MM 28: Liquid and Amorphous Metals

Time: Wednesday 10:15–12:45 Location: SCH A 118

MM 28.1 Wed 10:15 SCH A 118

Relation between decoupled α and β relaxation processes and medium-range ordering in $Pd_{40}Ni_{40}P_{20}$ bulk metallic glasses — •Manoel Wilker da Silva Pinto, Mark Stringe, Dražen Radić, Harald Rösner, and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Individual annealing treatments at $0.8T_g$ and $0.9T_g$ on $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass samples were performed in a differential scanning calorimeter to either activate mainly β or both α and β relaxation processes. Prior to and after these measurements the samples were heated into the supercooled liquid in order to establish a comparable reference relaxation state.

The medium-range order of the different stages of the amorphous structures were investigated by fluctuation electron microscopy and compared with that of the as-cast state. The results indicate that first, a defined structural reset was achieved when heating into the supercooled liquid; however, with increased strain due reduction of excess volume. Second, the annealing treatment at $0.8T_g$ increases the volume fraction of medium-range order again with annealing time and third, a depletion of the volume fraction is observed after annealing at $0.9T_g$.

MM 28.2 Wed 10:30 SCH A 118

Analysis of the relaxational behavior of PdNiS — •Maximilian Demming[1], Nico Neuber[2], Martin Peterlechner[1], Ralf Busch[2], and Gerhard Wilde[1] — [1]University of Münster, Münster, Germany — [2]Saarland University, Saarbrücken, Germany

In this work we examine a sulfur-containing bulk metallic glass, PdNiS. The impact of sulfur is investigated with a focus on the thermodynamic behavior and the comparison with the well-known PdNiP bulk metallic glass. Several samples from the same initial state were annealed at a certain temperature below Tg for different annealing times in order to adjust distinct relaxation states. After isothermal annealing in a differential scanning calorimeter (DSC), a calorimetric study was carried out to examine the relaxation behavior. Especially the so-called overshoot during heating the samples through the glass transition was evaluated, since it is one of the most prominent signals which depends on the thermal history of a metallic glass. Additionally, low temperature heat capacity measurements were performed to quantify the so-called boson peak. The boson peak can be related to soft vibrational modes, and thus it is characteristic to the relaxational state of a metallic glass and it is affected by the thermal history of a glass. All methods combined deliver a picture of the relaxational behavior under pre-Tg annealing of this Sulphur-containing metallic glasses.

MM 28.3 Wed 10:45 SCH A 118

Unravelling the origin of the anomalous thermal expansion in Fe-based bulk metallic glasses — •Alexander Firlus[1], Mihai Stoica[1], Gavin Vaughan[2], Stefan Michalik[3], Robin E. Schäublin[1], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, ETH Zurich, 8093 Zurich, Switzerland — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [3]Diamond Light Source Ltd., Didcot, UK

Fe-based bulk metallic glasses (BMGs) are known for their soft-magnetic properties but their magnetic interactions also give rise to an anomalous thermal expansion, called the Invar effect. In the ferromagnetic state, their coefficient of thermal expansion is reduced by a factor of four. This phenomenon has been observed in all ferromagnetic Fe-based BMGs at the macroscopic scale, but due to the lack of long-range order the physics of this effect needs to be described at the atomic scale. Although it is now widely accepted to be of magnetic origin, the contributions of the different atomic species to the Invar effect have been unknown. We studied the atomic-scale thermal expansion of multiple quaternary BMGs by in situ X-ray diffraction. The anomalous thermal expansion is visible in all diffraction patterns and can clearly be associated with the disordered Fe network. Through variations of the minor alloying elements, we elucidated the effect of different atomic species and provide a framework in which their respective influence on the Invar effect can be understood.

MM 28.4 Wed 11:00 SCH A 118

Rejuvenation engineering in metallic glasses by complementary stress and structure modulation — •Daniel Şopu[1,2], Florian Spieckermann[3], Simon Fellner[1], Christoph Gammer[1], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria — [2]Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany — [3]Department of Materials Science, Chair of Material Physics, Montanuniversität Leoben, Austria

Residual stress engineering is very widely used in the design of new advanced lightweight materials. For metallic glasses the attention has been on structural changes and rejuvenation processes. Here, based on high energy scanning X-ray diffraction strain mapping, transmission electron microscopy (TEM) and microindentation we distinguish between structural and elastic fluctuations, the two key factors for the observed extreme rejuvenation in triaxial compression. TEM characterization shows that structural rejuvenation under room temperature deformation relates to shear-induced softening and dilatation (large volumetric strain). High energy scanning X-ray diffraction strain mapping reveals large elastic fluctuations in metallic glasses after deformation under triaxial compression. Microindentation hardness mapping hints to a competing hardening-softening mechanism after compression and further reveals the complementary effects of stress and structure modulation. Molecular dynamics simulations provide an atomistic understanding of the complex shear band activity in notched metallic glasses and the related fluctuations in the strain/stress heterogeneity.

MM 28.5 Wed 11:15 SCH A 118

Enhancing mechanical properties by introducing surface grooves in metallic glasses — •Xudong Yuan[1], Daniel Şopu[1,2], Kaikai Song[3], and Jürgen Eckert[1,4] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, Leoben A-8700, Austria — [2]Institut für Materialwissenschaft, Fachgebiet Materialmodellierung, Technische Universität Darmstadt, Otto-Berndt-Str.3, Darmstadt D-64287, Germany — [3]School of Mechanical, Electrical and Information Engineering, Shandong University (Weihai), Weihai 264209, China — [4]Department of Materials Science, Chair of Materials Physics, Montanuniversität Leoben, Jahnstraße 12, Leoben A-8700, Austria

The correlation between the mechanical properties and surface defects in metallic glasses (MGs) is investigated by surface ultrasonic bonding experiments and molecular dynamics simulations. The strength together with the compression ductility of Zr65Cu15Ni10Al10 MG can be enhanced by introducing surface grooves. Induced grooves and pre-shear bands (SBs) lead to the formation and interaction of multiple SBs during compression, which consequently enhances ductility. Additionally, the thermal-induced nanocrystallization, together with generated free volume and residual stresses around the grooves contribute to the emergence of hierarchical structure and stress heterogeneity, which delays the propagation of dominant SB and enables the improvement of strength and plasticity of MG.

