Spectral Phonon Relaxation Time Calculation Tool Based on Molecular Dynamics

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ABSTRACT

Thermal conductivity is an important material property which affects the performance of a wide range of devices from thermoelectrics to nanoelectronics. Information about phonon vibration modes and phonon relaxation time gives significant insight into understanding and engineering material’s thermal conductivity. Although different theoretical models have been developed for studying phonon modes and relaxation time, extensive knowledge of lattice dynamics and molecular dynamics is required to compute phonon modal frequencies and relaxation times. Therefore, a computational tool which can take simple inputs to calculate phonon mode frequencies and relaxation time will be beneficial. Through this research work, such computational tool has been developed. A computational style ‘compute sed’ has been added to Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). It computes the Spectral Energy Density (SED) for each mode of vibration. Two different MATLAB scripts perform Fourier Transform and fit the results to a Lorentzian form to calculate phonon mode frequency and relaxation time. The computational tool is validated by comparing its results with previously obtained results. After the verification, the computational tool has been deployed in nanoHUB.org which can be utilized by users around the globe.

KEYWORDS

Phonon, thermal conductivity, LAMMPS compute style