag–Pd–Cu–Si bulk metallic glass (BMG) system has received considerable attention as jewelry material due to its extraordinary premium-white gold color, the absence of allergen constituents such as Ni, Cr, and Co, twice the hardness of cold worked or age hardened conventional white gold alloys, melting temperatures below 400 °C, less than 0.5% solidification shrinkage and a good processing ability. However, this system is affected by non-uniform tarnishing that is detrimental to its application. This behaviour is typical for a mixture of elements with very different nobility, where preferential oxidation and partitioning are common processes observed upon reaction with environment [1, 2]. Based on thermodynamic considerations we have judiciously added Ga and/or Sn to the aforementioned system and developed novel 18-karat premium-white gold BMG compositions with improved tarnishing resistance [3]. We report here upon the strategy applied to develop the novel compositions and their processing and performing ability for jewelry and dentistry applications combined with first field trials (Figure 1) as well as their limits and possible further solutions.

Figure 1: Results of a 60d wearing test of three rings [4]

KEYWORDS: Bulk metallic glasses, Synthesis, Alloy development, Tarnishing, Jewelry

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

HRTEM investigation of nanocrystals and magnetic structure of FeNi-based BMGs

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Fe-based bulk metallic glasses (BMGs) have attracted great attention due to their soft magnetic properties along with high strength at the expense of plasticity [1]. A newly developed $Fe_{50}Ni_{30}P_{13}C_7$ based BMG overcome this limitation by showing extensive compressive plasticity [2]. The large plasticity observed in the newly developed monolithic BMGs raise a question about the contribution of atomic-scale effects. Nanocrystals on the order of 1-1.5 nm in size are observed within Fe-based bulk metallic glass using aberration-corrected high resolution transmission electron microscopy. Furthermore, we report the details of magnetic structure of the partially crystalline and amorphous alloys of the same compositions produced by different casting conditions and link the findings to the nanostructure using the combination of Lorenz Transmission Electron Microscopy (TEM) with recently developed Virtual Bright Field Differential Phase Contrast method (VBF-DPC) [3]. While the first method allows in-situ study of the dynamic of the magnetic structure under external magnetic field, VBF-DPC gives quantitative information. Magnetic structure of partially crystalline BMG shows two distinguished magnetic configurations correlated with amorphous and crystalline phases. Domain structure of the amorphous regions within homogenously dispersed nanocrystals is determined by only shape anisotropy, while the domain structure of the regions with micron-sized crystallinity is the result of completion between shape and crystalline anisotropy.

KEYWORDS: Bulk Metallic Glasses and composites, Nanostructured materials

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Sub-Ablation Femtosecond Laser Processing of Nanocrystalline Alloys and Metallic Glasses

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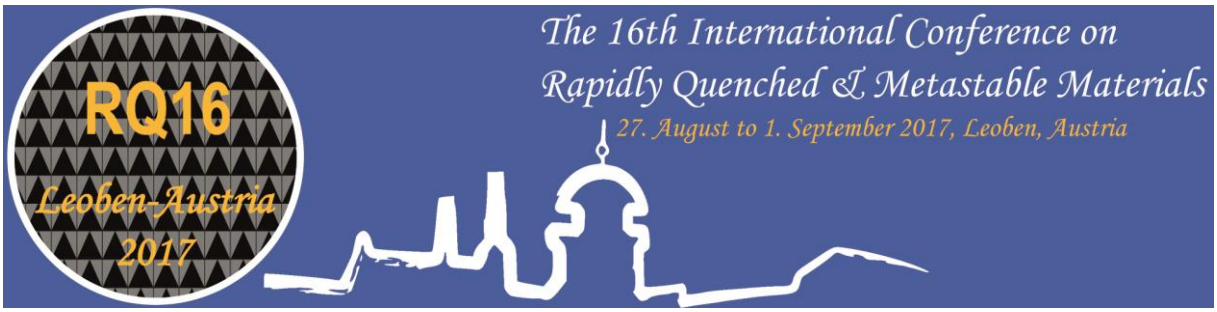
Far from equilibrium materials, exemplified by nanocrystalline (NC) metals and metallic glasses (MGs), are distinct from traditional engineering materials due to their high degree of structural disorder. MGs exhibit global atomic disorder, whereas NC materials exhibit disorder constrained to grain boundary regions. The mechanical behavior of MGs is quite sensitive to the structural state of this disorder – how rejuvenated, i.e. liquid-like, or relaxed the structure is. The ability to control the structural state of MGs via numerous processing routes shows tremendous promise for the control of deformation homogeneity, including suppression of catastrophic shear localization. The effect of local disorder in NC materials manifests in ways reminiscent of fully amorphous materials: mesoscale shear localization, high hardness, pressure-dependent yielding, etc. Furthermore, in the limit of grain sizes <50 nm, NC metals exhibit unique deformation mechanisms relative to their coarse-grained counterparts owing to the high concentration of grain boundaries and their predominance in governing plasticity. Relaxation processes in NC materials, such as low temperature annealing, have been shown to decrease GB energy for a given crystallographic configuration. This reduction in GB energy leads to enhanced mechanical strength, akin to relaxing the structural state of a MG. However, rejuvenation-type processes have not been observed in NC materials and thus limit the tunability of its properties. Here, we use femtosecond laser processing as a unique far-from-equilibrium process that can generate complex stress states due to ultrafast electronic excitation and subsequent relaxation events. We study the influence of sub-ablation threshold femtosecond laser pulses on location-specific properties of NC materials using small scale mechanical testing. Experiments on both NC Al-O and Cu-Zr alloys indicate that sub-ablation femtosecond laser pulses cause a dramatic reduction in hardness accompanied by negligible changes in grain size. Parallels between our results and rejuvenation processes in glassy systems will be discussed in the context of controlling the far-from-equilibrium metastable configuration through novel processing routes.

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



C7-High-Entropy Alloys 2

Design of advanced metastable titanium alloys for functional biomedical devices

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In this communication, the design and the properties of newly developed metastable beta titanium alloys containing biocompatible elements are presented. They show particularly interesting mechanical properties for biomedical applications. Indeed, it was observed that in a given composition domain, the metastable beta microstructure is transformed into a stress-induced alpha" martensite when an external stress is applied leading to a superelastic effect. These Ni-free alloys can then be envisaged to replace the TiNi shape memory alloy for the fabrication of biomedical smart devices such as coronary stents, orthopaedic staples or orthodontic wires. On the other hand, this superelastic effect is accompanied by a very significant reduction of the elastic modulus, which is very beneficial for the medical devices in osseous site such as hip prostheses or dental implants, for which the stress shielding effect must be avoided. With these alloys, the challenge consists to optimize the chemical composition, the micro and the nanostructure at different scale and the mechanical properties in order to propose new highly biocompatible titanium alloys possessing the functional properties adapted to medical devices of dedicated use. Thus, mechanical properties including superelasticity and plasticity were investigated in relation with the different deformation mechanisms observed (stress-induced martensite transformation, twinning and dislocation slip).

KEYWORDS: nanostructured materials, biomedical materials, high performance materials

Presentation Method (Invited/Regular Oral/Poster): Invited

Insights into the thermal stability and deformation behavior of the CrMnFeCoNi high-entropy alloy revealed by nanoindentation

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Recently, it has been shown for different High Entropy Alloys that these might show some microstructural instabilities during annealing resulting in a multi-phase structure, which occurs especially rapid in the nanocrystalline conditions and after prolonged times in the coarse-grained states, as shown for the Cantor alloy CrMnFeCoNi. To gain more insights into the corresponding mechanical properties of differently annealed samples, nanoindentation was used from room temperature to 400 °C and revealed drastic changes in hardness, and strain-rate sensitivity but also in the Young's modulus. The equiatomic face-centered cubic high-entropy alloy CrMnFeCoNi was tested in the nanocrystalline state (grain size ~50 nm) as well as in the cast and homogenized coarse-grained state (grain size ~150 μm). Besides a strong increase in the Young's Modulus due to precipitation formation in the nc-conditions by annealing, a significant scatter in the randomly distributed coarsen-grained states was also found [1]. Further tests in single crystalline regions showed additionally a strong elastic anisotropy and for further detailed analyses a grain with <100>-orientation was selected by electron back scatter diffraction for nanoindentation.

In general, it was found that hardness decreases more strongly with increasing temperature than Young's modulus especially for the coarse-grained state. The modulus of the nanocrystalline state was slightly higher than that of the coarse-grained state, since the latter was tested in the elastically softer <100> orientation. For the coarse-grained sample a strong thermally activated deformation behavior was found up to 150 °C, followed by a diminishing thermally activated contribution at higher testing temperatures. For the nanocrystalline state, different deformation mechanisms are proposed over the tested temperature range. At low temperatures, the governing processes in the nanocrystalline state are similar to those in the coarse-grained condition but, with increasing temperature, dislocation-grain boundary interactions apparently become more dominant. Finally, at 400 °C, where decomposition of the single-phase nanocrystalline alloy occurs, a further reduction of the activation volume was observed. This can be rationalized by a reduction of the deformation controlling internal length scale caused by precipitate formation in conjunction with a diffusional contribution.

KEYWORDS: High Entropy Alloy, Nanoindentation, Thermally activated deformation behavior.

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Presentation Method (Invited/Regular Oral/Poster): Invited

Experimental measurement of pseudo-binary phase diagram of FeCoCrNi-Cu complex concentrated alloys

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One of the biggest difficulties to study on complex concentrated alloys (CCAs) is an absence of precise information on its phase transformation. That is because it is hard not only to expect the exact phase diagram with existing calculation techniques, but also to understand the phase transformation route owing to complex interactions among constituting elements [1]. Meanwhile, some FCC CCA systems including Cu as a constituting element with phase separating behavior were reported. Cu has a strong tendency not to form a single solid solution but to be separated with other 3d transition metals such as Fe, Co, Cr and Ni, since it has large positive enthalpy of mixing with others. In other words, Cu generally forms a stable/metastable miscibility gap with other 3d transition metal elements except Ni at binary conditions.

In the present study, we will report how to measure experimentally pseudo-binary phase diagram of FeCoCrNi-Cu CCAs. Based on the positive enthalpy of mixing between Cu and other 3d transition metals, we inferred that Cu would exhibit phase separation behavior with other constituting elements even at higher configurational entropy condition. First, we drew a pseudo-binary phase diagram with FeCoCrNi CCA and Cu solid solution as the terminal phase by CALPHAD calculation. After then, we carefully figured out phase transformation paths which are needed to determine the phase diagrams such as invariant reaction lines, solubility limits, phase transformation temperatures and so on by a series of experiments. Through these attempts, we can manipulate phase transformation behavior systematically through measuring pseudo-binary phase diagram in FeCoNiCr-Cu phase separating alloy system, which will make an important progress of one step forward in CCA research.

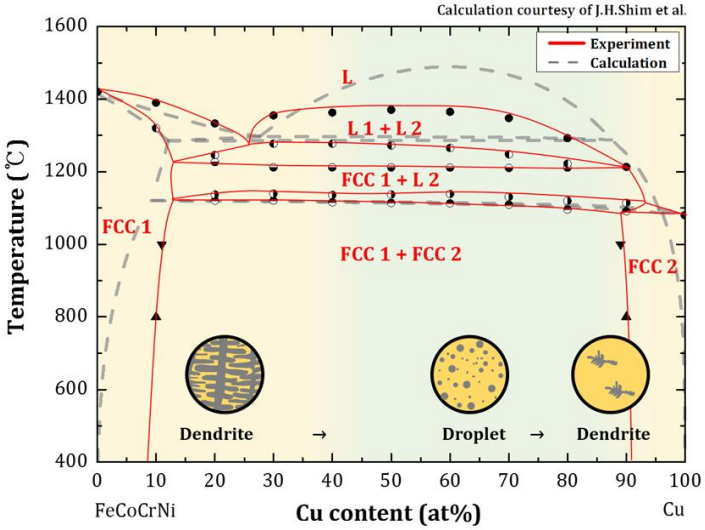

Fig1. Pseudo-binary phase diagram of FeCoCrNi-Cu CCAs

KEYWORDS: **Complex concentrated alloy**, Pseudo-binary phase diagram, CALPHAD, Experimental measurement

1. Chung-Jin Tong, Yu-Liang Chen, Jien-Wei Yeh,Su-Jien Lin, Swe-Kai Chen, Tao-Tsung Shun, Chun-Huei Tsau, Shou-Yi Chang, *Metallurgical and Materials Transactions A*, **36** (2004)

Presentation Method (Invited/Regular Oral/Poster): Regular oral

Microstructure and mechanical properties of Ta-Nb-V-(Ti,W,Mo) high entropy alloys by mechanical alloying and spark plasma sintering

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High entropy alloys (HEAs) usually contains more than 5 metallic elements with nearly equiatomic ratios, but can crystallized as a single phase as solid solution. HEAs have recently drawn remarkably attentions among the scientist due to properties such as high temperature strength, high corrosion, promising resistance to wear oxidation. Many HEAs have been made in the form of bulk by casting process. Recently, HEAs by mechanical alloying (MA) and subsequent consolidation process has been attracted attention due to the unique advantage of mixing elements with large difference among their densities and resulting in homogeneous microstructures [1].

In this study, we report the microstructure and mechanical properties of the $Ta_{20}Nb_{20}V_{20}Mo_{20}W_{20}$, $Ta_{20}Nb_{20}V_{20}Ti_{20}W_{20}$ and $Ta_{20}Nb_{20}V_{20}Mo_{20}Ti_{20}$ HEAs prepared powder metallurgy. The starting materials were Ta, Nb, V, W, Mo and Ti elemental powder with (99.9%) high purity and particle size of ~45 ㎛. The HEAs synthesized by high energy ball milling followed by spark plasma sintering. Structural characterization was performed using X-ray diffractometry (XRD) and scanning electron microscopy (SEM) with energy dispersive spectrometer (EDS). Compressive strength of HEAs was measured at room temperature with a strain rate of $1x10^{-4}s^{-1}$.

KEYWORDS: High entropy alloys, Ball milling, Mechanical alloying, Sintering

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Synthesis and Characterization ofAlCoCrFeNi high entropy alloy (HEA) processed by mechanical alloying and microwave sintering

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High entropy alloys with simple solid solution structures are emerging as advanced class of materials. In contrast to conventional alloys, high entropy alloys contain multiple principle elements, often five or more in equiatomic or near equiatomic ratios [1-3].These alloys have very interesting cocktail effects on the properties due to high entropy, sluggish diffusion and lattice distortion effects. HEAs are reported to possess excellent properties like higher hardness, strength as well as improved wear, oxidation, good corrosion resistance and other functional properties.In the present work AlCoCrFeNi high-entropy alloy was selected for the study. This alloy was prepared with equiatomic proportions of elemental powders by mechanical alloying in a high energy planetary ball mill (Retsch) PM400 up to 30 hours. Structural and microstructural characterizations were carried out by X-ray diffraction (XRD) with CuKα radiation, scanning electron microscopy (SEM) and transmission electron microscopy (TEM TECNAI G^2) techniques.The NETZSCH DSC 404F apparatus was used to check the thermal stability of the alloy powders. In this alloy system, major body-centered cubic (BCC) structure with lattice parameter of 2.8911Åwas observed. It should be noted that, alloy system is having BCC structure, elements like Fe and Cr are stronger elements which are more open structure with high melting point. Thermal analysis of this alloy system suggested that exothermic peaks at 601ºCmight be associated with the formation of new phase. Green pellets were then sintered at 900ºC by microwave heating for 30 min. at 2.45GHz. Two phase microstructure of BCC (a=2.860Å) and FCC (a=3.582Å) was observed in the bulk consolidated HEA. The sintered samples showed microhardness value of 539±16 HV. This HEAs also exhibits very interesting soft magnetic property with 70.05 emu/g saturation magnetization. Phase formation of this alloy was interpreted through detailed Miedema calculations.

Keywords:-High entropy alloy, Mechanical alloying, Microwave heating, Functional properties, Mechanical properties

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

A strategy for overcoming strength-ductility trade off in BCC high-entropy alloy

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Over the last decade high-entropy alloys (HEAs) has attracted significant attention in the metal community. HEAs are single-phase multi-component alloy with the composition of approximately equal atomic concentrations. Contrary to design concept of traditional alloy, HEAs are designed to be composed of multicomponent elements in an equiatomic or near equiatomic ratio to induce high configurational entropy, which stabilize the single solid solution phase. Recently, BCC HEAs composed by Group-4 to Group-6 elements (Ti, Zr, Hf, V, Nb, Ta, Cr, Mo and W) were reported to exhibit superior mechanical properties at high temperature above 1000 ℃ comparing conventional Ni-based superalloy. [1,2] However, it is known that the HEAs containing mainly Group-6 refractory elements (Mo and W) suffer from poor ductility at room termperature, while HEAs without Group-6 refractory elements show poor strength at high tempearture. To devleop HEA with high strength at high temperature and favorable ductiltiy at room temperature, a new BCC HEA systems were designed. It is known that valence electron concentration (VEC) of BCC alloys has negative relationship with ductiltiy, but elements with high mismatch of shear modulus as well as atomic radius (Mo and W) are responsible for high strength of the alloy. To develope an alloy with balanced strength and ductiltiy, Ti-V-Nb-Ta-(Mo, W) system, whose VEC is 5.0 in equiatomic composition, was selected. HEAs in equiatomic and near equiatomic composition in the system were predicted to form single BCC phase by CALPHAD method via calculation of phase diagram, and experimentally confirmed to have single BCC phase. Mechanical properties at room temperature were determined by compression test. Indeed, ductiltiy and strength of the HEAs were quantitatively analyzed in terms of VEC and solid solution hardening. Our results could provide an effective guideline for tailoring mechanical properties of BCC high entropy alloy and developing promising HEAs for high temperature structural materials.

KEYWORDS: high entropy alloy, refractory element, valence electron concentration, mismatch, mechanical property

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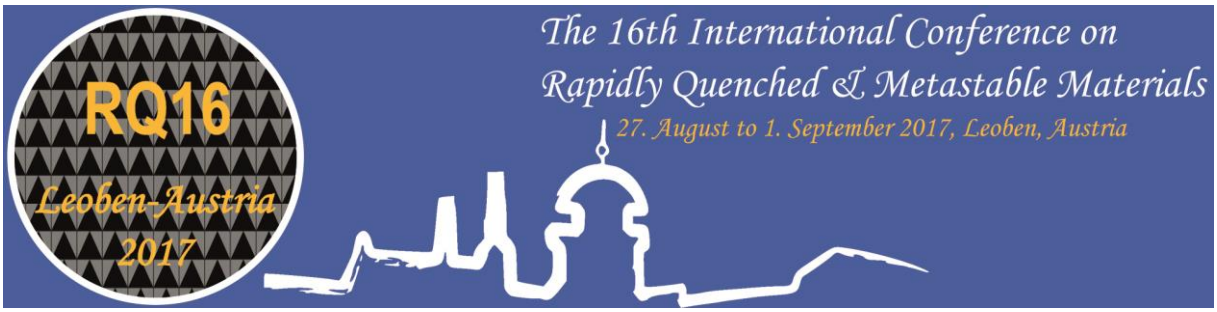
Presentation Method (Invited/Regular Oral/Poster): Regular Oral



A8-Metallic glass 12: Structure & kinetics

Shear bands in metallic glasses: atomic transport, propagation and relaxation behavior

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Plastic deformation of metallic glasses is mostly localized in plate-like mesoscopic defects, so-called shear bands. Their propagation often initiates catastrophic failure. Yet, small compositional variations ("minor alloying") as well as structural heterogeneities can affect their propagation revealing different interaction mechanisms that are summarized in a qualitative mechanism map that categorizes the various processes that may occur in the course of the interaction between shear bands and structural heterogeneities.

Although the occurrence of shear bands is well known and often determines the mechanical performance of the material, their actual physical properties remain fairly unknown. Here, experimental data on the rate of atomic diffusion within shear bands have been obtained using the radiotracer method on post-deformed specimens. Additionally, novel TEM-based methods served to experimentally determine the local specific volume as well as the local degree of medium-range order and the local chemical composition quantitatively. Moreover, local strain fields at shear bands have also been analyzed and the impact of shear deformation and relaxation on the low-temperature heat capacity anomaly known as the "Boson peak" has been addressed, revealing complex dependencies on time, temperature and strain. Relaxation experiments showed an unexpected temporal evolution of the shear bands, including so-called cross-over behavior. The experimental results are discussed with respect to the underlying mechanism during the early stages of shear band activation and their temporal evolution as well as on the properties characterizing these "defects" in deformed metallic glasses.

KEYWORDS: Bulk Metallic Glasses, Shear Bands, Mechanical properties and behavior

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Presentation Method (Invited/Regular Oral/Poster): Invited (keynote) Oral

In-situ methods to study electro-mechanical behavior of flexible electronic materials

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Electrical, mechanical and interfacial properties of thin metal films on compliant polymer substrates are important to understand in order to design reliable flexible electronic devices. Thin films of Cu and Au on polyimide (PI) and polyethylene terephthalate (PET) substrates were examined for their use as interconnects in flexible electronic devices. Using in-situ tensile straining with atomic force microscopy (AFM), X-ray diffraction (XRD), and confocal laser scanning microscopy (CLSM) mechanical and interfacial behavior can be examined. AFM and CLSM can provide information about crack spacing and film delamination, while XRD experiments are utilized to determine the lattice strains and stresses present in the films. If these in-situ techniques are combined with in-situ 4-point-probe (4PP) resistance measurements, the influence of the mechanical damage on the electrical properties can be correlated. This combination of multiple in-situ investigations are particularly useful when studying the electro-mechanical behavior under fatigue conditions where some materials can have an improvement of the electrical conductivity after a few hundred cycles. Mechanisms behind these phenomena as well as methods to measure the adhesion of metal-polymer interfaces found in flexible electronic devices will be discussed.

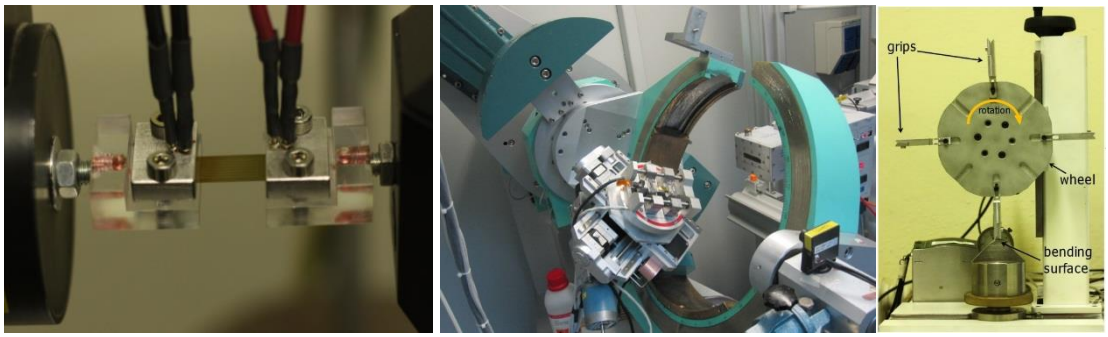

Fig 1. Various tensile and bending stages are used to measure the electro-mechanical behavior of flexible material systems. Examples of in-situ resistance (left), in-situ X-ray diffraction (middle) and cyclic bending (right) are just a few techniques used.

Presentation Method (Invited/Regular Oral/Poster): Invited

In-situ investigation of cracking and stress corrosion cracking in Zr-based bulk metallic glass

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Bulk metallic glasses (BMGs) show extraordinary high strength due to their amorphous structure and the inherent lack of structural defects mediates plasticity [1, 2]. However, this outstanding characteristic is usually a trade-off that is paid with a nearly complete absence of tensile ductility, because BMGs fail catastrophically by localized shear band formation [1]. Therefore, a wealth of investigations on BMGs with respect to shear bands, plasticity and its improvement has been done, e.g. [1-4]. Much less investigations were dedicated to fracture, crack propagation and fracture mechanisms [5] as well as to mechanical failure under corrosive environments [6, 7]. Zr-based BMGs are susceptible to pitting corrosion in halide containing solutions, e.g. [8]. In this work and in earlier investigations the glassy Zr52.5Cu17.9Al10Ni14.6Ti5 alloy (Vit 105) was chosen in order to study corrosion, stress corrosion cracking (SCC) and corrosion fatigue [6-10]. Under stress induced pitting corrosion conditions, i.e. between anodic pitting and repassivation potentials, the SCC behavior of Vit 105 was investigated on full cross section rectangular bars in a specialized 3-point bending SCC setup [6-8]. In result of these earlier studies a phenomenological model on pit-to-crack transition and crack propagation under SCC conditions was proposed [6]. The present study concentrates on notched bars of Vit 105 with geometries which are as close as possible to ASTM 399 conditions in order to further investigate the present SCC failure mechanisms and to validate the proposed model [6]. These works continue with the same setup and protocol and are further enriched by optical and scanning electron microscopy observations during in-situ 3-point bending of similarly notched specimens without corrosive environment (Fig. 1). The analysis will also focus on fracture surface features in relation to lateral shear band patterns. These two complementary approaches are used in order to enhance the general understanding of crack propagation and fracture mechanisms as well as the special implications encountered during SCC under anodic polarization.

