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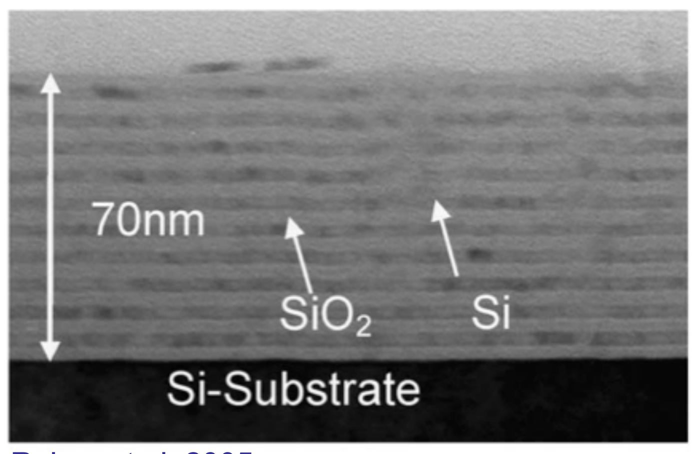
Introduction

- Superlattices are periodic nanostructures with promising ability to manipulate the thermoelectric figure of merit (ZT) by tuning thermal conductivity

$$ZT = \frac{\Omega S}{k}$$

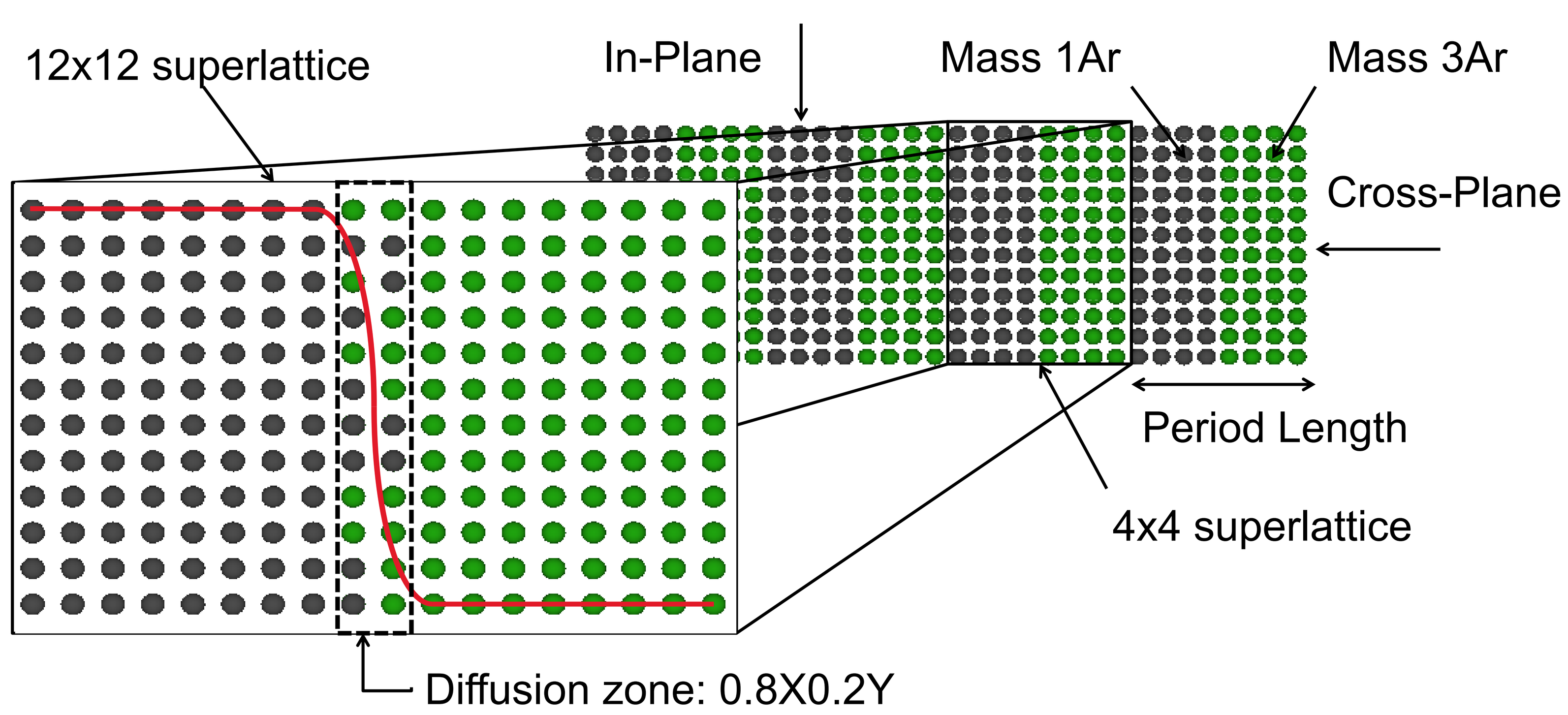


Rolver et al. 2005

Objective

Use Lennard – Jones Argon at 20K with a mass ratio of 1:3 to investigate

