MM 3: Liquid and amorphous materials I

Time: Monday 10:15–11:15 Location: H4

MM 3.1 Mon 10:15 H4

Neutron scattering investigatons on melts of Al-Ni and Zr-Ni alloys — •Dirk Holland-Moritz[1], Andreas Meyer[1], Helena Hartmann[1], Sebastian Stüber[2], and Fan Yang[2] — [1]Institut für Materialphysik im Weltraum, DLR-Köln, Germany — [2]Physik Department E13, TU-München, Germany

This work presents investigations on the short-range order of stable and deeply undercooled melts of binary Al-Ni and Zr-Ni alloys. The liquids were containerlessly processed and undercooled by use of the electromagnetic levitation technique which was combined with the technique of elastic neutron scattering at the diffractometer D20 of the Institut Laue-Langevin (ILL) in order to determine the static structure factor. The scattering contrast was varied by isotopic substitution. By means of this partial structure factors were determined. For the case of $Zr_{64}Ni_{36}$ alloys strong indications for the existence of a chemical order are found.

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MM 3.2 Mon 10:30 H4

Interplay of Structure and Dynamics in liquid and undercooled AlNi melts — •Sebastian Stüber[1], Andreas Meyer[2], Dirk Holland-Moritz[2], Helena Hartmann[2], and Tobias Unruh[3] — [1]Physik Department E13, TU München — [2]Institut für Materialphysik im Weltraum, DLR Köln — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Garching

AlNi melts show a chemical short-range order (CSRO), dependent on the Ni concentration [1]. For lower temperatures, this CSRO becomes more pronounced. To increase the available temperature range further, we used electromagnetic levitation. This container-free method enabled significant undercooling (up to 266 K) for several hours.

The AlNi melts were studied using inelastic neutron scattering. The quasielastic line was fitted by a scaled Lorentzian, whose HWHM corresponds to the inverse of the mean relaxation time τ_q. With this a q-dependent diffusivity $D(q) = 1/(\tau q^2)$ can be defined, for the hydrodynamic limit $q \to 0$ one gets the (Ni) self-diffusion coefficient D as a function of temperature.

The q-dependent diffusivity $D(q)$ provides information about the correlation between the diffusive motion and the CSRO, visible at intermediate q values. Using $D(q)$ we will discuss the process of diffusive atomic motion in AlNi melts, under the pronounced influence of CSRO.

[1] S.K. Das *et al.*, Appl. Phys. Lett. **86**, 011918 (2005).

MM 3.3 Mon 10:45 H4

Struktur und Dynamik von flüssigem Titan: Computersimulation, Modenkopplungstheorie und Experiment — •Jürgen Horbach — Institut für Physik, Universität Mainz, Staudinger Weg, D-55099 Mainz

Mittels Molekulardynamik-Computersimulationen wird die Struktur und Dynamik von Titan in der Nähe des Schmelzpunktes, d.h. bei der Temperatur $T = 1970\,\mathrm{K}$, untersucht. Dabei verwenden wir als Modell ein Potential vom "embedded atom"-Typ [1]. Der statische Strukturfaktor $S(q)$ aus der Simulation ist in sehr guter Übereinstimmung mit experimentellen Daten [2,3]. Wir verwenden den simulierten Strukturfaktor $S(q)$ als Input für eine Rechnung im Rahmen einer Modenkopplungstheorie, aus der die von der Frequenz ω abhängigen, dynamischen Strukturfaktoren $S(q,\omega)$ vorhergesagt werden. Wir zeigen, dass die dynamischen Strukturfaktoren aus der Theorie in semiquantitativer Übereinstimmung mit der Simulation sind.

[1] R. Zope, Y. Mishin, Phys. Rev. B **68**, 024102 (2003).

[2] G. W. Lee, A. K. Gangopadhyay, K. F. Kelton, R. W. Hyers, T. J. Rathz, J. R. Rogers, D. S. Robinson, Phys. Rev. Lett. **93**, 037802 (2004).

[3] D. Holland-Moritz, O. Heinen, R. Bellissent, Th. Schenk, Mat. Sc. Eng. A, in press (2006).

MM 3.4 Mon 11:00 H4

Thermophysical properties of Si, Ge and Si-Ge melts under microgravity — •Suresh Mavila Chathoth, Bernd Damaschke, and Konrad Samwer — I. Physikalisches Institut, Universitaet Göttingen, 37077 Göttingen, Germany

The liquid Si and Ge are highly reactive materials. Especially the liquid Si is known to reactive with almost all materials. To have an accurate values of thermophysical properties of these melts container less processing is required. The container less processing can be realized by electromagnetic or electrostatic levitation. These ground based levitation techniques have demerits of gravity driven convection and accuracy of the data depend on convection currents. The thermophysical properties of Si, Ge and Si-Ge alloy melts have been investigated in the TEMPUS facility on board of Zero-G plane during the parabolic flights. Unlike metallic alloys [1] which can melt in a magnetic field, Si, Ge and Si-Ge are semiconductors in their sold state a laser pre-heating was necessary to melt these samples. The melted droplets were video taped and from the images the thermal expansion and surface tension of the samples were evaluated. Absence of gravity driven convection a separation of the influence of gravity induced convection become possible by comparing the data with ground based experiments. The work was supported by BMBF/DLR under grant No. 50WM0541.

[1] B. Damaschke, D. Oelgeschlaeger, J. Ehrich, E. Dietzsch, and K. Samwer, Rev. Sci. Instrum. **69**, 2110 (1998).