Funding from the DFG in the framework of SPP-1594 under grant number GE 1106/11 is gratefully acknowledged.

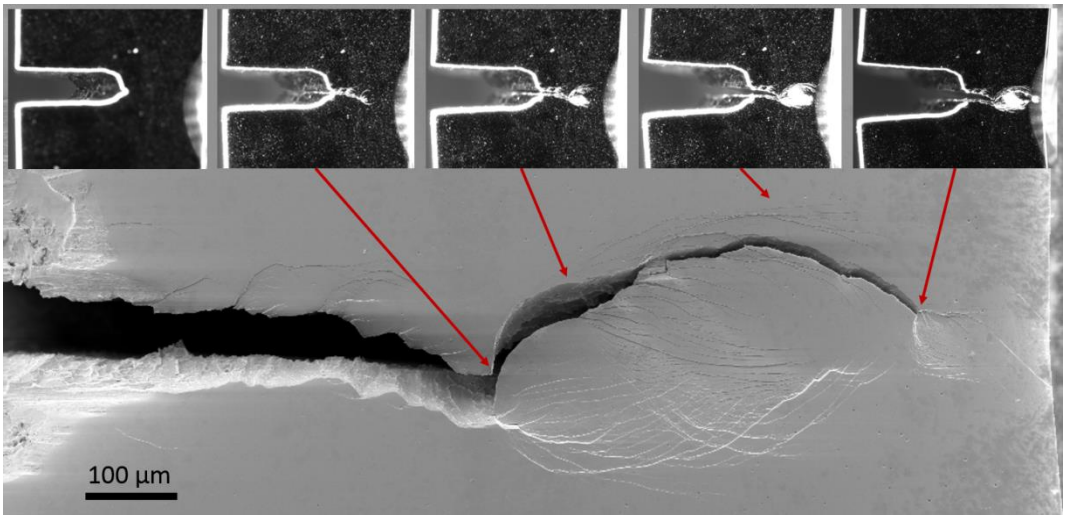

Fig1. Snap shots of in-situ cracking under 3-point bending of a notched Vit 105 BMG specimen.

KEYWORDS: bulk metallic glass, chemical and physical properties, fracture, stress corrosion interactions.

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Transverse excitations in a Pd-Ni-Cu-P alloy of the liquid and supercooled liquid phases

Shinya Hosokawa[1], Masanori Inui[2], Yukio Kajihara[2], Tetsu Ichitsubo[3], Hidemi Kato[3], Kazuhiro Matsuda[4], Koji Kimura[5], Satoshi Tsutsui[6], Alfred Q. R. Baron[7]

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In liquids, transverse acoustic (TA) phonon modes were believed to be undetectable because the shear force in the long special range is very weak. In the terahertz frequency region, however, there is a solid-like cage effect on the *nm* scale that acts as a restoring force for the TA waves. In the previous inelastic x-ray scattering (IXS) experiments on liquid metals [1-3], low-energy excitation modes were clearly observed between the quasielastic peak and the longitudinal acoustic (LA) peak in the dynamic structure factors, $S(Q,\omega)$. Since the lifetime of the cages may become drastically longer in the glass forming metallic liquids, we try to carry out IXS experiments on supercooled and liquid $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ alloy having the best glass-forming ability at present [4] to investigate the TA excitations in metallic melts further.

Figure 1 shows the IXS spectra of supercooled liquid (left) and liquid (right) $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$. Strong LA modes are seen as the red arrows having clear dispersion relations. The TA modes seem to exist between the quasielatic line and the LA peak as the blue arrows. The analyses are now in progress using a damped harmonic oscillator model and a generalized Langevin formula, and the detailed results of microscopic elastic properties will be presented at the conference.

The IXS experiments were performed at BL35XU of the SPring-8 with the approval of the Japan Synchrotron Radiation Research Institute (Proposal Nos. 2013A1138, 2013B1298, and 2014A1059).

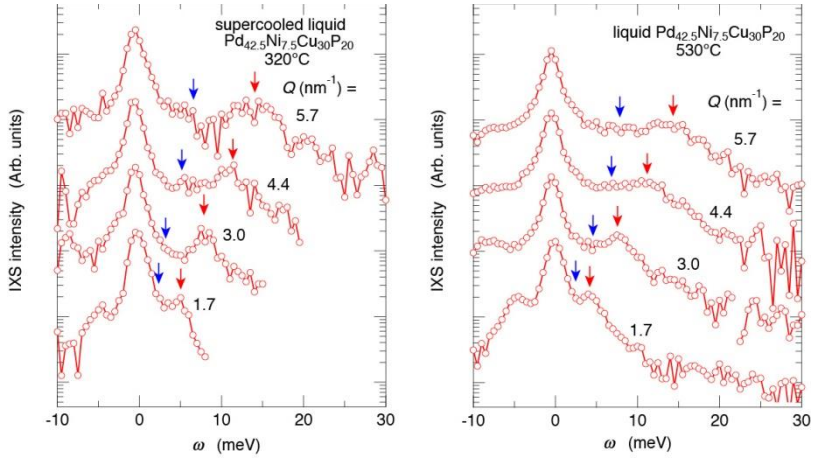

Fig1. I XS spectra of supercooled liquid (left) and liquid (right) $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$.

KEYWORDS: Melt structure and relaxation studies; Chemical and physical properties

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Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Different Sub-T_g Relaxation Patterns in Metallic Glasses far from Equilibrium

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We investigate the sub-T_g relaxation patterns (RPs) in CuZrAl and LaAlNi glass ribbons (GRs) by using the hyperquenching-sub-T_g annealing-calorimetric approach [1-3]. Different from the monotonic relaxation pattern observed in rare-earth based metallic GRs, the abnormal three-steplike sub-T_g relaxation pattern has been observed in CuZrAl ternary glasses. It has been found that the presence of this three-steplike sub-T_g RPs of CuZrAl closely relates to the fictive temperature T_f where the supercooled liquids are frozen in during cooling. Only in a certain range of T_f (or cooling rate for fabrication), this thermodynamic anomaly can be observed. Accompanied with this thermodynamic anomaly, we have observed a three-stage evolution of structures with the increase of annealing degree on CuZrAl GRs. It indicates a dramatic change of the MRO clusters around 1.3 T_g upon cooling in supercooled liquids, which is due to the competitions among the MRO clusters composed of different locally ordering configuration [3, 4]. This accords well with the models based on the competitions between the low-temperature and high-temperature clusters used in the terms of the fragile-to-strong (F-S) transition. In order to further clarify the generality and the origin of this remarkable abnormal thermodynamic phenomenon, the sub-T_g relaxation patterns (RPs) was also detected in other Cu-based metallic GRs. It has been found that this abnormal RPs can be observed in binary CuZr and ternary CuZrAl glasses, rather in quaternary CuZrAlNi. It shows that the anomaly of sub-*T*g relaxation pattern could not be simply attributed to the large difference in the enthalpy of mixing between different elements in alloys. By using a high-temperature torsional oscillating viscometer, the existence of the liquid-liquid phase transition (LLPT) depicted by anomalous viscosity drop during cooling in superheated liquids is also been observed in CuZr and CuZrAl melts. In accordance with this dynamic anomaly well above the liquidus temperature, the thermodynamic evidence in these alloys has also been detected above T_l. A close link between the abnormal three-steplike sub-T_g relaxation pattern in GRs and the LLPT in their corresponding melts has been discovered. This work helps to better understand the complex structural evolution from superheated to glassy solids approaching *T*g.

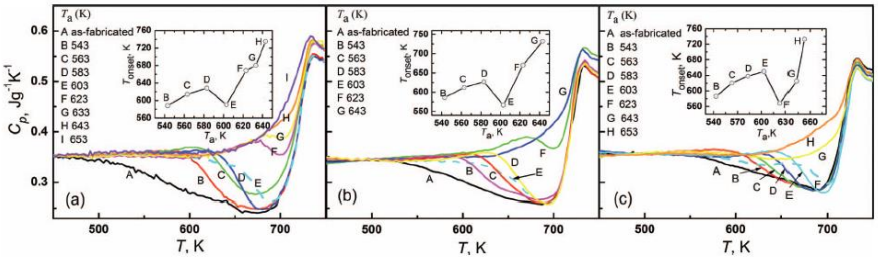

Fig1. Non-monotonic enthalpy relaxation of $Cu_{46}Zr_{46}Al_8$ metallic glasses.T_a points to the annealing temperature.

(a) 35m/s;(b)25m/s;(c)17m/s

KEYWORDS: metallic glass, relaxation, liquid-liquid transition.

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Presentation Method (Invited/Regular Oral/Poster): Regular oral

Thermodynamics, kinetics, and sub-T_g relaxations of Mg-based bulk metallic glasses

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Mg-based bulk metallic glasses are known since the early nineties [1] and have been compositionally varied and optimized [2,3] to reach massive critical casting diameters of up to 27 mm [3]. In the present work, four of these alloys are characterized using calorimetry (DSC, MDSC), thermomechanical analysis (TMA), as well as dynamic-mechanical analysis (DMA).

DSC temperature scans as well as specific heat capacity (C_p) measurements allow to establish the excess Gibbs free enthalpy functions ($\Delta G^{l-x}(T)$), which increase relatively slow with ongoing undercooling. This indicates low driving forces towards crystallization. Small offsets between the C_p curves of glass and supercooled liquid at T_g suggest rather densely packed liquids with sluggish kinetics. The kinetic properties are further investigated via three-point beam bending using a TMA. The obtained sets of isothermal equilibrium viscosities are fitted with the VFT equation and the Adam-Gibbs equation. Strong liquid behavior in terms of the fragility concept is found, with D* values between 20 and 27. The good glass forming abilities of these alloys are interpreted in this context.

Sub-T_g relaxation events and their activation energies are investigated by isochronal DMA temperature scans with various applied frequencies. In addition, these events are observed during modulated DSC measurements (MDSC), where the influence of the thermal history is studied by comparing scans of as-cast samples and slowly cooled samples. It is found, that the signals vanish irreversibly after cooling the sample slowly from the supercooled liquid state into the glassy state.

The definition of the Johari-Goldstein-type secondary relaxation as a general feature of metallic glasses has become increasingly popular in recent literature [4]. Though, some present findings are atypical for this relaxation type, like e.g. the relatively high activation energies or also the massive influence of the thermal history on the signal intensity.

These results accord with recent literature [5], where the sub-T_g events are interpreted as part of the structural relaxation process. This overall interpretation is adopted with some differences in detail, which are discussed.

KEYWORDS: metallic glasses, bulk metallic glasses, heat capacity, thermodynamics, kinetics, fragility, structural relaxation, sub-T_g relaxations, secondary relaxations, calorimetry, dynamic-mechanical analysis, thermomechanical analysis

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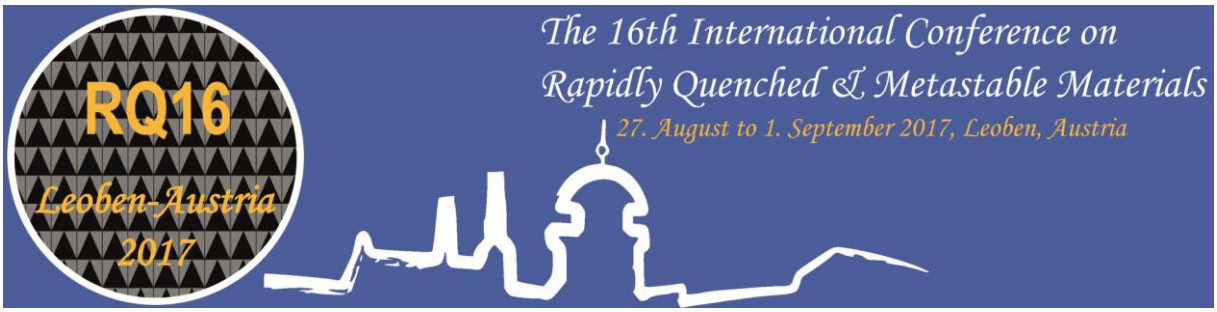
Presentation Method (Invited/Regular Oral/Poster): Regular Oral



B8-Severe plastic deformation 3

Structural instabilities during deformation of nanostructured materials

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Nanostructured materials can nowadays be easily processed by various methods such as deposition or severe plastic deformation. In any case, the resulting microstructure can be considered as highly metastable, not only due to a limited thermal stability, but also during deformation. In such fine grained metals, grain boundaries can no longer be treated as static objects, but will migrate during deformation. Under certain circumstances this can lead to dramatic grain growth and so a change of the mechanical properties. We will show examples of such mechanically induced grain boundary migration under quasi-static and cyclic loading. Results from quasi in-situ experiments which allow to directly track the response of individual grains with respect to the external load will be presented and allow conclusions about the mechanisms and driving forces of mechanically induced grain boundary migration.

Presentation Method (Invited/Regular Oral/Poster): Keynote

Limiting factors for deformation-induced supersaturation during severe plastic deformation

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Mechanical alloying by severe plastic deformation can be used to synthesize alloys with solubilities far beyond equilibrium. This processing method has already been successfully applied to different immiscible systems [1-5], but the underlying processes and the key parameters controlling deformation-induced supersaturation have not been entirely clarified until now.

In this work, various material systems – from crystalline/crystalline, amorphous/crystalline to amorphous/amorphous- have been systematically analyzed and the limiting factors for mechanical intermixing have been determined. Contrary to single-phase materials system-related characteristics like initial hardness, volume fraction and geometrical arrangement of the different phases can play a significant role and influence the complex deformation processes. The degree of supersaturation in the different material systems was determined by X-Ray measurements as well as atom probe tomography and correlated in detail to microstructural changes by scanning and transmission electron microscopy. It is shown that the amount of mixing strongly depends on the homogeneity of the deformation process and is thus affected by the strength differences of the constituent phases. Deformation of material systems with large hardness mismatch results in strong local plasticity in the soft phase. Material systems with phases with similar ductility predominantly co-deform. In some systems a strong tendency for shear band formation is also observed. A clear correlation between the degree of strain-induced supersaturation and the dominating deformation mechanisms is observed.

Funding of this work has been provided by the European Research Council under ERC Grant Agreement No. 340185 USMS.

KEYWORDS: metastable materials, nanostructured materials, bulk metallic glass composites, severe plastic deformation.

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Presentation Method (Invited/Regular Oral/Poster): Invited

Microstructure evolution of ZrCuAgAl metallic glass processed by high pressure torsion

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Metallic glasses (MGs) possess many outstanding properties such as great strength, a high elastic limit and good resistance to corrosion that stem from their disordered atomic configuration [1]. However, the limited ductility due to the early catastrophic failure during plastic deformation is the major obstacle for their applications as structural materials. Recently, high pressure torsion (HPT) has been widely developed to increase ductility of MGs, with the tendency to impose extremely high strains compared to other severe plastic deformation (SPD) processes, such as rolling and shot-peening [2]. However, understanding the changes of the microscopic structure of MG as a result of HPT deformation, and how they affect the macroscopic physical properties still remains unclear.

In this work, we compared the thermal stability and mechanical properties between the as-cast and deformed samples. And we investigated the changes of the microscopic structure of $Zr_{46}(Cu_{4.5/5.5}Ag_{1/5.5})_{46}Al_8$ bulk MG after the HPT deformation by scanning transmission electron microscopy (STEM) methods, including fluctuation electron microscopy (FEM) to get the information of medium range order [3]; and RDF-imaging for short-range structural mapping around the shear bands area of the HPT-processed sample [4].

KEYWORDS: metallic glass; microstructure

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Presentation Method: Regular Oral

Powder metallurgy of W-Cu material synthesized by hot consolidation process

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W-Cu composite materials synthesized by powder metallurgy have shown excellent properties and microstructure for the development of fusion reactors as a plasma facing component. Plasma facing components (PFCs) consist of a plasma facing and a heat sink material. These have to fulfill different functions that require different material properties, for example high melting point of tungsten and excellent thermal conductivity of copper. But it is difficult to prepare and sustain in high heat loads because of high residual and thermal stresses induced at the interfaces due to vast difference in thermal expansion coefficients, $15.4x10^{-6}$/K (W) to $4.5x10^{-6}$/K (Cu). In order to reduce residual stresses at the interface, W-Cu functionally graded material (FGM) was prepared by spark plasma sintering process (SPS), which acts as an interlayer to decrease thermal-induced stress effectively and to avoid delamination and damage. SPS is a pressure sintering method, based on high temperature plasma momentarily generated in the gaps between powder particles. The process offers significant advantages with various kinds of new materials and consistently produces a highly dense compact in a shorter sintering time and of finer grain than conventional methods.

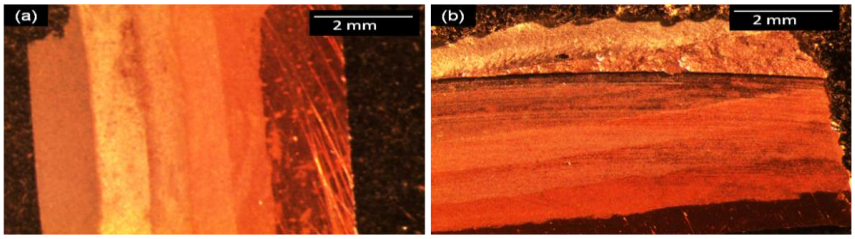
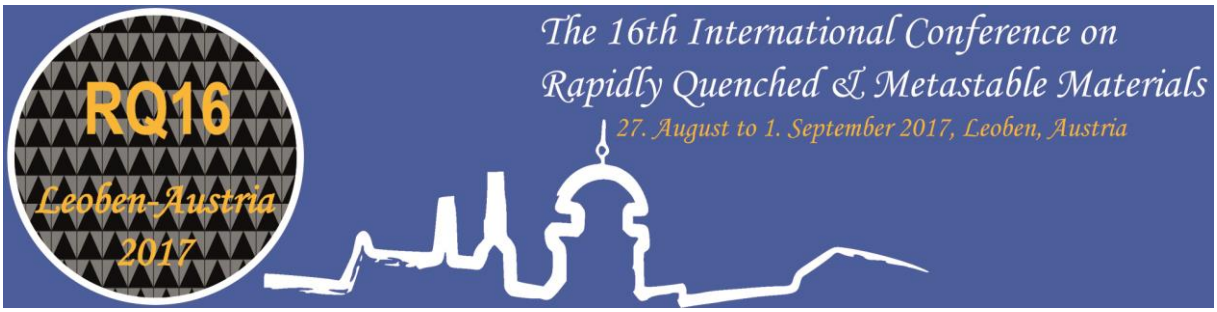


Figure : Stereomicroscopy image showing different layers of the spark plasma sintered sample. (a) 950^0C and (b)1000^0C**.**

In present work seven-layered W/Cu FGM (100W, 80W-20Cu, 60W-40Cu, 50W-50Cu, 40W-60Cu, 20W-80Cu, 100Cu (wt%) with each layer having thickness 1 mm) were fabricated by a spark plasma sintering process at a pressure of 60MPa. Sintering was performed in three different temperatures (i.e. 950^0C, 1000^0C, 1050^0C) for 5min at constant temperature. The influences of sintering temperature on relative density, hardness and microstructure at various layers of sintered samples were investigated. The experimental results indicated that the graded structure of the composite could be well densified after the SPS process. The polished layer surface were analysed by optical microscope and scanning electron microscope. Scanning electron microscopy and energy dispersive X-ray spectrometer analysis showed that the graded structure can be retained at a sintering temperature of 1050^0C and the fine microstructure within each layer can be also maintained due to the short sintering time. The sample sintered at 1050^0C exhibited excellent mechanical and physical properties with higher hardness 239±5 Hv and maximum densification has been achieved 94.45% of their theoretical density.

Keywords: Powder metallurgy, Functionally graded material, Mechanical properties; Spark Plasma Sintering; Plasma Facing Components

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



C8-Undercooled melts & rapid solidification

Advanced Structure Analysis of Hard Magnetic Al-Mn Alloys

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The need for rare-earth free or at least rare-earth-poor hard magnets emphasizes the focus on alloy systems based on Fe-Pt, Co-Pt, Bi-Mn and Al-Mn [1]. In Al-Mn alloy the main issue is, alongside with the development of suitable technology to obtain $Al_{45}Mn_{55}$ alloy with sufficient purity and in reasonable quantity, the formation of the optimal amount of the ferromagnetic τ-AMnl phase. For practical reasons and possible production upscale, metallurgical preparation of a master alloy and its rapid quenching into ribbon or flake form with subsequent suitable thermal treatment seems among the most suitable.

As shown in our previous work [2], as-quenched ribbon contains a mixture of ε- and τ-phases, the ε-phase being a majority phase created in the process of rapid quenching. This work presents among other a minor phase unobserved so far by the XRD analysis, Fig1. Isothermal annealing in the temperature region between 650 – 713 K for several tens of minutes has been shown to lead to transformation of the ε-phase into τ-AlMn phase which already exhibits acceptable hard magnetic properties, especially magnetic coercivity and energy product.

The structure of both types of $Al_{45}Mn_{55}$ phases has been crystallographically investigated previously [3]. However, experimental verification of the validity of atomic scale models has not been verified yet. In addition, the process controlling the transformation from of ε- to τ-phase has not been clarified and it is not known whether the process is of the martensitic type or whether the transformation takes place by nucleation and growth of the forming ε-phase [4]. The τ-phase formation has also been assumed be accompanied by micro-twinning associated with stress relaxation at the growth front [5].

We shall try to investigate the local chemical order of the phases present in rapidly quenched $Al_{45}Mn_{55}$ in as-quenched state and after thermal treatment and to assess the issue of controlling mechanisms of ε- to τ-phase transformation by in-situ transmission electron microscopy.

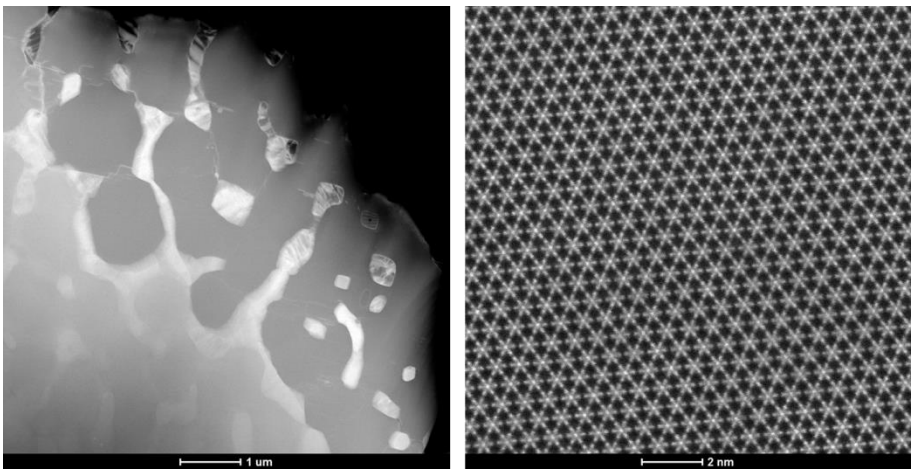

Fig1. DF STEM micrograph of the as-quenched state of $Al_{55}Mn_{45}$ alloy (left), HAADF STEM micrograph of the unidentified ε –AlMn grain inclusion (right) appearing in the left image as the bright areas.

KEYWORDS: Al-Mn magnetic alloy, rapid quenching, .

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Presentation Method (Invited/Regular Oral/Poster): Keynote

Metastable Ti-based alloys for biomedical use

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Current research on materials for load-bearing metallic implants in trauma surgery and orthopaedics focusses on new Ti alloys with significantly lower stiffness values than those of clinically used materials combined with high strength and hardness and excellent biocompatibility. These alloys are expected to reduce the problems of stress shielding and implant failure as well as to suppress complications which are related to the release of metal ions due to corrosion [1]. In this regard, two types of alloys which are only composed of non-toxic constituents are subject of current studies. Firstly, these are alloys in the metastable Ti-Nb system which stabilize a beta-phase and yield Young's moduli ≤60 GPa while strengthening can be achieved by thermomechanical processing [2]. Secondly, Ti(-Nb)-Zr-Si metallic glasses with very high hardness and moderate elastic moduli are developed [3]. As these materials are foreseen for permanent implants, a major demand is the generation of bioactive surface states enabling optimum osseointegration.

