KFM 20: Structurally and Chemically Complex Alloys (joint session MM/KFM)

Time: Wednesday 17:15–18:00 Location: C 230

KFM 20.1 Wed 17:15 C 230

Synthesis and atomic transport properties in pseudo-binary ordered B2 aluminides — •Mohan Muralikrishna Garlapati[1], Christian H. Liebscher[2], Murty B.S.[3], Gerhard Wilde[1], and Sergiy V. Divinski[1] — [1]Institute of Materials Physics, University of Muenster, 48149-Muenster, Germany — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [3]Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, 600036-Chennai, India.

The present study highlights a novel alloy design of HEAs to fabricate fully ordered pseudo-binary multicomponent and ordered aluminides and is focused on the underlying diffusion behaviour. Microstructure and sublattice ordering in the multicomponent alloys starting from binary to hexanary B2 aluminides are studied. A radiotracer technique using the 57Co, 59Fe, 54Mn, 63Ni and 65Zn radioisotopes is employed to measure the diffusion rates of individual elements. Diffusion in the multicomponent (n>4) B2 ordered alloys is found to be enhanced in comparison to stoichiometric binary AlNi. However, the addition of Co or Fe to AlNi slows down (Co) or enhances (Fe) the diffusion rates. The measured diffusivities are compared to the literature data and the effect of chemical complexity and the B2 ordering on diffusion are discussed.

KFM 20.2 Wed 17:30 C 230

Short range order in compositionally complex NiCoMnTi alloys — David Koch[1], Benedikt Beckmann[1], Oleh Ivasko[2], Martin von Zimmermann[2], Oliver Gutfleisch[1], and •Wolfgang Donner[1] — [1]Institute of Materials Science, Technical University of Darmstadt , 64287 Darmstadt, Germany — [2]Deutsches Elektronen-Synchrotron DESY, D-22607 Hamburg, Germany

Analyzing the chemical order in compositionally complex alloys can be challenging and may become complicated by low elemental contrast. One such compositionally complex material is the all-d-Heusler alloy NiCoMnTi. These alloys exhibit a tunable magneto-structural phase transition, where the high-temperature phase has a long-range B2 structure that can be adjusted through proper thermal treatment. The typical long-range $L2_1$ structure found in classical p-metal Heusler alloys cannot be stabilized. In this report, we present data on short-range order in this system, which can be probed through diffuse X-ray scattering. To achieve this, we grew single crystals via abnormal grain growth and conducted synchrotron high-energy X-ray diffraction experiments to obtain high-quality diffuse scattering data. This data was then reconstructed into reciprocal space maps for interpretation.

KFM 20.3 Wed 17:45 C 230

Mechanical Alloying of High-Entropy Alloys: Insights from Molecular Dynamics Simulations — •Marie Charrier, Yulia Klunnikova, and Karsten Albe — Technical University of Darmstadt, Materials Modelling Division, Otto-Berndt Straße 3, 64206 Darmstadt, Germany

Mechanical alloying is a promising technique for producing high-entropy alloys. In this work, we explore intermixing processes and the formation of the solid solution starting from principal elements Co, Fe, Ni, Cr and Al in their respective lattice structures.

Severe plastic deformation is mimicked in Molecular Dynamics simulations by cyclic compressive loading of nanocrystalline samples inducing a quasi-hydrostatic stress state. The influence of grain orientation, grain size and temperature on structural evolution and chemical mixing is investigated. The structural and chemical complexity is increased by varying interfaces (from planar, bicrystalline to multiple, randomly oriented grains) and the number of components, respectively.

Independent of the starting configuration, we observe grain refinement and an HCP/BCC-FCC phase transformation within a few cycles, while chemical homogeneity is reached only at higher strains. These processes strongly depend on temperature and grain size, while the grain orientation plays a minor role. The final structures exhibit a large number of defects, in agreement with experimental observations. In general, the results provide atomic level insights into the mechanisms of mechanical alloying.