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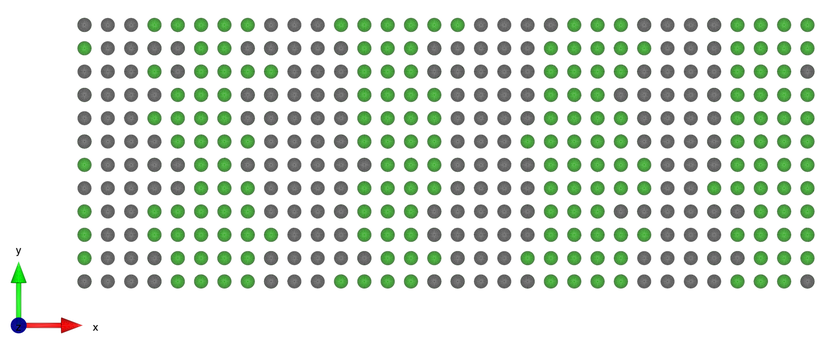
Introduction

- Superlattices are periodic nanostructure

Objective

- Cross-Plane vs In-Plane
- Effects of interspecies diffusion



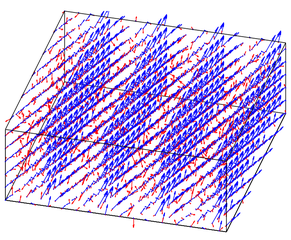
Methodology

Atomic velocities sampled from Molecular Dynamics

$$\dot{u}(jl,t)$$

Eigenvectors and group velocities from Lattice Dynamics

$$e(j,\kappa,\nu)$$



Normal mode coordinates obtained from projecting atomic velocities onto eigenvectors

$$\dot{Q}(j,\kappa,t)=\frac{1}{\sqrt{N}}\sum_{jl}\sqrt{m_j}e^{(-i\kappa\bullet r(jl))}e(j,\kappa,\nu)\bullet\dot{u}(jl,t)$$

Autocorrelation and Fourier Transform of Q yields the power spectrum of Lorentzian form

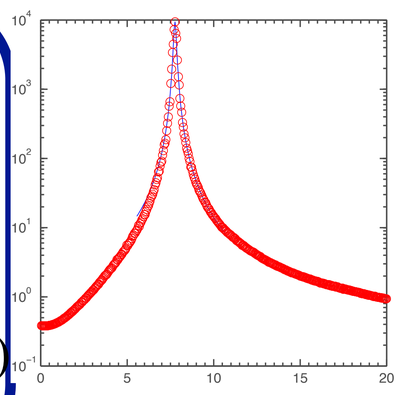
$$\int_{-\infty}^{\infty}\lim_{T\to\infty}\left[\frac{1}{T}\int_0^T\dot{Q}(j,\kappa,t+t')\dot{Q}(j,\kappa,t')dt\right]e^{-i\omega t}\,dt=\frac{\Gamma(\kappa,\nu)/\pi}{(\omega_0(\kappa,\nu)-\omega)^2+\Gamma(\kappa,\nu)}$$

Fitting the Lorentzian yields the phonon lifetime

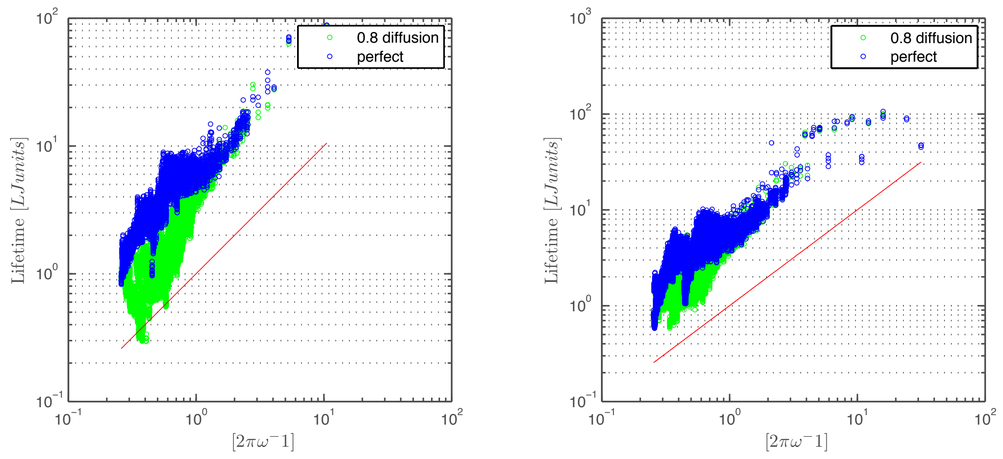
$$\tau(\kappa,\nu)=\frac{1}{2\Gamma(\kappa,\nu)}$$

