MM 36: Liquid and Amorphous Metals

Sessions: Local structure and crystallization; Mechanical deformation of metallic glasses

Time: Thursday 10:15–13:00 Location: H46

MM 36.1 Thu 10:15 H46

The effect of temperature and composition on resistivity of Bi-Ga and Ga-In binary alloys — •Yuri Kirshon[1], Guy Makov[1], and Eyal Yahel[2] — [1]Ben-Gurion University of the Negev, Beersheba, Israel — [2]NRCN, Beer-Sheva, Israel

The electrical resistivity of liquid metals and alloys is a probe of the electronic and structural properties of the system. The present study focused on the development of an experimental apparatus to measure the electrical resistivity of liquid metals and its application to selected metal and alloy systems. The presentation consists of two parts: the first reports on the design of the experimental measuring system, with some emphasis on the importance of component materials. The second part reports on measurements of resistivity in pure Bi, Ga and In, also, Bi-Ga and Ga-In binary alloys were tested as well. The resistivity of the alloys was measured for selected compositions over wide range of temperatures. In all the studies the absolute resistivity was determined up to an error of 3% and the results are with good agreement with previous studies. A clear linear correlation between resistivity and temperature is obtained for tested pure metals and some tested alloys. For Bi-Ga the resistivity and its temperature coefficients are found to vary smoothly with composition as suggested by simple theoretical models. In contrast, for Ga-In alloys the composition dependence is non-monotonous. In addition, the near eutectic alloys display anomaly which point toward a structural transition in the liquid.

MM 36.2 Thu 10:30 H46

Impact of Glass Transition on Crystallization Kinetics of Phase-Change Material Ge2Sb2Te5 — •Julian Pries[1], Shuai Wei[1], Matthias Wuttig[1,2], and Pierre Lucas[3] — [1]Institute of Physics IA, RWTH Aachen University, Germany — [2]Peter Grünberg Institute (PGI 10), Forschungszentrum Jülich, Germany — [3]Department of Materials Science and Engineering, University of Arizona, United States

Phase-Change materials (PCMs) can be switched in nanoseconds between the amorphous and crystalline phase. In combination with the pronounced change of physical properties like electrical resistivity or optical reflectivity upon this transition, PCMs offer a wide potential for memory applications. A deep understanding of crystallization kinetics is essential for increasing the data transfer rate of such devices. Here, crystallization kinetics of the prototypical PCM Ge2Sb2Te5 is investigated. Combining conventional and Flash DSC opens a heating rate interval of over six orders of magnitude. The resulting crystallization data reveals a sharp transition from a high to a low Kissinger activation energy of crystallization when exceeding the critical heating rate. Moreover, pre-annealing affects this activation energy at low, but not at high rates. Utilizing Fluctuation Electron Microscopy and JMAK-simulations uncovers the origin of this behavior: The manifestation of glass dynamics and glass transition in crystallization behavior. Accordingly, Ge2Sb2Te5 crystallizes from the glass at low and undercooled liquid phase at high heating rates. The presence of this transition has major consequences for estimating the performance of PCM memory.

MM 36.3 Thu 10:45 H46

Crystallization behavior of a bulk metallic glass-former — •Mark Stringe, Joachim Bokeloh, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, D-48149 Münster

Crystallization plays a crucial role not only regarding the production of metallic glasses, but also concerning the stability of these systems. This stability is linked to the corresponding ability of atoms to rearrange. The movement of atoms is also affecting the glass forming ability and thus the crystallization of the undercooled liquid.

With a variation of scanning rates of calorimetric measurements it is possible to analyze crystallization kinetics. The measurements are performed with conventional differential scanning calorimetry (DSC). Higher scanning rates are realized using a custom-built fast DSC according to the concept of C. Schick et al. [1]. With this fast scanning calorimetry (FSC) samples with a mass of the order of micrograms are measured with scanning rates up to 10.000 K/s.

An AuCuSiAg bulk metallic glass with low melting point is analyzed. In FSC it is possible to reach cooling rates to quench a glass in-situ. Thus the critical cooling rate can be determined directly and activation energies for crystallization of the supercooled liquid are obtained from Kissinger analyses.

Depending on the degree of undercooling, the system shows a change in the crystallization behavior of the undercooled liquid suggesting a change in kinetics.

[1] Zhuravlev E, Schick C, Thermochimica Acta 505 (2010) 1-13

MM 36.4 Thu 11:00 H46

Quasi-discontinuous change of the density correlation length at the fragile-to-strong transition in a bulk-metallic-glass forming melt — •Sergey V. Sukhomlinov and Martin H. Mueser — Universität des Saarlandes, 66123 Saarbrücken, Germany

Many bulk-metallic-glass (BMG) forming melts undergo a fragile-to-strong transition (FST), which is accompanied by a small but noticeable peak in the specific heat c_p. However, density and local structure at the FST appear to change only continuously. Because of the peak in the c_p, the FST is sometimes interpreted as a smeared-out phase transition. This motivated us to study how the specific heat, dynamical and structural properties of a selected BMG depend near the FST temperature on the system size using computer simulations.

