MM 18: Liquid and Amorphous Materials II

Time: Tuesday 14:00–15:30 Location: SCH/A315

MM 18.1 Tue 14:00 SCH/A315

Influence of Phosphorus Content on the Symmetry and Correlation Length of the Medium-Range Order in Pd-Ni-P Bulk Metallic Glasses — •Hongshuai Li, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Pd-Ni-P metallic glass is known as an excellent glass former, which enables systematic investigation of how variations in phosphorus (P) content affect its structural characteristics. In this study, we investigate the influence of P concentration on the dominant correlation length and the local symmetries of motifs within Pd-Ni-P metallic glass using fluctuation electron microscopy (FEM) and angular correlation microscopy. In FEM, the relationship between normalized variance and probe size can be used to examine the medium-range order (MRO) in amorphous materials. Our experimental results reveal that, as the composition deviates from the eutectoid composition Pd40Ni40P20, the correlation lengths associated with the dominating motifs undergo significant changes. Moreover, the volume fraction of the medium-range order increases as the P content diverges from the eutectoid composition. Regarding the symmetry analysis, the P content exerts a strong impact on the four-, five-, and six-fold symmetries. Specifically, as the P content moves away from the eutectoid composition, five-fold symmetry becomes prominent relative to the four- and six-fold symmetries.

MM 18.2 Tue 14:15 SCH/A315

Decoupling Structural and Mechanical Behavior in CuZr Metallic Glasses — •Askar Kvaratskheliya[1], Jürgen Eckert[1,2], and Daniel Şopu[1,3] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Technical University of Leoben, Leoben, Austria — [3]Technical University of Darmstadt, Darmstadt, Germany

Although lacking of long range order symmetry, metallic glasses (MG) possess a high degree of short- and medium-range order that governs their macroscopic properties. Particularly, in case of CuZr MG, network of five fold symmetry clusters defines the degree of local order. These motifs resist shear, stabilize energy minima, and inhibit strain localization. In this study, we systematically decouple the contributions of distinct motif perturbations by simulating irradiation-induced structural states through targeted atomic dilution. Specifically, we construct post-irradiation analogs of $Cu_{64}Zr_{36}$ MG by systematically removing atoms according to their local motifs. This approach enables decoupling of the influence of local topology from the overall degree of rejuvenation. We investigated how perturbation of specific motifs alters relaxation, stress distribution, and mechanical strength. Recent advances in high-performance computing have enabled a clear shift toward large-scale, high-throughput molecular dynamics workflows. Leveraging this paradigm, we performed an extensive parameter sweep consisting of hundreds of independent molecular dynamics simulations, systematically varying temperature and structural perturbation protocols.

MM 18.3 Tue 14:30 SCH/A315

Influence of Xe swift heavy ions irradiation on the mechanical properties of PdNiP bulk metallic glasses — •Maren Jeromin[1], Marilena Tomut[1,2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str.10, 48149 Münster — [2]GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt

Pd40Ni40P20 bulk metallic glass samples that had been subjected to different relaxation states were investigated by nanoindentation and laser scanning microscopy (LSM) for irradiation effects induced by swift heavy ions. The samples were irradiated with 630 MeV Xe-ions at the UNILAC accelerator at GSI in Darmstadt. During irradiation, the samples were partially covered with honeycomb- patterned masks to enable direct comparison between irradiated and non-irradiated areas. LSM revealed a distinct swelling step at the mask boundary, whose height increased with ion fluence and varied systematically with the relaxation state of the material. The observed swelling is attributed to ion track formation, where localized melting and rapid re-solidification generates excess volume due to cooling rates exceeding the initial quenching rate. Nanoindentation measurements demonstrated a fluence-dependent decrease in hardness; however, the hardness of irradiated regions consistently remained higher than that of pristine samples. These findings offer new insight into the structure modification of bulk metallic glasses under medium-mass swift ion irradiation, where elastic collision effects increasingly compete with ion track formation governed by electronic energy-loss processes.

