MM 8: Intermetallic Phases II

Time: Monday 11:30–12:30 Location: H5

MM 8.1 Mon 11:30 H5

Perturbed γ-γ angular correlation studies of selected 211-MAX phases using ^{111}In probes — •Daniel Jürgens[1], Michael Uhrmacher[1], Hans Hofsäss[1], and Jose Mestnik-Filho[2] — [1]Georg-August-Universität Göttingen, II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Instituto de Pesquisas Energeticas e Nucleares, 05422-970 São Paulo, Brazil

MAX phases are nanolaminated layered carbides and nitrides, which feature an unusual set of the best attributes of both metals and high-performance ceramics. These compounds can be good electrical and thermal conductors, behave elastically stiff as well as high thermal shock resistant. To investigate the local structure of these phases, the technique of perturbed angular correlation (PAC) was used for material characterization beside x-ray diffraction and electron microscopy. Radioactive ^{111}In ions, decaying by a γ-γ cascade were implanted into the samples, sensing as *spies* their local environment via hyperfine interactions. The PAC method was applied to Nb_2InC, Ti_2AlN, Cr_2GeC and Nb_2AsC. Spectra were taken after different annealing steps to determine strength and symmetry of the electric field gradients (EFG) as a fingerprint for probe atoms on a specific lattice site and local surrounding. In each material an axial symmetric EFG was found with a characteristic quadrupole coupling constant ν_Q variing between 250 MHz and 350 MHz. Regarding to the question of lattice location of the In-probes we demonstrate that they occupy the A-site by comparing the experimental results with ab initio DFT calculations using the FP-LAPW+LO method implemented in the WIEN2k package.

MM 8.2 Mon 11:45 H5

Crack front propagation by kink formation — •Frohmut Rösch and Hans-Rainer Trebin — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

In a brittle material a travelling crack generates an upper and a lower fracture surface, which meet at a one-dimensional crack front. From a macroscopic point of view there is no reason why this curve should deviate from a straight line, contrary to the atomistic point of view, where a crack propagates by successive rupture of cohesive bonds.

We investigate fracture of the C15 $NbCr_2$ Friauf-Laves phase on an atomic level by means of molecular dynamics simulations. The numerical experiments highlight that crack fronts in general do not form a straight line and propagate by kink-pair formation at low loads (EPL 87 (2009) 66004). This mechanism should be relevant for crack propagation in any ordered brittle solid.

MM 8.3 Mon 12:00 H5

Magnetic properties of Pr_2PdSi_3 single crystals — •Yiku Xu[1,2], Fei Tang[3], Matthias Frontzek[3], Wolfgang Löser[1], Günter Behr[1], Bernd Büchner[1], and Lin Liu[2] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]State Key Laboratory of Solidification Processing, Northwestern Polytechnical University,Xi'an, Shaanxi 710072, PR China — [3]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany

Ternary R_2TSi_3 intermetallic compounds (R = Rare Earth, T = Transition Metal) with hexagonal AlB_2-type crystallographic structure are known because of their interesting physical properties. Pr_2PdSi_3 single crystals were grown by a vertical floating zone method. The compound exhibits congruent melting behavior at a liquidus temperature of about 1770°C. Single crystalline samples show a huge anisotropy at low temperatures due to the crystal electric field effect and order antiferromagnetically below the Néel temperature $T_N = 2.17$ K. This value approximately obeys the linear de Gennes scaling for this class of compounds. The [0 0 1] orientation was identified as the magnetic easy axis at room temperature. At lower temperature (≈ 20 K) magnetic easy and hard axes interchange with each other. Two additional magnetic phase transitions were observed at temperatures below 1 K.

MM 8.4 Mon 12:15 H5

Lattice dynamics in complex metallic alloys — •Holger Euchner[1], Marc de Boissieu[3], and Marek Mihalkovič[2] — [1]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Stuttgart, Germany — [2]Slovak Academy of Sciences, Bratislava, Slovakia — [3]Science et Ingénierie des Matériaux et Procédés, INP Grenoble CNRS UJF, Saint Martin d'Hères Cedex, France

We report on the vibrational properties of a series of complex metallic alloys with different degrees of structural complexity.

Dynamic structure factor and vibrational density of states, obtained from inelastic X-ray and neutron scattering, are compared to both ab initio calculations and molecular dynamics simulations. This comparison is used to discuss the impact of structural complexity, as present in complex metallic alloys, on vibrational dynamics and physical properties, like specific heat and thermal conductivity.