15 min. break

MM 28.6 Wed 11:45 SCH A 118

Atomic transport in heavy ion irradiated amorphous PdNiP near the glass transition temperature — •Saba Khademorezaian[1], Marilena Tomut[1,2], Maximillian Demming[1], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]2GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany

The influence of ion irradiation on Ag diffusion in Pd40Ni40P20 bulk metallic glass was investigated by the tracer diffusion technique at temperatures below the glass transition. Bulk samples of Pd40Ni40P20 relaxed states were irradiated with 4.8 MeV/u Au, U, and Ca ions at the UNILAC accelerator at GSI Darmstadt. The achieved fluences were in the range of 5e10 to 1e13 ions/cm2. The diffusion rates of 110mAg isotopes after irradiation with heavy ions, Au and U, were found to be monotonously increasing with increasing total fluence. For the light ions, Ca, the diffusion enhancement shows an unexpected non-monotonous, cross-over behavior. The results are discussed re-

lating the impacts of irradiation with swift heavy ions on structure modifications and the atomic kinetics in a bulk metallic glass.

MM 28.7 Wed 12:00 SCH A 118

Nanostructural investigations on thin film nanoglasses using different TEM techniques — •Hendrik Voigt[1], Evgeniy Boltynjuk[2], Aaron Rigoni[1], Horst Hahn[2], Harald Rösner[1], and Gerhard Wilde[1] — [1]University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Karlsruhe Institute of Technology, Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Nanoglasses as a relatively new family of amorphous alloys present an attempt to tailor the structure of glasses to improve their properties. The concept of nanoglasses is based on the introduction of glass-glass interfaces into the amorphous material, mimicking the effect that defects have in crystalline matter. Different transmission electron microscopy (TEM) techniques were used to investigate the microstructure of Cu60Zr40 columnar thin film nanoglasses. Nanobeam diffraction pattern (NBDP) analysis and energy dispersive X-ray spectroscopy (EDX) were employed to investigate differences in the excess free volume and chemical composition. NBDP acquired over an extended region of interest were used to perform an angular correlation analysis revealing different symmetry motives compared to a compositionally equivalent homogenous glass. Additionally, time-of-flight secondary ion mass spectroscopy (ToF SIMS) measurements discovered an increase in diffusivity in the nanoglasses. All the results shown here provide clear evidence for the existence of glass-glass interfaces with two structurally different phases present in the nanoglass.

MM 28.8 Wed 12:15 SCH A 118

Properties of Sodium Borosilicate Glasses via Dynamics Simulations with Ultra-Fast Machine-Learning Potentials — •Hendrik Krass[1], Benedikt Ziebarth[2], Wolfgang Mannstadt[2], and Matthias Rupp[3] — [1]University of Konstanz, Konstanz, Germany — [2]Schott AG, Mainz, Germany — [3]Luxembourg Institute of Science and Technology (LIST), Belvaux, Luxembourg

Glasses are of scientific interest and have many industrial applications. However, their investigation and development are limited by the duration and costs of experiments. The computational study of glasses can in principle overcome these limits, but current atomistic glass models are either fast but not accurate enough (classical empirical potentials) or accurate but too slow (ab initio potentials). Machine-learning potentials (MLPs) trained on ab initio reference calculations promise to be both fast and accurate enough.

We investigate the suitability of "ultra-fast potentials" (UFPs) [1]—a class of MLPs that are data-efficient, physically interpretable, sufficiently accurate for applications, can be parametrized automatically, and are as fast as the fastest traditional empirical potentials—to study glasses. For this, we compute structure and properties of interest via dynamics simulations with UFPs and compare them against state-of-the-art models and experimental values for sodium borosilicate glasses, a prototypical glass system.

[1] Stephen R. Xie, Matthias Rupp, Richard G. Hennig: Ultra-Fast Interpretable Machine-Learning Potentials, arXiv 2110.00624, 2021.

MM 28.9 Wed 12:30 SCH A 118

An atomic scale inspired phase-field approach to model fracture in amorphous silica — •Gergely Molnar[1], Gaylord Guillonneau[2], Guillaume Kermouche[3], and Etienne Barthel[4] — [1]Univ Lyon, CNRS, INSA Lyon, LaMCoS, UMR5259, 69621 Villeurbanne, France — [2]Univ Lyon, Ecole Centrale de Lyon, CNRS, LTDS, UMR CNRS 5513, 69134 Ecully, France — [3]Mines Saint-Etienne, CNRS, UMR 5307 LGF, Centre SMS, 42023 Saint Etienne, France — [4]ESPCI, CNRS, SIMM, UMR7615, 75231 Paris, France

In the last decade, phase-field models have gained great popularity in fracture simulation. These models regularize the sharp crack using an internal length-scale by diffusing the damage into the material. This work was set out to investigate the competition between homogeneous plastic deformation, shear banding, and brittle failure in amorphous silica. The molecular dynamics inspired finite element model uses the phase-field approach to model fracture, while a pressure-dependent yield criterion accounts for densification and shear plasticity. The talk presents a proof of concept to model plasticity and crack propagation in micrometer size silica samples.