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Phonon anharmonicity from ab initio calculations

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Applying principles similar to those used in creation the harmonic PHONON software, a novel nonperturbative approach of the anharmonic lattice dynamics of crystals is proposed. The method treats a crystal as an ensemble of supercells, each with atoms displaced from equilibrium positions, such that the created POSCAR mimics the atomic configuration arising from all allowed excited phonons with amplitudes determined by the requested temperature. Next, using VASP and PhononA softwares the computed phonon dispersion curves are averages over created atom configurations to show the anharmonic phonon peaks and their finite widths and shifts. The method also allows to treat directly the soft modes. The thermal conductivity can be estimated after adopting the Green-Kubo formalism to the present non-perturbative method. Anharmonic results for fcc-Pb, bcc-W, cubic-Si, fcc-MgO, mineral-$MgSiO_3$, AlN, MgB_2 and soft mode in NiTi will be shown. The calculated anharmonic behaviour of MgB_2 superconductor is well reproduced with the proposed method, including the giant width of E_{2g} phonon branch in agreement to its x-ray measurements.

For other crystals, when available, the results are compared to measured data.

The complete formulations of the harmonic and anharmonic theories is only shortly presented. The details can be found in the recent paper of the author, Phys.\ Rev.\ B {\bf 98}, 054305 (2018). The method is highly parallel and computationally very fast, since using VASP, in general it requires only single run of ionic loop for each atomic configuration POSCAR. Typically, a comprehensive anharmonic study of a material takes less than a˜(few) day(s).

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