Reduction effect on thermal conductivity of Silicon by defect structures investigated from atomistic level

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Introduction

Lattice defects such as vacancies, voids, or dislocations are inevitably present in any material of technological interest. Such defects break the crystal structures’ symmetry which makes the analysis using lattice dynamics methods challenging. Non-equilibrium molecular dynamics (NEMD) simulations are conducted to investigate how monoatomic vacancies and nano-voids influence the lattice thermal conductivity of silicon. To develop a fundamental understanding of these observations, the spectral energy densities (SED) for all phonon branches obtained from 2D Fourier transformation of the atomic trajectories are analyzed, which demonstrates the feasibility of using MD to evaluate thermal transport in defected non-metal materials.

- **Model:** Pre-induced vacancies and nano-voids (with 0.1% - 10% volume fraction) are randomly distributed.
- **NEMD:** Thermal flux is imposed by Müller-Plath method [1], that is the particles in the cold (green) and hot (red) regions are chosen for exchanging kinetic energies to create the temperature gradient. Three-body Stillinger-Weber atomic potential [2] for silicon is used.

Method

- Fourier Law
  \[ \kappa = -\frac{1}{3} \rho c \nabla T \]
  \( \kappa \): thermal conductivity; \( J \): thermal flux; \( \nabla T \): temperature gradient

Results

Spectral energy density

\[ \Phi(k, \omega) = \sum_{\alpha \beta} \left| \langle \phi_{\alpha}(x, t) | \phi_{\beta}(x, t) \rangle \right|^2 \]

Phonon relaxation time is given as the half-width at the half maximum of the Lorentzian function [7].

Conclusion

- Reduction of thermal conductivity is mainly attributed to the phonon relaxation time.
- Smaller defect sizes have stronger scattering effect on phonon transportation. Small defect volume fractions cause a strong effect on phonon.
- Flat region in phonon relaxation curves indicates the saturation of the scattering effect which is attributed to the averaged defect distances and the domain size.