For a ternary BMG former ($Zr_{0.606}Cu_{0.29}Al_{0.104}$), in contrast to the expectations for a phase transformation, we observed that the larger the system the smaller the peak in c_p. This result, along with size dependence of other properties, is difficult to reconcile with the interpretation of the FST being a (smeared-out) phase transformation.

The results from structural analysis showed a smooth evolution of radial distribution functions (RDF) at small distances through the FST. However, the long-range density correlation length increases (quasi-) discontinuously at the FST as revealed by an Ornstein-Zernike-based analysis of the RDF. Likewise, the temperature derivative of the Zr-Zr mean nearest-neighbor distance decreases (quasi-) discontinuously at the FST. These observations add to the rich phenomenology of FSTs lacking a theoretical understanding.

MM 36.5 Thu 11:15 H46

Effect of Co microalloying on thermodynamic and kinetic properties of a $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass — •René Hubek[1], Mikhail Seleznev[2], Isabelle Binkowski[1], Martin Peterlechner[1], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Togliatty State University, Togliatty, Russia

The physical properties of bulk metallic glasses are subject of intense research especially with respect to their mechanical behavior. Recently, it was shown that the mechanical properties of a $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass could significantly be enhanced through cobalt microalloying [1].

In this report we are focusing on the low-temperature heat capacity and shear band diffusion measurements. The results are discussed in comparison to the reference $Pd_{40}Ni_{40}P_{20}$ glass [2, 3]. The effect of plastic deformation and post-deformation annealing on the excess heat capacity at low temperatures, known as the "boson peak", is thoroughly examined. Furthermore, the influence of annealing and micro-alloying on the shear band diffusion is investigated.

These data are discussed with respect to the relaxation behavior and excess free volume distribution in the Co-free and Co-microalloyed PdNiP.

[1] N. Nollmann et al., Scripta Materialia 111 (2016), 119-122
[2] Y.P. Mitrofanov et al, Acta Materialia 90 (2015) 318-329.
[3] I. Binkowski et al, Acta Materialia 109 (2016) 330-340.

15 min. break

MM 36.6 Thu 11:45 H46

Origin of Large Plasticity in Fe50Ni30P13C7 Bulk Metallic Glass — •Baran Sarac[1], Yurii P. Ivanov[2], Mihai Stoica[3], and Jürgen Eckert[1,4] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]University of Cambridge, Cambridge UK — [3]ETH

Zurich, Zurich, Switzerland — [4]Montanuniversität Leoben, Leoben, Austria

Despite Fe-based bulk metallic glasses (BMGs) garner great interest owing to their combined high temperature thermal stability, soft magnetic properties along with high strength, the biggest barrier against a more widespread use is their negligible plasticity. A newly developed Fe50Ni30P13C7 BMG overcome this limitation via extensive compressive plasticity [1]. Using a combination of an aberration-corrected high-resolution transmission electron microscopy (HRTEM) and nanoindentation techniques, we identified a multi-stage deformation mechanism involving 1-1.5 nm sized homogeneously dispersed crystals and micro-scale heterogeneities [2]. Besides, we conducted a systematic set of simulations of the HRTEM images at varying sample thicknesses, and adopted a cooperative shearing model for the estimation of the shear transformation zone size of Fe50Ni30P13C7 BMG. The findings indicate that the controlled nanocrystal-induced plasticity with crystal sizes of several nanometers contributes to the remarkable shear observed under quasi-static compression and enhance the plasticity of the BMG through the initiation and impediment of STZs. [1] W.M. Yang et al., Sci Rep, 4, 6233 (2014) [2] B. Sarac, et al., Nat Commun, 9, 1333 (2018)

MM 36.7 Thu 12:00 H46

Dr — •Alexandra E. Lagogianni, Muhammad Hassani, and Fathollah Varnik — ICAMS, Ruhr-Universitaet Bochum

Probing the degree of heterogeneity within the shear band of a model glass Alexandra E. Lagogianni, Muhammad Hassani and Fathollah Varnik 1ICAMS, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany

We employ large scale molecular dynamic simulations to study the degree of heterogeneity within the shear band of a model sheared glass in the athermal limit. The heterogeneity, demonstrated as spatial variations of microscopic quantities such as density, local strain and viscosity, is tracked along the propagation direction of the shear band. The spatial evolution of these quantities inside the shear band shows a position-dependent nature and a sinusoidal-like pattern with a large characteristic length scale. By probing the correlations of the quantities at the stationary plastic region, we provide a quantitative analysis of the underlying mechanism and the local environment of the shear band. These correlations, captured by a simple glass forming model, are suggested to be a generic feature of metallic glasses rather than material-specific properties.

