MM 30: Liquid and Amorphous Metals

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

MM 30.1 Thu 10:15 H46

Controlling the degree of rejuvenation and strain-hardening in metallic glasses — •Daniel Şopu[1,2], Xudong Yuan[1], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Technische Universität Darmstadt, Germany — [3]Montanuniversität Leoben, Austria

The correlation between the degree of rejuvenation and strain-hardening in metallic glasses (MGs) is investigated using molecular dynamics simulations. By randomly removing atoms from the glass matrix, free volume is homogeneously generated and glassy states with different degrees of rejuvenation are designed and further mechanically tested. The highest rejuvenated state is defined by the dynamic balance between free volume generation and annihilation. The highest degree of rejuvenation correlates to the flow strain of the materials and the structure is similar to that found in shear bands. The free volume in the rejuvenated glasses can be annihilated under tensile or compressive deformation that consequently leads to structural relaxation and strain-hardening. Loading-unloading cycling tensile tests are simulated and the atomic-scale mechanism of strain-hardening in the highly rejuvenated MGs is highlighted.

MM 30.2 Thu 10:30 H46

Revealing the impact of Sulfur addition on the medium-range order and relaxation dynamics of metallic glasses — •Hendrik Voigt[1], Nico Neuber[2], Harald Rösner[1], Martin Peterlechner[1], Ralf Busch[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany — [2]Chair of Metallic Materials, Saarland University, Saarbrücken, Germany

The addition of Sulfur as an alloying element has been shown to enable or improve the glass forming ability of certain glasses drastically [1]. Despite growing knowledge of the impact that Sulfur has on the mechanical properties, the underlying structure and its dynamics are still not fully understood [2].

In this contribution the sample system Pd31Ni42S27 has been investigated with respect to medium-range order (MRO). For the MRO analysis multiple series of nanobeam diffraction patterns with varying probe sizes were acquired in order to conduct variable resolution Fluctuation Electron Microscopy (FEM). Furthermore, Electron Correlation Microscopy (ECM) was employed to analyse relaxation dynamics by the acquisition of a tilted dark-field time series. By the combination of these two techniques it appears that the size of the regions displaying strongly decelerated dynamics at room temperature correlate with the detected MRO. The results are discussed with respect to current models.

[1] A. Kuball et al., Scripta Materialia (2018) 73-76 [2] H. Jiang et al., Scripta Materialia (2021) 116923

MM 30.3 Thu 10:45 H46

Glass Formation and Shear Banding in High-Entropy Metallic Glasses: A Molecular Dynamics Study — •Marie J. Charrier, Daniel T. Utt, Arne J. Klomp, and Karsten Albe — Fachgebiet Materialmodellierung, Institut fuer Materialwissenschaft, Technische Universitaet Darmstadt

Bulk metallic glasses (BMGs) and High-Entropy Alloys (HEAs) both comprise a large number of elements but deviate strongly in their mechanical properties. BMGs are strong but brittle and usually derived from crystalline binary subsystems with deep eutectics and intermetallic phases. HEAs, on the other hand, show remarkable ductility, a small heat of mixing, and are thus typically not glass formers. The open question is whether a classically crystalline random solid solution HEA can be transformed into a BMG using appropriate processing. In this work, we use atomistic computer simulations to study the combination of the two materials classes, HE-MGs. Here, we are able to kinetically suppress crystallization in the CrMnFeCoNi alloy, which in the real world remains a crystalline single-phase solid solution using conventional quench rates. First, we investigate the thermodynamics of the glass transition and its dependence on quench rate. Second, the phase stability of the HE-MG is compared to the crystalline HEA. Third, the atomic-level structure is characterized in terms of chemical and structural short- and medium-range order. Last, we perform compressive and tensile testing on HE-MG samples to assess failure by homogeneous deformation or shear localization and compare the mechanical properties against a CoCrFeMnNi nanocrystal.

