

MM 26: Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids

Time: Thursday 10:15–11:45

Location: H10

MM 26.1 Thu 10:15 H10

Influence of sulfur on the amorphous structure, high temperature viscosity and solidification of Zr-based bulk metallic glass formers — ●BASTIAN ADAM, OLIVER KRUSE, LUCAS MATHIAS RUSCHEL, MAXIMILIAN FREY, NICO NEUBER, and RALF BUSCH — Chair of Metallic materials (LMW), Saarbrücken, Germany

The usage of the element sulfur in Bulk Metallic Glass (BMG) synthesis was recently introduced by Kuball et al. and lead to increased research interest into these new family of BMG [1]. Here we report on the influence of sulfur on the A2B type intermetallic composition (Zr₅₀Ti_{16.6}Ni_{18.3}Cu₁₅) that was characterized by container-less electromagnetic melting under microgravity within the 43rd & 44th TEMPUS parabolic flight campaigns by the German aerospace center (DLR). The investigation is accompanied by structural investigations of the amorphous solid and liquid that were conducted with the help of an electrostatic levitation device to observe the structure and solidification in an in-situ wide-angle scattering diffraction experiment at the German electron synchrotron (DESY) in Hamburg.

[1]A. Kuball, O. Gross, B. Bochtler, and R. Busch, Sulfur-bearing metallic glasses: A new family of bulk glass-forming alloys, *Scr. Mater.*, 2018.

MM 26.2 Thu 10:30 H10

Structure and dynamics of Ni-Nb alloy melts upon sulfur addition — NICOLAI GRUND¹, DIRK HOLLAND-MORITZ¹, SABA KHADEMOREZAIAN², LUCAS P. KREUZER^{1,3}, NICO NEUBER⁴, LUCAS M. RUSCHEL⁴, HENDRIK VOIGT², JOHANNA WILDEN¹, ●FAN YANG¹, SERGIY DIVINSKI², RALF BUSCH⁴, ANDREAS MEYER¹, and GERHARD WILDE² — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany — ²Institute of Materials Physics, University of Münster, Münster, Germany — ³Heinz Maier-Leibnitz-Zentrum, Technische Universität München, Garching, Germany — ⁴Chair of Metallic Materials, Saarland University, Saarbrücken, Germany

We investigated the change in the structure and dynamics of a Ni-Nb bulk metallic glass upon sulfur addition on microscopic and macroscopic scales. With the sulfur concentration of 3 at.%, where the composition Ni₅₈Nb₃₉S₃ exhibits the best glass forming ability in the investigated sulfur concentration range, both the equilibrium and undercooled melt dynamics remain almost unchanged. Only in the glassy state sulfur seems to result in less decoupled mass transport to the viscosity of the undercooled liquid, where the Ag tracer diffusion coefficient is slower in the ternary alloy. With the structural disorder introduced by alloying sulfur, the improved glass forming ability is attributed to geometrical frustration, where crystal nucleation requires a depletion of sulfur and hence long range diffusion, as long as no primary sulfur-containing crystalline phase is involved.

MM 26.3 Thu 10:45 H10

Probing Medium-Range Order in Metallic Glasses with 4D-STEM — ●BIRTE RIECHERS¹ and ROBERT MAASS^{1,2,3} — ¹Federal Institute of Materials Research and Testing (BAM), Germany — ²University of Illinois at Urbana-Champaign, USA — ³Technical University of Munich, Germany

Medium-range order (MRO) in metallic glasses (MGs) plays a crucial role for their applicability, as it significantly affects their mechanical properties. Important details of the MRO were revealed by micro-second long atomistic simulations, that have shed light on the temperature- and time-dependent evolution of MRO, especially in connection to the emergence of a network of specific structural motifs (JALCOM 821, 153209, 2020; *Acta Mater.* 267, 119730, 2024).

While these insights help to understand the effect of MRO evolution, the experimental validation remains challenging. To test these findings, we employ 4-dimensional scanning transmission electron microscopy (4D-STEM) (Ultramicroscopy 232, 113405, 2022) to analyze both the first and second diffraction shells of MGs. By examining the diffraction symmetries at these length scales, we aim to uncover the dominant structural features associated with MRO.

