Poster Presentation

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Structure of A-T-Al aluminides (A=actinide/lanthanide; T=transition metals)

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In the last years much attention has been given to accelerating the discovery of new materials with unique properties that could have technological implications. An example of such researches is study of materials with unique magnetic ordering and unconventional superconductivity exhibited by heavy fermion compounds. A-T-Al aluminides, where A = actinide, lanthanide or rare earth elements with 4f- or 5f-shells and T=transition metal, are part of this family of compounds. Atomic structure of many aluminides of this type is yet to be discovered since most of the researches are performed using "trial and error" approach, which could be time consuming. It would be of clear benefit to formulate a rule that could predict the relative stability of the structures that may form in the ternary Al-richest phases in the A-T-Al systems, since physical properties are intimately linked with the atomic structure. Such prediction will shorten the research time. This will be a valuable contribution to the materials genome initiative, providing a useful tool for scientists working in this field.
As a first steps towards achieving this goal - ThT2Al20 systems (where T=3d transition metal) were investigated [1-3]. It was proved both experimentally and theoretically that the symmetry of the Th-based ternary aluminides` structure changes abruptly as a function of atomic number, ZT, of T. At T=Mn the symmetry decreases from cubic CeCr2Al20-type (structure that crystallizes with ZT25). It was concluded that total spin magnetic moment of the transition metal can be used in order to foreseen the stable structure of the aluminide which will form [2].
Mn was identified as breaking symmetry element. In current research, we kept T=Mn and changed A in the AMn2Al20 alloys. The research was performed both experimentally (applying X-ray and electron crystallography) and using Density Functional Theory calculations. It was found that in the AMn2Al20 alloys - orthorhombic YbFe2Al10-type structure is the stable one when A=Th; cubic CeCr2Al20-type structure crystallizes when A=U and tetragonal CaCr2Al10-type structure is received with A=Gd, Y. Theoretical and experimental results are in perfect agreement. One of the most exciting aspects of this research is the structural relations between these structure types and their connection to the most widely studied ThMn12-type.
1) Bram, A.I., Venkert, A., Meshi, L. (2015). J. Alloys Compd. 641, 1–6.
2) Uziel, A., Bram, A.I., Venkert, A., Kiv, A.E., Fuks, D., Meshi, L. (2015) J. Alloys Compd. 648, 353–359.
3) Yaniv, G. & Meshi, L. (2016) J. Alloys Compd. 660, 496–502.
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