- Cross-Plane versus In-Plane thermal conductivity



- Effect of interspecies diffusion upon phonon mean free path

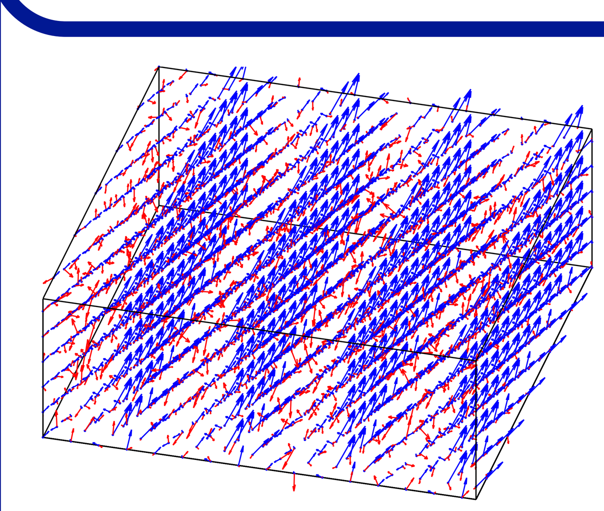
Methodology: Normal Mode Decomposition

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

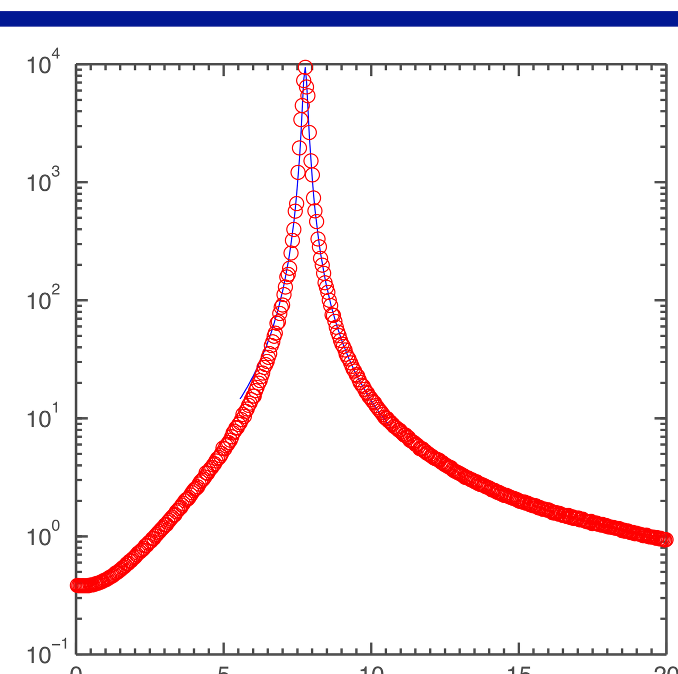
$$\dot{Q}(j,\kappa,t) = \frac{1}{\sqrt{N}} \sum_{jl} \sqrt{m_j}\, e^{(-i\kappa \cdot r(jl))} e(j,\kappa,\nu) \cdot \dot{u}(jl,t)$$