In this paper, advanced surface modification strategies for bioactivation of new metastable Ti alloys are presented. Oxidation treatments which yield a variety of oxide coatings with different morphologies and thicknesses from nano- to micron-scale dimensions are reviewed. It is demonstrated that the growth of oxide nanotubes by anodization in fluoride-containing electrolytes is possible for both alloy types, whereby tube diameter and length are controlled by the anodization parameters [4,5]. Plasma-electrolytic oxidation in strongly alkaline solution is applicable to Ti-Nb alloys and yields a complex layer structure with a thin compact inner layer and a thicker outer layer with micropores and microchannels [4]. For glassy Ti(-Nb)-Zr-Si alloys the thermal oxidation behaviour was investigated and a temperature-time frame could be identified for effective growth of an oxide layer under conservation of the amorphous state [6]. Besides that the coating of implant surfaces with bioresorbable bone-like hydroxyapatite (Hap) is considered as effective method for bioactivation. A new approach of electrodeposition of (Sr-substituted) Hap from water-based Ca-nitrate and ammonium dihydrogen-phosphate solutions is presented and the impact of processing parameters like temperature on the Hap morphology is discussed [7].

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KEYWORDS: metastable alloys, metallic glasses, biomedical materials, chemical properties

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Presentation Method (Invited/Regular Oral/Poster): Invited

Hydroxyapatite coated and non-coated novel Fe-Mn-Si-Pd biocompatible alloys, designed for biomedical applications

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Two new, potentially biodegradable, Fe-based alloys, Fe-10Mn6Si1Pd and Fe-30Mn6Si1Pd, were fabricated by arc melting and subsequent copper mould suction casting. The progressive changes in their microstructure, mechanical and magnetic properties during immersion tests in Hank´s solution were investigated. These alloys show relatively high nanoindentation hardness values (5.6 GPa and 4.2 GPa, for 10 and 30 wt% Mn, respectively), higher than the typical hardness of the 316L stainless steel, which constitutes one of the most common Fe-based reference materials for biomedical applications. The cytotoxicity of these alloys was also studied in view of their possible applications. The more hydrophilic Fe-10Mn6Si1Pd showed improved cell adhesion but its pronounced ion leaching had a negative effect on cell proliferation. In an attempt to increase the biocompatibility of this alloy, calcium phosphate coatings (CaP) were grown by pulsed current electrodeposition on Fe-10Mn6Si1Pd alloys. The mechanical behaviour of the coatings was studied by means of scratch testing and nanoindentation. As a general trend, the Young's modulus and hardness values of the electrodeposited coatings were lower than those reported for fully dense hydroxyapatite, independently of the deposition conditions, because of the porous morphology of the coatings. No signs of cracking or delamination were observed during nanoindentation or scratch tests.

KEYWORDS: Rapidly quenched materials, Coating, Mechanical properties, Biomedical materials

Presentation Method (Invited/Regular Oral/Poster): Invited

Rapid Dendritic Solidification and Physical Properties of Co-4.54%Sn Alloy with Broad Mushy Zone

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The high undercooling has a significant influence on the microstructural characteristics and physical properties of as-solidified alloys. Here we report that the dendritic growth and physical properties of Co-4.54%Sn alloy with broad mushy zone depend remarkably on the undercooling levels during rapid solidification. The maximum undercooling attains 208 K with glass fluxing method and 314 K($0.18T_L$) at free fall condition, and XRD analyses show that there are three phases of (αCo), βCo_3Sn_2 and (εCo) at the different undercoolings. The dendritic growth velocity of primary (αCo) phase is quite sluggish in highly undercooled liquid Co-4.54%Sn alloy because it has a broad solidification temperature range of 375 K($0.21T_L$). The maximum value is only 0.95 m/s at the undercooling of 175 K, then it decreases with the undercooling. The microstructure is refined visibly and the volume fraction of interdendritic βCo_3Sn_2 phase decreases with the increase of undercooling and the decrease of droplet diameter. EDS results show that the solute content of primary (αCo) phase exceeds 0.56 wt.%Sn once the temperature decreases below 1760 K according to the equilibrium phase diagram of binary Co-Sn alloy, and exhibits the obvious solute trapping effect under high undercooling. The microhardness displays the linear trend with undercooling, and it increases 1.5 times from 11 to 185 K undercooling. The electrical resistivity shows the nonlinear feature with increase of undercooling. Clearly, the nucleation rate increases rapidly with the increase of undercooling, which enhances the number of crystal nuclei and refines the microstructure obviously, therefore the grain boundary hinders the electronic transmission. Meanwhile, the magnetic conductivity and saturation magnetization decrease, whereas the remanent magnetization and coercivity increase with undercooling also due to the dendritic growth velocity and solute content enhancement in primary (αCo) phase during rapid solidification.

Keyword: rapid solidification, dendritic growth, microhardness, electrical resistivity, magnetic property

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

An Experimental Study of Thermophysical Properties for Liquid and Solid Binary Ti–Nb Alloys

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Owing to their strong chemical reactivity at high temperatures, the substantial undercooling of liquid Ti-based alloys is usually difficult to achieve. The electromagnetic levitation technique provides a containerless environment, and substantial undercoolings can be obtained in this way. Here, the thermophysical properties and rapid solidification of binary Ti-Nb alloys were investigated by electromagnetic levitation. Maximum undercoolings of 208 K ($0.10T_L$) and 203 K ($0.10T_L$) were achieved for liquid Ti-10at.%Nb and Ti-25at.%Nb alloys, respectively. The thermophysical properties of liquid Ti-Nb alloys were determined over a wide temperature range. The viscosity and density of undercooled liquid Ti-Nb alloys were also calculated by some well-known models using the measured data as input. Moreover, the relationship between dendritic growth velocity and liquid undercooling was determined as a power function, and the growth velocity of liquid Ti-10at.%Nb alloy attained over 10 ms^{-1} at the maximum undercooling of 208 K ($0.10T_L$). The microstructure evolution and solute redistribution mechanisms were studied through XRD, SEM and EDS analyses. The microhardness measurements were explored at various undercooling conditions. In addition, the thermal diffusivity and thermal conductivity of solid Ti-Nb alloys were also determined by laser flash method, and the measured results displayed a significant change in the experimental temperature range.

KEYWORDS: Ti-Nb alloy, high undercooling, thermophysical property, rapid solidification

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Rapid crystallization of undercooled liquid Ag-Si and Ag-Cu-Si alloys

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The crystallization of liquids is a common phenomenon in nature, and has attracted much attention in the fields of material science, chemical engineering, and biology. For metallic materials, crystallization can occur in undercooled metallic melts after nucleation. The microstructure formed during crystallization determines the property of materials. Therefore, it is essential to understand the crystallization process and then to control the microstructure in order to improve the performance of the materials. The drop tube technique provides a rapid solidification condition for dispersive metallic droplets during free fall. The information of nucleation and growth can be extracted from the thermal diagram using differential scanning calorimetry (DSC) method. In this presentation, the rapid crystallization of liquid silver, Ag-Si, and Ag-Cu-Si alloys is achieved by drop tube and DSC methods. Under the drop tube condition, the microstructures of Ag-Si and Ag-Cu-Si alloys are refined with the decrease of droplet diameters due to the increase of cooling rate and undercooling. Meanwhile, the isothermal and nonisothermal crystallization of pure silver, Ag-Si and Ag-Cu-Si alloys is investigated by DSC method. Different undercoolings have been achieved by setting the holding temperature or cooling rate for isothermal and nonisothermal crystallization, respectively. With the increase of undercooling, the solidification of silver, Ag-Si and Ag-Cu-Si alloys shows sharper exothermic peak in the thermal diagram. The transformed solid fraction is extracted to analysis the crystallization kinemics using Avrami equation. It is revealed that the Avrami exponent varies with the extent of crystallization for both the isothermal and nonisothermal conditions. This indicates that the growth mechanism changes at different stages of crystallization in pure silver, Ag-Si and Ag-Cu-Si alloys.

KEYWORDS: Drop tube, Ag-Cu-Si alloys, Avrami exponent, Thermodynamics and phase transformation studies, Chemical and physical properties

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Thermophysical Properties and Dendrite Growth Kinetics of Supercooled Liquid Refractory W-Ta Alloys

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Since its discovery by Fahrenheit in 1724, the supercooling phenomenon of liquids, which entraps a metastable liquid state even well below their freezing temperatures, is still fascinating scientists in diverse areas, such as the origins of nucleation, the hail prevention in meteorology, and the control of materials solidification. The supercooling of metallic liquids, which implies the thermodynamic activation barrier to be surpassed for crystallization, determines not only crystal growth kinetics but also phase selection process or the formation of metastable phases.

The high melting temperature and the physico-chemical contamination from container walls make it difficult to investigate the solidification process of liquid refractory metals by conventional methods. The containerless processing by electrostatic levitation not only eliminates the heterogeneous nucleation from container walls, but also displays satisfactory stability for levitated liquid metal. It is very suitable for measuring the thermophysical properties, such as density and surface tension, and investigating dendrite growth kinetics of metastable supercooled melts.

The liquid W and W-*x*%Ta (*x*=25,50,75) alloys were supercooled by up to 733K ($0.2T_m$) and 773K ($0.23T_L$) respectively. The measured density and the ratio of specific heat to emissivity displayed a linearly increasing tendency versus supercooling. The thermal dendrites in supercooled liquid tungsten achieved a maximum growth velocity of 41.3 $m \cdot s^{-1}$, and the concurrent recalescence process exhibited Johnson-Mehl-Avrami type kinetics. Liquid W-Ta alloys showed stronger supercoolability but a lower maximum dendrite growth velocity of only 35.2 $m \cdot s^{-1}$. The dendritic growth kinetics was always characterized by a power function relation to liquid supercooling. The microstructure of equiaxed grains transforms to the well-developed dendrites with the increase of supercooling. Grain refinement effect resulting from dendrite fragmentation took place at moderate supercooling regime in rapidly solidified W-Ta alloys.

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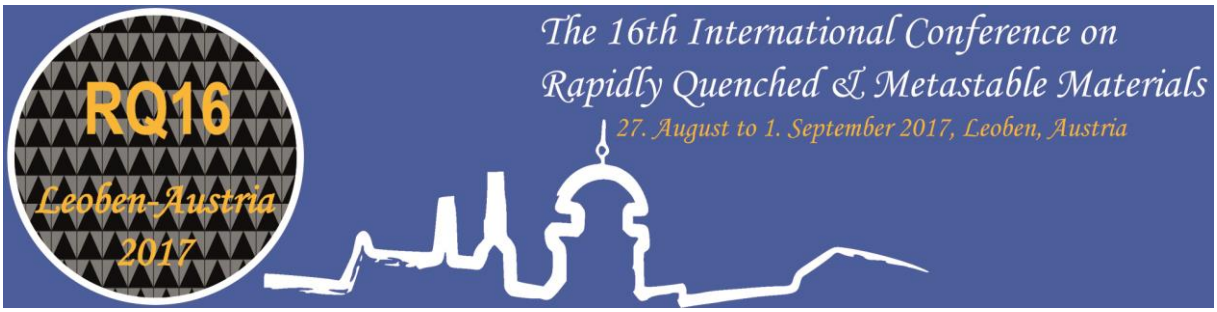
KEYWORDS: W-Ta alloy, Supercooling, Thermophysical properties, Dendrite growth, Electrostatic levitation.

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



D1-Thin film 1 & metallic glass: properties

Quantum mechanically guided materials design and experimentally guided quantum mechanical calculations of short range ordered thin film materials

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A paramount challenge in materials science is to design damage-tolerant glasses. Poisson's ratio is commonly used as a criterion to gauge the brittle-ductile transition in glasses. However, our data, as well as results in the literature, are in conflict with the concept of Poisson's ratio serving as a universal parameter for fracture energy. Here, we identify the electronic structure fingerprint associated with damage tolerance in thin film metallic glasses. Our correlative theoretical and experimental data reveal that the fraction of bonds stemming from hybridised states compared to the overall bonding can be associated with damage tolerance in thin film metallic glasses. [1]

Utilizing a similar computational approach We have systematically studied the effect of transition metal valence electron concentration (VEC) of amorphous $T_{0.75}Y_{0.75}B_{14}$ (a-$T_{0.75}Y_{0.75}B_{14}$, *T*= Sc, Ti, V, Y, Zr, Nb) on the elastic properties, bonding, density and electronic structure using *ab initio* molecular dynamics. As the transition metal VEC is increased in both periods, the bulk modulus increases linearly with molar- and mass density. This trend can be understood by a concomitant decrease in cohesive energy. *T'* = Ti and Zr were selected to validate the predicted data experimentally. A-$Ti_{0.74}Y_{0.80}B_{14}$ and a-$Zr_{0.75}Y_{0.75}B_{14}$ thin films were synthesized by high power pulsed magnetron sputtering. Chemical composition analysis revealed the presence of up to 5 at.% impurities, with O being the largest fraction. The measured Young's modulus values for a-$Ti_{0.74}Y_{0.80}B_{14}$ (301±8 GPa) and a-$Zr_{0.75}Y_{0.75}B_{14}$ (306±9 GPa) are more than 20% smaller than the predicted ones. The influence of O incorporation on the elastic properties for these selected systems was theoretically studied, exemplarily in a-$Ti_{0.75}Y_{0.75}B_{12.75}O_{1.25}$. Based on *ab initio* data, we suggest that a-$Ti_{0.75}Y_{0.75}B_{14}$ exhibits a very dense B network, which is partly severed in a-$Ti_{0.75}Y_{0.75}B_{12.75}O_{1.25}$. Upon O incorporation, the average coordination number of B and the molar density decrease by 9% and 8%, respectively. Based on these data the more than 20% reduced Young's modulus obtained experimentally for films containing impurities compared to the calculated Young's modulus for a-$Ti_{0.75}Y_{0.75}B_{14}$ (without incorporated oxygen) can be rationalized. The presence of oxygen impurities disrupts the strong B network causing a concomitant decrease in molar density and Young's modulus. Very good agreement between the measured and calculated Young's modulus values is obtained if the presence of impurities is considered in the calculations. The implications of these findings are that prediction efforts regarding the elastic properties of amorphous borides containing oxygen impurities on the at.% level are flawed without taking the presence of impurities into account. [2]

KEYWORDS: thin film fabrication, metastable materials, modelling

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Presentation Method (Invited/Regular Oral/Poster): Keynote

In situ small scale fracture experiments: A new tool for developing quenched materials

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The mechanical properties of engineering components can – in brittle systems – be decisively influenced by the local properties of individual phases and interfaces. *In situ* micromechanics allows for probing properties like yield strength and fracture toughness down to the sub-micron scale [1, 2]. Thereby, micro fracture experiments [3] are the ideal tool to assess the fracture properties of physical vapor deposited (PVD) metallic glasses [4].

Within the talk, the state-of-the-art in micro fracture experiments will be shown and discussed. The talk focusses on metallic glass thin films (including the ones from [4]) and silicon [2, 5] as model materials and will discuss the influence of sample size, sample geometry, notch shape and elastic anisotropy of the material.

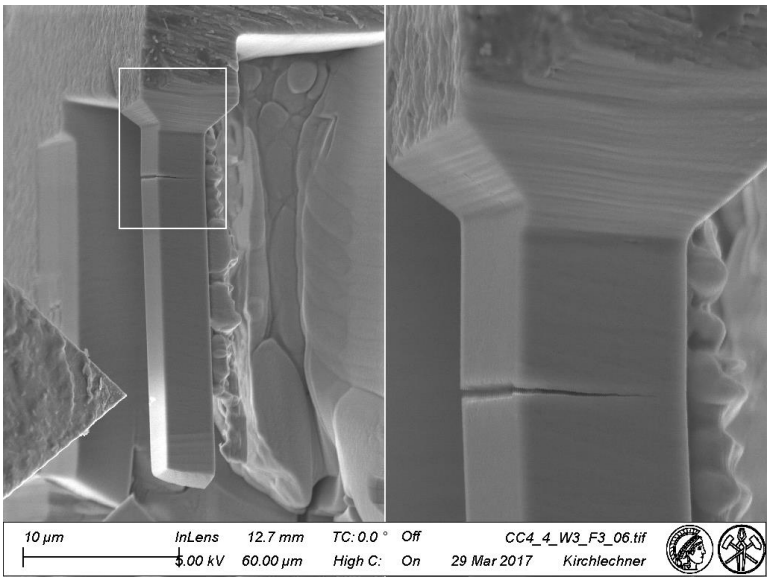

Fig 1. A fractured micro-cantilever.

KEYWORDS: Metallic glas, fracture, *in situ* microscopy

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Presentation Method: Invited

Structure and approach of the mechanical strength and deformation of nano porous silver prepared by de-alloying

Daria Barsuk[1], Alberto Moreira Jorge Junior[1,2,3], Mathilde Laurent Brocq[4] and Yannick Champion[1].

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Production of nanoporous materials by simple or electrochemical de-alloying is being used for several decades. Dealloying is one of the most common methods, which allows driving the structure formation by the power of the chemical solution and by the control of time and temperature. Nanoporous silver was produced by dealloying of an AgCuSi alloy in a HNO_3-HF-H_2O solution. AgCuSi alloy was prepared by melt spinning producing nanometer grain size more favorable to nanoligaments and steady amorphous structure formation during the etching process. The nanoporous material was characterized using FIB sectioning and computing 3D image reconstruction (Fig. 1). The procedure allows analyzing local curvature of internal surfaces that we would intend to correlate to catalytic properties [1]. Mechanical properties were then approached using nanoindentation. A depth-hardness dependence was analyzed and an analytical modeling was proposed to explain the observed trends. The results show that structural properties in terms of local ligament arrangement, local density and their variation with deformation can be approached and quantified.

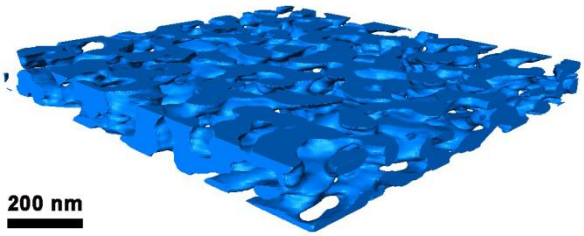

Fig1. FIB sectioning and 3D image reconstruction of nanoporous sylver prepared by de-alloying of AgCuSi alloy.

KEYWORDS: At least two keywords from the Conference Topics should be included.

1. D. Barsuk, A. Zadick, M. Chatenet, K. Georgarakis, N. T. Panagiotopoulos, Yannick Champion, Alberto Moreira Jorge Jr, *Materials and Design*, **111**, 528 (2016).

Presentation Method (Invited/Regular Oral/Poster): Invited

Effect of Au addition on the corrosion activity of Ca-Mg-Zn bulk metallic glasses in Ringer's solution

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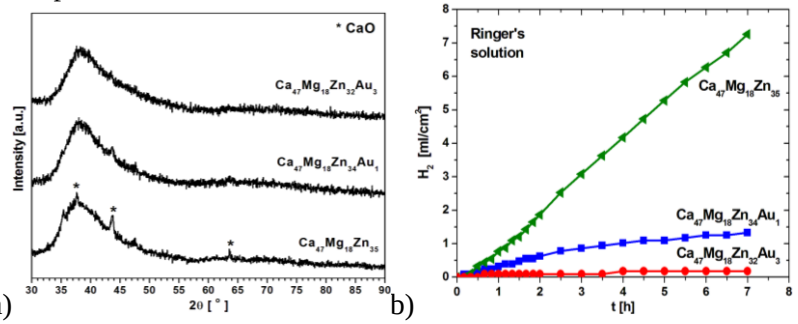
Ca-based metallic glasses due to their resorbable behavior and biocompatibility can be used as temporary resorbable implants [1,2]. Unfortunately, using of calcium alloys as biomaterials are limited by their rapid degradation. It is also known that the degradation of calcium alloys leads to the hydrogen evolution [3]. In some cases, the corrosion activity of calcium alloys may be decreased by introduction of alloying elements. Li et al. [4] reported that the dissoluble features of Ca-Mg-Zn glasses in water can be controlled by alloying additions. Therefore, the aim of the research is to study the effect of minor Au addition on the active behavior of bulk Ca-based metallic glasses in Ringer's solution.

The studies were performed on $Ca_{47}Mg_{18}Zn_{35-x}Au_x$ (x=0,1,3) (at.%) metallic glasses in the form of plates. The master ingots were remelted in a quartz crucible and then injected into a copper mold by the pressure casting to fabricate 1 mm thick plates [1]. The amorphous structure of the samples in the as-cast state was checked by X-ray diffraction (XRD) in the reflection mode using the Co *K*α radiation source. The corrosion behavior of the bulk glassy samples in the form of plates was studied by immersion tests in Baxter Ringer's solution (8.6 g/dm^3 NaCl, 0.3 g/dm^3 KCl, 0.48 g/dm^3 $CaCl_2 \cdot 6H_2O$).

The XRD measurements revealed that the as-cast samples were amorphous. The diffraction patterns show the broad diffraction halo centered at about 37º in 2θ range (Fig. 1a). However, small reflections come from calcium oxides can be noticed for $Ca_{47}Mg_{18}Zn_{35}$ alloy. Fig.1b shows the influence of Au content on the hydrogen evolution volume as a function of time. Studied samples exhibited significantly less hydrogen evolution volumes for $Ca_{47}Mg_{18}Zn_{34}Au_3$ (0.18 ml/cm^2), $Ca_{47}Mg_{18}Zn_{34}Au_1$ (1.32 ml/cm^2) alloys than $Ca_{47}Mg_{18}Zn_{35}$ glass (7.25 ml/cm^2). The hydrogen evolution of the glassy samples with minor Au addition indicated a potential of these alloys as new calcium alloys with improved corrosion resistance.



a) b)

Fig.1. X-ray diffraction patterns of $Ca_{47}Mg_{18}Zn_{35}$, $Ca_{47}Mg_{18}Zn_{34}Au_1$, $Ca_{47}Mg_{18}Zn_{34}Au_3$ bulk metallic glasses in as-cast state (a) and hydrogen evolution volume after corrosion test in Ringer's solution (b).

KEYWORDS: amorphous alloys, bulk metallic glasses, corrosion activity, hydrogen evolution
The work was supported by National Science Centre under research project no.: 2013/09/B/ST8/02129.

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Presentation Method: Regular Oral

In-situ Tensile Deformation of Thin Film Metallic Glasses

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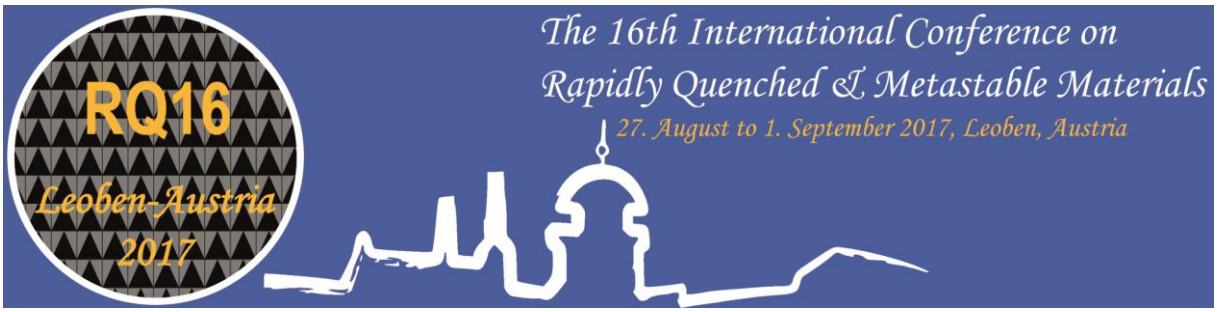
While crystalline metallic thin films have a long history as protective or functional coatings, their amorphous counterparts – so-called thin film metallic glasses – have only recently emerged as promising functional materials. Potential areas of application include actuators and sensors, as well as biomedical films. Due to their disordered structure, thin film metallic glasses do not show work-hardening behaviour and tend to fail catastrophically under tension by the formation of shear bands. To investigate this failure mechanism, we prepare binary crystalline and amorphous metallic thin films (thickness < 100 nm) by co-sputtering from elemental targets in an unbalanced DC magnetron sputtering device. The microstructural variation is achieved either by an adjustment of deposition temperature (e.g. amorphous CuZr at room temperature, crystalline CuZr at 650 °C) or a change in chemical composition (e.g. amorphous $Pd_{0.85}Si_{0.15}$, crystalline $Pd_{0.69}Si_{0.31}$).

