MM 9: Topical session: Dynamics, relaxation and deformation in deeply supercooled metallic liquids and glasses II - Undercooled Melts

Time: Monday 11:45–13:15 Location: IFW A

MM 9.1 Mon 11:45 IFW A

Short range order in liquid metals — Guy Makov[1] and •Eyal Yahel[2] — [1]Materials Dept, Ben-Gurion University of the Negev, Beer Sheva, Israel — [2]Physics Dept, NRCN, Beer Sheva, Israel

Evolution of short range structure in liquid metals as a function of temperature in the regime from supercooled to high temperature melt is studied within the quasi-crystalline model of liquid structure. Experimental data on elements of groups IV and V, many of which exhibit anomalous thermophysical properties are compared with molecular dynamics generated data on model systems.

The quasi-crystalline model allows quantitative characterization of the short range order in liquids by identifying a reference structure. It is found that the liquid pnictides are characterized by a short range order which reflects a Peierls distorted structure. This distortion decreases as the elements progress down the periodic table column V and explains the large change in coordination number from 3 to 8. Surprisingly the distortion is found to increase with temperature and correlates with the appearance of a sound velocity maximum with respect to temperature. Column IV elements exhibit a very different short range order which is found to remain constant with temperature, possibly indicating that the origin of the sound velocity anomaly in these systems is not related to any structural rearrangement of the liquid unlike in the pnictides. Simple models allow supercooling into the glassy state with modification of the short range order into intermediate states between the liquid and solid phases.

MM 9.2 Mon 12:00 IFW A

Influence of the Chemical Short-Range Order on the Atomic Dynamics in Binary Glass-Forming Melts — •Benedikt Nowak[1], Dirk Holland-Moritz[1], Fan Yang[1], Thomas Voigtmann[1], Tobias Kordel[1], Thomas Hansen[2], and Andreas Meyer[1] — [1]Institute of Materials Physics in Space, German Aerospace Center (DLR), 51170 Cologne, Germany — [2]Institut Laue-Langevin (ILL), 38042 Grenoble, France

The dynamical behaviour of atoms and their short-range order are crucial for understanding the glass-forming ability of metallic melts. To investigate the short-range order (SRO) we measured partial structure factors for the melts of Zr-Ni by combining electrostatic levitation with neutron diffraction and isotopic substitution [1]. Mode coupling theory (MCT) allows us to establish structure-dynamics relations using partial structure factors as an input [2]. The self-diffusion coefficients derived by MCT show the same trends with respect to composition and temperature dependence compared to experimental results.

MCT results highlight that diffusion is partly coupled, exhibiting a distinct composition dependence of the ratio of diffusion coefficients. Compared to a hard-sphere model, we show that such a composition dependent decoupling is due to the strong chemical interaction between Zr and Ni atoms. This can be understood by the fraction of different atomic nearest-neighbour pairs, derived from the measured partial structure factors.

[1] D. Holland-Moritz et al., PRB 79, 064204 (2009) [2] Th. Voigtmann et al., EPL 82, 66001 (2008)

MM 9.3 Mon 12:15 IFW A

Self-diffusion in liquid gold-silicon investigated using quasi-elastic neutron scattering — •Zach Evenson[1], Fan Yang[2], Giovanna Simeoni[1], and Andreas Meyer[2] — [1]Maier-Leibnitz Zentrum (MLZ) and Physik Department, Technische Universität München — [2]Institute for Materials Physics in Space, German Aerospace Center, Cologne

We use incoherent quasi-elastic neutron scattering to study the atomic dynamics of gold in a eutectic Au81Si19 melt. Despite the glass-forming nature of this system, the gold self-diffusivity displays an Arrhenius behavior with a low activation energy characteristic of simple liquids. At high temperatures, long-range transport of gold atoms is well described by hydrodynamic theory with a simple exponential decay of the self-correlation function. On cooling towards the melting temperature, structural relaxation crosses over to a highly stretched exponential behavior. This suggests the onset of a heterogeneous dynamics, even in the equilibrium melt, and is indicative of a very fragile liquid.

