MM 34: Liquid and Amorphous Metals I

Time: Wednesday 14:45–16:30 Location: IFW D

MM 34.1 Wed 14:45 IFW D

On systematics of the atomic structure of liquid and amorphous elements along the periodic table — •Peter Häussler — Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz

Over many years we systematically studied structure formation at very early stages, within the amorphous state. This state, as well as the liquid one are the precursors of any crystalline state. But, both are not really disordered, instead show a well defined spherically-periodic order (SPO), in the mean around any atom. This order can be seen as a precursor of planar order which is expressed by Bloch's theorem. The SPO is an effect of a self-organizing resonance between global subsystems as there are all the valence electrons on one side, and the forming static structure on the other. We learned that both subsystems may adjust to eachother for an optimal phase stability.

Here we report, starting with hydrogen (Z=1), on systematics in the static atomic structure of liquid and amorphous elements all along the Periodic Table of the Elements, up to bismuth (Z=83), highers are mostly unknown. With the *Resonance Model* we are able to explain major structural features of all the elements, independent whether they are metallically, covalently or van-der-Waals-like bonded, of atomical or molecular type. Main features of unknown structures as for e.g. liquid W, Ta, Mo can be predicted.

MM 34.2 Wed 15:00 IFW D

Supercooled and glass-forming liquids as Skyrmionic textures — •Andrei A. Leonov[1,2], U.K. Rössler[1], and A.N. Bogdanov[1] — [1]IFW Dresden — [2]Donetsk Institute for Physics and Technology

The concept of Skyrmionic textures in chiral magnetic systems [1] has been extended to continuum models for glass-forming liquids. These models describe the frustrated tiling of space by incompatible locally preferred clusters within a generalized elastic theory. The field theory for the local order-parameter includes antisymmetric couplings derived from the decurving of ideal template units into flat space[2]. As a qualitative new feature, we propose a softened modulus of the local intensity of the order parameter. The corresponding classical field theory allows for the stabilization of Skyrmionic localized states and extended textures [3]. The notion of a glassy structure as an entangled network of defect lines is replaced by the complex geometry of an elastic and frustrated continuum that can display both "rotation" or twisting and suppression of the ideal local order. The Skyrmions in the simplest version of the frustration models are close, but soft relatives of the hedgehog solutions in Skyrme's original SU(2) symmetric model for nucleons. It is argued that stable Skyrmions are formed at elevated temperatures in molecular liquids and that their condensation into frustrated textures underlies the stability of supercooled and glassy states. — [1] U.K.Rößler, A.N.Bogdanov, C.Pfleiderer, Nature (London) **442**, 797 (2007). [2] S. Sachdev, D.R. Nelson, Phys. Rev. B **32** (1985) 1480. [3] U.K.Rößler, A.N.Bogdanov, J.Non-Cryst.Solids **354**, 4198 (2008).

MM 34.3 Wed 15:15 IFW D

Stokes-Einstein relation in computer simulated bulk glass forming Cu33Zr67 melts — •xiujun han and herbert schober — IFF, Forschungszentrum Juelich, 52425 Juelich, Germany

The validity of Stokes-Einstein (SE) relation in glass forming Cu33Zr67 melts is checked by studying the relationship between viscosity and self-diffusion coefficient with molecular dynamics simulation. The atomic interaction of Cu-Zr is modeled by modified-embedded-atomic method (MEAM). The self-diffusion coefficient is calculated from mean squared displacements (MSD) and the viscosity is evaluated from Green-Kubo equation. It was found that at temperatures higher than 1500K, SE relation is valid. When the temperature is further decreased, SE relation breaks down, which is an indication of dynamical heterogeneity in the melts.

MM 34.4 Wed 15:30 IFW D

Density, surface tension and viscosity of ternary CuCoNi alloys — •Michael Schick, Jürgen Brillo, and Ivan Egry — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany

We selected the ternary system CuCoNi, which is a good candidate for improving the Giant Magneto Resistance (GMR) of conventional CuCo alloys, for investigation of thermophysical properties.

The latter play an important role in the numerical simulation of processing steps, e.g. casting processes. Along two perpendicular cuts through the ternary phase diagram, surface tension, density and viscosity have been determined as functions of temperature.

For surface tension and density measurements the well established electromagnetic levitation technique was used, which allows a containerless processing of the samples and therefore deep undercooling. Viscosities have been measured in our high temperature oscillating cup viscometer.

MM 34.5 Wed 15:45 IFW D

The hydrodynamic limit in liquid titanium: At which length and time scales is it valid? — •Jürgen Horbach and Andreas Meyer — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

A combination of neutron scattering experiments and molecular dynamics (MD) computer simulations is used to analyze the dynamic structure factor of liquid titanium near its melting temperature. First, we show that the simulation is in good agreement with neutron scattering, regarding the self part of the dynamic structure factor, $S_{\rm s}(q,\omega)$ (with q the wavenumber and ω the frequency). For both methods, we find that the width of the quasielastic line shows a hydrodynamic q^2 dependence for wavenumbers up to about $1.0\,\text{Å}^{-1}$, and thus the self-diffusion constant can be extracted in this q range. Second, MD simulations allow for an accurate calculation of the total dynamic structure factor, $S(q,\omega)$, over the full relevant range of q and ω. The latter function is compared to the analytically known hydrodynamic prediction that requires the shear and bulk viscosities as well as the thermal diffusion coefficient as an input. The latter transport coefficients are directly computed from the MD simulation. The comparison of the hydrodynamic $S(q,\omega)$ with the "exact one" allows for a quantitative determination of the q-ω range where hydrodynamics is valid.

MM 34.6 Wed 16:00 IFW D

Laser induced non-thermal melting of germanium — •Momar S. Diakhate[1], Harald O. Jeschke[2], and Martin E. Garcia[1] — [1]Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany. — [2]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany.

We study the ultrafast non-thermal melting in bulk germanium. By performing molecular dynamics simulations on time-dependent potential energy surfaces and also static frozen phonon calculations, both based on a non orthogonal tight-binding Hamiltonian, we describe the nonequilibrium melting process occurring in bulk germanium under ultrafast laser pulse excitation. The laser parameters are explicitly taken into account. We show that, upon laser heating, all transverse acoustic phonon modes becomes strongly affected and even destabilized, which drives the melting process. We calculate the time-dependence of the structural properties, in particular the structure factor, and predict the time-dependence of different Bragg-peaks. Our simulations yield nonthermal melting of Ge in less than 1ps after laser excitation.

MM 34.7 Wed 16:15 IFW D

Liquid Phase Separation in Gd-Zr and Gd-Ti Melts — •Steffen Schmitz, Hans-Günther Lindenkreuz, Norbert Mattern, Wolfgang Löser, and Bernd Büchner — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Phase-separated metallic glasses can be formed in complex alloys involving binary terminal systems with both, negative and positive enthalpy of mixing. The miscibility gaps of Gd-Zr and Gd-Ti melts are determined by electromagnetic levitation experiments. If Gd-Ti melts are undercooled below the binodal line samples exhibit the typical coarse phase separated microstructures. On contrary, in Gd-Zr samples quenched on a Cu-substrate both of the two primary phases, i.e. Gd and Zr, occurred in the matrix simultaneously with the eutectic microstructure. Therefore the existence of a metastable miscibility ap is supposed. The findings are compared with CALPHAD calculations of the binary phase diagrams. The consequences for the formation Gd-Zr-Cu and Gd-Ti-Cu metallic glasses by rapid quenching techniques

showing phase separation on the nanometre scale are briefly discussed.