Thermal Conductivity Predictions for Nanostructures by Phonon Free Path Sampling

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INTRODUCTION

Thermal Conductivity,

$$k = \sum_{\kappa} \sum_{v} C_{ph} \binom{\kappa}{v} v_g^2 \binom{\kappa}{v} \tau \binom{\kappa}{v}$$

Bulk Material:

-Phonon-phonon scattering

-Techniques like Lattice Dynamics Method

Nanostructures:

-Phonon-phonon and phonon boundary scattering

-Matthiessen rule

Matthiessen Rule

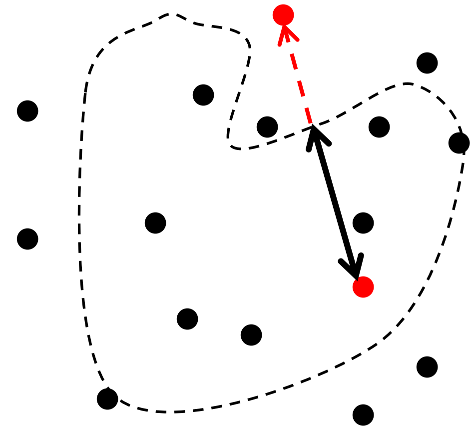
$$\frac{1}{\bar{\tau}_M\binom{\kappa}{v}} = \frac{1}{\bar{\tau}_{p-p}\binom{\kappa}{v}} + \frac{1}{\bar{\tau}_b\binom{\kappa}{v}}$$

- Based on average phonon properties
- Assumes independence of scattering mechanisms
- Irregular geometries and specular scattering:

$$\bar{\tau}_b\binom{\kappa}{v} = ?$$

Alternative Approach

$$\tilde{\tau}_{eff} = \text{minimum}(\tilde{\tau}_{p-p}, \tilde{\tau}_{b-p})$$

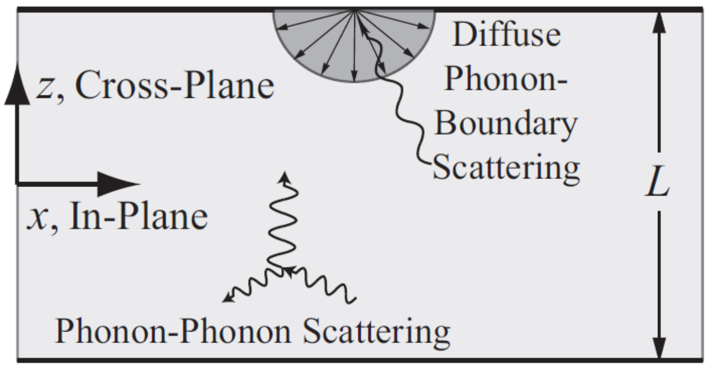


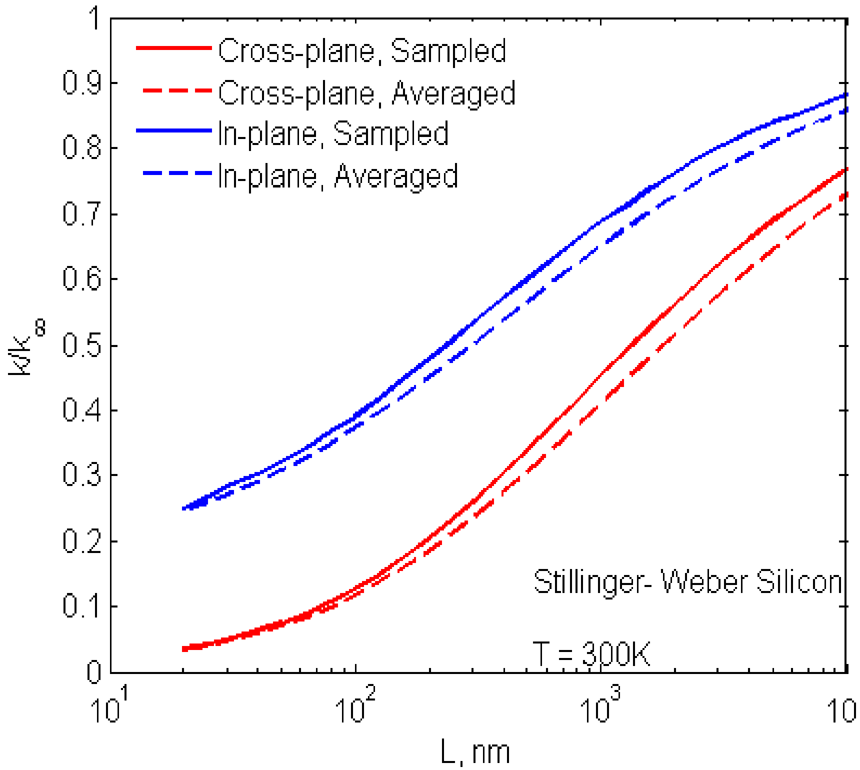
Sampled from Poisson distribution

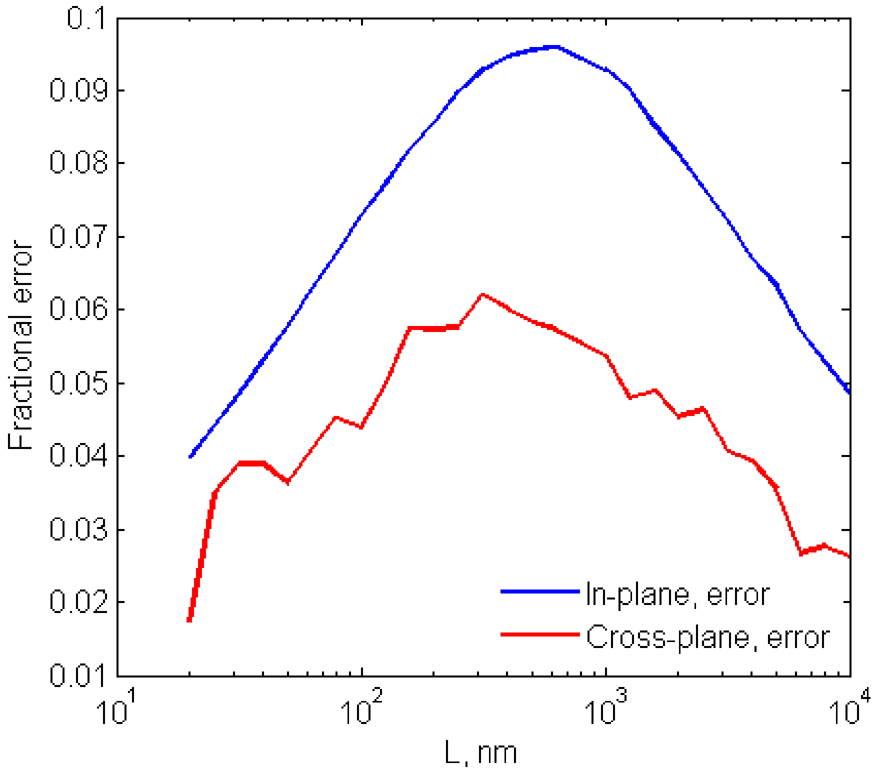
$$P(\tilde{\tau}) = \frac{1}{\bar{\tau}} e^{-\frac{\tilde{\tau}}{\bar{\tau}}}$$

Random sampling of phonons initial position inside the material

Results: Thin Film

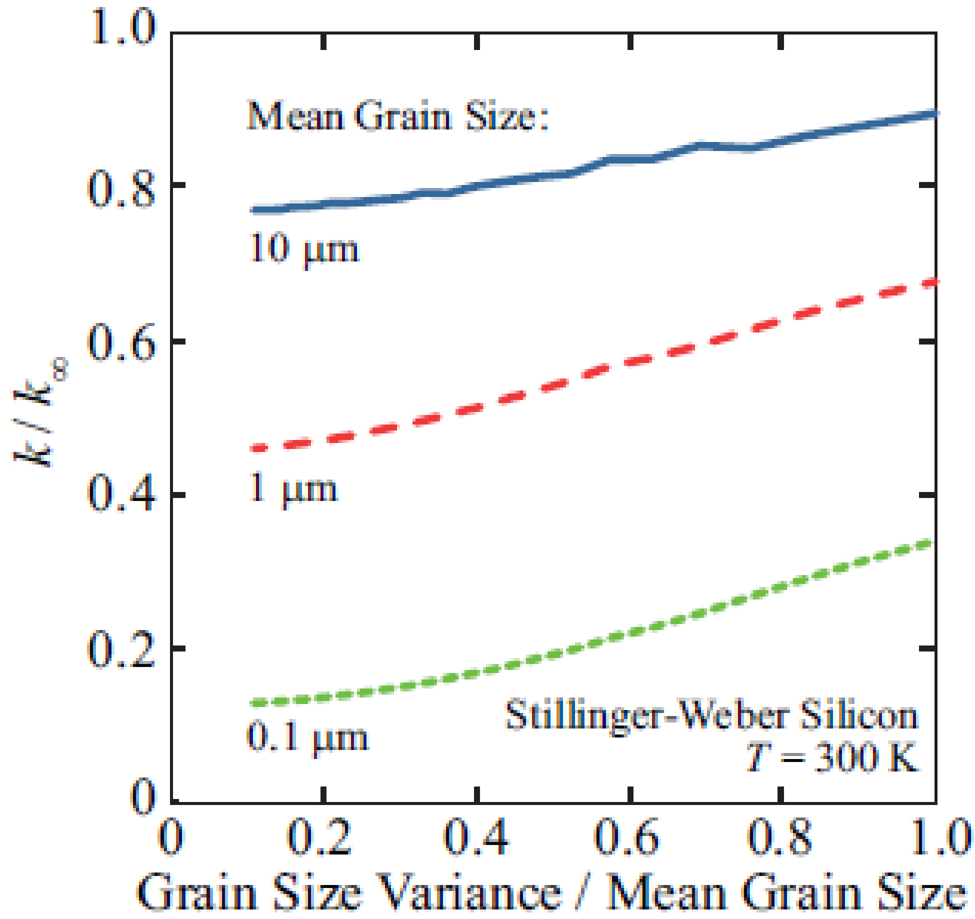






Thermal conductivity predictions for thin film

Results: Polycrystalline Material



Thermal conductivity predictions for polycrystalline material with spherical grains

Future work

- Porous thin films with cylindrical holes
- Understanding Lattice Dynamics calculations for generating bulk phonon properties

Thank You