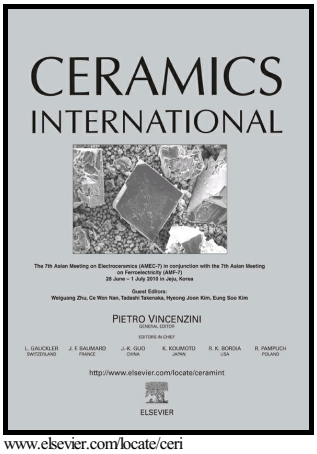

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Temperature dependent phase stability of $Ti(C_{1-x}N_x)$ solid solutions using first-principles calculations

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Abstract

We investigated lattice dynamic and temperature-dependent thermodynamic phase stabilities of $Ti(C_{1-x}N_x)$ solid solutions using first-principles calculations within the quasi-harmonic approximation. Phonon dispersion and density of states were obtained by the finite-element method. Special quasi-random structures were used to mimic the random distribution of carbon and nitrogen atoms in the sublattice of $Ti(C_{1-x}N_x)$. The reliability of the models and calculations were obtained by comparing the structural and elastic properties of $Ti(C_{1-x}N_x)$ with previous results. The random mixing of carbon and nitrogen atoms had a minor effect on the elastic properties, but greatly influenced the dynamic stability. Thermodynamic phase stability was investigated using the formation energy of the solid solutions. The phonon density of states with the quasi-harmonic approximation yielded accurate formation energies

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