MM 20: Topical Session: Thermophysical Properties of Bulk Metallic Glasses and Bulk Metallic Glass-forming Liquids

Time: Wednesday 15:45–18:30 Location: H10

Topical Talk MM 20.1 Wed 15:45 H10

Magnetic properties of Fe-based amorphous alloys produced by melt-spinning and selective laser melting — •Paola Tiberto — INRIM, Torino, Italy

Amorphous soft-magnetic materials play an important role as core constituents in improving the energy transformation efficiency of electrical machines and passive electrical components. Although the melt-spinning process remains the main technique for obtaining amorphous soft-magnetic ribbons with remarkable soft magnetic properties, new and efficient production methods based on additive manufacturing have been developed in recent years, enabling the direct synthesis of larger elements. Ribbons were obtained by a conventional melt-spinning process while 3D-printed samples were produced by additive manufacturing via Selective Laser Melting (SLM) using powder of the same alloy as a precursor. In this study, we investigate the hysteresis properties of amorphous Fe-Si-B-based alloys in ribbon shape and 3D-printed bulk samples produced by different casting techniques. The SLM processing conditions have been observed to play a crucial role in the microstructure of the printed parts and, therefore, in their magnetic properties, due to their dependence on morphology. The effect of different printing parameters on magnetic properties, such as laser power and scan speed, has been studied. This study highlights the critical link between microstructure engineering through manufacturing techniques and the resulting magnetic performance, offering insights into optimizing both for enhanced energy efficiency in magneto-electrical applications.

MM 20.2 Wed 16:15 H10

Advancements in Developing Fe-Based Metallic Glasses for Additive Manufacturing of Soft Magnetic Components — •Amirhossein Ghavimi[1], Maryam Rahimi Chegeni[1], Purbasha Sharangi[2], Uma Rajput[2], Gabriele Barrera[2], Enzo Ferrara[2], Paola Tiberto[2], Isabella Gallino[3], and Ralf Busch[1] — [1]Saarland University, Chair of Metallic Materials, Campus C6.3, 66123 Saarbrücken, Germany — [2]INRIM, Strade delle Cacce 91, Torino, Italy — [3]Department of Materials Science and Engineering, Metallic Materials, TU-Berlin, Ernst-Reuter-Platz 1, 10587 Berlin, Germany

This research aims to create suitable Fe-based soft-magnetic amorphous alloys for the 3D printing of motor components. Since a fully amorphous structure of the 3D-printed parts is expected to improve motor efficiency, i.e. increase magnetic softness and decrease energy losses, the glass-forming ability (GFA) is enhanced through the judicious change of the alloy chemical composition while maintaining competitive soft magnetic properties. The GFA of the compositions was studied by evaluating the critical casting thickness (dc) of the samples. Subsequently, XRD, DSC and DTA were used to characterize the structure and thermal behavior of the samples. The magnetic properties were determined by means of VSM in addition to the evaluation of losses. The eutectic zone of the Fe-Si-B system was experimentally determined. Evaluation of quaternary and quinary component alloys involved studying the effects of promising elements such as phosphorous and nickel on GFA and magnetic properties.

MM 20.3 Wed 16:30 H10

Ni-Nb-(Ta)-P-Based Bulk Metallic Glasses: The Origin of Glass Formation Based on Thermodynamics, Kinetics, Structure and Crystallization Behavior — •Lucas M. Ruschel and Ralf Busch — Chair of Metallic Materials, Saarland University, 66123, Saarbrücken, Germany

Ni-Nb-based bulk glass-forming alloys are among the most promising amorphous metals for industrial applications due to their incomparable combination of strength, hardness, elasticity and plasticity. A successful approach in alloy development is so-called minor alloying, where metallic glasses with improved properties and enhanced GFA are produced, if the proper minor alloying element is chosen for the respective base alloy. Here, minor additions of P to the binary Ni-Nb system increase the GFA up to a record value of 5 mm, which surpasses the binary $Ni_{62}Nb_{38}$ alloy by 150 %. The partial substitution of Nb by Ta further boosts the GFA up to 6 mm. To elucidate the origins of the significant improvement in GFA, key properties such as the thermodynamics and kinetics of the system are studied, including the driving force for crystallization and the kinetic slowdown of viscosity during the transition from the equilibrium liquid to the glassy state. The primary precipitating phase, critical for glass formation, is identified by high-energy synchrotron X-ray diffraction (HEXRD) under containerless electrostatic levitation conditions. Complementary low-temperature HEXRD experiments reveal the structural evolution across a wide temperature range, offering a comprehensive understanding of the mechanisms responsible for the enhanced GFA.