MM 36.8 Thu 12:15 H46

Size-dependent failure of the strongest bulk metallic glass — •Ruitao Qu[1,2], Dominik Tönnies[1], Lin Tian[1], Zengqian Liu[2], Zhefeng Zhang[2], and Cynthia Volkert[1] — [1]Institute of Materials Physics, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang, 110016, China

Upon reducing sample size into the sub-micrometer scale, the mechanical behavior of metallic glasses (MGs) is often changed dramatically. For instance, obvious tensile ductility and necking can be observed in nano-scale MGs, while they are rarely seen in bulk samples. Here we present our recent studies on the size effect of the deformation and failure behaviour of a Co-based MG, which exhibits the highest strength among all known bulk MGs. An obvious brittle-to-ductile transition accompanied by a drastic change of failure mode were observed on decreasing the sample size. The bulk compressive samples failed by splitting and shattering, similar to other brittle MGs, while the micrometer and sub-micrometer scale specimens demonstrated shear banding, typical of ductile MGs. In order to assess whether this size effect was caused by the reduced probability of the presence of defects in small-scale samples, we intentionally designed various micropillar specimens containing defects. However, no brittle failure was observed in the defective micropillars, even though the local maximum tensile stress in front of defects had far exceeded the critical tensile stress for splitting in bulk sample. A characteristic distance model for cleavage cracking initiation in brittle MGs is proposed to explain these observations.

MM 36.9 Thu 12:30 H46

Design of thin film metallic glasses with superior fracture toughness — •Simon Evertz[1], Ines Kirchlechner[2], Rafael Soler[2], Christoph Kirchlechner[2], Paraskevas Kontis[2], Volker Schnabel[3], Gerhard Dehm[2], Dierk Raabe[2], and Jochen M. Schneider[1] — [1]Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany — [2]Max-Planck-Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [3]Laboratory for Nanometallurgy, ETH Zürich, Vladimir-Prelog-Weg 5, 8093 Zurich, Switzerland

Damage tolerance, i.e. the combination of high yield strength and fracture toughness, is crucial for the application of metallic glasses as structural materials. One fingerprint for damage tolerance in metallic glasses is the fraction of hybridized bonds (Schnabel et al., Scientific Reports 6 (2016) 36556), which is affected by alloying $Pd_{57.4}Al_{23.5}Y_{7.8}M_{11.3}$ with M = Fe, Co, Ni, Cu, Os, Ir, Pt and Au. Based on these ab initio calculations, the minimum fracture toughness was identified for $Pd_{57.4}Al_{23.5}Y_{7.8}Ni_{11.3}$. Furthermore, it is shown that by correlating experimental fracture toughness data to the fraction of hybridized bonds scaling with the crystal orbital overlap population at the Fermi level, the fracture toughness can be estimated based on electronic structure data. The fracture toughness of $Pd_{57.4}Al_{23.5}Y_{7.8}Ni_{11.3}$ is predicted to be in the range of 90 to 150 $MPa.m^{0.5}$ exhibiting a plastic zone size of 0.1 to 1 mm, which is consistent with micro-mechanical beam bending experiments, where fracture was not observed.

MM 36.10 Thu 12:45 H46

Atomic-scale deformation in metallic glass nanolaminates with shape memory alloys — •Daniel Şopu[1,2], Karsten Albe[1], and Jürgen Eckert[2,3] — [1]Technische Universität Darmstadt, Otto-Berndt-Straße 3, D-64287 Darmstadt, Germany — [2]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, A-8700 Leoben, Austria — [3]Department Materials Physics, Montanuniversität Leoben, Jahnstraße 12, A-8700, Leoben, Austria

Crystalline-metallic glass laminates with shape memory alloys represent a class of material with enhanced mechanical performance superior to those predicted from a simple rule-of-mixtures. Here, we model the deformation behavior of metallic amorphous Cu64Zr36/crystalline B2 CuZr nanolaminate systems using molecular-dynamics computer simulations. First, a modeling strategy is developed to capture the autocatalytic chain-type deformation mechanism. We find that the deformation of the glassy and crystalline phases is a coupled process: martensitic transformation leads to shear band formation while the stress at the shear band tip induces martensitic transformation in the shape memory crystal. Moreover, the martensitic transformation changes the shear band morphology, stabilizes the shear flow and avoids a runaway instability. Finally, we differentiate the contributions of the aspect ratio, laminate thickness, volume fraction and structural rejuvenation to the plasticity. Therefore, tailoring the architecture of metallic glass laminates with shape memory phases may allow the development of materials that exhibit large tensile ductility.