PREDICTING THERMAL TRANSPORT IN NANOSTRUCTURES USING *AB-INITIO* CALCULATIONS

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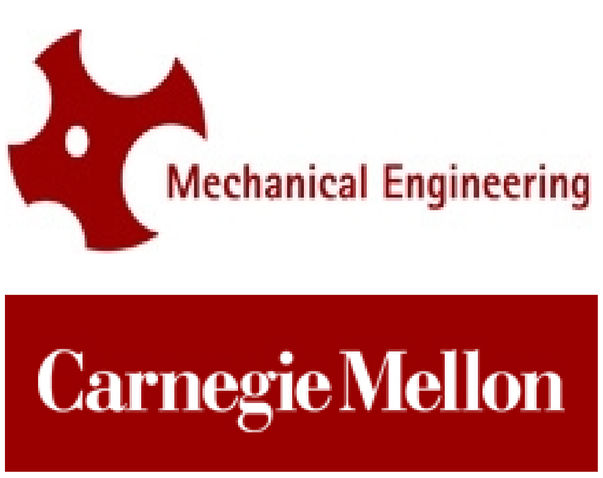
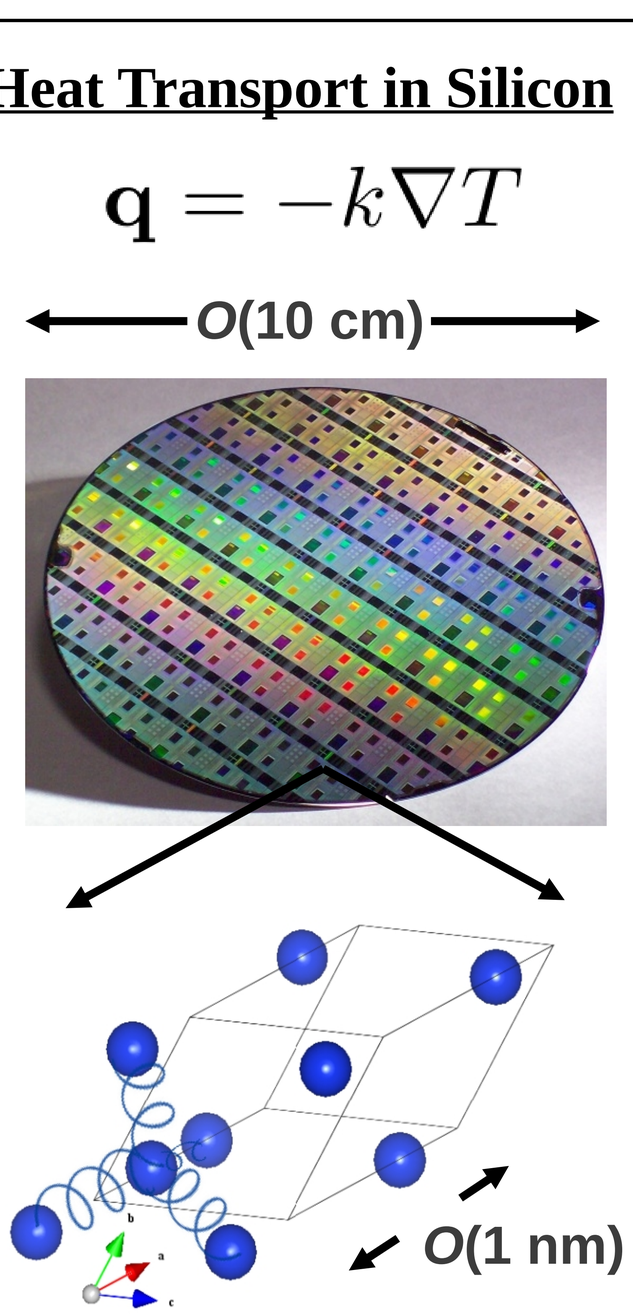
Heat Transport in Silicon

$$\mathbf{q} = -k\nabla T$$

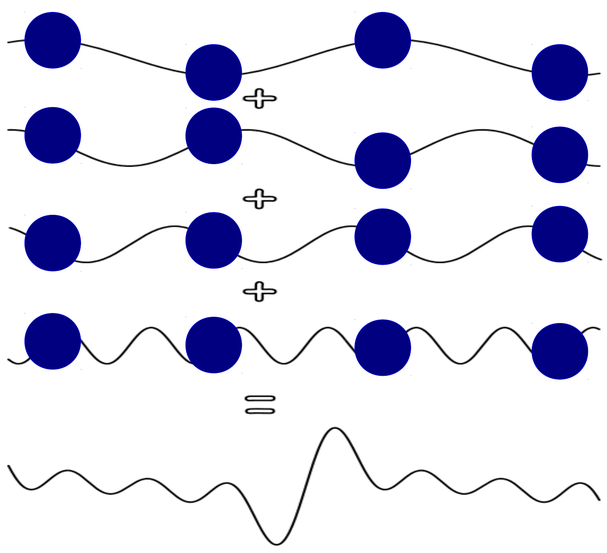
O(10 cm)





