MM 5: Liquid and Amorphous Metals - Kinetics and Modelling

Time: Monday 10:15–11:30 Location: IFW D

MM 5.1 Mon 10:15 IFW D

Nucleation rates of crystallization of a bulk metallic glass-former — •Mark Stringe, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, 48149 Münster, Germany

Crystallization plays a crucial role not only regarding the production of metallic glasses via melt quenching, but also concerning the stability of the resulting metastable systems. High scanning rates in calorimetric measurements are realized using a custom-built fast differential scanning calorimeter. With this fast scanning calorimetry (FSC), samples with a mass of the order of micrograms are measured with scanning rates up to the order of 10.000 K/s. This vast range of scanning rates enables an analysis of crystallization for different levels of undercooling. An AuCuAgSi bulk metallic glass with low melting point is analyzed. In FSC it is possible to reach cooling rates to quench a glass in-situ. Hence, the critical cooling rate can be determined directly. Thus, using FSC it is possible to obtain large datasets of measurement cycles. Statistical variations of the undercooling of the glass-forming alloy can be extracted from these datasets. Applying a Poisson process to the stochastic nature of nucleation, the activation barriers for nucleation of the crystalline phase are determined. Low activation barriers indicate a heterogeneous nucleation mechanism for crystallization of the FSC samples.

MM 5.2 Mon 10:30 IFW D

Kinetics of nucleation in undercooled binary and glass forming alloys — •Manoel W. da Silva Pinto, Mirko Gabski, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, WWU Münster, Deutschland

The undercooling and nucleation behavior of alloys was quantitatively analyzed via a statistical analysis that describes nucleation as a non-homogeneous Poisson process. The statistical analysis of calorimetric data, previously applied to pure metals and metalloids, was now applied to binary Cu-Ge alloys, and to two glass-forming systems: Au-Si and Pd-Ni-P. The results enable the discussion on nucleation of binary and ternary mixtures in the framework of a concentration dependency of nucleation rates and glass forming ability. The presented results suggest a change in nucleation behavior already at small concentration variations. Such variations are not considered in the current classical nucleation theory used to describe the kinetics of nuclei formation in binary mixtures or glass forming alloys.

MM 5.3 Mon 10:45 IFW D

Predicting the glass formation behavior of multi-principal element alloys — •Mirko Gabski, Martin Peterlechner, and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster

In contrast to conventional alloys, multi-principal element alloys consist of several constituents in similarly high concentrations. Examples for such alloys range from solid-solution high entropy alloys, like the Cantor alloy $Co_{20}Cr_{20}Fe_{20}Mn_{20}Ni_{20}$, to metallic glasses like $Pd_{40}Ni_{40}P_{20}$ or the commercially used Vitreloy $Zr_{40}Be_{22.5}Ti_{13.8}Cu_{12.5}Ni_{10}$. Both are of interest for research and commercial applications due to their favorable mechanical and chemical properties. Guo et al. showed that there is a correlation between the values of a set of thermodynamic and structural parameters of an alloy and the phases it forms[1]. In the present work this correlation is used to predict the glass formation behavior of multi-principal element alloys by calculating the relevant parameter set. The parameters are evaluated and the deduced critical cooling rate is compared to literature values on well-known glass formers.

[1] Guo, S. and C.T. Liu, Progress in Natural Science: Materials International, 2011. **21**(6): p. 433-446.

MM 5.4 Mon 11:00 IFW D

Micro-second molecular dynamics — structural relaxation and mechanical properties of a model glass system — •Peter Derlet[1] and Robert Maass[2] — [1]Condensed Matter Theory Group, Paul Scherrer Institute, Switzerland — [2]Department of Materials Science and Engineering and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, USA

Using molecular dynamics, we study the structural relaxation of a model binary Lennard-Jones glass over time scales spanning up to several tens of microseconds. These well-relaxed samples are then deformed to study the elastic and collective plastic shear activity under simple shear for a range of strain rates spanning six orders of magnitude. It is found that at the longer time-scales of deformation, significant thermally activated mobility and relaxation occurs in both the elastic and plastic deformation regimes. These results are discussed in terms of both the known elastic robustness of bulk metallic glasses, and the correlation between local structure and local plasticity.

MM 5.5 Mon 11:15 IFW D

Ultrafast melting of antimony after fs laser excitation: experiment meets fully ab-initio simulations — •Bernd Bauerhenne[1], Sascha Epp[2], Felipe Valencia[3], and Dwayne R. J. Miller[2] — [1]Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — [2]Max-Planck-Institut für Struktur und Dynamik der Materie, Luruper Chaussee 149, Geb. 99, 22761 Hamburg, Germany — [3]National University of Colombia, Cra 45, Bogota, Columbia

The time-resolved Bragg peak decay of a fs-laser pulse excited 30 nm thick antimony film was measured using x-ray pulses generated from a free electron laser. To predict this measured Bragg peak decay, we derived an electronic temperature (Te) dependent interatomic potential for antimony. For this, we fitted forces and energies obtained from ab-initio MD simulations of a thin antimony film at increased Te. Furthermore, we calculated the optical properities and the Te-depend electron-phonon coupling constant for antimony ab-initio. Utilizing the Te-dependent interatomic potential, the derived optical properites and the electron-phonon coupling constant, we performed MD simulations of a laser-excited 30 nm thick antimony film containing 9072 atoms. The calculated time-dependence of the Bragg-peaks shows very dood agreement with the experiment. Antimony melts within 600 fs for the highest considered laser intensity.