MM 30.4 Thu 11:00 H46

Cyclical structural relaxation of PdNiP and micro-alloyed PdNiPFe and PdNiPCo glasses — •Manoel W. da Silva Pinto, Mark Stringe, Katharina Spangenberg, Harald Rösner, and Gerhard Wilde — Institut für Materialphysik, WWU Münster

Relaxation phenomena in $Pd_{40}Ni_{40}P_{20}$ bulk metallic glasses (BMG) as well as in micro-alloyed forms of Co and Fe addition were investigated by calorimetry. The BMGs were submitted to different thermal treatments by varying temperatures and times. In order to identify distinct signatures of relaxation, the thermal and temporal evolution of enthalpic contributions to calorimetric signals were analyzed using different kinetic models. A possibility was found to control the formation and depletion of an endothermic signature before the glass transition by quenching and annealing procedures. From the evolution of the enthalpies with annealing time and from isothermal heat flow, time constants related to structural relaxation were obtained and supplemented by dynamical and structural TEM analyses. The obtained results are discussed with respect to existing models for glass relaxation.

MM 30.5 Thu 11:15 H46

Enhancing ductility and strain hardening by modulating residual stresses in metallic glasses — •Xudong Yuan[1], Daniel Şopu[1,2], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Technische Universität Darmstadt, Darmstadt, Germany — [3]Montanuniversität Leoben, Leoben, Austria

The correlation between the deformation behavior and the residual stress modulation in metallic glasses (MGs) is investigated using molecular dynamics simulations. Particularly, the influence of residual compressive stress and stress heterogeneity on the tensile deformation behavior of amorphous Cu64Zr36 alloys is investigated. Strain hardening together with enhanced tensile ductility in monolithic MGs can be attained by only modulating the internal stress without changing their local structure. The stress heterogeneity changes the shear band dynamics leading to the formation and interaction of multiple shear bands, which consequently enhances the macroscopic ductility. Additionally, the residual compressive stress offsets the external tensile stress, which delays shear band formation and enables strain hardening in uniaxial tensile tests.

15 min. break

MM 30.6 Thu 11:45 H46

Origin of the Invar effect in Fe-based bulk metallic glasses — •Alexander Firlus[1], Mihai Stoica[1], Stefan Michalik[2], Robin E Schäublin[1], and Jörg F Löffler[1] — [1]1 Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland.2 — [2]Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, UK

Generally, metals, including most ferromagnetic ones, have a constant coefficient of thermal expansion (CTE). However, a few magnetic alloys show an anomalously low CTE below their Curie temperature. At the Curie temperature it increases abruptly by up to one order of magnitude. This effect is known as the Invar effect. While it is rare in crystalline alloys, it is universally observed in ferromagnetic Fe-based bulk metallic glasses (BMGs). To this day, it is still unclear in which way the amorphous atomic arrangement creates the Invar effect and how it manifests at the atomic scale.

In this work we studied BMGs with only one magnetic atom species, Fe, by in-situ high-energy X-ray diffraction. This allows us to measure the thermal expansion at the atomic scale and to associate it with specific atomic pairs. Fe-Fe pairs are found to be responsible for the Invar effect at the atomic scale. Moreover, also full atomic shells, which contain all atomic species, show an abrupt increase in their thermal expansion. This proves that the Invar effect is not just a macroscopic effect but has clear origins at the atomic scale.

MM 30.7 Thu 12:00 H46

Coupling deformation mechanisms in metallic glass-high en-

tropy alloy nanolaminates — •Qi Xu[1], Daniel Şopu[1], and Jürgen Eckert[1,2] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Montanuniversity leoben, Leoben, Austria

The uniaxial tensile deformation behavior of metallic glass (MG) - high entropy alloy (HEA) nanolaminates is explored through molecular dynamics simulations. The combination of glassy and crystalline nanolayers results in misfit stresses at the interface that drive the partial crystallization of amorphous phase and the nucleation of short dislocations. Upon loading, the further stress-induced crystallization facilitates the nucleation and growth of dislocations along the interfacial regions and across the HEA plate, which advances the yielding of MG-HEA nanolaminate. The dislocations are absorbed into the amorphous plate via slip transfer across glass-crystalline interface that in turn triggers the activation of homogeneously distributed STZs. The co-deformation mechanism suppresses the formation of critical shear bands and increases the resistance to dislocation motion that, consequently, promotes enhanced ductility in MG-HEA nanolaminate. The strength combination of HEA and MGs and the complex deformation behavior may overcome the typical strength-ductility trade-off and make MG-HEA laminates promising candidates for a variety of structural and functional applications.