Energy Carriers: Phonons

$$k_{\mathbf{n}} = \sum_{\boldsymbol{\kappa}} \sum_{\nu} c_{ph}\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) \boldsymbol{v}^2_{g,\mathbf{n}}\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) \frac{\Lambda\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right)}{|\boldsymbol{v}_g|}$$



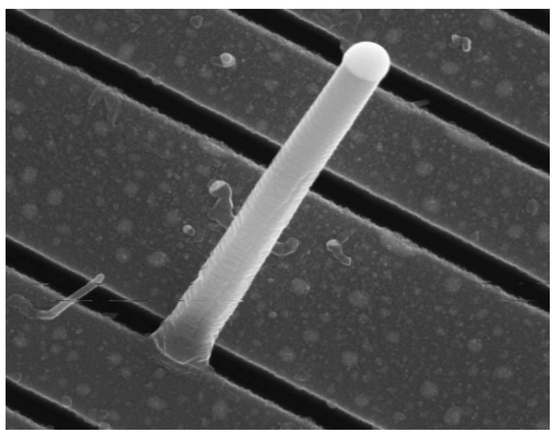
Group Velocity: v_g

Bulk Mean Free Path:

Λ_{p-p} = *O*(1 nm – 10 μm)

Heat Transport in Nanostructures

- Nanowires/rods



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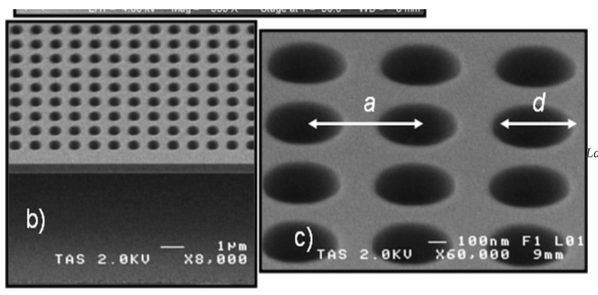
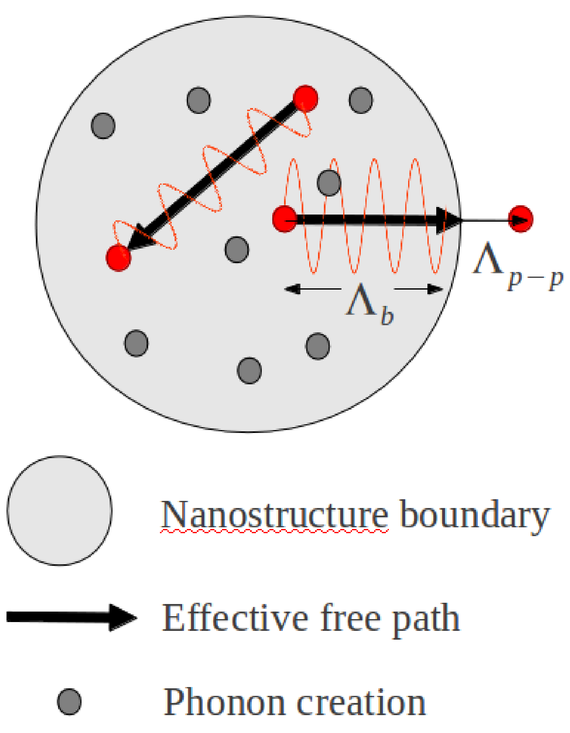
- Porous Silicon



Nano Letters **11**, 107-112 (2011).

Monte Carlo Sampling

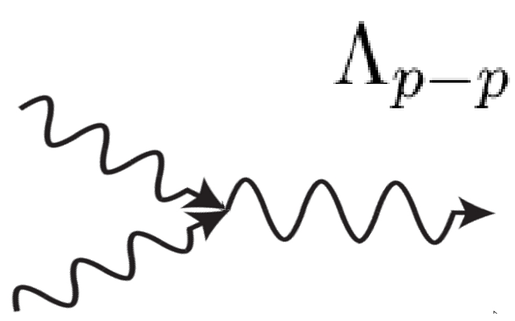
$$\Lambda_{eff} = min\left(\Lambda_{p-p}, \Lambda_b\right)$$



A. J. H. McGaughey and A. Jain, "Nanostructure thermal conductivity prediction by Monte Carlo sampling of phonon free paths." Applied Physics Letters 100 (2012) 061911.

