MS11 Hybrid approaches and validation (X-ray and electron microscopy)

Chairs: Felix Rey, Mathieu Botte

MS11-P1 Structural changes as a function of transition metal`s (T) type in the ThT_2Al_{20} alloys

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Strong inter-linkage exists between the physical/chemical properties-chemical composition and crystal structure of the materials. In order to gain improved properties - composition and/or structure should be changed. Such researches are normally done either via theoretical route (i.e. prediction) or experimental (i.e. “trial and error”). Experimental route is time and resource consuming. Prediction (basing on energy landscapes) is not always possible, especially when system of an interest exhibits complex electronic structure, such as A-T-Al (where A-actinide and T-transition metal) containing *f*-electron elements. In these systems, AT_2Al_{20} alloys were intensively studied with a purpose to find aluminides with heavy fermion properties. Our study concentrated on the ThT_2Al_{20} system (where T-*3d* transition metal) in order to formulate a general “rule of thumb” which will allow to estimate the symmetry of the Al-rich ternary structure forming in these systems. Such prediction will shorten the research time spent on search for the heavy fermion materials with interesting magnetic and electrical properties. We have proved experimentally (using a combination of X-ray diffraction and conventional electron microscopy) and theoretically (applying Density Functional Theory) that ternary aluminides structure’s symmetry changes abruptly as a function of atomic number of T (i.e. Z_T). At T=Mn, the symmetry decreases from cubic ($22 \le Z_T < 25$) to orthorhombic ($25 \le Z_T \le 27$). At $Z_T=28$ (i.e. T=Ni) three new structures were formed. Despite the prolonged heat treatment, equilibrium was not achieved. Applying Electron Diffraction Tomography method (known as EDT) for structure characterization of these phases - geometry of all phases was proposed. Full structure solution of the major $Th_2Ni_{10}Al_{15}$ phase was performed using manually collected EDT dataset. This phase was found to be orthorhombic, I*mmm*, with lattice parameters a=3.992Å, b=11.172 Å and c=17.343 Å. Although Th, as heavy scatterer, did smeared the Fourier difference map so that finding Al atom positions was not an easy task, all 54 atom positions in the unit cell were determined. It should be noted that despite the drastic compositional differences, the new $Th_2Ni_{10}Al_{15}$ phase can be related to the orthorhombic phase discussed above since they both belong to a family of so-called layered structures.

Keywords: Intermetallics, Alluminides, Structure solution, Electron Crystallography, DFT calculations, Symmetry