MM 26.4 Thu 11:00 H10

Structural evolution during annealing in a Zr-Cu-Al bulk metallic glass by X-ray absorption spectroscopy — ●ANDREA

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Understanding structural evolution in the time-temperature-transformation diagrams of bulk metallic glasses (BMGs) is crucial to tackle common challenges in glass science such as embrittlement and mechanical failure. Preliminary extended X-ray absorption spectroscopy fine structure (EXAFS) measurements carried out at the Zr and Cu K-edges on a typical Zr-Cu-Al system allowed following the evolution of element-specific bond lengths, static and dynamic disorder, and nearest-neighbor numbers as a function of temperature and time. Data on the as-cast BMG, on further annealed BMG at two different temperatures (0.9T_g and 1.02T_g) and at different holding times was collected (ex-situ) at the BM-08 beamline, ESRF, finally showing two different behaviors depending on the temperature used, which will be described in terms of EXAFS fitting parameters during the presentation.

MM 26.5 Thu 11:15 H10

Thermodynamic, kinetic and structural study of Pt42.5CuxNi36.5-xP21 alloy variations — ●ZIYU LING¹, MARYAM RAHIMI CHEGENI¹, NICO NEUBER¹, SERGEY KASATIKOV², AMIRHOSSEIN GHAVIMI¹, ANDREA FANTIN³, ISABELLA GALLINO⁴, and RALF BUSCH¹ — ¹Lehrstuhl für Metallische Werkstoffe, Universität des Saarlandes — ²Helmholtz-Zentrum Berlin für Materialien und Energie Elektrochemische Energiespeicherung — ³Bundesanstalt für Materialforschung und -prüfung, Berlin — ⁴Lehrstuhl für Metallische Werkstoffe, TU Berlin

The thermodynamic and kinetic properties of Pt_{42.5}Cu_xNi_{36.5-x}P₂₁ glass-forming liquids are studied via differential scanning calorimetry and Flash DSC (Mettler Toledo). The kinetic fragilities of the alloys are determined from relaxation times measured in a broad heating rates range using a T_g shift method and the relaxation time of the deeply undercooled liquids determined via a step-response method. Furthermore, the specific capacity heat (C_p) as a function of temperature for the glassy, liquid and crystalline state of the chosen alloys are determined. The thermodynamic fragility is assessed from the 'C_p jump' at T_g and the driving force for crystallization is calculated using fitting parameters of thermodynamic functions derived from C_p data. Then the glass forming ability of the alloy liquids is evaluated based on their critical cooling rates and TTT-diagrams. The interfacial energy is obtained by JMAK fitting with TTT-diagrams. Moreover, the alloy ribbons were investigated by synchrotron X-ray scattering experiments at DESY for structural study and by XPS and NEXAFS at BESSY for energy state information of each elements.

MM 26.6 Thu 11:30 H10

Temperature dependence of cooperative fluctuations in supercooled glass-forming metallic melts — ●JÜRGEN SCHAWÉ¹, MIN KYUNG KWAK², MIHAI STOICA¹, EUN SOO PARK², and JÖRG LÖFFLER¹ — ¹ETH Zürich, Laboratory of Metal Physics and Technology, Zurich, Switzerland — ²Seoul National University, Department of Materials Science and Engineering, Seoul, Republic of Korea

The behavior of a supercooled glass-forming metal alloy depends on the cooperative atomic fluctuations caused by the dynamic heterogeneities in the melt. These spatial and temporal heterogeneities form dynamic clusters, which are regions of cooperative rearrangement (CRR). The time and temperature dependence of the CRR characterizes the α -relaxation. In this study, the correlation length ξ , characteristic of the CRR, is derived for Pt_{57.4}Cu_{14.7}Ni_{5.3}P_{22.6} and Pd₄₃Cu₂₇Ni₁₀P₂₀ bulk metallic glasses by fast differential scanning calorimetry in a temperature range between the glass transition temperature T_g and T_g + 50K. It appears that while the composition of the alloy influences the macroscopic α -relaxation and vitrification kinetics, typically defined by T_g, as well as the limiting temperature of the Vogel-Fulcher-Tammann-Hesse equation and the fragility index, it has no significant influence on the correlation length of the cooperative atomic motions. In agreement with many other materials, ξ at T_g is about 3 nm for both metallic glasses. The temperature dependence of ξ correlates with the apparent activation energy of the α -relaxation and is the reason for their non-Arrhenius behavior.