Selected samples deposited on polymer substrates are analyzed in a tensile testing set-up with *in-situ* resistance measurements. The strain at which cracks start to form in the film can be determined exactly as the point where resistance starts to increase. Scanning electron microscopy of the strained samples provides more information on the failure mode. In amorphous samples, characteristic shear bands are evident with a 45° angle to the straining direction in addition to large cracks formed normal to the straining direction.

To further illustrate the crack formation and propagation, amorphous samples deposited on NaCl substrates are floated onto a grid in water. These metallic glass thin film foils are then subjected to qualitative *in-situ* tensile tests in a transmission electron microscope. Experimental results are compared to molecular dynamics simulations (Murali, PRL 107 2011). It is found that two different crack propagation modes, i.e. ductile and brittle, can be active in amorphous films, depending on the free volume ahead of the crack tip. This could be a potential future approach for tuning the fracture mode in amorphous metallic films.

KEYWORDS: Thin Films and Coatings, Metallic Glasses

Presentation Method (Invited/Regular Oral/Poster): Regular Oral



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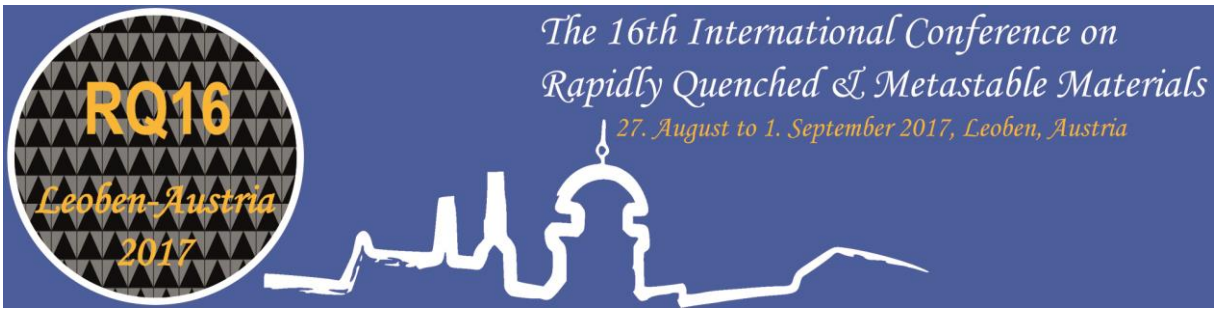

A9-Thin film 2

Reactive and non-reactive sputter deposition of MoO_x thin films

Julia Pachlhofer[1], Robert Franz[1], Enrico Franzke[2], Aitana Tarazaga Martín-Luengo[3], Alberta Bonanni[3], Harald Köstenbauer[2], Jörg Winkler[2], Christian Mitterer[1]

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Due to their unique optical, electrical and chemical properties, oxide-based thin film materials are widely used in industrial applications. In particular, depending on their oxidation state, molybdenum oxides (MoO_x) are characterized by a wide variation of electrical and optical properties, ranging from the non-transparent appearance with metal-like electrical conductivity of MoO_2 to the transparent and electrically insulating behaviour of MoO_3. Tuning chemical bond characteristics might thus enable to adjust their electrical and optical properties in a wide range, making them interesting candidates for optical and electronic applications.

Within this work, MoO_x thin films were synthesized by dc magnetron sputter deposition using two different approaches: (*i*) reactive sputtering from a Mo target in an Ar/O_2 atmosphere, where the partial pressure of oxygen was used to adjust the chemical composition of the films, and (*ii*) sputtering from MoO_x targets in a non-reactive process. For reactive sputter deposition from Mo targets at moderate O_2 partial pressures, amorphous-like films dominated by MoO_2 bonds with electrical conductivity similar to metallic Mo and high optical absorbance of up to 70 % were obtained. Exceeding a critical O_2 partial pressure results in formation of crystalline and highly transparent, but insulating MoO_3-dominated films [0,0]. Since such reactive deposition processes using high oxygen partial pressures are disadvantageous for large-scale synthesis of thin films due to process instabilities, in a second approach synthesis of MoO_x thin films by non-reactive dc magnetron sputter deposition using MoO_x targets was explored. The films obtained in the non-reactive mode exhibited an amorphous structure dominated by MoO_2 bonds with properties similar to those grown by the reactive process. Small additions of O_2 to the process gas yielded the same transition in structure and properties of the films as in the reactive mode; however, at a significantly lower O_2 partial pressure [0]. In general, the use of oxide targets in dc magnetron sputter deposition of MoO_x films offers an efficient and reliable alternative to films sputtered reactively from metal targets and might thus enable their use in a wide range of optical and electronic applications.

KEYWORDS: Thin films and coatings, Nanostructured materials.

J.M. Pachlhofer, C. Jachs, R. Franz, E. Franzke, H. Köstenbauer, J. Winkler, and C. Mitterer, *Vacuum* **131**, 246 (2016).

J.M. Pachlhofer, A. Tarazaga Martín-Luengo, R. Franz, E. Franzke, H. Köstenbauer, J. Winkler, A. Bonanni, and C. Mitterer, *J. Vac. Sci. Technol.* A **35**, 021504 (2017).

J.M. Pachlhofer, A. Tarazaga Martín-Luengo, R. Franz, E. Franzke, H. Köstenbauer, J. Winkler, A. Bonanni, C. Mitterer, submitted for publication.

Presentation Method (Invited/Regular Oral/Poster):Keynote

Revealing the interface effects in hard coatings at the atomic level

Zaoli Zhang

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Transition metal nitrides have found wide-spread applications in the cutting- and machining-tool industry due to their extreme hardness, thermal stability and resistance to corrosion. The increasing demand of these nitrides requires an in-depth understanding of their structures at the atomic level. This has led to numerous experimental and theoretical researches [1-2].

In this paper, we will firstly present the recent results on the atomic and electronic structures of the interface between various metal nitride mono-layer films (CrN, VN and TiN) on MgO and Al_2O_3 substrate using C_S-corrected high resolution transmission electron microscopy (HRTEM), scanning TEM, electron energy loss spectroscopy (EELS), quantitative atomic measurements, and theoretical calculations. Interfacial detailed atomic and electronic structures are revealed. Interface induced phenomena between nitride films and substrates are unveiled [1-4]. The emphasis will also be placed on the nitrogen vacancy effect at the interface. The study brought about some interesting results.

The second example will be on nanolayers. CrN/AlN nanolayers exhibit a peak in hardness of ~40 GPa under certain bilayer period (Λ). These improvements in mechanical properties in comparison with their monolithic counterparts have a close relationship with the existence of a metastable face-centered cubic (*fcc*) AlN phase which can be epitaxially stabilized in thin films. Here, interplanar spacing oscillations in cubic CrN/AlN multilayers were experimentally observed by using spherical aberration-corrected HRTEM, and were corroborated by first principles calculations. Electron spectroscopy and microscopy were employed to analyze the strain distribution in the multilayers and obtain generalized relationships between the electronic structure on the one hand, and (non-)stoichiometry or strains in the multilayers on the other hand. The present study provides atomic-scale insights in the mechanisms of extraordinary strength pertaining to the CrN/AlN multilayers [3].

KEYWORDS: hard coatings, atomic resolution TEM, electron energy loss spectroscopy (EELS)

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3. The author would like to thank David Holec, Rostislav Daniel and Christian Mitterer (Montanuniversität Leoben), Matthias Bartosik and Paul H.Mayrhofer (TU Wien) for helpful discussions and preparing the film materials. Thanks are also given to Gerhard Dehm (Max-Planck-Institut für Eisenforschung, Düsseldorf) for inspiring discussion.

Presentation Method (Invited/Regular Oral/Poster): Invited

Metastable single-phase rock salt structure VAlN thin films grown by Al^+ subplantation

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J.M. Schneider[2]

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Conventional design approaches for transition metal nitride coatings with improved thermal and chemical stability are based on alloying with Al. The solubility of Al in NaCl-structure transition metal nitrides is, however, limited which presents a great challenge to increase Al concentration substantially, while avoiding precipitation of thermodynamically-favored wurtzite-AlN phase (*w*-AlN), detrimental to mechanical properties.

Here, we use VAlN as a model system to demonstrate a new concept for the synthesis of a metastable single-phase NaCl-structure thin films with Al content far beyond solubility limits obtained with conventional plasma processes. This is achieved by separating the film-forming species in time and energy domains through synchronization of the pulsed substrate bias with intense periodic fluxes of energetic Al^+ metal ions during reactive hybrid high power impulse magnetron sputtering (HIPIMS) of Al target and direct current magnetron sputtering of V target in Ar/N_2 gas mixture.[1] 70-μs-long bias pulses with an amplitude of -300 V are applied synchronously with the Al^+-rich portion of HIPIMS discharge, to increase implantation depth of ionized Al. At all other times the substrate is floating at -10 V, which suppresses ion mixing due to gas ion bombardment and leads to VN-rich surface even for the case where time-averaged Al flux significantly exceeds that of V. Thus, single-phase cubic VN crystallites dominate the surface and provide a template for subplanted Al^+ metal ions to crystallize in the metastable NaCl structure rather than to nucleate second phase *w*-AlN. We show that Al subplantation enables an unprecedented 42% increase in metastable Al solubility limit in $V_{1-x}Al_xN$, from x = 0.52 obtained with conventional method to 0.75. High Al-content cubic VAlN films grown by the Al^+-subplantation technique exhibit fully-dense nanostructure and excellent mechanical properties with hardness in the range of 28-30 GPa for Al fractions on the cation lattice as high as 84%. The elastic modulus is with 325±5 GPa in excellent agreement with density functional theory calculations, and approximately 50% larger than the coating deposited by DCMS. This substantial improvement with respect to the conventional techniques opens the way for synthesis of supersaturated single-phase alloy thin films combining excellent mechanical properties with high oxidation resistance. Extensions of the presented method to other materials systems are expected to be straightforward.

* presenting author, grzgr@ifm.liu.se

KEYWORDS: metastability, thin films, nitrides, magnetron sputtering, HIPIMS

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Presentation Method (Invited/Regular Oral/Poster): Invited

Enhanced Atomic Interdiffusion of immiscible elements Fe/Cu in amorphous FeZr/CuZr multilayers

Tao Feng[1*], Ming Sun[1], Guo Peng[1], Si Lan[1], Horst Hahn[1,2], Herbert Gleiter[1,2]

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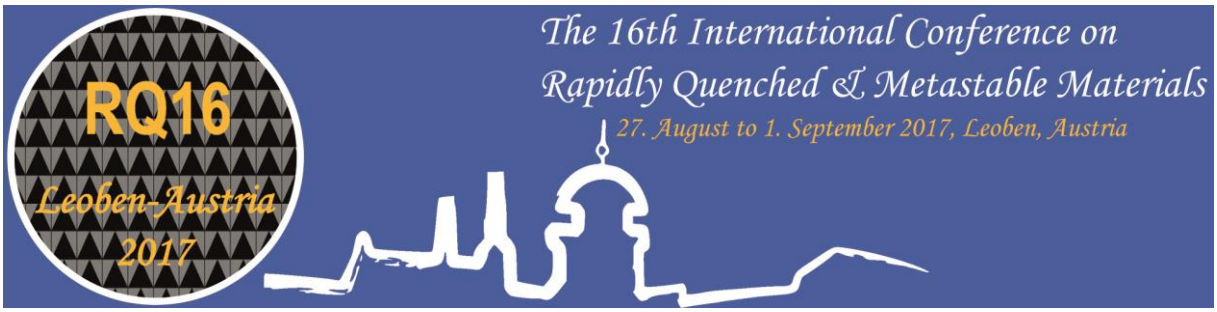
The FeZr/CuZr multilayer thin film metallic glasses (TFMGs) were prepared by magnetron sputtering technique. The amorphous structure and morphology of the multilayer TFMGs were confirmed by X-ray diffraction (XRD), high-resolution and scanning transmission electron microscopy (HRTEM/STEM) characterization. Atom probe tomography (APT) with 3D reconstruction function was employed to analyze the atomic interdiffusion at the interface of the FeZr/CuZr multilayers before and after annealing at 573K for 60 min. The concentration profiles of the original and annealed samples demonstrated a pronounced diffusion of Zr occurred between the amorphous FeZr and CuZr layers. Furthermore, a remarkable enhanced interfacial atomic diffusion in the amorphous FeZr/CuZr multilayer thin films has been found, which is at least 4 times larger than the literature data at room temperature. Besides the extra interfacial energy in multilayer thin films, the reasons of the extraordinary enhancement of intermixing of immiscible elements Fe/Cu may be contributed by the thermodynamic instability of metallic glasses and the excess volume existing in metallic glasses which gives rise to the diffusion behavior. As the atomic interdiffusion in amorphous multilayers is much stronger than that in crystalline counterparts, it may open a way to control or tailor the properties of multilayer TFMGs.

KEYWORDS: thin film metallic glasses (TFMGs); amorphous multilayer; interdiffusion; Atom probe tomography (APT)

Presentation Method (Invited): Regular oral



B9-Additive manufacturing & powder metallurgy

Microstructures and Mechanical Properties of Bulk Ultrafine and Fine Structured Metallic Materials from Powders

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Bulk ultrafine and fine structured metallic materials including metal matrix nanocomposites can be fabricated by thermomechanical consolidation and rapid melting-solidification of metallic powders including nanostructured metal matrix nanocomposite powders fabricated by various processes such as high energy mechanical milling. The microstructures of the consolidated materials are affected by the microstructures, compositions and sizes of the powder particles and the consolidation or rapid melting-solidification conditions, and in the meantime, the microstructure of the fabricated materials dictate their mechanical properties and fracture behavior. For ultrafine and fine structured metallic materials fabricated by thermomechanical consolidation of metallic powders, one of the key microstructural characteristics is the interparticle boundaries (IPBs) which have not been transformed into grain boundaries or interfaces. If they are present in the microstructure, and their strength is lower than the yield strength or flow stress of the consolidated material, the IPBs can play a critical role in determining the fracture stress and ductility of the material. If the strength of IPBs is only slightly higher than the flow stress of the consolidated, the IPBs may still significantly affect the tensile ductility of the material, since the incompatibility of powder particles' plastic deformation may cause stress concentration at IPBs, leading to formation of cavities. For fine structured metallic materials fabricated by rapid melting-solidification of metallic powder particles, metallurgical defects such as lack of coalescence and cavities can dictate the mechanical properties of the fabricated material. This talk will present and discuss the major results from our team's work on microstructures and mechanical properties of different ultrafine and fine structured materials fabricated by thermomechanical consolidation and rapid melting-solidification of metallic powders including nanostructured metal matrix nanocomposite powders. The roles played by the IPBs and the metallurgical defects in materials fabricated by rapid melting-solidification of a mentioned above will be discussed.

Presentation Method (Invited/Regular Oral/Poster):Keynote

SLM from a metallurgical point of view - influencing parameters, microstructures, defects and development of new alloys

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Selective Laser Melting (SLM) follows the physical principles of laser welding. Laser energy, scan speed, hatch distance, scan strategy and other factors determine the rapid thermal cycle and cooling rate, resp. and consequently the microstructure, porosity, mechanical properties, appearance of defects and distortion or residual stresses. The typical procedure to find optimal processing conditions will be demonstrated and the resulting microstructures of some engineering alloys will be shown. The question of laser weldability and avoidance of welding defects will be discussed in detail. Variations of the as-build structures by post weld heat treatment and HIP-treatment and their influence on the mechanical properties will also be shown exemplarily. Finally, structures in the fusion zone of hybrides of steel/Al and Cu/Al will be discussed and the development of new alloying systems will be considered in an outlook.

KEYWORDS: Selective laser melting, microstructure and properties, hybride structures

Presentation Method (Invited/Regular Oral/Poster): Invited

Additive manufacturing of strong and ductile Cu-15Ni-8Sn

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Cu-15Ni-8Sn specimens are manufactured by selective laser melting (SLM) from gas-atomized powders and their microstructures and mechanical properties have been analyzed by mean of optical microscope, electron probe microanalysis, scanning electron microscopy and tensile-test facility. The relative density of SLM samples increase with increasing power density and reach peak value of 99.4% without any post-treatment. Room-temperature tensile tests reveal a remarkable mechanical behavior. The sample of 99.4% relative density shows yield and tensile strengths of about 522MPa and 653MPa, respectively, along with fracture strain of 17%. The result is also compared to those samples fabricated by traditional powder metallurgy. The high strength and excellent ductility of Cu-15Ni-8Sn can be ascribed to the refined microstructure resulting from the high cooling rate imposed by laser processing, further demonstrating the effectiveness of SLM for the production of materials with enhanced mechanical performance.

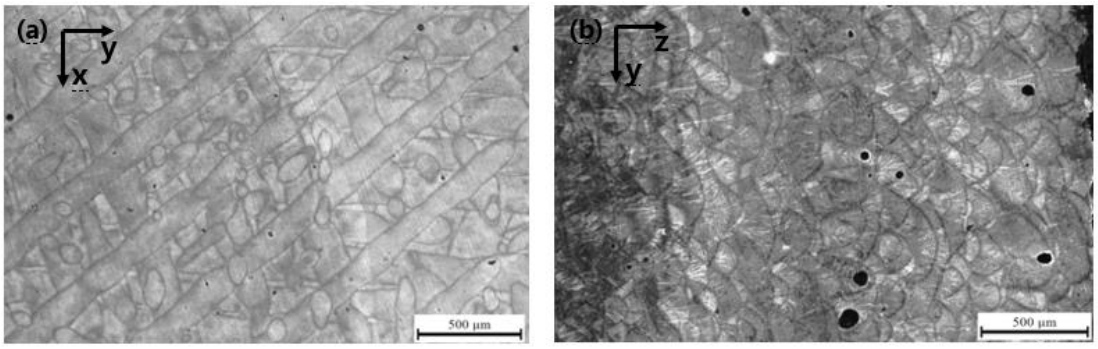

Fig.1. Optical micrographs of microstructures of Cu-15Ni-8Sn fabricated by SLM in (a) horizontal and (b) vertical direction

KEYWORDS: Additive manufacturing, Cu-15Ni-8Sn, selective laser melting

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Presentation Method (Invited/Regular Oral/Poster): Invited

Synthesis of Gas Atomized Titanium Powder for Additive Manufacturing

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Recently, additive manufacturing has been rapidly developing in the many fields of manufacturing industry such as aerospace, National defense, auto mobile, and medical industry. Titanium (Ti) is regarded as most important material for additive manufacturing because of its advantages such as high strength to weight ratio, ductility and biocompatibility. Conventionally, it is difficult to synthesize Ti powder for additive manufacturing due to constraints like powder shape, impurity content and oxide inclusions. On the contrary, synthesis of Ti powder by gas atomization process seems a valuable choice to overcome these problems. In this study, the authors designed cold crucible based gas atomization system of Ti and Ti based alloys and fabricated Ti powders by optimizing process parameters such as nozzle design, spray angle, gas pressure etc. Detailed characterization was performed to analyze surface morphology, impurity content, microstructure and mechanical properties. It was found out that powder produced through this route has far less impurity content than Ti powder obtained through conventional route. Also, the shape of powder was spherical.

KEYWORDS: Additive manufacturing, Ti powder, atomization process, powder synthesis, cold crucible

Presentation Method (Invited): Regular oral

Electrical and Mechanical Properties of Gas Atomized Copper-Iron Metastable Alloys

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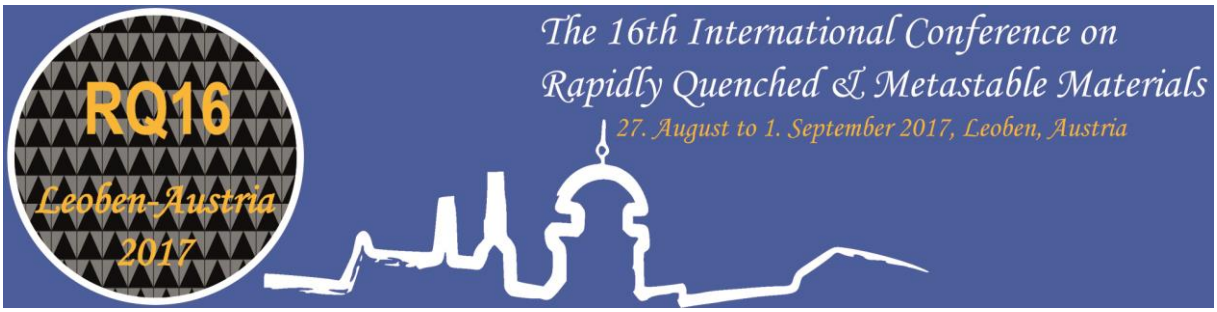
With the increase in global demand for highly functionalized materials, there is a continued interest in exploiting material properties of metals either individually or in the form of alloys. Copper-Iron alloy is considered unique with its remarkable combination of strength and electrical conductivity. Due to low cost of iron, this alloy is expected to replace alloys like Cu-Ag and Cu-Nb. Copper-iron alloy with composition of 10 at% Fe was prepared by a gas atomization process and consolidated by spark plasma sintering. After consolidation, samples were extruded with varying extrusion ratios followed by heat treatment in vacuum to promote the precipitation of iron from the copper matrix. In order to explore the correlation of electrical and mechanical properties with powder size dependent microstructural features, a detailed microstructural characterization was performed using scanning electron microscopy, X-ray diffraction and electron backscattered diffraction. A curve of optimum tensile strength against electrical conductivity was determined. It was found that sample with powder size measuring ≤ 24 μm lies at the top of tensile strength against electrical conductivity as contrast to other powder sizes due to enhanced precipitation of Fe from Cu matrix.

KEYWORDS: Powder synthesis and consolidation, microstructure, Fe-rich phase, misorientation, physical properties.

Presentation Method: Regular oral



C9-Rapid Solidification 3

Dendrite Growth in undercooled Melts of glass-forming Metallic Alloys

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Electrostatic levitation is applied to containerless undercool droplets in size of about 3 mm under ultra-high-vacuum conditions. The droplets are heated by a laser and the temperature is measured contactless by a pyrometer. A high speed camera is used to record the advancement of the crystallization front when propagating through the undercooled melt. In such the dendrite growth velocities are measured as a function of undercooling. Due to the avoidance of heterogeneous nucleation on container walls and processing in an ultra-high purity environment a very large undercooling range becomes accessible. According to a work by Osava and Greer [1] all glass forming systems should obey a universal characteristics. The growth velocity should pass a maximum at a temperature T_{max} with a maximum growth velocity V_{max}. The parameters T_{max}, V_{max} and the glass temperature T_g correlate with the glass forming ability. That is well known for non-metallic glass formers but scarce information is existing for metallic glass formers. That is because these systems are difficult to undercool to temperatures respectively extreme undercoolings at which a maximum in the growth velocity can be observed. In the present work we investigate metallic glass forming systems with respect to their behaviour in this respect. We report on measurements on Zr-based alloys and report results of the growth velocity – undercooling relations from which both T_{max} and V_{max} are inferred from. These findings are discussed within the general classification scheme by Osava and Greer.