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

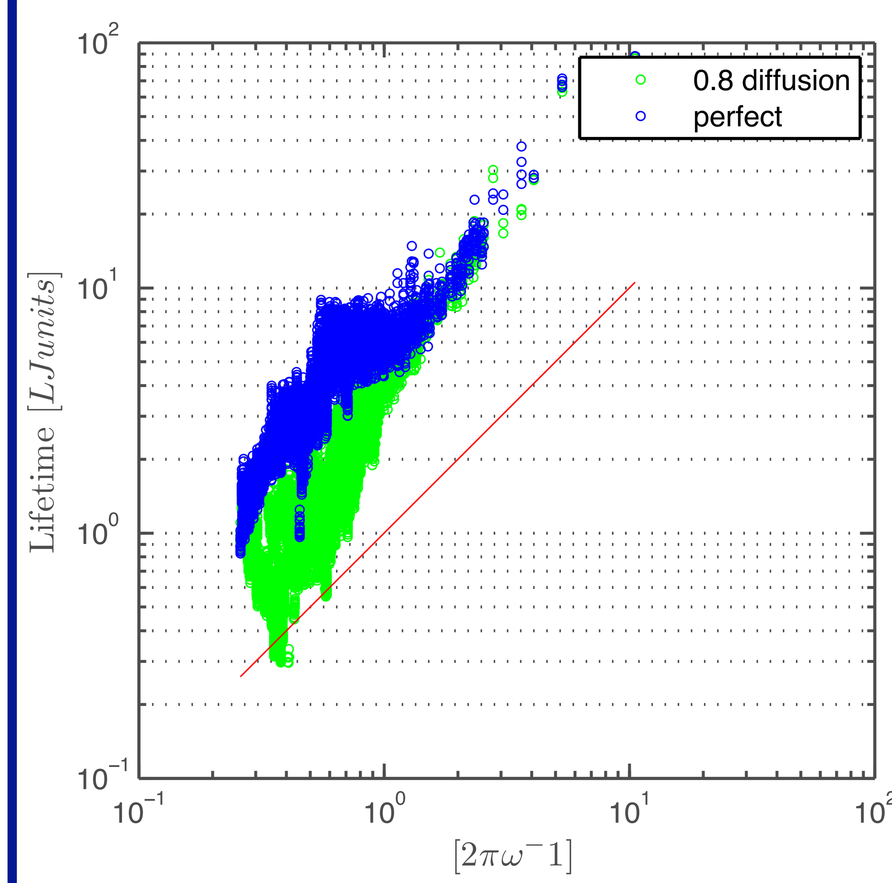
$$\int_{\infty}^{\infty} \left[\lim_{T\to\infty} \frac{1}{T} \int_0^T \dot{Q}(j,\kappa,t+t')\dot{Q}(j,\kappa,t')\,dt \right] e^{-i\omega t}\, dt = \frac{\Gamma(\kappa,\nu)/\pi}{(\omega_0(\kappa,\nu)-\omega)^2 + \Gamma(\kappa,\nu)}$$

