

## MM 10: SYM Phase Transformations in Metallic Melts IV

Time: Monday 16:30–18:00

Location: H 1058

MM 10.1 Mon 16:30 H 1058

**Quasielastic Neutron Scattering on Refractory Al-Ni melts** — ●SEBASTIAN STÜBER<sup>1</sup>, ANDREAS MEYER<sup>2</sup>, DIRK HOLLAND-MORITZ<sup>2</sup>, HELENA HARTMANN<sup>2</sup>, and TOBIAS UNRUH<sup>3</sup> — <sup>1</sup>Physik Department E13, Technische Universität München, 85747 Garching — <sup>2</sup>Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR) 51170 Köln — <sup>3</sup>Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München, 85747 Garching

In this talk we will present results of quasielastic neutron scattering at the time of flight spectrometer ToF-ToF of the FRM II used to study atomic dynamics in melts of binary Al-Ni alloys that are the basis of a large variety of high temperature applications. In order to undercool the melts deeply below the melting temperature and to avoid reactions with crucible materials, the liquids are containerlessly processed under high purity conditions by application of the electromagnetic levitation technique. Due to the containerless processing the measured dynamic structure factors are not affected by scattering from a sample container such that the quasielastic neutron scattering measurements were possible also at large momentum transfer. From the measured dynamic structure factors Ni self-diffusion coefficients are determined as a function of alloy composition and temperature. At constant temperature, the Ni self diffusivity is constant within a wide compositional range.

MM 10.2 Mon 16:45 H 1058

**Structure and dynamics of liquid Ni<sub>36</sub>Zr<sub>64</sub>** — ●DIRK HOLLAND-MORITZ<sup>1</sup>, OLIVER HEINEN<sup>1</sup>, ANDREAS MEYER<sup>1</sup>, SEBASTIAN STÜBER<sup>2</sup>, THOMAS VOIGTMANN<sup>1</sup>, TOBIAS UNRUH<sup>3</sup>, and THOMAS HANSEN<sup>4</sup> — <sup>1</sup>Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — <sup>2</sup>Physik Department E13, Technische Universität München, 85747 Garching, Germany — <sup>3</sup>Forschungsneutronenquelle Heinz Maier Leibnitz (FRM II), Technische Universität München, 85747 Garching, Germany — <sup>4</sup>Institut Laue-Langevin, 38042 Grenoble, France

We investigated the atomic dynamics and the static structure factor of Ni<sub>36</sub>Zr<sub>64</sub> melts. To undercool the liquids below the melting temperature and to avoid reactions with crucible materials, the melts are containerlessly processed under high purity conditions by electromagnetic levitation. This technique is combined with quasielastic neutron scattering at the time of flight spectrometer TOFTOF of the FRM II and with elastic neutron scattering at the diffractometer D20 of the ILL. Partial static structure factors have been derived via isotopic substitution. From the quasielastic neutron scattering studies the Ni self-diffusivity is determined. The partial static structure factors indicate a chemical short-range order in liquid Ni<sub>36</sub>Zr<sub>64</sub> and a topological short-range order that is different from the icosahedral short-range order found in most other metallic melts. The experimental results are discussed in the framework of mode coupling theory. We thank Deutsche Forschungsgemeinschaft for funding within the priority programme 1120 under contract Nos. HO1942/6-3 and ME1958/2-3.

MM 10.3 Mon 17:00 H 1058

**Computational optimisation of multi-component hard sphere liquids** — ●HELMUT HERMANN<sup>1</sup>, ANTJE ELSNER<sup>1</sup>, VALENTIN KOKOTIN<sup>1</sup>, KRISTIN LOCHMANN<sup>2</sup>, and DIETRICH STOYAN<sup>2</sup> — <sup>1</sup>Institute for Solid State and Materials Research, IFW Dresden, P.O.Box 270116, D-01171 Dresden, Germany — <sup>2</sup>Freiberg University of Mining and Technology, Institute of Stochastics, Agricolastr. 1, D-09596 Freiberg, Germany

The atomistic simulation of multi-component metallic melts is a difficult task since there are no realistic interaction potentials for systems consisting of more than three species. Therefore, the generalised Bernal's model for liquids is used as an approach to the structure of multi-component liquid and amorphous metallic alloys. Varying size distribution and chemical composition, parameter ranges are determined leading to maximum values of the mean packing fraction. This generalised Bernal's model is combined with Miedema's macroscopic atom model for predicting enthalpy effects in alloys. The results of the simulations correspond at least qualitatively to empirical rules of high glass forming ability of multi-component metallic melts.