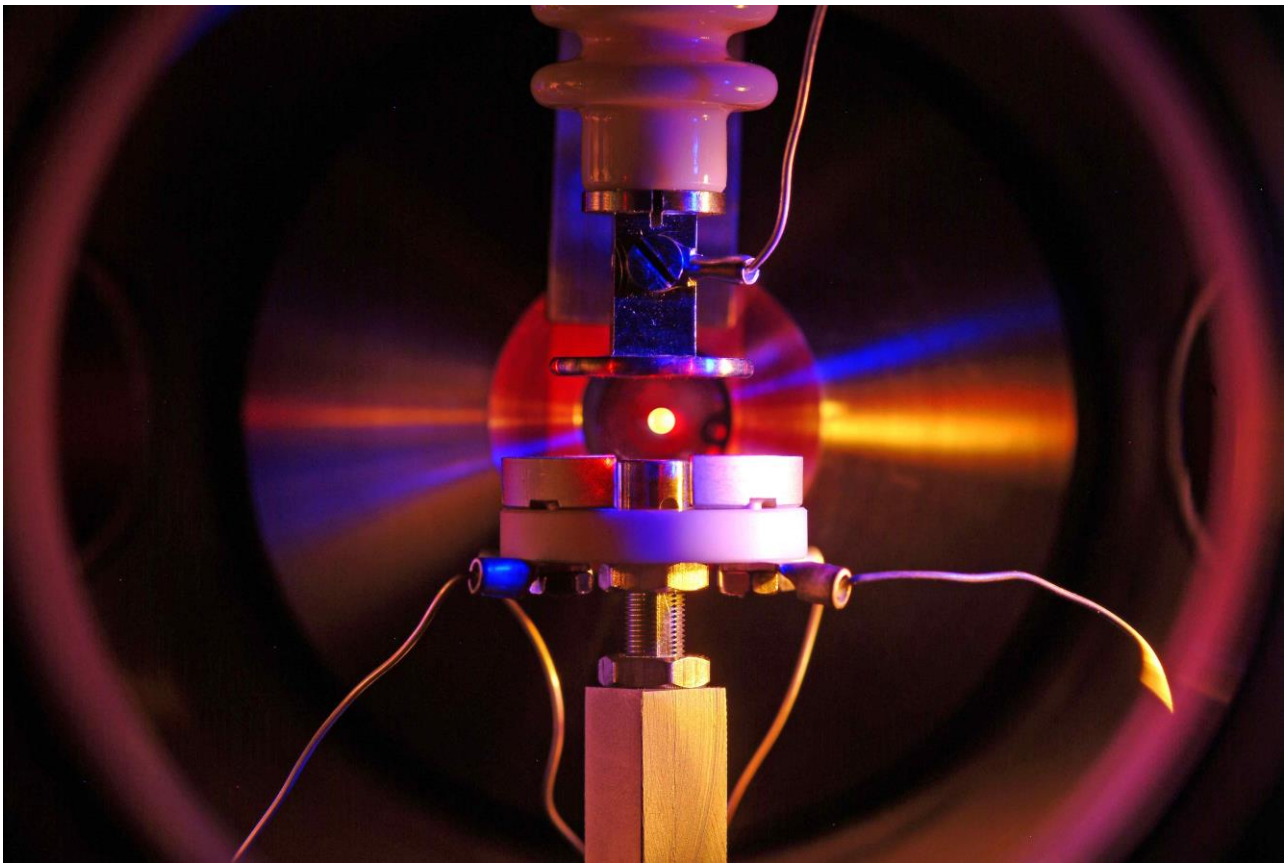

Fig1. Electrostatic levitation of droplet in size of 3mm under ultra-high-vacuum condition.

KEYWORDS: Dendrite growth, undercooled melt, glass forming alloys, containerless processing

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Presentation Method (Invited): Keynote

Correlation between thermodynamics and kinetics upon first-order phase transformation

Liu Feng

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We deduced and proposed the correlation between thermodynamics and kinetics based on the study of first-order phase transformation, which includes thermodynamics and kinetics of rapid solidification of undercooled single-phase alloy, formation kinetics of amorphous alloy, casting aluminum alloys based on the integration of non-equilibrium solidification and solid state transformation, interface migration during diffusional phase transformation, dynamic recrystallization during TMCP, thermodynamics and kinetics of solid-state phase transformation with accommodating mismatch, martensitic transformation of pure iron via Bain path, prediction of ferrite microstructure during TMCP of HSLA steel, thermodynamics and kinetics of martensitic transformation during TMCP of HSLA steel, and α/γ transformation in cold rolled steel.

Based on the above preliminary work, correlation between thermodynamics and kinetics during grain boundary migration, grain growth and thermal stability of nano-crystalline materials, grain growth and densification of nano-phase ceramics during sintering were established. On this basis, the multi-scale model for microstructure evolution during first order phase transformation was developed, which were then applied to predict the macrostructure evolution during γ/α transformation of Fe-C alloys.

Presentation Method (Invited/Regular Oral/Poster): Invited

Hydrogen and amorphous alloys: friends or foes?

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Experimental observations point towards contrasting effects of Hydrogen on the properties of amorphous alloys. For example, while Hydrogen addition to a Zr-based metallic glass yields better glass forming ability and improves its ambient temperature compressive ductility, it has no effect on Pd-based metallic glasses and diffuses out rapidly. As these observations are very difficult to be comprehensively explained at the atomic level, we performed extensive ab initio molecular dynamics to simulate the structure of two Zr and Pd-based metallic glasses with and without minor additions of Hydrogen. Further density functional theory calculations were performed to reveal their electronic structure and assess the nature of chemical bonding therein. It was found that Hydrogen promotes heterogeneity in the local structure and while in the Zr-based alloy it results in a dynamic arrest, in the Pd-based alloy it decreases the electronic states with lower energies. The outcomes point toward a competition between topology, dynamics and electronic structure to determine the macroscopic properties of the glass.

Presentation Method (Invited/Regular Oral/Poster): Invited

Melt Spinning based Metal Alloy Microfibers

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Moyu Watari[1], Guenter Stephani[2], Juergen Binzer[2], Joachim P. Spatz[1]

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Metal microfibers have a wide range of applications, e.g. as filters, fiber reinforced composites, electrodes, catalysts, sensors, or magnetic shielding materials. Until now the formation of metal microfibers with a width of less than 10μm from different metal alloys and in large quantity was a challenge or simply not possible. Here, we present a melt spinning based process for producing metal microfibers from different metal alloys. The rapid cooling of the metal melt enabled the processing of amorphous metal fibers from alloys which are only knowing as being crystalline. This way, amorphous, nanocrystalline or crystalline metal microfibers with cross-sections down to 5μm and lengths of several centimeters were produced in large quantities from different metals including magnetic cobalt based alloys. The microfibers were characterized for different material properties such as elasticity, hardness, crystallinity, and magnetic properties. Some demonstrate ultra-soft magnetic properties with coercivity of about H_c=0.1 Oe. Magnetic behavior of the alloy after heat-treatment is also investigated.

KEYWORDS: amorphous metal; soft magnetic; microfiber

Presentation Method (Invited/Regular Oral/Poster): Regular Oral

Nanoglasses – expanding our views of the amorphous state

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[2]Herbert Gleiter Institute of Nanoscience, Nanjing University of Science and Technology, Nanjing, China

Metallic nanoglasses, prepared by compaction of amorphous nanoparticles within the size range of 8 to 10 nm, are constituted of two distinctly different amorphous components, the cores of the former nanoparticles and an interfacial component. For the investigated systems, the core component has been found to be structurally identical to the structure of amorphous materials prepared by rapid quenching from the melt (RQ). The interfacial component, however, is structurally different exhibiting a large amount of free volume and a medium range order that is substantially different from the core regions. The results, based on extensive studies of Mössbauer spectroscopy, small angle X-ray scattering, synchrotron studies (radial distribution functions), atom probe tomography, positron annihilation studies, and others, indicate that amorphous structures, at least for metallic systems, allow for the introduction of a large fraction of free volume, resulting in amorphous structures being different from those in the RQ state. As a consequence of this difference in structure, the mechanical, magnetic and thermal properties are altered drastically. As examples, amorphous $Fe_{90}Sc_{10}$ and $Cu_{50}Zr_{50}$, have been examined. $Fe_{90}Sc_{10}$ is paramagnetic at room temperature in the RQ state and ferromagnetic below 120 K, however, in the nanoglass state exhibits a Curie temperature (T_c) well above room temperature. Mechanical deformation is altered as well. The nanoglass samples do not exhibit shear band formation, while RQ samples fail catastrophically under mechanical loads. Furthermore, scanning calorimetry studies show an increased crystallization temperature of the nanoglass compared to the RQ material of the same composition.

In an attempt to increase the fraction of the amorphous interfacial component by reducing the size of the primary nanoparticles, a cluster ion beam deposition system was used. Furthermore, the mechanical compaction employed for the larger nanoparticles was replaced by an energetic impact of the cluster ions (1.000 atoms each) onto a substrate, a process that allows for the easy modification of the consolidation conditions, all under ultra-high vacuum conditions. For all impact energies, varied between 600 eV and 12 keV, it was found that the $Fe_{80}Sc_{20}$ samples were fully amorphous, However, the magnetic properties varied drastically. The results indicate that the fraction of the interfacial component has increased substantially.

In any case, nanoglasses offer a opportunity to alter the mechanical, magnetic and thermal properties of metallic amorphous structures. Furthermore, the established concepts of the amorphous structure should be reconsidered.

Presentation Method (Invited/Regular Oral/Poster): Plenary

Fragility in Metallic Liquids and Glass Formation

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[2]*Department of Physics, Harbin Normal University, Harbin, Heilongjiang Province 150025, China.*

How structural changes in liquids correlate with changes in the dynamical properties, and what role this may play in glass formation and the glass transition are outstanding questions. Although it is widely believed that the dynamical behavior is linked to the atomic structure of the liquid, it has been difficult to demonstrate this experimentally. Liquids can be described by their *kinetic fragility*, typically defined from the rate of increase of the viscosity as a function of the inverse temperature scaled to the glass transition temperature, T_g (i.e. T_g/T). The viscosities of *strong* liquids more closely follow Arrhenius behavior, with an activation energy that changes little with temperature. The activation energy for *fragile* liquids is small at high temperature, but increases dramatically upon approaching T_g. Corresponding structural changes in the liquid have been difficult to determine. While the viscosity of the liquid changes by orders of magnitude with temperature, changes in the static structure factor, $S(q)$, or pair correlation function, $g(r)$, are almost negligible. With the recent development of containerless processing methods and the introduction of intense X-ray and neutron sources, these changes can now be accurately measured in deeply supercooled liquids.

Here, we focus on fragility in metallic liquids. The results of experimental studies on containerless-processed liquids clearly demonstrate a link between fragility and the rate of structural ordering [1]. A new scaling temperature, T_A, is experimentally identified, which based on the results of molecular dynamics simulations corresponds to the onset of cooperative flow in the liquid [2]. Recent experimental and molecular dynamics (MD) results show that the rate of short-range and medium-range structural ordering in the liquid accelerates below T_A, [3]; experimental data are discussed that confirm this. For all metallic glass-forming liquids studied $T_g \sim T_A/2$, suggesting a connection between the onset of cooperative dynamics and the glass transition [4], a conclusion supported by MD results [3]. The connections between fragility and structure and the correlation with other physical properties suggest that fragility could be a function of the interatomic potential. Recent experimental and molecular dynamics results are presented to confirm this [5].

Fragility is often (although not universally) believed to correlate with glass formation. By analyzing a large data-base of metallic glasses, Johnson et al. [6] recently proposed an expression for the critical casting thickness (d_{max}) in terms of the reduced glass transformation ($T_{rg}= T_g/T_l$), and the fragility parameter, m. Since the need to measure T_g and m requires first making the glass, this method is not best suited for identifying possible new glasses. By adapting their approach, however, we have developed an expression that is based on only liquid data. This is discussed and results are compared with experimental data.

This research was partially supported by the National Science Foundation (*DMR 15-06553*) *and NASA* (*NNX16AB52G*).

KEYWORDS: Melt structure and relaxation studies; Bulk metallic glasses and composites

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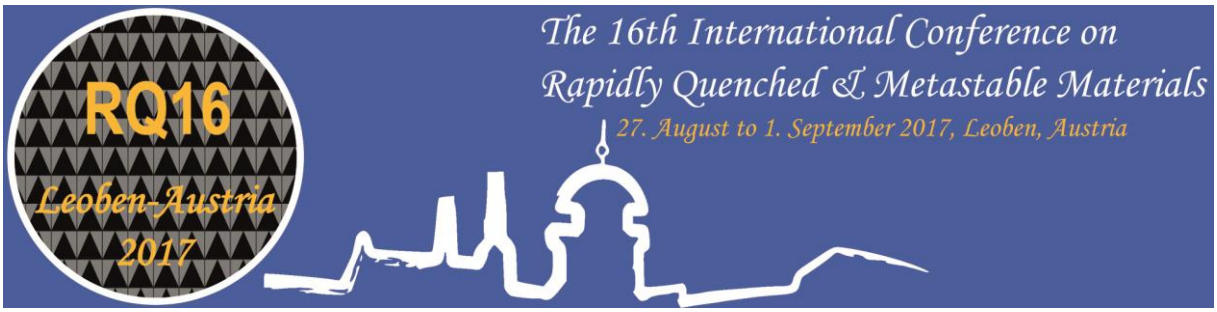
Presentation Method (Invited/Regular Oral/Poster): Plenary



Poster Sessions

A comparison of thermodynamic and kinetic fragilities of bulk metallic glass forming liquids

Maximilian Frey[1], Ralf Busch[1], Isabella Gallino[1]

[1]*Chair of Metallic Materials, Saarland University, Saarbrücken, Germany, Email: maximilian.frey@uni-saarland.de*

Glass formers are found in various classes of liquids, e.g. molecular or metallic ones. By undercooling them sufficiently fast, crystallization can be avoided. Instead, their viscosity increases with decreasing temperature until a kinetic arrest occurs, known as the glass transition. When comparing the equilibrium viscosities of various liquids in an Angell plot, which is an Arrhenius plot with an abscissa scaled by T_g, different curve behaviors can be observed. These can be classified in terms of the fragility concept via the steepness of the curves at T_g [1]. Systems that feature a steep course of the equilibrium viscosity are termed fragile liquids, while those showing low steepness are termed strong liquids. Strong behavior often correlates with high glass forming ability, since strong liquids feature higher viscosities as fragile ones in the temperature range between liquidus and glass transition, thereby kinetically impeding crystallization. The course of the equilibrium viscosity of a liquid can be described by various equations, e.g. the empirical Vogel-Fulcher-Tammann equation or also by the Adam-Gibbs theory [2]. The latter one connects kinetics with thermodynamic aspects by describing viscosity via the configurational entropy of the liquid.

The temperature dependent excess entropy of a liquid in reference to the crystal is a purely thermodynamic value, consisting of a vibrational, but also a configurational component. In analogy to kinetic considerations, its steepness at the glass transition temperature can be used to quantify thermodynamic fragility.

Martinez and Angell compared thermodynamic and kinetic fragilities of glass formers using the F parameter concept [3]. Thereby, a wide spectrum of fragilities was covered, reaching from ultra-strong to extremely fragile. A global one-to-one correspondence between both fragility definitions was found. However, metallic glass formers were not included in this comparison.

In the present work, thermodynamic and kinetic fragilities of various bulk metallic glass formers are compared to each other. The needed data is taken from literature. It is found that the previously established linear connection of thermodynamics and kinetics is blurred out into a widespread pattern. So, due to the rather narrow fragility range (typically D* values between 10 and 25), the previously observed one-to-one correspondence cannot be found by regarding only metallic glass formers. Instead, alloys with similar composition are often grouped together in the thermodynamic-kinetic-fragility landscape. This can be likely addressed to their comparable vibrational part of the excess entropy.

KEYWORDS: metallic glasses, bulk metallic glasses, thermodynamics, kinetics, fragility

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Presentation Method (Invited/Regular Oral/Poster): Poster

A new indicator of thermoplastic formability reflecting the stability of Newtonian viscous flow in supercooled liquid region

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One of the most attractive merits of glass-forming alloys is viscous flow in the supercooled liquid region. Throughout the supercooled liquid region, metallic glass relaxes into a metastable liquid and deforms homogeneously by viscous flow. This unique property has been employed for various applications in a simple, cost-effective, near-net shape thermoplastic forming (TPF) processes including nano-molding, extrusion, etc. Therefore, investigation of viscous flow is essential to get critical perspective for the deformation of metallic glass.

Meanwhile, the viscous flow of BMGs in the supercooled liquid region can be Newtonian or non-Newtonian, depending upon testing temperature and strain rate. When the forming is conducted at high stress and low temperature levels, the flow becomes non-Newtonian and stress sensitivity of deformation drops rapidly with mechanical flow instabilities such as necking, resulting in significant decrease of TPF ability. Therefore, stability of Newtonian flow should be considered as an important constraint of TPF ability. However, unlike other properties, we still lack a conceptual approach to evaluate the stability of Newtonian viscous flow of metallic glass. Hence, it is essential to establish a simple approach being able to be quantified easily to assess the stability of Newtonian flow of metallic glass for various glass-forming alloys.

In the present study, we aim at providing an extended concept to understand the nature of TPF ability considering the structural, mechanical stability of Newtonian viscous flow during TPF process. We will systematically discuss the relationship between several factors and the stability of Newtonian viscous flow. Indeed, we propose a new indicator for thermoplastic formability to quantify the stability of Newtonian viscous flow in supercooled liquid region as a function of characteristic temperatures of glass formation. This finding is not only scientifically important, but also significant practical implication.

KEYWORDS: metallic glass, thermoplastic forming ability, Newtonian viscous flow, fragility, new indicator

Presentation Method (Invited/Regular Oral/Poster): Poster

A strategy for overcoming strength-ductility trade off in BCC high-entropy alloy

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Over the last decade high-entropy alloys (HEAs) has attracted significant attention in the metal community. HEAs are single-phase multi-component alloy with the composition of approximately equal atomic concentrations. Contrary to design concept of traditional alloy, HEAs are designed to be composed of multicomponent elements in an equiatomic or near equiatomic ratio to induce high configurational entropy, which stabilize the single solid solution phase. Recently, BCC HEAs composed by Group-4 to Group-6 elements (Ti, Zr, Hf, V, Nb, Ta, Cr, Mo and W) were reported to exhibit superior mechanical properties at high temperature above 1000 ℃ comparing conventional Ni-based superalloy. [1,2] However, it is known that the HEAs containing mainly Group-6 refractory elements (Mo and W) suffer from poor ductility at room termperature, while HEAs without Group-6 refractory elements show poor strength at high tempearture. To devleop HEA with high strength at high temperature and favorable ductiltiy at room temperature, a new BCC HEA systems were designed. It is known that valence electron concentration (VEC) of BCC alloys has negative relationship with ductiltiy, but elements with high mismatch of shear modulus as well as atomic radius (Mo and W) are responsible for high strength of the alloy. To develope an alloy with balanced strength and ductiltiy, Ti-V-Nb-Ta-(Mo, W) system, whose VEC is 5.0 in equiatomic composition, was selected. HEAs in equiatomic and near equiatomic composition in the system were predicted to form single BCC phase by CALPHAD method via calculation of phase diagram, and experimentally confirmed to have single BCC phase. Mechanical properties at room temperature were determined by compression test. Indeed, ductiltiy and strength of the HEAs were quantitatively analyzed in terms of VEC and solid solution hardening. Our results could provide an effective guideline for tailoring mechanical properties of BCC high entropy alloy and developing promising HEAs for high temperature structural materials.

KEYWORDS: high entropy alloy, refractory element, valence electron concentration, mismatch, mechanical property

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Presentation Method (Invited/Regular Oral/Poster): Poster

Consolidation of amorphous powder by thermoplastic forming and mechanical testing

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Bulk metallic glasses combine extraordinary strength with a large elastic limit, thus making them interesting for industrial applications. However, large scale production of parts is complicated by very specific production requirements, including rapid quenching from the liquid state for casting processes. In order to overcome the part size limitations induced by those high cooling rates, the production process of an amorphous pre-material and the forming of the final part can be decoupled by production and subsequent consolidation of amorphous powder.

In the present work, an amorphous powder of the commercially available Zr-based glass forming alloy AMZ4 ($Zr_{59.3}Cu_{28.8}Al_{10.4}Nb_{1.5}$) [1] is consolidated by a thermoplastic forming (TPF) process. During the TPF process, the glassy powder is heated into the supercooled liquid state, where its viscosity drops drastically and stress induced flow of the particles causes a binding of the powder sample. Here, we focus on the implementation of a TPF process on the way to an industrial production process. The powder is pressed in reusable molds under a high purity argon atmosphere to avoid oxidation of the Zr-based powder. Various time and temperature protocols for the TPF process are tested and evaluated regarding the powder compaction and the conservation of the amorphous structure. Compact and amorphous samples are obtained and are subsequently tested by three-point beam bending. The results show that the pressed samples are still outperformed by as cast bulk material in bending, however reach the hardness of bulk material.

KEYWORDS: Bulk metallic glasses, Powder consolidation, Mechanical properties

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Presentation Method (Invited/Regular Oral/Poster): Poster

Correction to the Wills-Harrison approach: Influence on the Fe-based liquid alloys thermodynamics

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Some years ago, we applied the Wills-Harrison (WH) [1] approach in conjunction with the variational method of the thermodynamic perturbation theory to calculate thermodynamic properties of Fe-Co and Fe-Ni liquid alloys [2, 3].

Later, we introduce the correction to the WH model due to the non-diagonal coupling between *d* electrons on different atoms and applied this correction to investigate the WH effective pair interactions in liquid Fe, Co and Ni [4].

Here, the influence of this correction on the thermodynamics of Fe-Co and Fe-Ni liquid alloys near their melting temperatures at different component concentrations is studied.

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KEYWORDS: Thermodynamics and phase transformation studies; Chemical and physical properties.

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Presentation Method (Invited/Regular Oral/Poster): Poster

Crystallization behavior of the $Al_{86}Ni_8Y_6$ metallic glass forming alloy upon rapid cooling

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Al-based metallic glasses are of special interest for lightweight technology because of their low density in combination with unique mechanical properties. Glassy alloys in the Al-Ni-Y system show tensile strength of about 1 GPa and hardness values of about 300 HV [1] resulting in a specific strength of roughly 0.3 (GPa cm³)/g. In comparison, commercially used, crystalline aluminum alloys such as Al 356.0 (Al-7Si-0.3Mg) show a tensile strength of about 0.3 GPa (depending on the microstructure) [2] and hence a specific strength of only 0.15 (GPa cm³)/g. However, the glass forming ability of Al-based metallic glasses is still limited preventing the industrial use of these alloys.

In this study, the crystallization behavior of $Al_{86}Ni_8Y_6$ upon quenching from the equilibrium liquid is investigated and the crystalline phases competing with glass formation are identified. $Al_{86}Ni_8Y_6$ is one of the best ternary Al-based glass formers [3,4]. Contrary to previous studies suggesting α-Al as the primary phase upon rapid cooling, this study reveals that glass formation is limited by the formation of the primary precipitating ternary intermetallic compound $Al_{23}Ni_6Y_4$. The nucleation of $Al_{23}Ni_6Y_4$ appears to be triggered by oxide particles present in the melt acting as heterogeneous nucleation sites which cannot be prevented in Y-containing alloys. Once the primary phase $Al_{23}Ni_6Y_4$ has been formed, further crystallization of the Ni and Y depleted melt occurs as α-Al.

The corresponding results are shown and discussed with respect to their effects on the glass formation in the ternary Al-Ni-Y system providing new strategies for the development of novel glass forming compositions in this system.

KEYWORDS: Bulk Metallic Glasses; Synthesis and Processing; Alloy Development;

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Presentation Method (Invited/Regular Oral/Poster): Poster

Development of Copper Alloys with β-Phases for Mechanical Properties

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Copper alloys such as high-strengthened brasses have been used as wear-resistance materials for iron-based parts. The copper alloys with β-phases have been recently required in the synchronizer rings or bearings of automobile parts in order to withstand harsh environments. Higher hardnesses and strengths have been generally shown in the copper alloys with β-phases than those than α-phases. Therefore, the copper alloys with the mixed phases of α-phase and β-phase have been used in the conventional wear-resistance for controlling formability and moderate strength. However, it is currently inevitable that the fraction of β-phases in copper alloys should be increased with controlling grain sizes homogeneously in order to enhance the hardness and the strength of copper alloys. We designed the copper alloys consisting of zinc, aluminum, nickel, etc. by zinc equivalent equation and manufactured them by casting and extrusion processes. It could be obtained from this study that the strength of copper-zinc alloys with β-phases was more than 655MPa and the hardness was above 200Hv, which could be obviously compared to 540MPa and 160Hv of copper-zinc alloys with α-phases and β-phases.

KEYWORDS: copper, alloy, α-phases, β-phases,

Presentation Method (Invited/Regular Oral/Poster): Poster

Effect of additional element on microstructure and mechanical properties of Ti-based ultrafine eutectic alloy

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Ti-based nano-structured dendrite eutectic composites have been engendered considerable interest due to their good mechanical and physical properties such as high strength, high toughness, corrosion resistance and wear resistance compared to conventional microcrystalline materials [1~~5]. It is responsible for outstanding mechanical properties featured by the volume fraction, size, morphology, chemical composition difference and distribution of the constituent phases with different length scale, which consist of the micron-scale dendrites and the ultrafine eutectic matrix. In particular, interaction of the soft dendrite and nano-scale eutectic matrix during deformation can achieve a novel high strength composites combined with large plasticity [6~8]. In this study, the high strength $(T_{82}Sn_{18})_{100-x}Nb_x$ (x=0~15) ultrafine eutectic composites with large plasticity are developed. Nb is selected because it is known as β -Ti stabilizer and Nb has large solubility in Ti than Sn. The addition of Nb in the Ti-Sn eutectic composite has a strong effect to decrease the size of the duplex colony and to increase the volume fraction of the β -Ti solid solution phase. Finally, the alloy is composed of a single β –Ti solid solution phase. These micro-structural evolutions in Ti-Sn-Nb alloys are effective to improve both strength and plasticity. In particular $(Ti_{82}Sn_{18})_{100-x}Nb_x$ alloy with x=11 exhibit excellent combination of the high yield strength (~1327 Mpa) and large plasticity (~36.5 %) at room temperature compression.