Fitting the Lorentzian yields the **phonon lifetime**

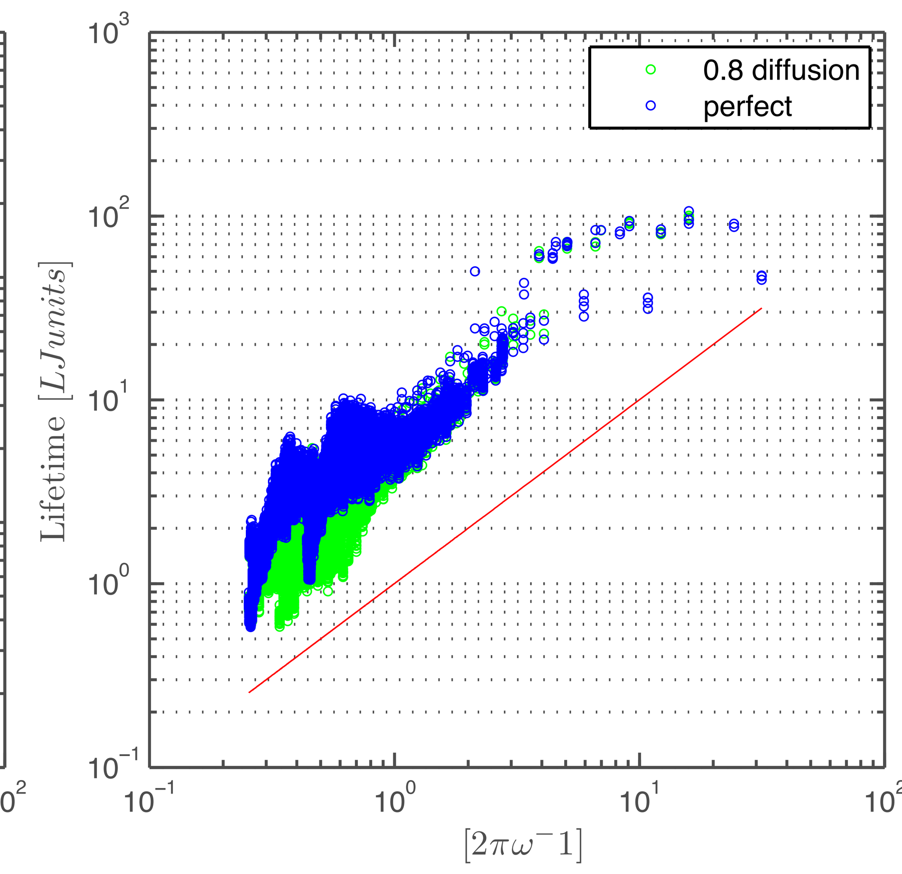
$$\tau(\kappa,\nu) = \frac{1}{2\Gamma(\kappa,\nu)}$$