MM 18.4 Tue 14:45 SCH/A315

A ReaxFF study of the covalency-driven cracking-to-shearing transition in metal-metalloid glasses — •Shansi Liao[1], Jürgen Eckert[1,2], and Daniel Sopu[1,3] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Technical University of Leoben,Leoben, Austria — [3]Technical University of Darmstadt, Darmstadt, Germany

Revealing the atomistic origins of failure in amorphous solids remains challenging. In metal-metalloid glasses, mechanical response is strongly governed by the breaking and reformation of covalent bonds which cannot be adequately captured by non-reactive interatomic potentials. Here, large-scale reactive molecular dynamics simulations using a ReaxFF potential that includes angular constraints for covalent bonding reveal a composition-dependent transition from cleavage cracking to shear banding in model CuSi glasses. During loading, a highly connected, rigid Si-rich network suppresses strain delocalization, generating mechanically unstable regions characterized by shear-induced reductions in coordination number and severe distortions of Si-Si-Si bond angles. These unstable regions serve as energetically favorable pathways along which the crack advances. As Cu content increases, reduced angular rigidity promotes widespread shear transformation and shear-band-mediated plasticity. In contrast, the modified embedded-atom method potential, which intrinsically overestimates the angular flexibility of the Si-rich networks, fails to reproduce this transition. Our results show that angular rigidity of the interatomic potential is a key descriptor of plasticity in metal-metalloid glasses.

MM 18.5 Tue 15:00 SCH/A315

Macroscopic response of $Pd_{40}Ni_{40}P_{20}$ Bulk Metallic Glasses to GeV ^{238}U Ion irradiation — •Richard von Destinon, Maren Jeromin, Marilena Tomut, and Gerhard Wilde — Institut für Materialphysik, Universität Münster, Münster, Germany

Ion tracks formed by localized heating due to intense electronic excitations of the target atoms offer new pathways to tailor the mechanical properties of bulk metallic glasses. In this work, we investigate the effects of swift heavy ion irradiation on macroscopic behavior such as the hardness, swelling and strain-rate sensitivity on the well-characterized bulk metallic glass $Pd_{40}Ni_{40}P_{20}$. The samples were thermally relaxed at $0.94T_g$ and subsequently irradiated with 1.14 GeV U ions at the UNILAC accelerator at GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt. By using aluminum degraders of different thicknesses, the energy loss of the ions at the sample surface and their corresponding penetration depths were systematically varied. Characterization was carried out using Laser Scanning Microscopy (LSM) as well as nanoindentation with displacement depths up to 0.3 μm. The results show a pronounced increase of swelling as well as a decrease in hardness with increasing irradiation fluences. The strain-rate-sensitivity increases at higher fluences, suggesting that the increased structural heterogeneity within the irradiated metallic glass alters the local stress distribution, affecting the shear band propagation.

MM 18.6 Tue 15:15 SCH/A315

Compositional and Surface Variations in Sasanian Early Islamic Glasses from Gorgan, Ray, and Istakhr — •Farahnaz Bayat Nejad[1], Mohammadamin Emami[2], Rémy Chapoulie[3], and Farzaneh Bayat Nejad[4] — [1]Islamic Azad University, Central Tehran Branch, Tehran, Iran — [2]Art University of Isfahan, Isfahan, Iran — [3]Archéosciences Bordeaux, UMR 6034 CNRS, Université Bordeaux Montaigne, Pessac, France — [4]Islamic Azad University, Central Tehran Branch, Tehran, Iran

This study investigates the compositional and microstructural characteristics of Sasanian*Early Islamic glasses from Gorgan, Ray, and Istakhr. Laser-Induced Breakdown Spectroscopy (LIBS), Scanning Electron Microscopy with Energy-Dispersive X-ray Spectroscopy (SEM-EDX), and Hyperspectral Imaging (HSI) were used to assess elemen-

tal composition, surface morphology, and colorant phases. Distinct variations in Ca/K/Na ratios reflect differences in raw materials and production recipes across the three sites. SEM-EDX reveals heterogeneous corrosion layers and localized devitrification, especially in Istakhr samples with silica-rich alteration crusts. HSI spectra identified absorption features of Fe**, Mn, and Cu** chromophores associated with glass coloration. These results provide insight into technological choices and raw material exchange networks in Late Antique Iran, demonstrating the power of non-destructive, multi-analytical methods in archaeometric glass research.