MM 9.4 Mon 12:30 IFW A

Ni-diffusion in a liquid and undercooled NiSi alloy — •Franz Demmel — ISIS Facility, Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK

Understanding the dynamics of liquid metals and alloys can be relevant for technological applications like solidification and welding. Here the Nickel self-diffusion coefficient was measured in a Ni75Si25 alloy in the liquid and undercooled state covering a temperature range of 1400K to 1900K. Quasielastic neutron scattering on a 2.7 mm diameter spherical sample was used to deduce the Ni self-diffusion coefficient. The experiment was performed by applying aerodynamic levitation with CO2 laser heating. That containerless technique allowed an undercooling of about 100K over 4 hours of measurement time. The temperature dependence of the diffusion coefficients follows an Arrhenius type behavior. The derived activation energy for the diffusion process is about 10% larger than in pure Nickel and is probably the reason for the moderately slower self-diffusion coefficients compared to pure Ni. Surprisingly, molecular dynamics simulations predicted a change in dynamics from an Arrhenius-type behavior to a power-law for temperatures as high as twice the glass transition temperature [1]. Our data are compatible with a power-law behavior for the Ni self-diffusion [2]. [1] Y.J. Lu, H. Cheng and M. Chen, J. Chem Phys 136 214505 (2012) [2] F. Demmel, L. Hennet, S. Brassamin, D.R. Neuville, J. Kozaily and M. Koza, Phys Rev B 94 (2016) 014206

MM 9.5 Mon 12:45 IFW A

Dynamic viscosity of Ge-Sb-Te alloys in liquid and supercooled liquid state — Hans Weber[1,2], Mathias Schumacher[3], Pal Jovari[4], Werner Skrotzki[2], Riccardo Mazzarello[3], and •Ivan Kaban[1] — [1]IFW Dresden, Institute for Complex Materials, Germany — [2]TU Dresden, Institute of Structural Physics, Germany — [3]RWTH Aachen University, Institute for Theoretical Solid State Physic, Germany — [4]Institute for Solid State Physics and Optics, Budapest, Hungary

Dynamic viscosity of binary Ge-Te and ternary Ge-Sb-Te alloys is measured by the oscillating-cup method and calculated by ab-initio molecular dynamics (AIMD) simulations. Binary alloys around Ge15Te85 eutectic composition show a strong deviation from Arrhenius plot at about 100-150 K above the melting temperature. In contrast, viscosity of GeTe and Ge-Sb-Te alloys shows Arrhenius behavior in the liquid and weakly supercooled liquid state, whereas it seems to be strongly non-Arrhenius at larger supercoolings. Atomic dynamics and glass-forming ability will be discussed in relationship to the structure of the alloys studied.

MM 9.6 Mon 13:00 IFW A

Self-diffusion in liquid Al-Ge investigated with quasi-elastic neutron scattering — •Sandro Szabo[1,2] and Zachary Evenson[1,2] — [1]Research Neutron Source FRM II, Garching, Germany — [2]Technische Universität München, Munich, Germany

Self-diffusion of atoms in liquid metals can be investigated on an absolute scale with quasi-elastic neutron scattering (QENS). For the Al-Ge system accurate modeling of solidification processes and mass transport in general suffers due to the lack of experimentally determined temperature-dependent diffusion coefficients. We investigate the self-diffusion of Ge in liquid Al-Ge in a wide temperature range at and below the melting point of the respective pure elements. QENS measurements were carried out at the multi-disc chopper time-of-flight spectrometer TOFTOF at the research neutron source Heinz Maier-Leibnitz (FRM II). The QENS results show a standard deviation of the self-diffusion coefficients of only 4 %, which is significantly more precise when compared to classical measurements in long capillaries. In all investigated Al-Ge alloys, the self-diffusivity of Ge follows an Arrhenius behavior over the entire investigated temperature range. At the melting point of pure Ge, the self-diffusivity of Ge in the investigated alloys is higher by some 22-28 % than that of pure Ge. This is in line with existing findings concerning dendrite growth in this system during solidification. Accurate calculations of mass flow, which were previously impeded by the lack of accurate diffusion data, might now be possible.