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Unified cluster expansion method applied to the configurational thermodynamics of cubic $Ti_{1-x}Al_xN$ BJÖRN ALLING, IFM, Linköping University, ANDREI RUBAN, MSE, Royal Institute of Technology, Sweden, AYAT KARIMI, IPMC, École Polytechnique Fédérale de Lausanne, Switzerland, LARS HULTMAN, IGOR ABRIKOSOV, IFM, Linköping University — We study the thermodynamics of cubic $Ti_{1-x}Al_xN$ using a unified cluster expansion approach for the alloy problem [1]. The purely configurational part of the alloy Hamiltonian is expanded in terms of concentration and volume-dependent effective cluster interactions. By separate expansions of the chemical fixed lattice, and local lattice relaxation terms of the ordering energies, we demonstrate how the screened generalized perturbation method can be fruitfully combined with a concentration-dependent Connolly-Williams cluster expansion method, getting the best out of both two schemes that are traditionally used separately. Utilizing the obtained Hamiltonian in Monte Carlo simulations we access the free energy of $Ti_{1-x}Al_xN$ alloys and construct the isostructural phase diagram. The results show striking similarities with the previously obtained mean-field results: The metastable c-TiAlN is subject to coherent spinodal decomposition over a large part of the concentration range, e.g., from x 0.33 at 2000 K.

[1] B. Alling, A. V. Ruban, A. Karimi, L. Hultman, and I. A. Abrikosov, PHYSICAL REVIEW B 83, 104203 (2011)

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