Title

Harmonic ensemble lattice dynamics of crystals with thermal and configurational disorder

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Abstract

The Born-von Kármán (BvK) model parameterizes the vibrations of atoms in a crystal lattice by Taylor-expanding the potential in which the atoms move. The empirical coefficients of the second-order term are force constant matrices that can be computed using physics simulations or extracted from experiments. The BvK model assumes periodic boundary conditions, but these are not rigorously met when the atoms are displaced from their ideal lattice positions, for example, due to temperature, or when different types of atoms are randomly assigned to those ideal lattice positions, known as configurational disorder. Here we describe a methodology we have developed to treat both crystal symmetry-breaking phenomena approximately and compare it to methods that rely on computing the coefficients of higher-order terms of the Taylor expansion.