First principle study of the solubility of Zr in Al

Emmanuel Clouet
emmanuel.clouet@cea.fr

The experimental solubility limit of Zr in Al is well-known. Al_3Zr has a stable structure DO_{23} and a metastable one $L1_2$. Consequently there is a metastable solubility limit for which only few experimental data are available. The purpose of this study is to obtain by $ab-initio$ calculations the solubility limit of Zr in Al for the stable as well as the metastable phase diagrams.

The cohesive energies of about thirty ordered compounds $Al_xZr_{(1-x)}$, all based on a fcc underlying lattice, have been caculated with the FP-LMTO (Full Potential Linear Muffin Tin Orbital). By taking into account all the relaxations allowed by the symmetry, we find that the DO_{23} structure is the stable one for Al_3Zr.

This set of results is then used with the cluster expansion in order to fit a generalized Ising model through the inverse method of Connolly-Williams. There are different ways to consider or not volume relaxations as well as relaxations of the unit cell shape and of the atomic positions which lead to different sets of coefficients for the Ising model.

This allows us to calculate in the Bragg-Williams approximation the configurational free energy at finite temperature. According to the previous FP-LMTO calculations the free energy due to electronic excitations can be neglected. For the vibrational free energy we compared for ordered phases results obtained from the elastic constants and the Debye model and those obtained from a calculation of the phonon spectrum.

All these different steps lead to a calculation of the solubility limit of Zr in Al which is found to be lower than the experimental one. The solubility limit in the metastable phase diagram is calculated in the same way and can thus be compared to the stable one.