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Generalization of first-principles thermodynamic model: Application to hexagonal close-packed ε-Fe3N - DTU Orbit (08/11/2017)

Generalization of first-principles thermodynamic model: Application to hexagonal close-packed ε-Fe_3N

A complete first-principles thermodynamic model was developed and applied to hexagonal close-packed structure ε-Fe_3N. The electronic structure was calculated using density functional theory and the quasiharmonic phonon approximation to determine macroscopic thermodynamic properties at finite temperatures was generalized in terms of the partition function for any lattice of interest. Specially, thermal expansion of the hexagonal close-packed ε phase with two independent lattice parameters was studied by means of the present model and first-principles phonon calculations. The present predictions of thermal expansion of ε-Fe_3N are in good agreement with experimental data.

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