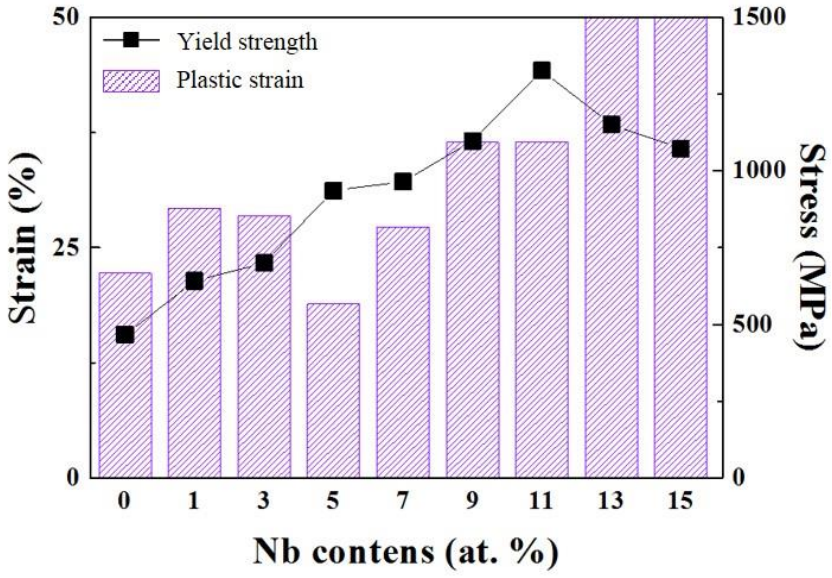

Fig1. Yield strength and plastic strain of as-cast $(Ti_{82}Sn_{18})_{100-x}Nb_x$ alloys

KEYWORDS: nanostructured materials, eutectic alloy, Ti-based alloy, mechanical properties

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Presentation Method (Invited/Regular Oral/Poster): Poster

Effect of amorphous alumina on the high temperature deformation behavior of B2 Aluminides

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In the present study, the nanocrystalline B2 aluminides (FeAl and NiAl) are synthesized using the mechanical alloying of their constituent elemental powders (Fe, Ni and Al). The ball milled powders were then heat treated and consolidated using spark plasma sintering. The dense sintered aluminide pellets were found to contain amorphous alumina [1]. Thus, the composite developed was studied for their high temperature deformation. The Hall-Petch plots were used to evaluate the alumina influence on the mechanical behavior of B2 aluminides. Also, the creep studies on dense samples were carried out at 973-1073 K and at different stresses 100-500 MPa. The creep deformation mechanisms were identified from the analysis based on the stress exponent and transmission electron microscopy studies. FeAl was found to have more creep resistance than NiAl. In both the compositions, glide was found on {011}. However, the major deformation vector was <111> in case of FeAl and for NiAl <001>, <011> along with <111> were found to be active.

KEYWORDS: Mechanical alloying; Microstructure; Deformation

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Presentation Method (Invited/Regular Oral/Poster): Poster

Effect of minor alloying elements addition on the glass forming ability of Ni-Ti-Cu-Zr alloy exhibiting superior superelasticity after crystallization

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Shape memory alloys or superelastic alloys, such as TiNi, β-Ti(Nb), β-CuZn, undergo a reversible martensite phase transformation when the energy barrier to lattice-invariant shear is higher than the barrier to the phase change. Superelasticity is a reversible deformation motion of domain boundary which shows very large elastic strain limit by lattice shear and twinning at above austenite transformation finish temperature. Among the well-known superelastic alloys, the TiNi alloy shows martensitic transformation from B2 to B19' accompanying high recovery strain under loading-unloading condition.

Metallic glass alloys generically show high yield strength but low plastic deformability due to absence of proper deformation mechanism. Many research groups have been trying to overcome the low level of plasticity by introducing a heterogeneity in the glass matrix to relax shear localization. Such metallic glass composites based on reversible B2-type shape memory alloy, such as CuZr and CuTi, are known to exhibit transformation induced plasticity (TRIP) which originates from deformation-induced martensitic transformation. Though the large recovery strain and high energy absorption ability of the B2-TiNi phase, there has been no report on the TiNi phase reinforced glass matrix composite due to low glass forming ability of the alloy system.

In this study, with an aim to improve the glass forming ability of TiNi-based metallic glass alloy, the quaternary Ti-Ni-Cu-Zr alloys with equiatomic (Ti,Zr)/(Ni,Cu) ratio, such as $Ti_{35}Ni_{35}Zr_{15}Cu_{15}$ and $Ti_{30}Ni_{35}Zr_{20}Cu_{15}$ were chosen as the base composition and the effect of minor element addition of 1 ~ 5 % Ga, Ge, Sn, P, B and Fe was systematically investigated. In order to compare the effective glass forming ability of each alloy, three types of specimens including thin ribbon (thickness≈ 50 μm) by melt-spinning, and thin plate(thickness ≈ 300 μm) and rod(diameter ≈ 1&2mm) by copper mold casting were fabricated. The alloys with fully amorphous state were obtained from the melt-spun ribbon containing the minor alloying element. The quinary alloys containing the minor alloying element show increased super-cooled liquid region in comparison to the quaternary alloy. However, the increase of the super-cooled liquid region was not enough to show the enhancement of the glass forming ability. The crystalline alloys containing 1 at% of Ga, Ge, Sn show large recovery strain ~7.5 % along with increased loading plateau stress. The detailed results on glass forming ability, microstructure and mechanical behavior in various TiNi-based alloys will be presented.

KEYWORDS : Glass forming ability, Superelasticity, NiTi

Presentation Method (Invited/Regular Oral/Poster): Poster

Effect of scan strategy and annealing on microstructure and properties of 316L stainless steel synthesized by selective laser melting

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Selective laser melting (SLM) is progressively becoming one of the prominent additive manufacturing routes for the synthesis of high-performance materials due to the ability to produce three-dimensional components of virtually any geometry and intricacy through an additive layer-by-layer strategy directly from powders/wires. Furthermore, due to the high cooling rate of the process, SLM offers the possibility to produce metastable phases and microstructures that are not accessible by conventional solidification techniques. Additional microstructural modifications can be achieved by properly varying the scan strategy and by annealing the SLM part at different temperatures. In this work, 316L stainless steel specimens have been produced by SLM using different scan strategies. Structural characterization followed by microstructural characterization as well as mechanical and wear properties have been investigated in detail and compared to the corresponding samples produced by conventional casting. Finally, the effect of annealing at different temperatures on the properties has been systematically studied by analyzing the microstructural changes as a function of annealing temperature.

Keywords: Additive manufacturing; metastable material; laser melting; AISI316L

Presentation Method: Poster

Effects of wheel material on amorphous ribbon formation in Planar Flow Casting in air

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Planar Flow Casting is well known as industrial technique for rapid quenching to produce amorphous ribbon used mainly as soft magnetic materials. It is clear that behavior of melt puddle formed on the surface of quickly rotating wheel by molten alloy impinged determines the quality of amorphous ribbon. We have succeeded in observing the melt puddle clearly in Planar Flow Casting in air. Now we have been researching the effects of process parameters on the behavior of melt puddle which influences formation mechanism of amorphous ribbon.

Various process parameters, for example distance between nozzle and wheel surface, ejection gas pressure and wheel surface velocity had been researched. However, research on the effects of wheel material does not appear to have been extensively studied. So, this work was carried out to examine the effects of wheel material on amorphous ribbon formation and we would like to report the results.

In this work, Cu based alloy and various metals are used as wheel. $Ni_{78}Si_8B_{14}$ alloy (melting point is 1313 K) is used for casting. The alloy melted to 1623 K by induction heating in quartz crucible is impinged on wheel of 300 mm diameter and 50 mm thickness through rectangular nozzle of 0.6 x 20 mm by argon gas pressure of 20 kPa. The distance between nozzle and wheel surface is 0.3 mm.

Relationships between wheel material and quality of amorphous ribbon are discussed from the results obtained in experiments of changing two process parameters; wheel surface velocity and wheel material.

KEYWORDS: Processing, Rapid solidification, Rapidly quenched materials

Presentation Method : Poster

Enhancement of glass forming ability of superelastic Ni-Ti-Cu-Zr alloy

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Unlike crystalline alloys, metallic glass exhibits high level of toughness and elastic limit due to its unique random atomic structure. In addition, metallic glass exhibits high level of formability when it is heated up to supercooled liquid region (SCLR), which enables precise thermo-plastic forming of metallic parts down to nm scale. However, since metallic glass exhibits low level of plasticity due to the absence of slip system, its application as structural materials has not been successful so far. There have been many efforts to solve the problems by introducing heterogeneity in the glass matrix. A large number of in-situ and ex-situ bulk metallic glass composites (BMGCs) with crystalline phase with high plasticity embedded in the glass matrix have been investigated. Recently, among such BMGCs, shape memory alloy phase reinforced BMGC receives an attention, since it shows deformation-induced martensitic transformation which enhances the level of plasticity.

Especially, B2-type CuZr shape memory alloy has been utilized for fabricating high plasticity BMGC, since even binary Cu-Zr alloy has superior glass forming ability (GFA) enough to fabricate mm scale (BMGC). Although B2-type NiTi alloy is known exhibit superior superelasticity which provides high level of recovery strain at room temperature, it has not been to fabricate BMCC due to inferior GFA of Ni-Ti based alloys. One way to utilize the advantage of superelastic NiTi alloy is to cast the Ni-Ti based alloy in amorphous state for precise thermoplastic forming at SCLR followed by full crystallization into superelastic alloy with high level of strength and recovery strain. For this purpose, it is required to design Ni-Ti based alloy system with enhanced GFA.

In this study, to improve GFA of Ni-Ti based alloy system, Ni and Ti in equi-atomic % Ni-Ti alloy have been replaced with Cu and Zr, respectively. To evaluate the GFA, the samples with the thickness of ~50㎛ and ~ 300 ㎛ were prepared using melt-spinning and melt-suction-casting, respectively. Among the alloy compositions of $Ni_{50-x}Ti_{50-y}Cu_xZr_y$ ($5 \leq x, y \leq 20$), $Ni_{33}Ti_{30}Cu_{17}Zr_{20}$ exhibit the highest GFA enabling the formation of partially amorphous 300 ㎛ thickness sample. Addition of small amount of Si was found very effective in enhancing GFA. The alloy with composition of $(Ni_{0.35}Ti_{0.3}Cu_{0.15}Zr_{0.2})_{98}Si_2$ exhibited fully amorphous structure in 300 ㎛ thickness sample. The B2-type $Ni_{35}Ti_{30}Cu_{15}Zr_{20}$ alloy sample with the diameter of 2 ㎜ fabricated by suction-casting showed ~8.9 % recovery strain (10% strain) at room temperature under compressive loading-unloading condition.

KEYWORDS : superelastic alloy, metallic glass

Presentation Method (Invited/Regular Oral/Poster): Poster

Fabrication of mono-dispersed amorphous $Fe_{76}Si_9B_{10}P_5$ particles by container-less solidification process and their soft magnetic property

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The urgent worldwide demand of energy saving requires miniaturized electrical equipment with improved energy efficiency [1]. Fe-based amorphous materials including metallic glasses have recently attracted much attention due to their high magnetic susceptibility, very low coercivity and high electrical resistance. In this study, we aim to prepare $Fe_{76}Si_9B_{10}P_5$ metallic glassy particles with high homogeneity and a low content of nucleation sites by the container-less solidification process called pulsated orifice ejection method (POEM) [2], and to investigate their nano-crystallization behaviors by heat treatment and their soft magnetic properties.

Monodispersed $Fe_{76}Si_9B_{10}P_5$ particles with a high sphericity were successfully prepared by our POEM. Soft magnetic properties of as-quenched and heat treated particles were evaluated by VSM measurement with a single particle. Fig. 1 show the B-H curves of a single particle after and before demagnetizing field correction with N=1/3, powder, and ribbon sample. In case of as-quenched single particle, the relationship between magnetic field and magnetization showed straight liner just before the saturation. Saturation magnetization was increased up to 1.64 T as a maximum by optimum annealing. $Fe_{76}Si_9B_{10}P_5$ particles fabricated by container-less solidification process could easily generate homogeneous nano-crystalline phase and their increment of saturation magnetization by heat treatment was higher than that of the ribbon (1.57 T).

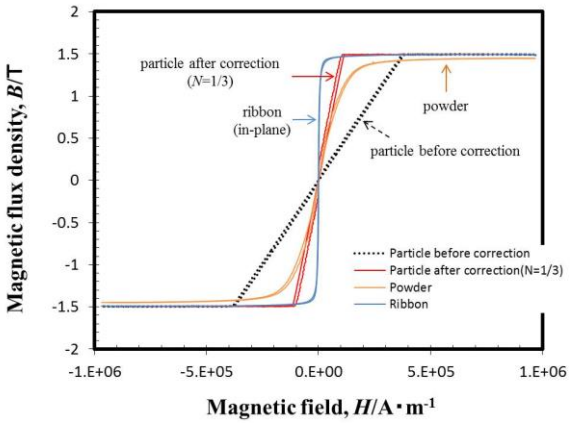

Fig. 1 B-H curves of a single particle after and before demagnetizing field correction with N=1/3, powder, and ribbon sample (as-quenched) .

KEYWORDS: Fe-based amorphous, container-less rapid solidification, nano-crystallization, soft magnetic material.

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Presentation Method (Invited/Regular Oral/Poster): Poster

Fractal abnormal grain growth in Pd_xAu_{100-x} — the rule or the exception?

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Although abnormal grain growth has been investigated for more than 70 years, our understanding of its underlying mechanisms remains quite fragmented. The situation is particularly unsatisfactory for nanocrystalline materials, in which coarsening is often observed to proceed by a subset of grains growing at a much higher rate than their immediate neighbors. Usually, the larger (*i.e.* abnormal) grains are roughly equiaxed in shape, and their boundaries are smooth. But in nanocrystalline specimens of $Pd_{90}Au_{10}$ produced by inert gas condensation, we find the fast-growing grains to be almost dendritic in appearance, with highly irregular perimeters (Fig. 1). Not only are the resulting grain morphologies suggestive of a "tentacle-like" growth process, but the perimeters themselves manifest a scaling behavior that lends itself to description via a fractal dimension D_f. Applying the well-established box-counting method to electron backscatter diffraction (EBSD) images of abnormal grains in $Pd_{90}Au_{10}$, we find an average D_f of about 1.2, which is comparable to the dimension of mathematical fractals like the Koch snowflake (D_f = 1.26). To gain insight into the origin of fractal grain boundary migration in nanocrystalline PdAu, we have investigated annealing-induced microstructural evolution as a function of both heating rate and dwell temperature, with additional experiments planned to encompass variation of the Au concentration. We compare the results with ideas from nucleation theory and attempt to connect the findings to standard models for abnormal grain growth.

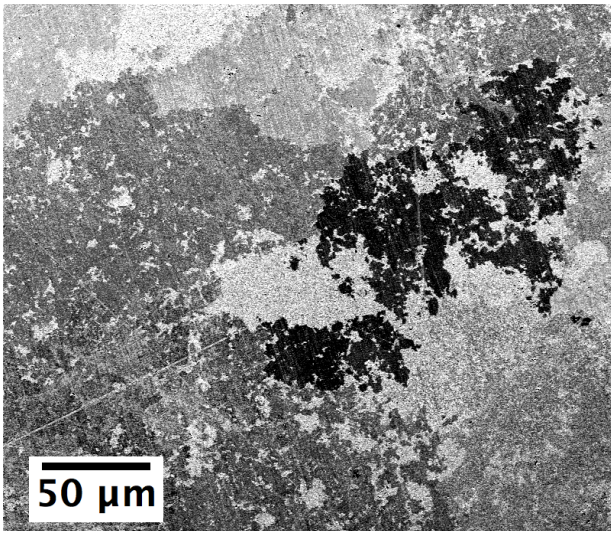

Fig. 1. SEM image of a polished surface of inert-gas-condensed $Pd_{90}Au_{10}$ following heat treatment at 200°C for 15 min. Abnormal grains (black and gray) manifest fractal-like perimeter morphologies.

KEYWORDS: abnormal grain growth; fractal microstructure; nanostructured material; inert gas condensation.

Presentation Method: Poster

Gas-pressure infiltrated Al-based MMC with $Ni_{60}Nb_{20}Ta_{20}$ metallic glass: Characterization by Analytical Transmission Electron Microscopy

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The utilization of metallic glass melt-spun ribbons to reinforce lightweight materials provides improved mechanical properties of the resulting metal-matrix-composites [1]. For the reinforcement in this work a multicomponent ball-milled melt-spun ribbon of a metallic glass, $Ni_{60}Nb_{20}Ta_{20}$, is used, having a crystallization temperature of 721 °C [2]. Those metallic glasses have superior properties such as improved strain limit or high strength, compared to regular metallic alloys, yielding to improved mechanical properties of the composite. The ribbons have a thickness of around 50 µm, and a length between 200 to 600 µm (after ball milling and sieving). As matrix a eutectic AlSi12 alloy with low melting point (580 °C) is used, which features excellent casting properties. The composites are fabricated by a liquid metal infiltration process. The processing temperature is near to the glass temperature of the metallic glass. The mean volume fraction of the glassy reinforcement is 30 %.

In order to understand the processing – structure – property relations, X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Scanning Transmission Electron Microscopy (STEM) combined with Energy Dispersive X-Ray analysis (EDX), and electron diffraction is applied to investigate mainly the interface between the AlSi12 matrix and $Ni_{60}N_{20}Ta_{20}$ glass. The targeted TEM-sample preparation of the interface between matrix and metallic glass reinforcement is done by Focused Ion Beam (FIB). STEM and EDX mainly answer the question, if diffusion occurs between matrix and reinforcement during the processing.

Electron diffraction shows diffraction peaks of the crystalline matrix and amorphous diffraction ring for the metallic glass reinforcement. The analytical results are summarized in Figure 1. The line profiles perpendicular to the interface show a transition zone at the interface, with a diffusion of Nb into the matrix, enrichment of Ta in the interface, and a decrease of Ni in the transition zone. Also a slight diffusion of Al into the metallic glass is observed at the interface. Parallel to the interface, a slight concentration variation of Nb and Ta, and a distinct variation of Ni is observed.

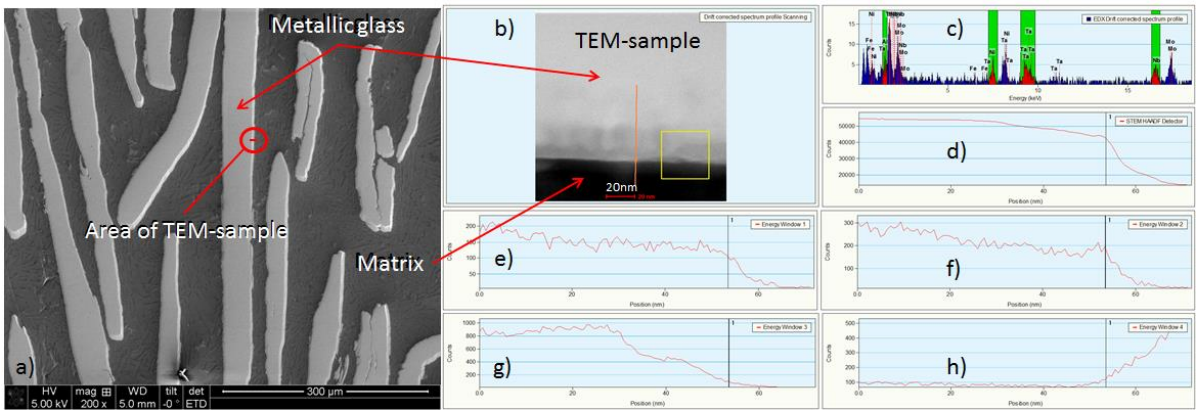

Fig1. a) SEM image, showing the metallic glass reinforcement embedded in the matrix and the position of the TEM-sample. b) Drift-corrected STEM-dark field image of the area of interest. The orange line corresponds to the trace of acquired EDX-line profiles, the yellow square is the square used for drift correction during acquisition. c) EDX-spectrum of the interface. d) Intensity profile of the STEM-image. e) Elemental distribution of Nb. f) Elemental distribution of Ta. g) Elemental distribution of Ni. h) Elemental distribution of the matrix element Al.

KEYWORDS: Metal matrix composites, $Ni_{60}Nb_{20}Ta_{20}$ metallic glass, interface, scanning transmission electron microscopy (STEM), focused ion beam (FIB), Energy Dispersive X-Ray analysis (EDX)

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Presentation Method: Poster

Influence of milling parameters on the formation of c-LLZO by mechanochemical processing

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Garnet type cubic $Li_7La_3Zr_2O_{12}$ (c-LLZO) is regarded as a promising material for solid state electrolyte for Li-ion batteries. The aim of this work was to study the influence of milling parameters on the formation of c-LLZO by mechanochemical processing. During the studies many milling parameters were subjected to changes, like type of mill (planetary or shaker), ball-to-powder weight ratio (45:1 and 15:1), vial and balls material (Al_2O_3 and ZrO_2), milling time (from 10 min to 10 h) and addition of process control agent (ethanol). The phase composition changes upon milling were monitored by X-ray diffraction, while powder size and morphology – by SEM observations. The influence of changeable parameters on phase composition of the powders after milling was analysed.

KEYWORDS: mechanical alloying, energy materials, high performance materials

Presentation Method (Invited/Regular Oral/Poster): Poster

Influence of Preparation Conditions on the Microstructure and Magnetic Properties of Rapidly Quenched Cold-Drawn and Glass-Covered FINEMET Thin Wires

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FINEMET microwires present a special interest for basic research as well as for applications due to their magnetic and magnetoelastic properties.

The aim of this paper is to present a comparative study on the evolution of microstructure, magnetic and magnetoelastic properties of cold drawn, glass-covered and 'glass-removed' microwires, having in view their potential use for low field or acoustic magnetic sensors. FINEMET ($Fe_{73.5}Si_{13.5}B_9Cu_1Nb_3$) wires with diameters of 30, 20 and 10 μm were prepared by cold-drawing successively an amorphous wire with the initial diameter of 105 μm, which was obtained by in-rotating-water quenching method. For comparison, glass-covered samples of the same composition, with the metallic wires diameters of 30, 20 and 10 μm and the total diameter of 38-40 μm, have been prepared using the glass coated rapid solidification technique. The 'glass-removed' microwires were obtained by removing mechanically the glass from the glass-covered microwires. All samples were annealed in vacuum for one hour at temperatures between 300°C and 600°C, to reduce the stresses induced during the preparation and to favor the formation of the optimum nanocrystalline structure, specific to FINEMET alloys.

The relative magnetic permeability of the glass-coated and 'glass-removed' microwires shows a maximum value of $0.6x10^5$ and respectively $1.3x10^5$ for an annealing temperature of 550°C. For the same annealing temperature the permeability of the cold-drawn wire is higher, i.e. $1.6x10^5$. The nanocrystalline phase, responsible for the obtained high magnetic permeability, is already formed and influenced by the residual stresses remnant from the cold drawn process, as confirmed by the UHR-TEM images, which show a nanocrystalline structure with nanograins between 6 and 18 nm, embedded in an amorphous residual matrix.

The magneto-impedance (MI) response and the sensitivity of the MI amplitude to tensile stresses show higher values for all diameters of the cold-drawn wires as compared with glass-coated and 'glass-removed' ones. Additionally, the values are larger for the wires with thinner diameters. The cold-drawn microwires of 10 μm in diameter show a sensitivity of the MI to force of 22 %/mN for an excitation frequency of 100 MHz and applied forces up to 10 mN. The complex action of intrinsic quenched-in stresses, cold drawing induced stresses, applied stresses, and annealing induced structural changes offers a wide range of possibilities for tailoring the magnetic characteristics of these materials for applications in magnetic sensors for the detection of mechanical deformations.

This work was supported by the Nucleu Programme (Project PN 16 37 02 02). A. Damian acknowledges the financial support offered by the POSDRU project (Contract nr. 159/1.5/S/133652).

