AB-INITIO CALCULATIONS OF THE BCC Mo-Fe PHASE DIAGRAM

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The so-called ab-initio electronic structure calculations, within the framework of the Density Functional Theory, are now considered a reliable and powerful tool to describe the atomic scale properties of materials. When combined with a statistical mechanics approach, this has also proven to be very useful in phase diagram calculations, being able to provide information on systems for which there is a lack of experimental data, aiming the development of new metallic alloys.

Here, the metastable phase diagram of the BCC phase in the Mo-Fe (molybdenum - iron) system is calculated using the formalism developed in Refs.[1,2,3]. We use the Cluster Variation Method (CVM), in the irregular tetrahedron approximation (a truncated cluster expansion) combined with the Full Potential – Linear Augmented Plane Wave (FP-LAPW) method, as embodied in the wien2k code. Particular attention is given to the sensibility of the obtained phase diagrams to basic choices commonly used in the theoretical electronic structure calculations allowed in the wien2k code . All ab-initio diagrams show a miscibility gap, which is in qualitative agreement with the metastable phase diagram calculated using the currently available CALPHAD assessment of the BCC phase [4]. Nevertheless, as already observed in other systems, the temperature scale of the ab-initio diagrams are too large and are incompatible with the experimental phase equilibria . Here we trace the influence of the different ab-initio calculations and the reliability of the derived theoretical phase diagrams.

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