Vacancy formation energy in alloys: an example of TiAlN

Ferenc Tasnadi\textsuperscript{1}, Magnus Odén\textsuperscript{1}, Igor A. Abrikosov\textsuperscript{1}

1) IFM Linköping University

Corresponding author: Ferenc Tasnadi (ferenc.tasnadi@liu.se)

Beyond the equilibrium thermodynamic and mechanical properties of materials their non-equilibrium kinetic behaviours are in capital importance for modern industrial applications. Vacancy mediated microstructural evolution is of major importance in high temperature applications, e.g. in modern coatings used as protection of metal cutting inserts such as TiAlN-alloys.

We present a technique for simulations of vacancy formation in alloys using a supercell approach. In contrast to elemental materials or ordered compounds, calculation of the vacancy formation energies requires concentration and configurational corrections. We establish the fact that there is a distribution of vacancy formation energies with large variation depending on the local chemical environments of the vacancies.

Using a cluster expansion on the derived formation energies, we demonstrate the major importance of the first two metallic coordination shells in TiAlN. We introduce a three-dimensional representation of the vacancy formation energies and we show to very good approximation, the vacancy formation energies arrange themselves around a plane. Using the least-squares fitted equations of these planes and 6480 randomly generated local environments we argue that in disordered alloys vacancies should occur in local environments that correspond to the lowest formation energies rather than distributed statistically.