KEYWORDS: microstructure, magnetic properties, rapidly quenched metallic materials

Presentation Method (Invited/Regular Oral/Poster): Poster

Interdiffusion and metastable phase formation in Ag/Al multilayer thin films studied by atom probe tomography

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Multilayer thin films exhibit unusual phase formations due to their unique microstructural properties compared to bulk materials, where the early-phase formation and phase evolution can be far from equilibrium conditions [1]. The knowledge and control of the mass transport and nucleation regimes are fundamental for guiding theoreticians towards a microscopic description of the solid-state reaction mechanisms and to avoid drawbacks in multilayer thin films applications. Especially in the case where individual layer thicknesses approach a few nanometers comprehensive experimental investigations are still missing.

In this work, we selected Ag/Al films deposited by DC magnetron sputtering, due to the simple Ag-Al phase diagram as well as negligible coherency stresses that derive from similar lattice constants of the Ag and Al crystal structure. The diffusion kinetics and phase formations were investigated as a function of individual layer thickness and the deposition conditions using conventional calorimetry (DSC), X-Ray diffraction, scanning-transmission electron microscopy, and atom probe tomography (APT). APT was extensively used in this study as it offers a superior capability to characterize local compositions, defect segregations, and concentration gradients in three dimensions with sub-nm resolution [2].

The magnitude of interdiffusion is found to be inversely proportional to the period thickness and is reduced by using low sputtering power [3]. Enthalpy values for the γ-hcp phase formation upon annealing are measured using DSC as a function of period and sputtering power. The formation of a metastable AgAl-hcp phase (50:50) was detected in periods of 10 nm thickness during annealing, where the stability and growth of the metastable phase was found to be highly dependent on the nominal composition of the thin films. Such metastable phase was previously predicted by theoretical studies [4].

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Presentation Method (Invited/Regular Oral/Poster): Poster

Investigation of $(Ti_{65}Fe_{35})_{100-x}(Bi_{53}In_{47})_x$ hypereutectic alloys with β-Ti dendrite

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Eutectic alloys exhibit a high strength because of the interaction between dislocation and lamellar interface [1,2]. However, one of the critical drawbacks in these eutectic alloys is the limited plasticity at room temperature[3]. To improve plasticity, the development of ultrafine eutectic alloys containing microstructural heterogeneity, i.e. eutectic composites having micron-dendrites as toughening phase, has been investigated[4]. The deformation mechanism of these alloys is the interaction of the slip and shear bands. So, these alloys effectively diminish the localization of the shear stress thus improving the plasticity. In the similar, the formation of chemical heterogeneity in the bimodal eutectic increases the ductility because the formation of different constituent phases in the eutectic colony boundaries prevent to catastrophic failure[5].

In this study, we researched the formation of a bimodal eutectic with chemical heterogeneity containing toughening phase by mixing Ti-Fe and Bi-In. The influence of addition of $Bi_{53}In_{47}$ eutectic alloy on microstructure and mechanical property of $Ti_{65}Fe_{35}$ hypereutectic alloy, i.e. $(Ti_{65}Fe_{35})_{100-X}(Bi_{53}In_{47})_X$, is investigated. These eutectic alloy was prepared by arc melting under Ar atmosphere. From these alloys, rods with 5mm diameter and 50mm length were made by suction casting. The microstructure of the samples was analyzed by scanning electron microscopy (SEM). X-ray diffraction (XRD) was performed for structural characterization. Mechanical property of these alloy was examined by compression test at room temperature.

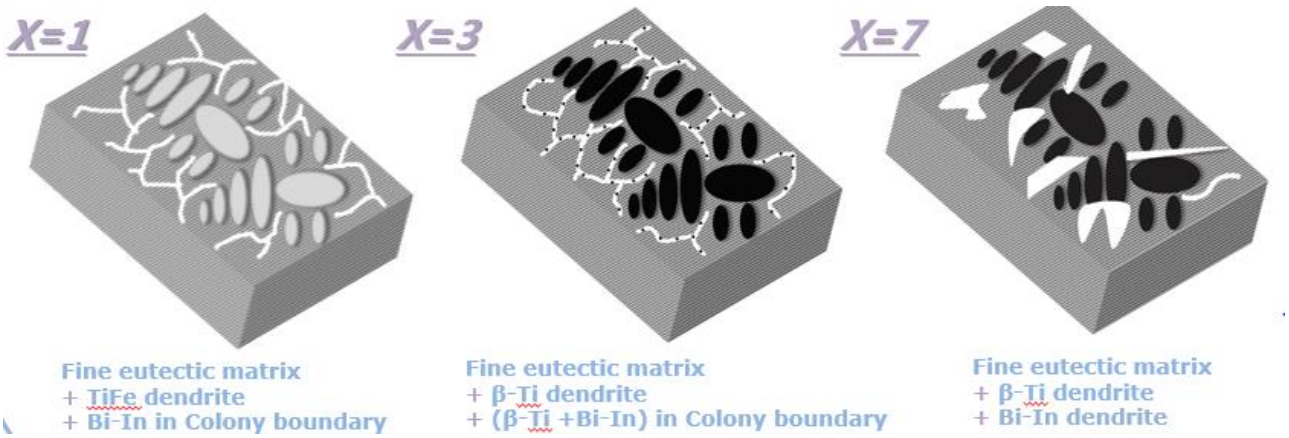

Fig1. Microstructure of $(Ti_{65}Fe_{35})_{100-x}(Bi_{53}In_{47})_x$ (x= 1, 3, 7) alloys

KEYWORDS: Eutectic alloy, Chemical heterogeneity, β-Ti alloy

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Presentation Method (Invited/Regular Oral/Poster): Poster

Investigation on Gd-based metallic glass alloys for magnetic refrigerant development

Yea Bin Moon[1], Yun Jung Hwang[1], Sung Hwan Hong[1], Hae Jin Park[1], Young Seok Kim[1], Young Hoon Lee[1], Yeon Beom Jeong[1] and Ki Buem Kim[1*]

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Conventional gas compression refrigeration is in need of alternative technology, because many problems of environmental and energy efficient. In order to overcome these drawbacks, the magnetic refrigeration based on the magnetocaloric effect (MCE) has become a promising alternative for gas compression refrigeration [1-2]. The MCE is a magneto-thermodynamic phenomenon in which the temperature changes as the material is exposed to changing magnetic fields. The heavy rare earth (RE) metals and RE-based alloys, such as Gd, Gd-Si-Ge, Dy-Al, La-Fe-Si and so on, have shown giant MCE [3-6]. Among these alloy, Gd-based alloys have a wide range of applications, because of Gd possesses the highest magnetic moment as well as highest effective exchange coupling around room temperature [5]. However, the polycrystalline Gd metal or Gd-based alloys with MCE undergo repetitive thermal expansion by temperature change, which induce catastrophic failure of the materials by the thermal strain on the grains and the stress accumulation at the grain boundaries during operation. Thus, it is necessary to develop a nano-crystalline magnetic refrigerant. Metallic glasses with a characteristic of metastable phase can easily form the homogeneous nano-crystalline structure [7]. Therefore, it is possible to develop nano-crystalline MCE alloys with excellent properties by using Gd-based metallic glass alloys with giant MCE.

In this study, we have selected Gd-based glass forming alloy system with MCE and attempt to extend the glass forming range on the alloy system by addition of alloying element [8-10]. The alloying elements were selected based on the empirical rule, and the glass-forming range of present alloys system were investigated by systemic structural and thermal analyses. In addition, we also investigated the crystallization behavior of metallic glass alloys. The phase identification of the metallic glasses and the nano-crystallized alloys was ascertained by X-ray diffraction (XRD) using Cu *K*α radiation. And thermal properties and crystallization behavior of metallic glasses were carried out using a differential scanning calorimeter (DSC) at the continuous heating rate of 0.333 K/s.

KEYWORDS: Metallic glasses, Magnetocaloric effect, Gd-based metallic glasses, Glass-forming ability

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Presentation Method (Invited/Regular Oral/Poster): Poster

Light weight FCC complex concentrated alloys with TRIP behavior

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Complex concentrated alloy (CCA) called “high entropy alloy” is an alloy system which is constituted with multi-principal elements [1]. Due to complex interactions among the constituting elements, this system shows higher configurational entropy than other conventional alloys, which means it is favorable to maintain stable solid solution at high-temperature rather form intermetallic compounds or intermediate phases. Moreover, CCA has received lots of attentions as a new metallic material due to its superior properties including relatively high strength and low thermal conductivity. Meanwhile, to overcome the intrinsic limitations of mechanical property in steel, twin induced plasticity (TWIP) or transformation induced plasticity (TRIP) behavior by controlling stacking fault energy (SFE) has been studied for a prolonged period. Thus, the combination between CCA and TWIP or TRIP property is one of the promising approaches to obtain unique mechanical property.

In the present study, we develop a new light weight CCA with TRIP behavior by manipulating SFE via minor addition of Al in 3d transition metal-based CCAs. To optimize the composition, first, we have carefully calculated the $\Delta G_{fcc\text{-}hcp}$ of phase transformation between fcc to hcp by CALPHAD method and optimized alloy compositions with enough low SFE to show TWIP or TRIP behavior. After then, we systematically control the addition of Al, which can reduce the density but increase SFE, in the optimized compositions. Indeed, our results provide a useful guideline how to improve mechanical properties by weight lightening as well as TWIP/TRIP behavior in CCAs.

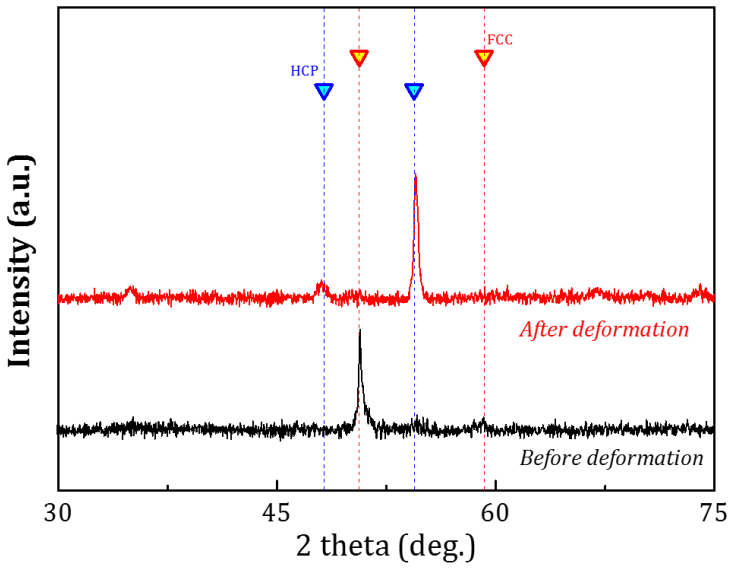

Fig1. XRD patterns before and after deformation. Austenite (FCC) phase is transformed to martensite (HCP) phase by severe plastic deformation.

KEYWORDS: Complex concentrated alloy, CALPHAD, TWIP/TRIP behavior, Al addition, Lightening method

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Presentation Method (Invited/Regular Oral/Poster): Poster

Low Temperature Peculiarities of Plastic Deformation of Several Bulk Metallic Glasses

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Mechanical behavior and failure peculiarities of the several bulk metallic glasses (BMG): $Zr_{64.13}Cu_{15.75}Ni_{10.12}Al_{10}$, $Zr_{57.4}Cu_{17,9}Ni_{13.4}Al_{10,3}Nb_1$, $(Zr_{57.4}Al_{0.1}\ Ni_{0.05,}\ Cu_{0,30})_{99}Y_1$, $Zr_{46.8}Ti_8Cu_{7.5}Be_{27.5}$ were studied in uniaxial compression at temperatures in the range 300-4.2 K. Several regularities of the low temperature plastic deformation have been found:

a) during temperature decrease from 300 to 170 K the type of plastic deformation changes from serrated to smooth;
b) high propagation rate of macroscopic shear bands (~ 10^3 m/s), observed at 300 K, is decreasing with decrease of the temperature to 170 K;
c) plasticity of the BMGs increasing with the temperature decrease, and maximum plasticity is observed near 77 K;
d) at 4.2 K the macroscopic plastic deformation is not observed and propagation of the shear band has catastrophic, avalanche-type character;
e) the typical ductile fracture ("vien" patterns) are observed at the fracture surfaces in whole studied temperatures in the range (300-4.2 K).

The registered regularities are discussed in terms of temperature dependence of shear bands quantity, responsible for macroscopic plastic deformation of the metallic glasses, and determined by nucleation probability and mobility of the shear transformation zones in the alloy's microstructure.

KEYWORDS: Bulk Metallic Glasses, Low Temperature.

Presentation Method: Poster

Magnetic Properties of Amorphous Alloys of Rhenium with Rare-Earth Metals

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During the last decades, amorphous alloys based on rare-earth metals (REM) are of great interest due to their unique magnetic properties. In this work we report on the experimental investigation and Monte Carlo simulation of magnetic properties of binary amorphous alloys of REM with nonmagnetic 5d-transition metal (rhenium) which were not studied so far.

Amorphous alloys of the Re_{100-x}-T^{4f}_{x} (T^{4f} = Gd, Tb, Dy, Ho, Er), (x=20-91 at. %) systems were produced by three-electrode ion-plasma sputtering method. At the low temperatures in these alloys in a wide compositional region the sharp maximum on temperature dependence of dynamic magnetic susceptibility and irreversibility of magnetization are observed. The observed magnetic phase transition is typical for spin glasses. The dependence of the transition temperatures T_f on the concentration of magnetic ions are linear functions. The slope of these lines decreases with increasing of the number of 4f-electrons of REM. The Re_{100-x}-Gd_x amorphous alloys at the intermediate concentrations (x=33-65 at. % Gd) turn into the reentrant spin-glass state.

All the phase transitions take place if the concentration of the REM atoms exceeds some critical value x_c=8-20 at. %. The existence of the critical concentration can be explained within the frame of percolation theory. The spin-glass transitions take place only if the percolation cluster of the REM atoms is formed.

Using the Monte Carlo method in the frame of the Heisenberg model, the computer simulation of magnetic properties of Re-Tb and Re-Gd amorphous alloys was carried out. The temperature dependencies of spontaneous magnetization, Edwards–Anderson order parameter and magnetic susceptibility were calculated. The magnetic phase diagrams for the pure amorphous Tb and for the Re-Tb amorphous alloys were constructed. With increasing concentration of Tb atoms, the transition temperature linearly increases, which is in a good agreement with the experimental results. Also the magnetic phase diagrams for the pure amorphous Gd and for the Re-Gd amorphous alloys were constructed. The magnetization curves, hysteresis loops, remanent magnetization, coercive field, spin-spin correlation functions at different temperatures are also calculated. The magnetization relaxation after switching-off the external magnetic field was also studied. Our results qualitatively agree with the experimental results obtained for amorphous alloys based on rare-earth metals.

KEYWORDS: Thin films and coatings, Chemical and physical properties.

Presentation Method (Invited/Regular Oral/Poster): Poster

Magnetism and magnetostriction in amorphous $Fe_xSi_{0.8}Mo_{18}B_{15.5}$ meltspun ribbons

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The scope of this work is to investigate the magnetic properties at room temperature of cores with high saturation polarization made from **$Fe_xSi_{0.8}Mo_{18}B_{15.5}$** as a function of the frequency of the applied field. To confirm the values for magnetic saturation polarization Js, a small flake of material was required for PPMS measurements while the measurement of the hysteresis under different discrete tensile stresses required a long ribbon sample. The ring shaped samples for hysteresis measurements were also made as tape-wound cores and were subjected to a triangular H-field in a frequency range from 1 to 50 Hz. The ribbons were available in the as cast state as well as in a heat treated state.

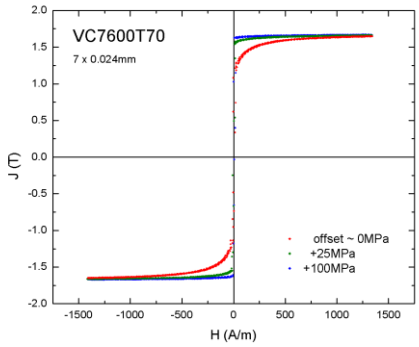

Fig. 1: Stress-dependent ribbon measurement on the narrow-band VC7600T70 sample (Hmax ~11000 A/m)

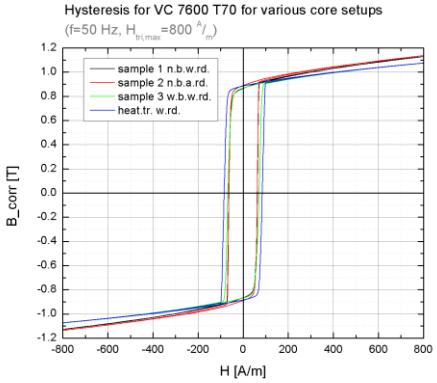

Fig. 2: hysteresis for triangular H-field on VC7600T70 with various core setups

The achieved results regarding the magnetic properties (hysteresis, losses, magnetostriction, etc.), microstructure and chemical composition of the tapes will be discussed.

Keywords: magnetostriction, soft magnetic alloys, Fe-based BMGs, core loss; soft magnetic properties; hysteresis loop measurements, meltspun tapes

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Presentation Method (Invited/Regular Oral/Poster): Poster

Mechanical behavior of super-elastic phase dispersed metallic glass composites

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Metallic glass alloys generically show high yield strength but low plastic deformability due to the absence of deformation mechanism. To overcome the low level of plasticity, many research groups have reported ex-situ and in-situ metallic glass composites to relax shear localization by introducing a heterogeneity in the glass matrix. In the case of in-situ metallic glass composites, nanocrystalline ductilization (ex, β phase in Zr-based metallic glass) and transformation-mediated ductilization (ex, B2 phase in CuZr-based metallic glass) have been suggested as the solution for ductility improvement in metallic glass for several decades. However, since the crystalline phases embedded in the amorphous matrix are, in most cases, stable up to high temperature, the type of the microstructure in in-situ metallic glass composites is strongly dependent on the cooling rate during fabrication. Therefore, the processing parameters during fabrication needs to be strictly controlled, thus the selection of proper microstructure in in-situ metallic glass composites still remains as a difficult task.

TiNi-B2 phase is stable at the room temperature and has proper properties such as excellent super-elasticity which can be useful as a second phase in-situ metallic glass composites. In spite of such superior characteristics, Ti-Ni based metallic glass composites have received less attention than Cu-Zr or Cu-Ti based metallic glass composites due to their inferior glass forming ability. Generally, metallic glasses have good thermo-plastic forming ability in the super-cooled liquid region, enabling to fabricate metallic glass parts by nano imprinting or surface patterning. Therefore, if the crystallization product from the Ti-Ni based metallic glass precursor is TiNi-B2 phase, the superelastic property can be achieved at room temperature.

In this study, a part of Ti and Ni are replaced with Zr and Cu maintaining equiatomic (Ti,Zr)/(Ni,Cu) ratio to improve the glass forming ability as well as to obtain isomorphous B2 phase as the crystallization product. Among the alloys investigated, the Ti35Zr15Ni35Cu15 alloy showed high glass forming ability which enabled the successful fabrication of fully amorphous ribbon with ~ 100 μm in thickness and ~ 10 cm in width by melt-spinning process. The amorphous ribbon was fully crystallized into single B2 phase by heating up to 600℃ without forming any other crystalline phase. To verify mechanical properties of the B2 phase alloy, compression test was performed using 2 mm diameter rod sample fabricated by suction casting. The result shows superior superelasticity with the recovery strain of ~ 6 %. The detailed results on the mechanical properties of super-elastic phase dispersed metallic glass composites will be presented.

KEYWORDS: composite, super-elasticity

Presentation Method (Invited/Regular Oral/Poster): Poster

Micro-sized Superelastic FeNiCoAl-based Alloys Prepared by Rapid Quenching from the Melt

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Recently, a new material that can resume its original shape in temperatures ranging from -196 to 249°C as compared to -20 to 80 °C reported before for this type of materials has been developed by Tanaka and co-workers through conventional forging and ageing[1]. The alloy presents superelastic strain of 13%, twice the maximum superelastic strain obtained in the Ni-Ti alloys.

This work reports results on the magnetic behavior of novel materials with high ductility, excellent magnetic characteristics and superelastic properties in the shape of micro-sized rapidly quenched FeNiCoAl(Ta,B) microwires prepared by in-rotating water quenching technique with diameters of around 200µm. Subsequent mechanical treatments have been applied by cold-drawing down to 50µm, followed by thermal treatments at 800°C for 1 hour. Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), thermomagnetic, and magnetic measurements have been performed to assess the structural and magnetic differences between the cold-drawn as-cast samples and samples annealed at 800°C for one hour.

In the as-cast state the wire shaped $Fe_{43.5}Ni_{28}Co_{17}Al_{11.5}$ and $Fe_{40.95}Ni_{28}Co_{17}Al_{11.5}Ta_{2.5}B_{0.05}$ present an amorphous-like structure which transforms into a polycrystalline structure by both cold-drawing (elongated grains) and subsequent annealing at 800°C for 1h (almost spherical grains). The relatively large grains observed, with a fine precipitates structure of tens of nanometers are attributable to γ '-$(FeNiCo)_3(AlTa)$ phase that occupies a relatively small volume, has spherical shape and are coherent with the austenitic phase matrix. Tantalum can be observed at grain boundaries. Thermomagnetic curves staring at 5K, at low fields of 20 Oe, present a maximum which is decreasing after cooling from 200K to 180 K for the as-cast cold drawn wire and from 130K to 100 K for the annealed wire and a Curie temperature of around 400K. Superelastic tensile stresses of up to 2.5 % have been achieved in the annealed FeNiCoAlTaB wires. Potential uses of superelastic alloys also include stents, catheters or guide wires in medicine due to their small dimensions.

KEYWORDS: Biomedical and energy materials, High performance materials.

Y. Tanaka, Y. Himuro, R. Kainuma, Y. Sutou, T. Omori, and K. Ishida, *Science* **327,** 1488 (2010).
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Presentation Method (Invited/Regular Oral/Poster): Poster

Microstructure evolution of ZrCuAgAl metallic glass processed by high pressure torsion

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Metallic glasses (MGs) possess many outstanding properties such as great strength, a high elastic limit and good resistance to corrosion that stem from their disordered atomic configuration [1]. However, the limited ductility due to the early catastrophic failure during plastic deformation is the major obstacle for their applications as structural materials. Recently, high pressure torsion (HPT) has been widely developed to increase ductility of MGs, with the tendency to impose extremely high strains compared to other severe plastic deformation (SPD) processes, such as rolling and shot-peening [2]. However, understanding the changes of the microscopic structure of MG as a result of HPT deformation, and how they affect the macroscopic physical properties still remains unclear.

In this work, we compared the thermal stability and mechanical properties between the as-cast and deformed samples. And we investigated the changes of the microscopic structure of $Zr_{46}(Cu_{4.5/5.5}Ag_{1/5.5})_{46}Al_8$ bulk MG after the HPT deformation by scanning transmission electron microscopy (STEM) methods, including fluctuation electron microscopy (FEM) to get the information of medium range order [3]; and RDF-imaging for short-range structural mapping around the shear bands area of the HPT-processed sample [4].

KEYWORDS: metallic glass ; microstructure

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Presentation Method (Invited/Regular Oral/Poster): Poster

Nanocrystalline NiAl intermetallic produced by mechanical alloying followed by hot-pressing consolidation

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An elemental Ni50Al50 powder mixture was subjected to mechanical alloying. Structural investigations revealed that a nanocrystalline NiAl intermetallic phase was formed during the milling process. The mechanically alloyed powder was consolidated at 1000 °C for 180 s under the pressure of 7.7 GPa. The bulk material was characterised by structural investigations (XRD, SEM) as well as by hardness and density measurements. It was found, that the quality of consolidation with preserving a nanocrystalline structure is satisfactory and the hardness of the produced material is relatively high.

KEYWORDS: Mechanical alloying, Powder and nanopowder synthesis and consolidation, Nanostructured materials.

Presentation Method (Invited/Regular Oral/Poster): Poster

Optimization of Ti-based coating layer as various deposition time with PVD method

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Recently, coating materials and technologies of tools are desired in many areas such as aerospace, automobile industries because it can be increased mechanical properties, abrasion resistance and tool life prominently [1]. To be satisfied with these characterizations, nitride coating layer has been widely studied in recent years because of high hardness and good wear resistance [2]. These properties are exhibited by the densification of coating layer as the formation of nitride. Among the nitride coatings, titanium nitride films have been widely used in many industrial areas due to their high mechanical properties and good abrasion resistance. In addition, Ti-based bulk metallic glass alloy which has higher hardness and elastic modulus than commercial alloys generally has been developed [1]. To make the coating layer which has superior hardness and elastic modulus, it is necessary that elements which can form nitride easily selected as the composition of Ti-based metallic glasses alloy.