Bulk Phonon Properties

Phonon-Phonon Scattering



3-phonon process

- Conservation of energy:

$$\omega\left(\begin{smallmatrix}\boldsymbol{\kappa}\\ \nu\end{smallmatrix}\right) + \omega\left(\begin{smallmatrix}\boldsymbol{\kappa}'\\ \nu'\end{smallmatrix}\right) = \omega\left(\begin{smallmatrix}\boldsymbol{\kappa}''\\ \nu''\end{smallmatrix}\right)$$

- Lattice translational invariance:

$$\boldsymbol{\kappa} + \boldsymbol{\kappa}'' = \boldsymbol{\kappa}'' + \boldsymbol{G}$$

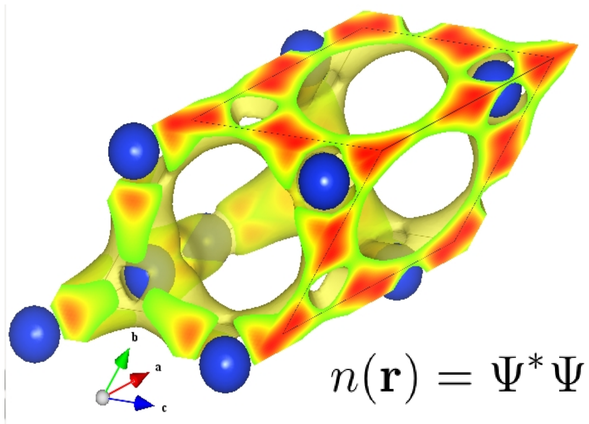
Ab-Initio Calculations VASP

- Phonon-Phonon interactions:

$$\Phi\begin{pmatrix}\boldsymbol{\kappa} & \boldsymbol{\kappa}' & \boldsymbol{\kappa}''\\ \nu & \nu' & \nu''\end{pmatrix}$$

- Calculated by Density Functional Theory:

$$\hat{H}\Psi = [\hat{T} + \hat{V}_{Har} + \hat{V}_{ext} + \hat{V}_{xc}]\Psi$$



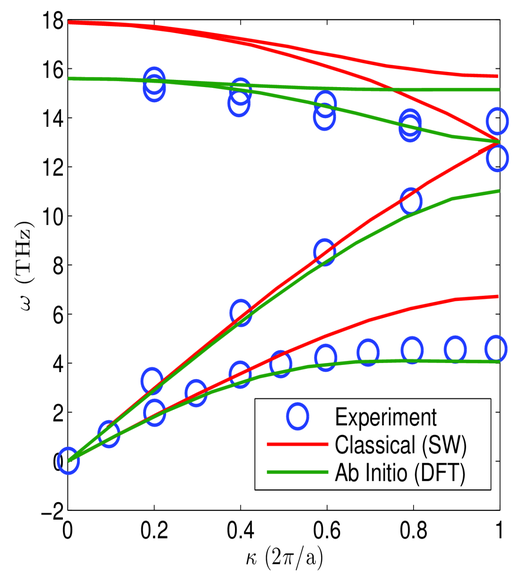
$$n(\mathbf{r}) = \Psi^*\Psi$$

http://www.vasp.at/

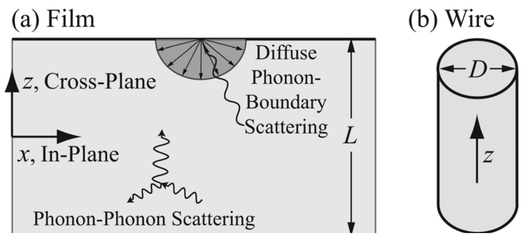
Accurate Predictions

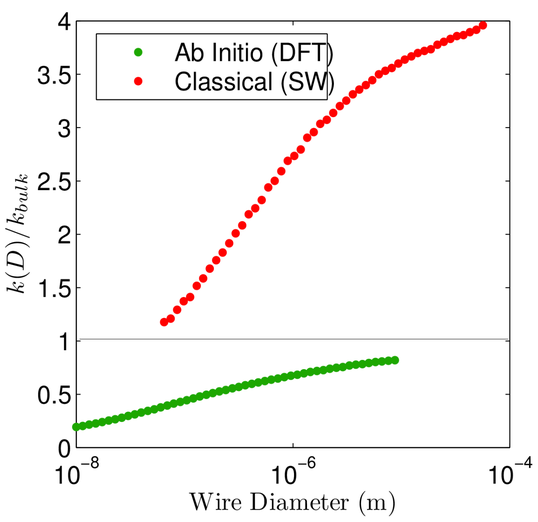
Group Velocity

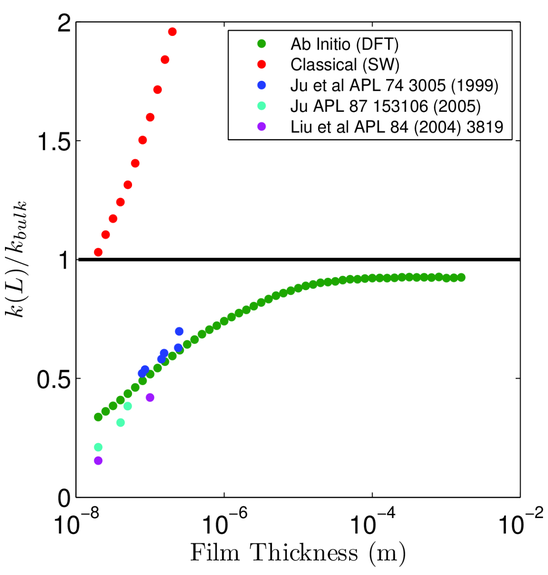
$$v_g = \partial\omega/\partial\boldsymbol{\kappa}$$



Effective Mean Free Path:







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