Computational Search for Dynamical Stability of Body-Centered Cubic Crystals in Chemical Space Using Multi-Objective Genetic Algorithms

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Abstract

Understanding the mechanical stability of crystalline solids is fundamental for advancing materials design. This study investigates the dynamical stability of body-centered cubic (BCC) crystals using the Born-von Kármán (BvK) model of lattice dynamics, where effective harmonic force constants represent interatomic interactions. A computational framework integrating a multi-objective genetic algorithm (MOGA) with Phonopy was developed to explore the stability landscape in BvK force-constant domain of BCC crystals. The algorithm optimizes BvK force constants up to second-nearest neighbors, while force constants for higher coordination shells are considered zeros, computes phonon dispersion relations using Phonopy, and evaluates fitness based on dynamical-matrix eigenvalues, translational invariance, and absence of imaginary phonon modes.

The implemented MOGA (PyGAD) simultaneously optimizes phonon smoothness and stability, enabling convergence toward regions of the force-constant domain that produce dynamically stable dispersions. The proposed computational framework was validated through comparison with experimental phonon dispersion data for BCC Fe, V, and Cr. Simulations were performed on the NERSC high-performance computing (HPC) platform to explore the BCC crystal stability map across the mass–lattice constant parameter space.

This work demonstrates a computationally efficient framework that integrates harmonic lattice dynamics, phonon simulations, and evolutionary optimization. The proposed approach accelerates the identification of mechanically stable configurations and provides a foundation for extending phonon-based stability searches to more complex alloys and crystal systems, contributing to the broader goal of materials discovery.