MM 20.4 Wed 16:45 H10

Mechanical Behavior of Phase-Separated Zr-Al-Fe-Y Metallic Glasses for Prospective Implant Applications — •Devinder Singh[1,2], Parthiban Ramasamy[1], Anna Sophie Jelinek[3], Christoph Gammer[1], Zaoli Zhang[1], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, 8700, Leoben, Austria — [2]Amity School of Applied Sciences, Amity University Uttar Pradesh, Lucknow 226028, India — [3]Department of Materials Science, Montanuniversität Leoben, Jahnstraße 12, 8700, Leoben, Austria

Phase separation arises from the substitution of Y in Zr70-xAl12.5Fe17.5Yx (x=0-25 at.%) metallic glasses (MGs), resulting in the formation of nano-amorphous domains within a glassy matrix. The glasses with $x > 10$ show a typical liquid phase separation-induced two-glassy phase (Zr-rich and Y-rich) morphology with droplet-like microstructures. Atom probe tomography (APT) analysis confirms the formation of nanometer-sized Y-enriched clusters for x=15 and 20. The micro-hardness and nano-hardness are found to be in the range of 4.58-5.73 GPa and 5.22-6.11 GPa. The Zr-based MGs exhibit Young's moduli in the range of 81-91 GPa, which are lower than that of Co-Cr-Mo, 316L SS and Ti-6Al-4V commercial implant alloys. Evaluation of the cytocompatibility of the MG ribbons reveals high metabolic activity and well-spread human gingival fibroblast (HGF) cells on the surface of x=10 and 15 samples. Thus, the two glassy-phase Zr-based MGs free of toxic elements (Ni and Cu) exhibit suitable mechanical properties and biocompatibility for implant applications.

15 min. break

Topical Talk MM 20.5 Wed 17:15 H10

Diffusion and nucleation in Al-Ni melts using machine-learned MD simulations — Johannes Sandberg[1,2,3], Leon F. Granz[2,3], and •Thomas Voigtmann[2,3] — [1]Universitë Grenoble-Alpes, Grenoble, France — [2]Heinrich-Heine-Universität, Düsseldorf, Germany — [3]Deutsches Zentrum für Luft- und Raumfahrt, Köln, Germany

The microstructure that forms during solidification of metallic melts greatly influences the material properties. It depends crucially on the microscopic transport properties, and the initial phase selection in the cricial nucleus. Simulation of these phenomena faces two contradictory demands: while the relevant length and time scales match well that of classical molecular dynamics simulations, the sensitive dependence on details of the interatomic interactions is only captured in much smaller-scale quantum-mechanical simulations. In recent years, machine-learned interaction potentials have helped to reconcilce these requirements, allowing MD simulations to be performed with almost DFT-like accuracy.

I will present results that we have obtained using high-dimensional neural network potentials (HDNNP) to the case of Al-Ni melts and nucleation processes therein. Crucially, we assess the performance of the HDNNP by comparing to structural and dynamical experimental data of the liquids at different compositions. This reveals also how the level of DFT closure chosen in the quantum-mechanical simulations used to train the network influences the prediction of thermophysical quantities.

MM 20.6 Wed 17:45 H10

Study of solidification behaviour of undercooled Zr-Ni-Cu melts — •Chu Yu[1,4], Fan Yang[2], Dirk Holland-Moritz[2], Yindong Fang[1,4], Ivan Kaban[3], Stephanie Lippmann[4], and Peter K. Galenko[1] — [1]Otto Schott Institute of Material Research, Friedrich Schiller University Jena, Jena, Germany — [2]Institut für Material-

physik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Cologne, Germany — [3]Leibniz IFW Dresden, Institute for Complex Materials, Dresden, Germany — [4]Institute of Applied Physics, Friedrich Schiller University Jena, Jena

We investigate the solidification behaviour of the glass-forming $Zr_{50}Cu_{35}Ni_{15}$ alloy employing different levitation techniques. The primary phase solidified from the undercooled melt has been found to be independent of the degree of undercooling up to a level beyond the hypercooling limit, as observed by time-resolved X-ray diffraction. The crystal growth velocity has been measured employing electromagnetic levitation (EML), where solidification occurs under stronger fluid-flow conditions compared to previous studies employing electrostatic levitation (ESL). In both cases the observed growth velocity increases with increasing undercooling, before reaching a plateau at undercoolings between 260-320 K. However, at small undercooling the growth velocities measured with EML are slightly higher than that in ESL. The solidification kinetics is discussed in terms of different crystal growth models, taking into account the effect of fluid flow. The works is supported by DFG, DLR, ESA via MULTIPHAS-project Nr. 50WM1941, and ProChance-exchange Program of the FSU Jena.

Topical Talk MM 20.7 Wed 18:00 H10

The effect of composition on the thermodynamics, structure, mechanical properties and atomic motion of (Pd-Pt)42.5Cu27Ni9.5P21 alloys — •Ralf Busch — Saarland University, Saarbrücken, Germany

According to basic hard sphere models Pt should replace Pd in the Pd42.5Cu27Ni9.5P21 alloy. But Pt42.5Cu27Ni9.5P21 shows significant structural differences compared to the Pd based alloy. To study the differences, we prepared a series of (Pd-Pt)42.5Cu27Ni9.5P21 alloys replacing Pd with Pt. We assess the thermodynamic functions revealing that the driving force for crystallization increases with the increase of the Pt content, which is in line with the decreasing critical casting thickness. The Pt-richer alloys are thermodynamically more fragile than the Pd-rich alloys, which is revealed by a larger specific heat capacity and a faster drop of the configurational entropy in the Pt-richer alloys. High energy XRD (HEXRD) studies reveal that the structure of the Pt rich alloys is dominated by its change in medium range order whereas the Pd-rich alloy is dominated by extraordinary short range order. The mechanical properties change drastically from a ductile behavior on the Pt-rich side to an embrittlement with increasing Pd content and decreasing Pt concentration. Nano-indentation investigations together with the HEXRD studies reveal that the embrittlement with increasing Pd-content can be connected to the structural changes. We used XPCS to study the atomic dynamics of the alloys as a function of temperature and wave vector.