The thermal conductivity

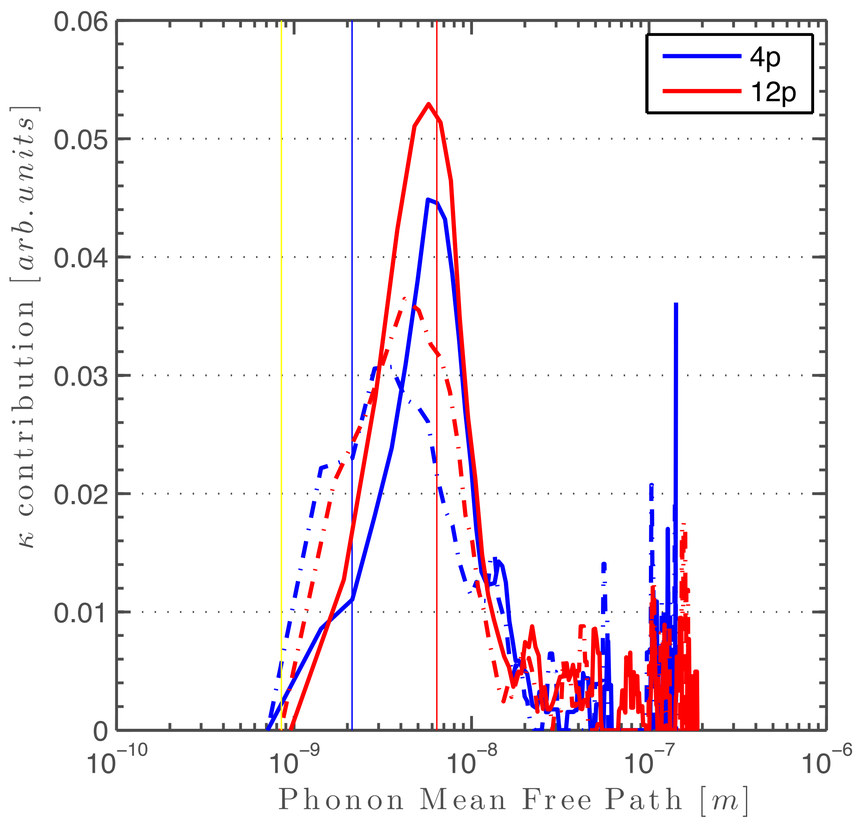
$$k_i=\sum_{\nu}\sum_{\kappa}c(\kappa,\nu)v_{g,i}^2(\kappa,\nu)\tau(\kappa,\nu)$$



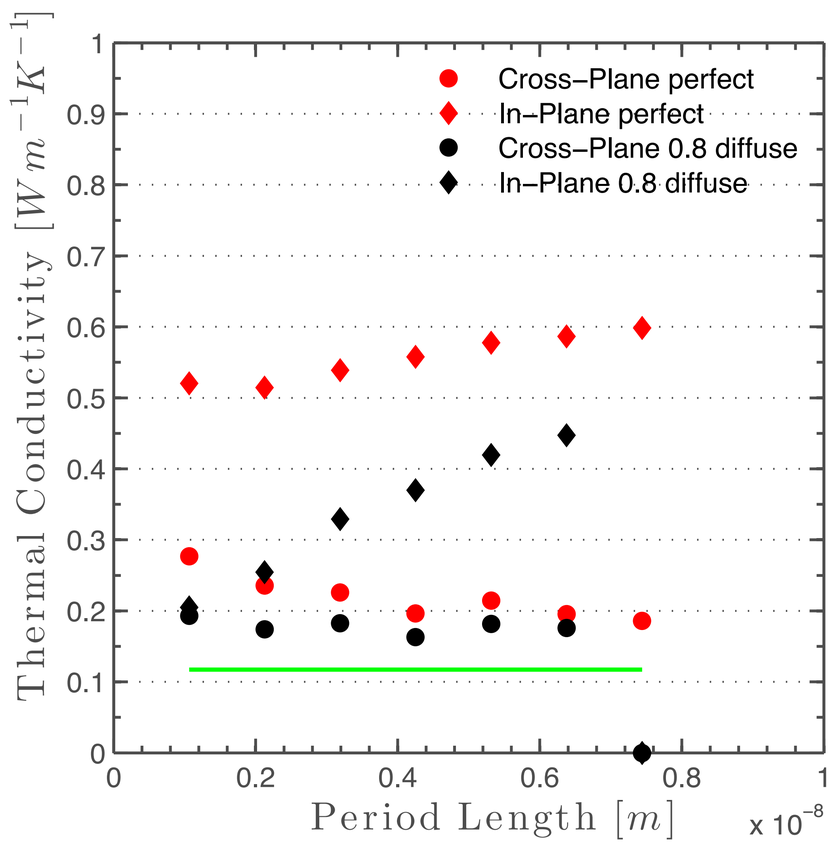
Results



Effect of interspecies diffusion on phonon lifetimes.



Effect of interspecies diffusion upon thermal conductivity depence upon MFP.



Effect of interspecies diffusion upon cross-plane and in-plane thermal conductivity.

Conclusions