In this study, Ti-Cu-Ni-Zr was chosen as the composition of Ti-based coating layer which is the composition of metallic glass alloy [3]. Also, Al known to have good mechanical properties was selected for the formation of many nitrides. To develop the coating layer, the experiment was conducted by reactive magnetron sputtering equipment. Ti-Cu-Ni-Zr target and Al target were used to make the coating layer by co-sputtering method. Ti-Cu-Ni-Zr-Al was deposited on the surface of tungsten carbide (WC) which is used as commercial alloy. To understanding the deposition rate of coating layer, we controlled the deposition time which has an effect on the thickness and microstructure of coating layer to check deposition rate of Ti-Cu-Ni-Zr-Al coating layer. To identify phase identification, microstructure of cross-section view and mechanical properties, the X-ray diffraction, FE-SEM and Nano-indentation analysis were carried out.

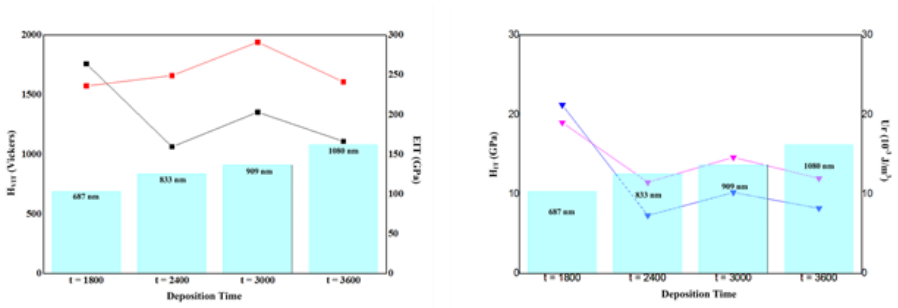

Fig1. Comparison of mechanical properties of Ti-Cu-Ni-Zr-Al-N coating layer with various deposition time

KEYWORDS: Sputtering, Microstructure, Nano-indentation, Hard coating

Yen Jin, Young-Gu Kim, Jong Ho Kim, Do Kyung Kim, Journal of Korean Ceramic Society 42, 455 (2005)

Li Chen, Yong Du, Fei Yin, Jia Li, International Journal of Refractory Metals and Hard Materials 25, 72 (2007)

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Presentation Method (Invited/Regular Oral/Poster): Poster

Oxidation behavior of Ti-Zr-Ni-Cu quaternary metallic glass

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Metallic glasses showing supercooled liquid region can be fabricated into a part with complex shape and surface patterns using various types of thermoplastic forming (TPF) process. In the process MG is heated into the supercooled liquid first and then is deformed by forced viscous flow. For optimization the TPF process, it is important to understand the oxidation behavior of MG during rapid heating because oxidation can occur readily during the process and the resulting oxide scales bring negative effects on viscous flow.

In the present study, we are reporting the oxidation behavior of $Ti_{40}Zr_{10}Ni_{40}Cu_{10}$ metallic glass (MG). The alloy was selected because it shows a reasonably good glass forming ability enabling fabrication into a glass state by melt spinning and the resulting metallic glass transforms into single B2 crystalline structure exhibiting superelastic behavior with large recovery strain of ~ 6.7 %. Thermal and oxidation behaviors of the metallic glass were analyzed during continuous heating with a heating rate of 40 K/min by differential scanning calorimetry (DSC) under argon atmosphere and thermogravimetric analysis (TGA) with a dry air (20 cm^3/min), respectively. Cross sectional microstructure of heated samples was examined in detail using STEM and TEM and depth-profiles of composition was examined using X-ray photoelectron spectroscopy (XPS).

The as-solidified MG showed a glass transition temperature (T_g) of 730 K and crystallization temperature of 771 K, resulting in SLR of 41 K, and a native glassy oxide film with thickness of about 5 nm and weak Ni segregation beneath the oxide layer. During heating the specimen, the thickness of oxide scales increased and various types of layered structure appeared depending on heating temperature. The specimen heated to 673 K, far below Tg, showed amorphous Ti(Zr) oxide layer of about 50 nm in thickness and Ni enriched layer between oxide and glassy substrate. The specimen heated to 733 K, just above Tg, showed oxide scale microstructure consisted of 3 layers: amorphous Ti(Zr) oxide layer of about 50 nm in thickness, Ni_3Ti layer with typical thickness of 15 nm and lamellar layer consisted of amorphous oxides and Ni_3Ti phases. The specimen heated to 873 K, far above T_x, showed oxide scale microstructure consisted of 4 layers: tetragonal $Ti(Zr)O_2$ oxide layer of about 50 nm in thickness, Ni_3Ti layer with typical thickness of 15 nm and lamellar layer consisted of crystallized oxides and Ni_3Ti phases and layer of internal oxidation on Ni(Cu)-Ti(Zr) B2 phase. These changes of oxide scale microstructure with heating temperature will be discussed in terms of selected oxidation, stabilization of amorphous TiO_2 structure by Zr substitution and diffusions of oxygen.

KEYWORDS: Ti-Ni based metallic glass, oxidation behavior

Presentation Method (Invited/Regular Oral/Poster): Poster

Preparation Method of Porous Titania(TiO_2) Thin Film using Cellulose Nanocrystal

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Titania is a very fundamental semiconductor material for photocatalysis, photovoltaics, and their composites. The more efficient performance of titania-based devices requires deposition of porous titania thin films possessing high specific surface area. To form the micro-sized pores in the titania thin films, inorganic templates such as ceramics or polymers are mainly utilized generally. However, removal of the solid inorganic templates without damaging the base material is challenging normally. Consequently, biomaterials are very attractive as pore generators since they can provide a variety shapes and sizes and they can be removed easily. This study mainly utilizes cellulose and chemically hydrolyzed cellulose nanocrystal(CNC) to prepare the mesoporous titania thin films. As a template, CNC can be self-combusted when the thin films are calcined at high temperature, so any subsidiary process to remove the template is unnecessary. By varying the titania-to-CNCs ratio, it is possible to handle the pore volume, pore size, pore anisotropy and specific surface area. Produced chemically purified cellulose(W-50, average particle size ~45μm, KC Flock) was used to extract the CNCs by acid hydrolysis method. Then, we established the standard of the mass ratio of CNCs compared with titania precursor(titanium(IV) ethoxide(TEOT)). After spin-coating on the ITO glass by using synthesized CNC-TiO_2 solution, we induced the CNCs to be combusted naturally to form the pores when calcined at high temperature. The content of CNC was classified by the mass ratio of tetravalent titanium(Ti^{4+}) of TEOT divided by CNC. By controlling the CNC content, we obtained 117.3 to 221.6 m^2/g of the specific surface area at various calcination temperature increased at least 220% than non-porous titania film.

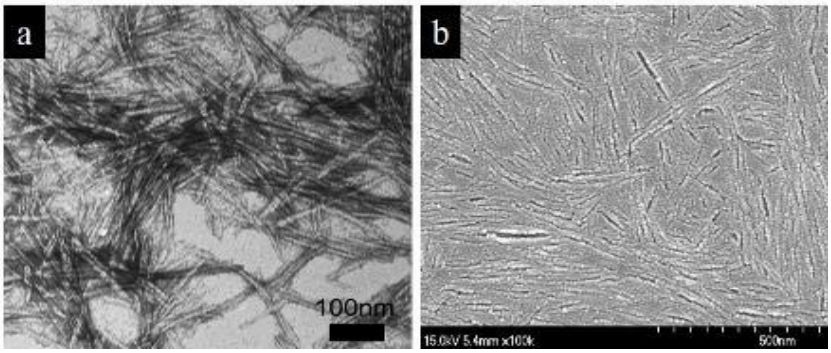

Fig. (a) TEM Image of Cellulose Nanocrystal (b) Surface Morphology of Cellulose-Templated Porous Titania Film

KEYWORDS: Photocatalyst, porous titania thin film, cellulose nanocrystal

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Presentation Method (Invited/Regular Oral/Poster): Poster

Rapidly Solidified Amorphous and Nanocrystalline $Fe_{73.5}Cu_1Nb_3Si_{13.5}B_9$ Nanowires

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Nanocrystalline wires and microwires prepared from rapidly quenched amorphous precursors exhibit a distinctive structure, which appears due to a well-defined annealing that triggers crystalline grains to nucleate and subsequently grow within the amorphous matrix. A typical alloy composition in which such a structure was emphasized and extensively investigated is $Fe_{73.5}Cu_1Nb_3Si_{13.5}B_9$, known as FINEMET. Magnetic materials with such combined structure - crystalline and amorphous - exhibit remarkably soft magnetic properties, due to the specific interaction between the two phases, i.e. the nanosized crystalline grains and the residual amorphous matrix, which leads to an averaged out vanishing overall magnetostriction [1]. These wires have typical diameters between 1 and 120 μm, being thus unsuitable for novel, state-of-the-art purposes, such as domain-wall-based magnetic logic applications.

Therefore, in this work we focus on the preparation and investigation of $Fe_{73.5}Cu_1Nb_3Si_{13.5}B_9$ wires with diameters at the submicron scale (< 1 μm), all the way down to the nanoscale (~ 100 nm), aiming to assess the origins of their peculiar characteristics, primarily the difference between the higher optimum annealing temperature found in these nanocrystalline ultrathin wires (600°C) and the optimum annealing temperature reported in nanocrystalline wires and microwires (550°C). We have also investigated the relation between their structure and properties, as the former evolves from amorphous to nanocrystalline, with a significant impact on the axial magnetization process. The domain wall propagation has been also studied, given its importance for the newly sought domain wall logic applications.

We proposed a simple, yet effective phenomenological model to explain the characteristics of the FINEMET nanowires and submicron wires, which is based on the interplay between the value of their specific exchange length and the changes in the inter-grain distance and grain size following the various stages of annealing. Accordingly, the exchange length is significantly affected by the small transverse dimensions involved in the rapid solidification process, being much smaller in the FINEMET nanowires compared to the thicker microwires and conventional wires with similar composition. Hence, a structure with comparable characteristics in terms of grain size and inter-grain distance, would not result in the same macroscopic magnetic behavior at the nanoscale. To reach similarly soft magnetic properties at the nanoscale, further annealing is essential.

The results are important for understanding the specific properties of the nanocrystalline structure at the nanoscale, and allow one to adequately design and tailor the properties of these novel materials for sensing and domain wall logic applications.

Acknowledgements-Work supported by the Romanian Ministry of Research and Innovation through the Nucleu Program (Project PN 16 37 02 02).

KEYWORDS: Materials - nanostructured materials; Properties and applications - physical properties.

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Presentation Method (Invited/Regular Oral/Poster): Poster

Selected properties of nanometric TiO_2 coating on biodegradable Mg alloys

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Magnesium based alloys have very poor corrosion resistance due to high chemical activity of the magnesium. The physical and mechanical properties of such materials used, for example, for biomedical implants get worse with progressive corrosion [1, 2]. This disadvantage has an impact on the limited use of magnesium and its alloys in aggressive environments such as living organism. Modifying the surface of magnesium alloys by deposition of organic and inorganic coatings is one of the most effective ways to prevent corrosion process [3, 4].

This paper presents one of the directions in the study of TiO_2 coating (with a thickness of about 100 nm) deposited on the MgZn2Ca1 alloy in as-cast state to improve its corrosion resistance. The thin coating was applied by magnetron sputtering method using the Kurt J. Lesker PVD 75 device. The coating process was carried out at the temperature of 100 °C for 75 min. The TiO_2 surface morphology was observed in the ZEISS Supra 25 scanning electron microscope. The Park Systems' AFM XE-100 atomic force microscope was used to observe the surface topography and conduct the roughness measurements. The measurements were done by non-contact mode. The analysis of the phase composition of studied material surface was carried out with the PANalytical X-Pert PRO X-ray diffractometer using the radiation of a Cu Kα. The corrosion resistance test of MgZn2Ca1 alloy and TiO_2 on master alloy was carried out in the Autolab PGSTA302N Multi BA potentiostat. In addition, immersion tests were conducted to measure the amount of hydrogen dissolution during 48 h for the coating and the substrate material. Electrochemical and immersion tests were performed in Ringer's solution, at 37 °C.

The nanometer TiO_2 coating deposited on the magnesium based alloy is compact and continuous. There were no defects in the form of cracks on its surface. The majority of coating surface irregularities does not exceed 25 nm (Fig. 1). The main surface roughness parameters have following values: Ra (Roughness average) is 11.94 nm, RMS (Root Mean Square) is 14.54. The analysis of potentiodynamic curves showed that the TiO_2 coating slightly improves the corrosion resistance of the MgZn2Ca1 alloy. The results of the open circuit potential (OCP) measurement suggest that the alloy with TiO_2 coating has the tendency to form a protective layer.

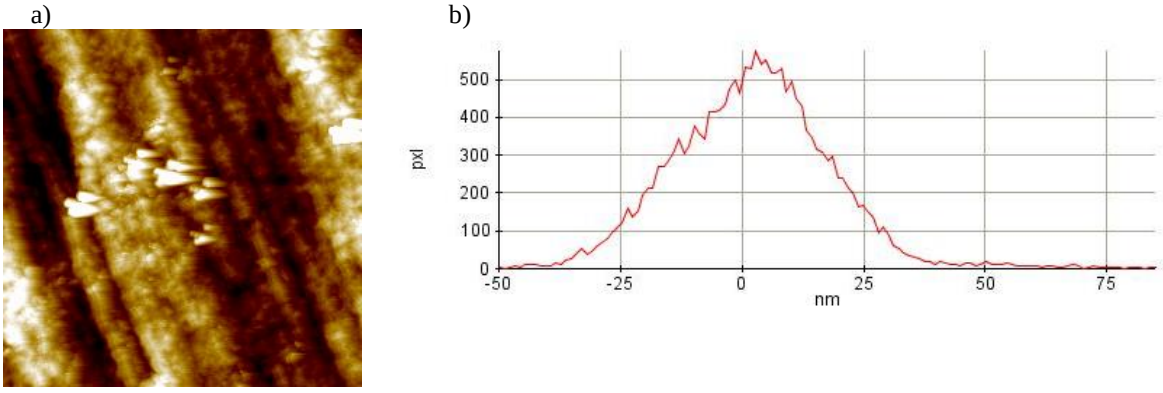

Fig.1. The AFM image of the TiO_2 coating: a) 2D surface topography image; b) distribution of surface irregularities of the TiO_2 coating.

KEYWORDS: thin film fabrication, fundamental research, nanometric TiO_2 coating, corrosion resistance.

The work was supported by the National Science Centre (project no.: DEC-2013/09/3/ST8/02129).

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Presentation Method (~~Invited~~/~~Regular Oral~~/Poster): Poster

Signature of the atomic structure in the thermophysical properties of flint and metallic glasses

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Flint glasses are silicates with large lead oxide content. From the experimental point of view, these glasses are the ideal network glass formers to compare metallic glasses with as they exhibit comparable glass transition temperatures. Despite the similar glass transition temperature, the structure of these two types of glass-formers is completely different. Flint glasses build network-like structures by connecting silicon and lead over bridging oxygen atoms with covalent or even ionic bonds, whereas metallic glasses are multicomponent atomic glass formers with non-directional metallic bonds and a less ordered clustered structure. The differences in the structure of these materials manifests in their thermophysical properties like the specific heat capacity and viscosity. For understanding the structure property relationship in glasses, three flint glasses with different lead content are investigated in terms of specific heat capacity and viscosity and compared to metallic glass formers.

KEYWORDS: Thermodynamics and phase transformation studies, Bulk metallic glasses and composites, Chemical and physical properties.

Presentation Method (Invited/Regular Oral/Poster): Poster

Structural and magnetic properties of magnetocaloric Gd-Si-Ge-(Mn) alloys by ball milling

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The magnetocaloric effect (MCE) is defined as heating or cooling of the magnetic material due to the application of magnetic field. This effect has been called adiabatic demagnetization for years, though this phenomenon is one practical application of the MCE in magnetic materials. Recently, there is a great deal of interest in using the MCE as an alternative technology for refrigeration. The magnetic refrigeration (MR) offers the prospect of an energy-efficient and environment friendly alternative to the common vapor cycle refrigeration technology in use today. The materials for MR technology have been intensively investigated and a lot of materials with excellent MCE have been developed in the last decades [1].

In this study, we report the structural and magnetocaloric effect in Gd-Si-Ge-(Mn) alloys by ball milling. The Gd-Si-Ge-(Mn) powders were prepared by the ball milling of arc-melted sample. The effect of milling time on the magnetocaloric effect of Gd-Si-Ge-(Mn) alloys has been investigated in detail. Structural characterization was performed using an X-ray diffractometry (XRD) with CuKα radiation and scanning electron microscope (SEM). Thermal behavior of MCE materials was measured by differential scanning calorimetry (DSC) and MCE was investigated by vibrating sample magnetometer (VSM).

KEYWORDS: Magnetocaloric effect, Ball milling, Gd-Si-Ge, Magnetic, Mechanical alloying

D.M. Rajkumar, M. Manivel Raja, R. Gopalan, and V. Chandrasekaran, *Journal of Magnetism and Magnetic Materials* **320**, 1479 (2008).

Presentation Method (Invited/Regular Oral/Poster): Poster

Structure and magnetic properties of Fe-based nanocrystalline soft magnetic alloys

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The series of alloys with nominal compositions $Fe_{79}Co_4Si_2P_2B_{12}Cu_1$, $Fe_{83}Si_2P_4B_{10}Cu_1$, $Fe_{82}Si_2B_{12}Cu_1Nb_3$, $Fe_{80}Co_3Si_2B_{12}Cu_1Nb_2$ and $Fe_{78}Co_4Si_2B_{14}Cu_1Nb_1$, (all in atomic %), were prepared by arc melting of high-purity elements (Fe, Co, Si, Cu, Nb) as well as Fe-P and Fe-B prealloys, in the atmosphere of Ar. The rapidly quenched ribbons were prepared by single roller melt spinning method. X-ray diffraction (XRD) was used to analyze the structure of the samples. The magnetic properties of the alloys were studied at room temperature using hysteresis loop tracer and vibrating sample magnetometer. Optimization of composition of the alloys was carried out to obtain high saturation induction (B_s) and low coercivity (H_c). An attempt to correlate the alloy composition, ribbon thickness, structure and magnetic properties was made. The thickness of the ribbons was between 20 and 36 μm. To obtain nanocrystalline ribbons, a series of 1 hour annealings were carried out at temperature ranging from 380 ºC up to 550 ºC. The measured coercivity of the alloys was from 23 to 57 A/m, and saturation induction was from 152 to 183 emu/g. The obtained results showed that the selection of chemical composition is trading between high magnetization and good glass forming ability, the two cannot be matched at the same time.

The temperature of crystallization stages depends on chemical composition, as expected. The optimum annealing temperature (Ta) of the alloys studied is between 475 °C and 575 °C. The coercivity of the $Fe_{79}Co_4Si_2P_2B_{12}Cu_1$ alloy increased from about 57 A/m (as-q state) to 104 A/m (T_a = 400 °C), later slowly decreased to 33 A/m (T_a = 475 °C - optimum) and finally reached the largest, excessive value of 4361 A/m (T_a = 550 °C). The coercivity of the alloys containing the same amount (83 %) of ferromagnetic elements behaves similarly. The coercivity of the $Fe_{83}Si_2P_4B_{10}Cu_1$ alloy increased insignificantly from 63 A/m (as-q state) to 65 A/m (T_a = 400 °C), then slowly decreased to 23 A/m (T_a = 475 °C - optimum) and finally rose to the highest value of 2137 A/m (T_a = 550 °C). These two alloys have relatively low coercivity and high saturation magnetization after annealing.

The best magnetic properties shows the $Fe_{83}Si_2P_4B_{10}Cu_1$ alloy (after annealing at 475ºC for 1 h): H_c = 23 A/m and M_s = 183 emu/g in nanocrystalline + amorphous state. Crystallization improved saturation magnetization, as compared to the alloys in an amorphous state, e.g. for $Fe_{82}Si_2B_{12}Cu_1Nb_3$, $Fe_{80}Co_3Si_2B_{12}Cu_1Nb_2$ and $Fe_{78}Co_4Si_2B_{14}Cu_1Nb_1$, M_s grew by 28, 17 and 8.5 %, reaching 169, 178 and 179 emu/g, respectively.

KEYWORDS: metallic glasses; soft magnetic properties; Fe based alloys; hysteresis loop measurements

Presentation Method (Invited/Regular Oral/Poster): Poster

Study on the microstructure and mechanical properties of equi-atomic substituted high-entropy alloys

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The conventional strategy for developing metallurgical alloys has been based mainly on one principal element. This alloy concept reaches the limit therefore the development of a new paradigm of advanced metallic materials of interest in high-entropy alloys (HEAs) is emerging. [1-6]

In previous study, describe the microstructure and mechanical properties of $(Ti_{33}Zr_{33}Hf_{33})$-$(Ni_{50}Cu_{50})$. Series of HEAs have been designed using an equiatomic substitution alloy strategy, so that their microstructure and mechanical properties could be compared to see the effect of different elemental contents. $(Ti_{33}Zr_{33}Hf_{33})_{60}(Ni_{50}Cu_{50})_{40}$ composites with equiatomic components show the best properties.

Based on these results, in this study, alloys with composition of equi-atomic substituted TiZrHfNiCu, TiZrHfNiCuCo, TiZrHfNiCuNb and TiZrHfNiCuFe high-entropy alloys (HEAs) were produced by suction casting method. The effects of addition elements on phase composition, microstructure and mechanical behaviors of the HEA were studied. The suction casted $Ti_{20}Zr_{20}Hf_{20}Ni_{20}Cu_{20}$ HEA exhibits single C14 Laves phase ($MgZn_2$-type) with fine homogeneous microstructure. When Co, Nb or Fe elements are added, morphologies are slightly modulated toward well-developed dendritic microstructure, phase constitutions are significantly changed from single Laves phase to mixed multi-phases as well as mechanical properties are also altered with increased plasticity and high strength. It is believed that modulated mechanical properties are mainly ascribed to the change of phase constitution and crystalline structure, together with the microstructural characteristics. This clearly reveals that the selection and addition of supplementary elements based on the formation rule for HEAs play an important role on the evolution of phase, microstructural morphology and mechanical properties of $Ti_{20}Zr_{20}Hf_{20}Ni_{20}Cu_{20}$ HEA. [7, 8]

KEYWORDS: High Entropy Allloys, equiatomic substitution, microstructure, mechanical properties

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Synthesis of Intermetallic Based Nanocomposites via Mechanochemical Route

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Mechanical deformation of powder particles during high energy ball milling can be utilized to promote solid-state chemical reaction between precursor powders at low temperature. This procedure is often referred as mechanochemical process in the literature. Due to the repeated cold welding and fracturing of powder particles during ball milling the product phase particles have nanoscaled size and disperse uniformly in the matrix. At the same time ball milling readily leads to the alloying of precursor elements and as a result formation of solid-solution, amorphous or intermetallic compounds depending on thermodynamics and kinetics of alloy system as well as milling conditions. Moreover, high energy ball milling is always accompanied by nanocrytallinity. All these processes lead to the in-situ formation of nanocomposite structures. In this paper the research findings of author's research group on application of ball milling for synthesis of intermetallic based nanocomposites are reviewed and discussed.

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The structure of equiatomic Ti-Y alloy after rapid quenching and its interaction with hydrogen and oxygen

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The structure of equiatomic Ti-Y alloy after melting and rapid quenching was studied. Initial ingots were melted by arc melting using non-consumable electrode; rapidly quenched strips with thickness nearly 30 microns were obtained by spinning. The structure was studied by XRD, metallography and electron microscopy. It was found that both after melting and quenching two-phase microstructure is formed in alloy. The microstructure consists of solid solutions, based on α-titanium and α-yttrium. For equiatomic as-cast alloy lattice parameters of titanium phase equal: a = 2,9553Å; c = 4,6989Å. In rapid quenched alloy lattice parameters of titanium phase equal: a = 2,956Å; c = 4,683Å. Lattice parameters of yttrium phase are equal a = 3,6545Å; c = 5,7470Å and a = 3,653Å; c = 5,738Å in as-cast and quenched states, respectively. The features of alloy microstructure formation are explained on the known phase diagrams.

It is shown that alloy hydrogenation causes to formation of cubic titanium and yttrium hydrides. Lattice parameter of TiH_2 phase was equal to a = 4,431Å and lattice parameter of YH_2 phase was equal to a = 5,210Å.

Annealing the alloy strips at temperature $T \geq 900$ ºC in air leads to formation of Y2Ti2O7-δ compound with pyrochlore structure. Influence of annealing temperature on crystallite size was studied.

KEYWORDS: Powder Synthesis, Rapid Quenching, Microstructure.

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