MM 9: Liquid and Amorphous Metals - Brittle-to-ductile Transition

Time: Monday 11:45–13:00 Location: IFW D

MM 9.1 Mon 11:45 IFW D

Invar effect in Fe-based bulk metallic glasses — •Alexander Firlus, Robin Schäublin, Mihai Stoica, and Jörg F. Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland

Ferromagnetic Fe-based bulk metallic glasses universally show a low coefficient of thermal expansion, which suddenly increases by a factor of ∼3 at the Curie temperature. This effect is known as Invar effect and it is usually seen in crystalline FeNi alloys. While it is clear that this is a magnetically driven effect, the physics behind it is still not understood. Up to now, the only explanations of the Invar effect are based on simulations and calculations that rely on a unit cell, but these have no base in amorphous materials. The strength of the Invar effect is particularly sensitive to the short-range order and Fe coordination. We thus aim to investigate the dynamics from the atomic scale to the macroscale for various alloys in different structural states. We correlate the structural data determined via transmission electron microscopy with studies on the magnetics to get a complete picture of the underlying mechanics of the Invar effect in Fe-based magnetic glasses.

MM 9.2 Mon 12:00 IFW D

How does a Cu-Zr-Al glass/crystal composite form in real time? — •Jiri Orava[1], Ivan Kaban[1], Xiaoliang Han[1], Olga Shuleshova[1], Ivan Soldatov[2], Olof Gutowski[3], Ann-Christin Dippel[3], Martin v. Zimmermann[3], Shanoob Balachandran[4], Michael Herbig[4], Yurii Ivanov[5], Alan L. Greer[5], and Dierk Raabe[4] — [1]IFW Dresden, Germany — [2]IFW Dresden, Germany — [3]DESY, Hamburg, Germany — [4]MPIE, Düsseldorf, Germany — [5]Department of Materials Science and Metallurgy, University of Cambridge, UK

Metallic glasses (MGs) have poor ductility, and due to the lack of atomic periodicity and microstructure, MGs mechanical properties cannot be controlled the same way as in crystalline materials. One approach to enhance ductility of MGs lies in introducing ductile nanometre-to-micrometre-size crystalline phases into a glass. This method has proven to be an effective way to improve the mechanical properties of such composites, particularly their plastic formability. We present a real time in-situ high-energy x-ray diffraction study of phases evolution during a controlled rapid-heating treatment, imposed at a rate ranging from ˜100-1000 K/s, and subsequent cooling of a Cu-Zr-Al metallic glass. We combine the synchrotron measurements with in-situ heating in TEM and with atom-probe tomography analysis of the final composite microstructures. The formation of crystalline phases beneficial to the ductility are clearly resolved and conditions under which these phases develop are formulated. We thank the DFG, contracts Ka-3209/9-1 and HE 7225/1-1, for funding.

MM 9.3 Mon 12:15 IFW D

Boron concentration induced Co-Ta-B composite formation observed in the transition from metallic to covalent glasses — •Simon Evertz[1], Stephan Prünte[1], Lena Patterer[1], Marshal Amalraj[1], Damian M. Holzapfel[1], Alexander Schökel[2], Marcus Hans[1], Daniel Primetzhofer[3], and Jochen M. Schneider[1] — [1]Materials Chemistry, RWTH Aachen University, Aachen, Germany — [2]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [3]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Due to their unique property combination of high strength and toughness, metallic glasses are promising materials for structural applications. As the behaviour of metallic glasses depends on the electronic structure which in turn is defined by chemical composition, we investigate systematically the influence of B content on glass transition, topology, magnetism and bonding for B contents between 2 and 92 at% in the $(Co_{6.8}Ta_1)_{1-x}B_x$ system. From an electronic structure and coordination point of view the B concentration range is divided into three regions: Below $38 \pm 5at\%$ B, the material is a metallic glass due to the dominance of metallic bonds. Above $67 \pm 5at\%$ the presence of an icosahdra-like B-network is observed. As the B concentration is increased above $38 \pm 5at\%$, the B-network evolves while the metallic coordination of the material decreases until the B concentration of $67 \pm 5at\%$ is reached. Hence, a composite is formed. It is evident that based on the B concentration the ratio of metallic bonding to icosahedral bonding in the composite can be controlled.

MM 9.4 Mon 12:30 IFW D

Cooling rate, temperature and applied strain rate effects on the brittle-to-ductile transition in metallic glasses — •Xudong Yuan[1], Daniel Şopu[1,3], and Jürgen Eckert[1,2] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Montanuniversität Leoben, Leoben, Austria — [3]Technische Universität Darmstadt, Darmstadt, Germany

The effects of cooling rate, temperature and applied strain rate on the tensile deformation behavior of Cu64Zr36 metallic glass (MG) are investigated using large-scale molecular dynamics simulations. An increase in quenching rate during sample preparation, as well as an increase of temperature or applied strain rate, affects the shear band nucleation and propagation processes and causes a brittle-to-ductile transition. High quenching rates lead to a low density of closed packed Cu-centered full icosahedra and by sampling of the saddle points on the potential energy surface we found lower barrier energy for local atomic rearrangement as compared to those MGs obtained at low quenching rates. High temperatures will increase the kinetic energy of the atoms, which leaves the atoms to easily rearrange and increases the probability of thermal activation of shear transformation zones. Finally, during deformation at high strain rates, the stored elastic energy has not enough time to redistribute through local elastic distortions along the maximum shear stress direction and, consequentially, the MGs deform homogeneously.

MM 9.5 Mon 12:45 IFW D

Temperature and chemical bonding effects on the brittle-to-ductile transition in metal-metalloid glasses — Franco Moitzi[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 relationship between the deformation behavior of metal-metalloid glasses and their intrinsic properties is studied using large-scale molecular dynamics simulations with hybrid interatomic potentials. Particularly, the influence of composition and temperature on the tensile deformation behavior of amorphous PdSi alloys is investigated. A transition from cracking perpendicular to the loading direction to shear banding can be achieved by increasing the temperature or decreasing the amount of silicon. A decrease in silicon content leads to fewer covalent bonds and, therefore, lower activation barriers for shear transformation zones and, consecutively, a high probability for shear band formation. On the other hand, at low temperatures these barrier cannot be overcome and cracking will dominate over shear banding. In this case, high activation barriers for local relaxation impedes stress redistribution into the glassy structure and, finally, cracking occurs. Additionally, the cracking path also depends on the degree of homogeneity. A corrugated fracture surface similar to experiment can be formed due to crack defection and cavitation ahead of the crack tip in chemically inhomogeneous samples. In contrast, a sharp cleavage-like fracture occurs for more homogeneous samples.