Assessment of a low-cost protocol for an ab initio based prediction of the mixing enthalpy at elevated temperatures: the Fe-Mo system

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I. Introduction

For a lot of applications in metallurgy and materials science, it is important to know whether the used components will mix or not. When the mixing under study is of a disordered nature — the atoms are distributed randomly over the lattice — the corresponding heat of formation is also called the enthalpy of mixing. It is shown that by means of ab initio calculations and a thermodynamical model we can predict this quantity without having need for time-consuming experiments.

II. Procedure

A limited number of ab initio calculations in combination with a simple Debye model allow us to predict a concentration- and temperature-dependent mixing enthalpy for a binary system. A set of distinct crystals is energetically evaluated by means of density functional theory (DFT). The use of quasiharmonic Debye theory and electronic computations then yields data at finite temperatures and arbitrary concentrations. The Fe-Mo system is taken as a test case, and our predictions are compared with phase diagram information and a recently measured heat of solution for Mo in Fe. Our results appear consistent with both cases. The presented methodology can be useful for making a quick survey of mixing enthalpies in a large set of binary systems, in particular in the dilute concentration ranges where tabulated data are often lacking and where CALPHAD-style modelling is less reliable.

III. Conclusions

A novel methodology for the prediction of mixing enthalpies is presented. It makes use of the excellent predictive power of current ab initio techniques. It allows us to quickly determine thermodynamical data for low-impurity level metals, as opposed to exhaustive experimenting.

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