Calculation of thermodynamic properties for metastable magnetic allotropes

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1 Introduction

A method for calculation of finite temperature thermodynamic properties for metastable magnetic allotropes has been developed. The method enables calculation of thermodynamic properties also for several dynamically unstable allotropes, which is not possible with classical quasi-harmonic approximations using phonon calculations. Here, the developed method has been used to study allotropes of Fe, Co and Ni.

Method

The method is based on quasi-harmonic (qh) calculations including electronic contributions (el). The Debye model \cite{Dugdale_MacDonald_1953} was used in combination with the Dugdale-MacDonald approximation \cite{Gruneisen_1953} of the Grüneisen parameter \cite{Gruneisen_1953}. A new method for estimation of the Curie temperature (T\text{C})\textsubscript{el} was used and magnetic disordering (mag) effects as described by Chen and Sundman \cite{Chen_Sundman_1995} were then added.

Metastable allotropes

1. For allotropes dynamically unstable at the equilibrium volume but stable at any other volume, the Debye temperature, T\text{D} of the allotrope, can be calculated using the Grüneisen parameter, \gamma.
2. For allotropes dynamically unstable at the equilibrium magnetic moment, \mu, but stable at other magnetic moments, T\text{D} of the allotrope can be calculated through extrapolation of ZPE(\mu).

This was used for bcc-Co.

Results

For each element (Fe, Co and Ni), the smaller diagrams show calculated Gibbs energies, G(T) (left columns) and isobaric heat capacities, C\textsubscript{v}(T) (right columns) of the allotropes bcc, fcc and hcp. All allotropes are ferromagnetic (FM) at 0 K, except fcc-Fe and hcp-Fe which are anti-ferromagnetic (AFM-D and AFM-II, resp.). The larger diagrams show G(T) for bcc, fcc and hcp, using the stable allotrope at room temperature as reference. All results are compared with the SGTE Unary database \cite{SGTE Unary}.

References

\cite{SGTE Unary} SGTE Unary (Pure Elements) TDB v5.1 supplied by Thermo-Calc Software AB

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