MM 10: Intermetallic Phases II

Time: Monday 16:00–16:45 Location: IFW B

MM 10.1 Mon 16:00 IFW B

Ordering and site occupancy of ternary elements in Fe_3Al — •Thomas Rademacher, Talaat Al-Kassab, and Reiner Kirchheim — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Ordered iron aluminides exhibit a number of advantageous properties, such as high-temperature strength, corrosion resistance and low cost. Therefore, iron aluminum based alloys are considered to replace in some cases high alloyed ferritic stainless steels, especially DO_3 - ordered Fe_3Al. The mechanical properties and high-temperature stability can be optimized when ternary elements are added.

In this study the site occupancy of ternary elements (4at.%V, 5at.%Cr, 5at.%Mn) has been investigated by means of Atom Probe Tomography (APT). A special analysis algorithm allows resolving the atom layers for different measurement directions which enables determining site preferences. Additionally, comparing the succession of layers with simulations the binding energies of the participating elements can be estimated.

MM 10.2 Mon 16:15 IFW B

Structural interrelations between cubic icosahedral approximants of the Ru-Sb-Zn system — •Bernd Harbrecht and Ding-Bang Xiong — Department of Chemistry, Centre of Materials Science, Philipps University, 35032 Marburg, Germany

Structural complexity in intermetallics comes in different guises, often not just as one phase rather than - as result of small energy differences between compositionally and structurally intimately related phases - in bundles of phases. Positional and substitution disorder may be one cause, long-range vacancy ordering another [1]. More attention has been paid recently to (in)commensurately complex alloy structures, quasicrystals QCs, and quasicrystal approximants QCAs, in which unusual rotational symmetries are relinquished that usual 3D translation symmetry can guide matter to the state of rest. We will present new examples of QCAs we found in the Ru-Zn-Sb system by partly substituting Sb for Zn and Ru in Ru13-δZn128-δ* (hP564-4(δ-δ*)[2], yielding icosahedral approximants of idealised composition Ru26Sb24Zn67 (cF936), Ru13Sb12Zn81, and Ru13Sb6Zn87 (cF848), homotypic to Mo7Zn40Sn12 [3]. The structures will be discussed in the light of the hierarchical approach by decorating high symmetry points with clusters instead with atoms, here with double-Mackay M127 and M119 snub cube clusters with and without additional glue atoms.

[1] S. Thimmaiah, B. Harbrecht, J. Alloys Comp. 2006, 417, 45. [2] C. Allio, B. Harbrecht, Z. Anorg. Allg. Chem. 2006, 632, 2142. [3] H. Hillebrecht, V. Kuntze, K. Gebhardt, Z. Kristallogr. 1997, 212, 840.

MM 10.3 Mon 16:30 IFW B

Characterization of MAX phases via hyperfine interactions — •Daniel Jürgens[1], Michael Uhrmacher[1], Hans Hofsäss[1], Agnieszka Kulinska[1,2], Jose Mestnik Filho[3], and Michel Barsoum[4] — [1]II. Physikalisches Institut, Universität Göttingen, 37073 Göttingen, Germany — [2]IFJ PAN, 31-342 Krakow, Poland — [3]Instituto de Pesquisas Energeticas e Nucleares, 05422-970 Sao Paulo, Brazil — [4]Dep. Mat. Science and Eng. Drexel University, Philadelphia, PA 19104, USA

$M_{n+1}AX_n$ phases, where n is 1, 2 or 3, are nanolaminated layered ternary carbides and nitrides, which feature a unique combination of the best attributes of both metals and high-performance ceramics. This class of solids possesses good electrical and thermal conductivities as well as high thermal shock resistance and damage tolerance.

The method of perturbed angular correlation (PAC), which is sensitive to hyperfine interactions, is used for material characterization on microscopic scale. ^{111}In was implanted as probe nuclei to measure the electric field gradients (EFG) in the *key-compounds* Ti_2InC and Zr_2InC to determine strength and symmetry of the EFG on the In-site or more general on the A-site. Regarding to the question of lattice location of In-probes in In-free MAX phases, PAC studies of Ti_2AlN and Cr_2GeC were performed to confirm the assumption occupying the A-site. The experimental results are compared with those from *ab initio* calculations using the FP-LAPW+LO method implemented in the WIEN2k code. Additionally investigations of annealing behavior, thermal stability and behavior under isostatic stresses are presented.