A method for fast approximation of the phonon density of states in crystals

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One method to calculate the phonon density of states of a crystal is to perform enough calculations to determine a system of equations to solve for the elements of the force constant matrix, use the force constant matrix to calculate the dynamical matrix, and then diagonalize the dynamical matrix. For larger and less symmetric crystals, many calculations may be required to complete this process. We develop a method to approximate the phonon density of states in crystals in order to reduce the amount of computation in the circumstances where full accuracy is not required. Using a smaller number of displacement and force sets calculated from the crystal structure along with sets generated on a random basis, we solve for the elements of the dynamical matrix in reciprocal space. To minimize the impact of the random information we force it to conform to known physical constraints such as having zero net displacement and force in configuration space. When applied to a simplified model including only nearest neighbor force constants the method is able to calculate the density of states due to the optical mode and top of the acoustic mode with reasonable accuracy. The existence of a band gap and its approximate size and position is also correctly predicted.