MM 9: SYM Phase Transformations in Metallic Melts III

Time: Monday 14:45–16:00 Location: H 1058

Invited Talk MM 9.1 Mon 14:45 H 1058

Atomic Diffusion in Liquid Alloys — •Andreas Meyer[1,2], Suresh Mavila Chathoth[2], Winfried Petry[2,3], Tobias Unruh[3], and Marek Koza[4] — [1]Institut für Materialphysik im Weltraum, DLR Köln — [2]Physik Department E13, TU München — [3]FRM-II, TU München — [4]Institut Laue Langevin, Grenoble

We investigate the atomic motion in liquids on Ni-, Pd-, and Zr- basis in order to clarify the microscopic transport mechanisms. High-resolution energy and momentum information from neutron scattering experiments allows to study how the atomic dynamics depends on structural properties, and in some special cases to derive the self diffusion coefficient of one particular component on an absolute scale. Results on binary alloys and multicomponent bulk glass forming melts, reveal non-trivial mechanisms of mass transport. We show that the relation between equilibrium melt structure and atomic transport is well described by a mode-coupling theory. Our findings are discussed in the context of results obtained by molecular dynamics simulations and long capillary diffusion experiments performed by other groups within the SPP 1120.

MM 9.2 Mon 15:15 H 1058

Influence of thermodynamic forces on diffusion in metallic melts measured by ex-situ and in-situ capillary techniques — •Axel Griesche[1,2], Michael-Peter Macht[2], and Günter Frohberg[3] — [1]Institut für Materialphysik im Weltraum, DLR, Linder Höhe, 51170 Cologne — [2]Dept. Materials, Hahn-Meitner-Institute Berlin, Glienicker Str. 100, 14109 Berlin — [3]Institute of Material Sciences and Technology, Technical University Berlin, Hardenbergstr. 36, 10623 Berlin

The Darken relation that correlates interdiffusion coefficients, self diffusion coefficients and thermodynamic factors was studied in different metallic melts. Interdiffusion and self diffusion in $Al_{80}Ni_{20}$, $Al_{77}Ni_{20}Ce_3$ and $Pd_{40}Cu_{15}Ni_{25}P_{20}$ melts have been measured above the liquidus temperature using classical capillary methods and a novel X-ray radiography method. The chemical diffusion profiles of the ex-situ technique were determined by means of EDS whereas for the in-situ technique the profiles were determined from absorption pictures. Self diffusion coefficients were determined from penetration profiles of stable enriched ^{62}Ni, ^{142}Ce, ^{108}Pd, and ^{65}Cu isotopes measured by ICP-MS and for Ni additionally by QNS. The thermodynamic factors of Al-based alloys were calculated from chemical potential data whereas the thermodynamic factor of Pd-alloys was estimated from partial mixing enthalpies. In liquid Al alloys the enhancement of chemical diffusion with respect to self diffusion correlates linearly with the thermodynamic factor. For Pd alloys the experimental findings are discussed only qualitatively.

MM 9.3 Mon 15:30 H 1058

Molecular dynamics computer simulation of crystal growth and melting in $Al_{50}Ni_{50}$ — Ali Kerrache[1], •Juergen Horbach[1,2], and Kurt Binder[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linder Höhe, 51147 Köln

The melting and crystallization of $Al_{50}Ni_{50}$ are studied by means of molecular dynamics computer simulation, using a potential of the embedded atom type to model the interactions between the particles. Systems in a slab geometry are simulated where the B2 phase of AlNi in the middle of an elongated simulation box is separated by two planar interfaces from the liquid phase, thereby considering different crystal orientations (100, 110, and 111). By determining the temperature dependence of the interface velocity, an accurate estimate of the melting temperature is provided. For the different orientations similar values around 0.002 m/s/K are found for the kinetic coefficient. This value is about two orders of magnitude smaller than that found for one-component systems. We discuss this finding in the framework of the Wilson-Frenkel model, considering also structure and diffusion dynamics in the vicinity of the liquid-crystal interface.

MM 9.4 Mon 15:45 H 1058

Entropy in Molecular Dynamics simulated AlyNi40-yZr60 melts. — •Helmar Teichler and Mohammed Guerdane — Inst. f. Materialphysik, Universität Göttingen, Göttingen, Germany

Entropy plays a major role in stabilizing melts against crystallization, and entropy (and enthalpy) release are the main phenomena that determine solidification. Despite its importance, little is known at present about the microscopic origin of entropy in melts, especially for complex multi-component metallic systems with steric and chemical short range order. Regarding this, exploiting ergodicity, we present here results from isothermal molecular dynamics simulations for the entropy in the pseudo binary AlyNi40-yZr60 series (y=0 - 40 at% Al), combining thermal integration along the temperature axis and Kirkwoods (1935) coupling parameter approach. In the simulations the AlNiZr model of Guerdane and Teichler (PRE 65, 014203 (2001)) is used.

We show in particular that our method provides entropy data with an internal reliability better than 0.01 kB. In the AlyNi40-yZr60 series, we find a slightly negative total entropy of mixing. The configuration entropy of the (trigonal prismatic) Ni40Zr60 melt at 2400 K turns out below that of liquid Zr while the configuration entropy of (binary polytetrahdral) Al40Zr60 melt lies above. These observations and the temperature dependence of the phenomena shall be discussed.