Results

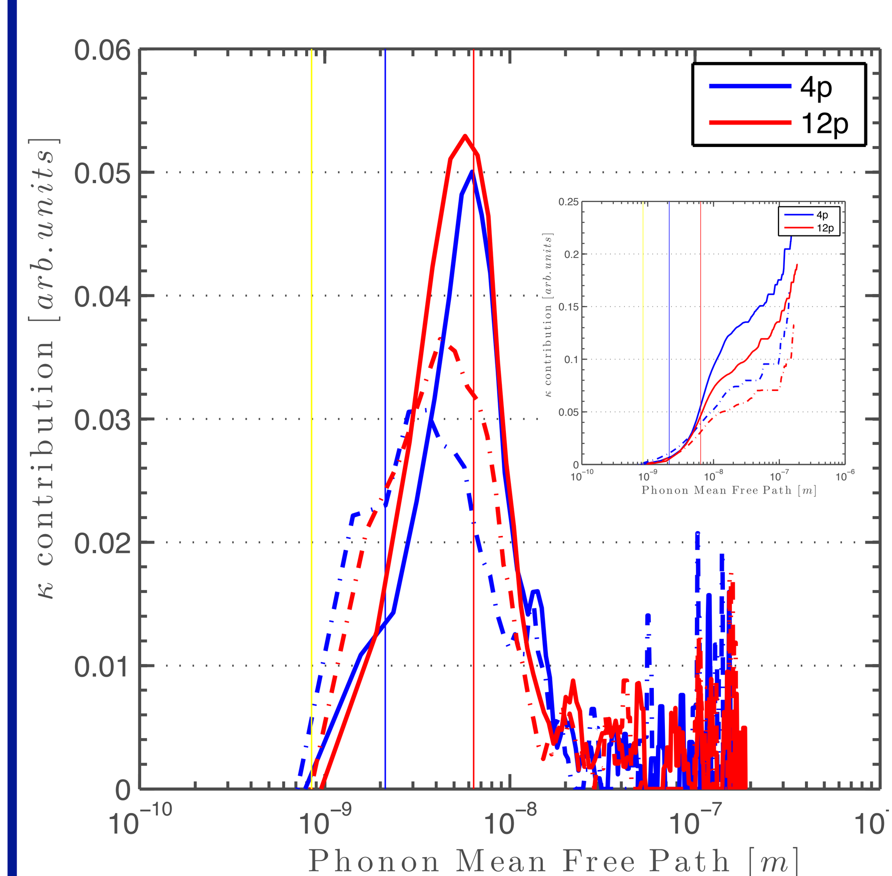


Phonon lifetimes in 4x4

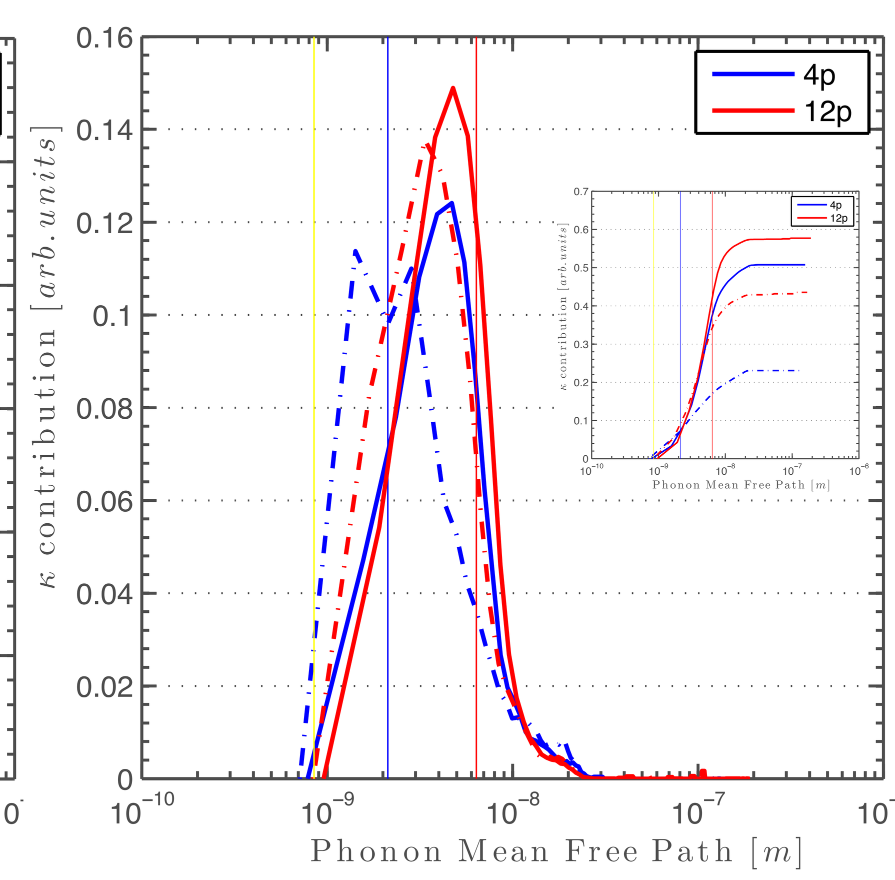


Phonon lifetimes in 12x12

$$\Lambda_i = v_{g,i}(\kappa,\nu)\tau(\kappa,\nu)$$

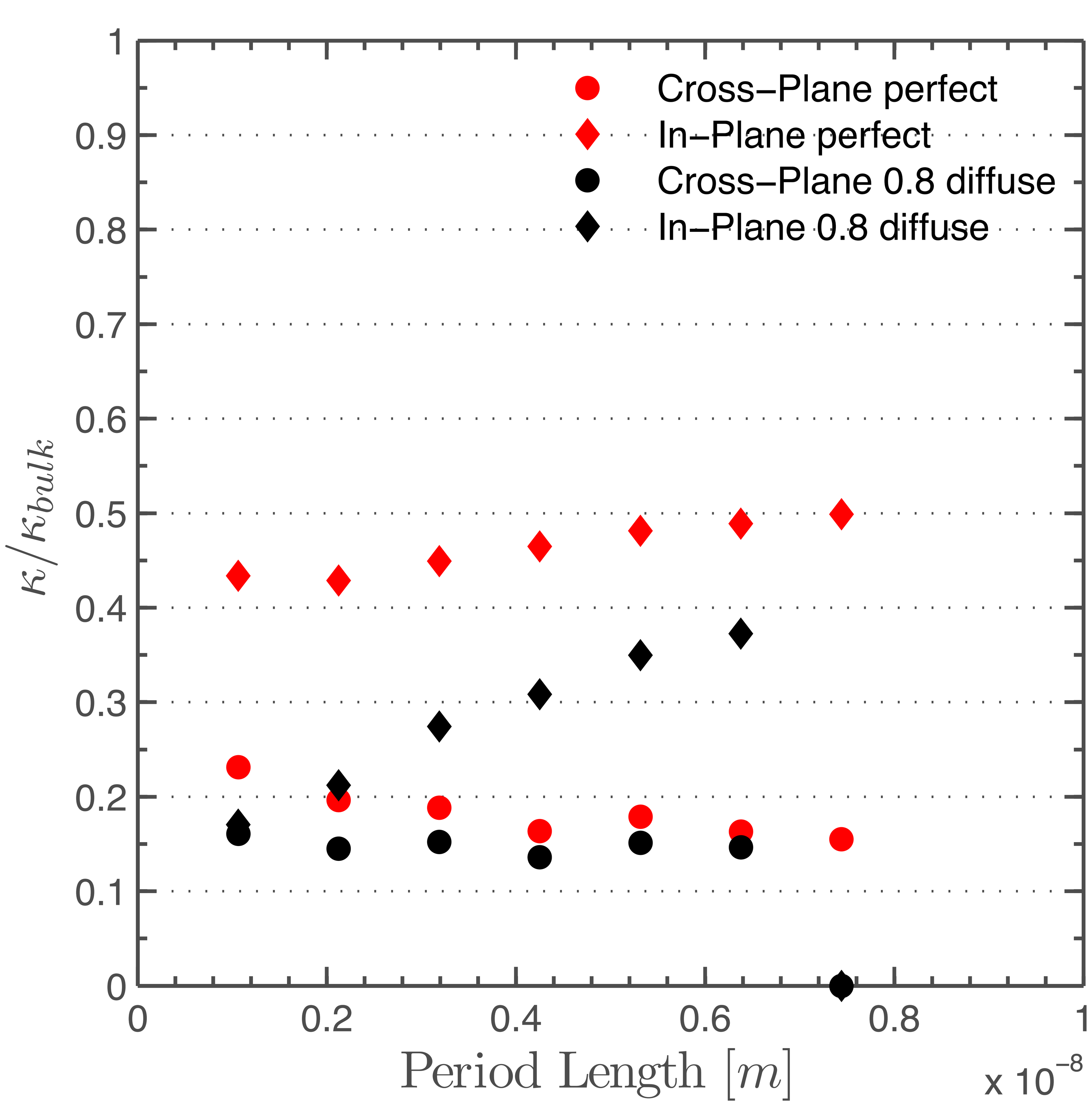


Cross-plane 4x4 and 12x12



In-plane 4x4 and 12x12

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



In-plane and cross-plane thermal conductivity as a function of superlattice period length.

Conclusions