MM 10.4 Mon 17:15 H 1058

**Crystal nucleation in colloidal model systems - Is Classical**

**Nucleation Theory still state of the art?** — ●HANS JOACHIM SCHÖPE<sup>1</sup>, GARY BRYANT<sup>2</sup>, and WILLIAM VAN MEGEN<sup>2</sup> — <sup>1</sup>Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland — <sup>2</sup>Department of Applied Physics, Royal Melbourne Institute of Technology, GPO Box 2476V, Melbourne 3001, Australia

A complete understanding of the solidification process (nucleation, crystal growth, ripening, vitrification) is one of the long-standing problems in condensed matter physics. The use of colloidal model systems provides an ideal controlled experimental system to reduce this lack of knowledge because the particle movement is much slower than in atomic systems and the crystallisation process can be monitored using optical investigations. Here we present systematic measurements of the solidification kinetics and of the phase behaviour as a function of the particle concentration in nominally one component colloidal model systems of spherical particles. Interestingly we observe a two step behaviour in the nucleation kinetics which was also recently observed in crystallization of proteins and simple atomic liquids.: (i) an induction stage where large numbers of precursor structures are observed; (ii) a conversion stage as precursors are converted to close packed structures. This behaviour is in contrast to the alternative of ordering and densifying at once as assumed in the classical picture of crystallization.

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MM 10.5 Mon 17:30 H 1058

**From solid solutions to the onset of compound formation and eutectic mixtures in binary charged colloidal suspensions** — ●THOMAS PALBERG<sup>1</sup>, NINA LORENZ<sup>1</sup>, and PATRICK WETTE<sup>2</sup> — <sup>1</sup>Institut f. Physik, Johannes Gutenberg Universität Mainz, — <sup>2</sup>Institut f. Materialwissenschaft im Weltraum, DLR, Köln

Aqueous colloidal charged sphere suspensions closely mimic the behaviour of metals on a mesoscopic model level. We here ask, whether this also holds for their binary mixtures. We studied the structure, elasticity and solidification kinetics of such mixtures as a function of mol fraction  $x$  and total particle density  $n$ . At an interaction ratio  $s = AA/BB = 1$  we observe solid solutions of bcc structure, with elasticity and solidification kinetics varying linearly with composition [1]. The onset of compound formation, with extended stability of the crystal phase and corresponding anomalies in elasticity and solidification kinetics occurs at  $s < 0.7$ . Most recently we found an eutectic behaviour for  $s = 0.55$  at  $x = 0.7$  with a strongly increased melt stability [2]. Close to the eutectic composition solidification kinetics are dramatically slowed. Our observations are discussed in relation to colloidal mixtures of different interactions (hard spheres, oppositely charged spheres) but moreover carefully analyzed in view of the possible extension of the role of colloids as model systems going from single component to binary systems.

[1] P. Wette, H. J. Schöpe, T. Palberg, J. Chem. Phys. 122, 144901 1-8, (2005).

[2] N.Lorenz, J.Liu, T. Palberg, Colloids Surf. A (at press 2007)

MM 10.6 Mon 17:45 H 1058

**Structural changes of undercooled melts in charged colloidal model systems** — ●PATRICK WETTE<sup>1</sup>, INA KLASSEN<sup>1</sup>, DIETER M. HERLACH<sup>1</sup>, DIRK HOLLAND-MORITZ<sup>1</sup>, THOMAS PALBERG<sup>2</sup>, and STEFAN VOLKHER ROTH<sup>3</sup> — <sup>1</sup>Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — <sup>2</sup>Institut für Physik, Universität Mainz, Staudinger Weg 7, 55128 Mainz, Germany — <sup>3</sup>DESY, HASYLAB, 22603 Hamburg, Germany

Colloidal model systems are often used to describe equilibrium properties of fluid and solid materials. Here we used them to study the short range order and the nucleation process in undercooled melts. We employed charged colloidal silica spheres in aqueous dispersion, which enables the precise adjustment of surface charge density and particle interaction via the controlled addition of sodium hydroxide leading to a rich phase behaviour. This colloidal system is characterized by convenient time scales between seconds and minutes and particle distances up to 500nm and is thus accessible by simple, yet powerful optical techniques. By contrast to metals heterogeneous nucleation can either be efficiently suppressed or, if present, clearly discriminated and separated from data evaluation. Microscopy and light scattering yield complementary information on equilibrium properties and crystallization

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kinetics from real and reciprocal space. Comprehensive measurements of structural changes of the melt with increased undercooling and the

corresponding changes of the solidification were carried out by means of the USAXS- technique at HASYLAB (Hamburg).