Mult-objective Genetic Algorithm for Body-Centered Cubic Crystal Stability

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This study carries out the advanced computational techniques to explore the mechanical stabilities of the Body-Centered Cubic (BCC) crystal structures in Born-von Kármán (BvK) reduced parameters space. The research employs a multi-objective genetic algorithm (GA) integrated with the BvK lattice dynamics model to optimize effective harmonic force constants which are crucial parameters for evaluating phonon dispersion and crystal stability. The GA fitness function focuses on optimizing the BvK parameters within the zeroth, first, and second coordination shells, while parameters beyond the fifth coordination shell are constrained to zero to reduce computational complexity and efforts significantly. Phonon dispersion relations are computed using the package *Phonopy*, which diagonalizes the dynamical matrix over the Brillouin zone grid points, enabling the assessment of mechanical stability conditions for each solution. This computational approach facilitates the exploration of the relationships between the force constants of the first and second nearest neighbors, providing insights into the stabilization mechanisms of BCC crystals. By mapping mechanical stability in BvK parameter space, this study aims to accelerate simulations and guide experimental efforts, thereby enhancing computational materials science methodologies for structural stability analysis.