MM 30.8 Thu 12:15 H46

Tracer diffusion of Fe and Zr in CuZr nanoglasses — •Christian Aaron Rigoni[1], Hendrik Voigt[1], Evgeniy Boltynjuk[2], Bonnie Tyler[3], Sergiy Divinski[1], Horst Hahn[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — [3]Physikalisches Institut, University of Münster, Germany

Metallic nanoglasses consist of nanometer-sized amorphous regions separated by amorphous interfaces. According to the current knowledge, the amorphous structure of these interfaces is different from that of the amorphous grains. This rather new class of material shows a different behaviour in comparison to conventional homogenous metallic glasses, e.g. a reduced density, a reduced number of nearest neighbor atoms, a different electronic structure, an increase in the ferromagnetic transition temperature and an increased thermal stability were reported. In the present work, tracer diffusion in CuZr nanoglasses and their homogenous amorphous counterparts is measured. For the investigation, a radiotracer technique via ion beam sputtering (89Zr and 55Fe radioisotopes) is applied as well as SIMS profiling using stable isotopes. The tracer diffusion measurements are demonstrated to represent a specific and sensitive probe of the structure modifications, and the results are compared to the observations made by TEM and APT.

MM 30.9 Thu 12:30 H46

Anomalous Liquids on a New Landscape: from Water to Phase-Change Materials — •Shuai Wei — Aarhus University, Aarhus, Denmark

A liquid that is cooled below its melting temperature, referred to as a supercooled liquid, can solidify into an amorphous rigid state (i.e., glass), if cooling is fast enough and crystallization is avoided. The phenomenology of supercooled liquids has been in general established. However, there are pronounced exceptions (e.g., water) which do not fall into the class of "normal" liquids but exhibit a transition behavior in their liquid states. The latest advances connect the unusual aspect of liquids to the properties of Phase-Change Materials (PCMs) that are the basis for non-volatile memory and neuromorphic technologies. Here we demonstrate that the "water-like" liquid anomalies exist in many alloys based on group-IV, V, VI elements including technologically important PCMs. Heat capacity, density, and thermal expansivity maxima were observed in the (supercooled) liquid states of those alloys. Structural changes were monitored using in-situ X-ray scattering and femtosecond X-ray diffractions. Dynamic properties were characterized by quasi-elastic neutrons scattering. Their anomalous behaviors can be rationalized in terms of liquid-liquid (metal-semiconductor, and fragile-strong) transitions. These transition behaviors have important implications for understanding the unusual phase switching behaviors in PCMs, in which amorphous phase can crystallize rapidly within tens of nanoseconds at an elevated temperature, while it retains excellent amorphous stability for 10 years at room temperature.

MM 30.10 Thu 12:45 H46

Thermophysical study of anomalies and transitions in liquid Bi-Ga and Ga-In systems — •Yuri Kirshon[1], Shir Ben-Shalom[1], Moran Emuna[2], Yaron Greenberg[2], Eyal Yahel[2], and Guy Makov[1] — [1]Department of Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel — [2]Physics Department, Nuclear Research Centre-Negev, Beer-Sheva 84190, Israel

Interest in the properties and applications of liquid metals has been reignited and leading to innovative new pathways. Work on low-melting alloys provided new products such as Galinstan liquid metal thermometers, self-healing electronic devices and cooling systems for high-temperature reactors. However, due to the experimental challenges, study of thermophysical properties of liquid binary systems remains limited. In particular, Bi-Ga and Ga-In alloys have attracted scientific interest due to possible changes in their liquid structure, reported recently [Q.Yu (2017), Z.Wang (2017), Y.Kirshon (2019)]. In the present contribution, we report on thermophysical measurements conducted on Bi-Ga and Ga-In alloys. Custom table-top resistivity and differential thermal analysis (DTA) setups are presented, including a demonstration of their capability to capture subtle transitions in the melts. We observed evidence of liquid-liquid crossover in the liquid Ga-In, measured both systems at a temperature range in good agreement with previous density measurements. In the Bi-Ga system, we probed the liquid-liquid miscibility gap and were able to obtain the latent heat and resistivity change during the liquid de-mixing process. Both results were in good agreement with previous reports.