MM 55: Liquid and Amorphous Materials II

Time: Thursday 10:15–11:45 Location: C 230

MM 55.1 Thu 10:15 C 230

Between amorphous and crystalline silicon: a revised paracrystalline model — •Louise A. M. Rosset and Volker L. Deringer — Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, Oxford, UK

The existence of paracrystalline silicon, characterized as a crystallite embedded in an amorphous matrix, has long been a topic of debate; the argument derives from hand crafted models and a limited exploration of configurational space, restricted by slow, inaccessible quench rates.

Using a computationally efficient machine-learning potential that unlocks slow quench rates comparable to experiment, we systematically sample the space of a-Si structures by simulated melt-quenching and build a large dataset of disordered silicon configurations. This extensive database points toward the existence of 'paracrystalline' disordered structures, characterized by localized diamond-like neighborhoods that affect medium-range properties. These configurations vary widely in structure and energy, and demonstrate better agreement with experimental results than previously proposed models.

This work highlights the use of data driven methods in elucidating fundamental structural questions using systematic sampling of the configurational space.

MM 55.2 Thu 10:30 C 230

Phase Separation in Ce-Al (Ga) Metallic Glasses — •Devinder Singh[1,2] 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, 226028 Lucknow, India — [3]Department of Materials Science, Montanuniversität Leoben, Jahnstraße 12, 8700, Leoben, Austria

In recent years, much attention has been given to phase separated metallic glasses (MGs) which provide a unique opportunity for designing alloys/ composites with hierarchical microstructure at different length scales. The structure and physical properties of phase separated MGs have characteristics different from those of other MGs. Many theoretical efforts have been undertaken to understand the origin of phase separation; yet the understanding of the mechanism is insufficient.

In this presentation, results of our recent studies on the role of Ga substitution in place of Al in Ce-Al (Ga) MGs will be discussed with the aim to understand the genesis of phase separation. The rationale of phase separation could not be explained in terms of enthalpy of mixing of the three possible binaries in this system. The X-ray absorption spectroscopy (XAS) spectra of Ce-based melt-spun ribbons have shown appearance of 4f0 delocalized states in Ga substituted alloys. Such a substitution has led to shortening of Ce-Ce distance in the alloys owing to chemical pressure leading to creation of two types of distinct major clusters. This work, therefore, opens up new direction of research for delineating issues pertaining to phase separation in amorphous systems.

MM 55.3 Thu 10:45 C 230

Correlations between the p content and medium-range order of bulk pd-ni-p metallic glasses — •Hongshuai Li[1], Martin Peterlechner[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Laboratory for Electron Microscopy, Karlsruhe Institute for Technology (KIT), Engesserstr. 7, 76131 Karlsruhe, Germany

So far, the understanding of a composition dependence of medium-range order (MRO) in metallic glasses is incomplete. Thus, structure-property correlations for glasses or the structural origin of often helpful *minor alloying* strategies remain unknown. In this study, we systematically investigated three as-cast ductile bulk Pd-Ni-P metallic glass samples, where the P content was deliberately varied from 17 to 21 at%. The medium-range order of these samples was characterized using variable-resolution fluctuation electron microscopy. Sampling with different parallel coherent probe sizes, so-called variable resolution FEM (VR-FEM), was performed. From the obtained normalized variance values of the experimental data the dominant MRO correlation lengths are determined. The results are discussed with respect to the compositional dependence of MRO in a given alloy system, i.e. without changes incurred by introducing additional chemical complexity.

MM 55.4 Thu 11:00 C 230

Atomic-scale model of the Invar effect in metallic glasses — •Alexander Firlus[1], Mihai Stoica[1], Pál Jóvári[2], Michalis Charilaou[3], Robin E. Schäublin[1], and Jörg F. Löffler[1] — [1]ETH Zurich, Switzerland — [2]Wigner Research Centre for Physics, Hungary — [3]University of Louisiana at Lafayette, USA

The disordered atomic arrangement of metallic glasses (MGs) provides them with a variety of unique properties such as high hardness, high strength and high elastic limit, and excellent soft-magnetic properties for Fe-based MGs. For all these properties, a microscopic explanation has already been provided, based on the disordered atomic arrangement of MGs. However, Fe-based MGs also universally exhibit the Invar effect, which reduces the coefficient of thermal expansion (CTE) in the ferromagnetic state to almost zero. Despite its universality, there has been no explanation on how the disordered atomic arrangement gives rise to the Invar effect.

We studied the atomic arrangement of quaternary MGs by in situ X-ray diffraction and absorption techniques over all length scales from the atomic to the macroscopic. Based on the experimental data we performed Reverse Monte Carlo modeling to obtain a series of 3D model structures to reveal how the magnetic interactions stabilize the atomic arrangement and lead to a reduced CTE. We find that all Fe atoms contribute to the Invar effect with their magnetic interactions, and that the structural disorder enables a local optimization of the potential energy landscape, which explains the universal occurrence of the Invar effect.

MM 55.5 Thu 11:15 C 230

Introduction of sulfur into the (Zr3Ti)(NiCu) system - characterization of a new group of Zr-based BMG containing sulfur — •Bastian Adam, Oliver Kruse, Lucas M. Ruschel, Maximillian Frey, Nico Neuber, and Ralf Busch — Lehrstuhl für metallische Werkstoffe, Saarbrücken,Deutschland

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 (Zr50Ti16.6Ni18.3Cu15) that was characterized by synchrotron diffraction of copper mold cast specimen to determine crystalline phases around the induced primary crystallization change. The addition enables the bulk glass forming ability (GFA) of up to 6 mm 2 at % to 3 at% sulfur. The devitrification behavior and the melting behavior was also studied by heating and melting of the samples in an in-situ synchrotron wide angle scattering experiment (WAXS) experiment utilizing a LINKAM THMS 600 furnace and a high temperature LINKAM TS1500 furnace. For the best glass former of the system the mechanical properties were investigated in terms of three-point beam bending determining the offset yield strength and breaking elongation of the alloy. [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 55.6 Thu 11:30 C 230

Interplay of capillary pressure and Bangham effect during imbibition in nanopores — •Juan Sanchez[1,2], Lars Dammann[1,2], Zhuoquing Li[1,2], Laura Gallardo[1,2], Robert Meissner[1], Howard Stone[3], and Patrick Huber[1,2] — [1]Hamburg University of Technology (TUHH) — [2]Deutsches Elektronen-Synchrotron (DESY) — [3]Princeton University

We conducted water imbibition experiments in mesoporous silica glass (Vycor) using optical imaging and high-resolution dilatometry. The interplay between surface stress release (Bangham effect) and tensile Laplace pressures on the nanopore walls led to two distinct deformation regimes. Capillary filling followed the Lucas-Washburn law, exhibiting continuous expansion of the mesoporous matrix with square-root-of-the-time dynamics. Complete pore filling resulted in the sudden matrix expansion due to the disappearance of Laplace pressure. This behavior was quantitatively described by a continuum mechanical model, considering the interplay of Bangham and Laplace pressure effects in a 3D network of cylindrical pores.

We further explored the Laplace pressure contribution by conducting imbibition experiments on unsealed porous monoliths under low humidity. In this scenario, both inward (imbibition) and outward (evaporation) flows occurred simultaneously. As the in- and out-flow rates balanced, a dynamic equilibrium (artificial tree configuration) with highly curved menisci at the liquid-gas interface was observed. As a result, there is no observable disappearance of the Laplace pressure during the dilatometry experiments.