Atomistic Green's Function Method: Density of States and Multi-dimensionality

Timothy S. Fisher
Purdue University
School of Mechanical Engineering, and
Birck Nanotechnology Center
tsfisher@purdue.edu

Based on:

W. Zhang, T.S. Fisher, N. Mingo, "The Atomistic Green's Function Method: An Efficient Simulation Approach for Nanoscale Phonon Transport," *Numerical Heat Transfer: Part B (Fundamentals)*, Vol. 51, No. 3/4, pp. 333-349, 2007.

Density of States Definitions

- Recall the phonon density of states that gives the number of modes per unit frequency per unit volume of real space

$$D(\omega) = \frac{1}{L^{\alpha=1}}\frac{dN}{d\omega} = \frac{1}{L}\frac{dN}{dK}\frac{dK}{d\omega} = \frac{1}{\pi}\frac{1}{d\omega/dK} = \left[\pi a\sqrt{\frac{g}{m}-\frac{\omega^2}{4}}\right]^{-1}$$

- Proof $\omega = 2\sqrt{\frac{g}{m}}\sin\left(\frac{Ka}{2}\right) \rightarrow \frac{d\omega}{dK} = a\sqrt{\frac{g}{m}}\cos\left(\frac{Ka}{2}\right)$

$$a\sqrt{\frac{g}{m}-\frac{\omega^2}{4}} = a\sqrt{\frac{g}{m}-\frac{g}{m}\sin^2\left(\frac{Ka}{2}\right)}$$

$$= a\sqrt{\frac{g}{m}}\cos\left(\frac{Ka}{2}\right)$$

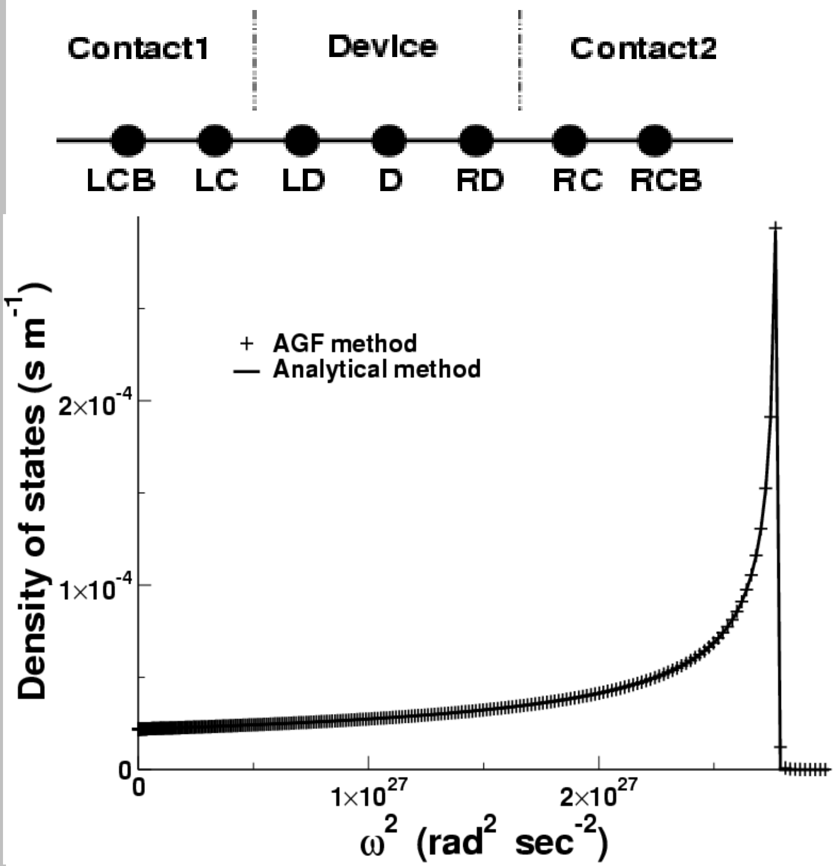
Relation to AGF

- The Green's function inherently contains the local density of states

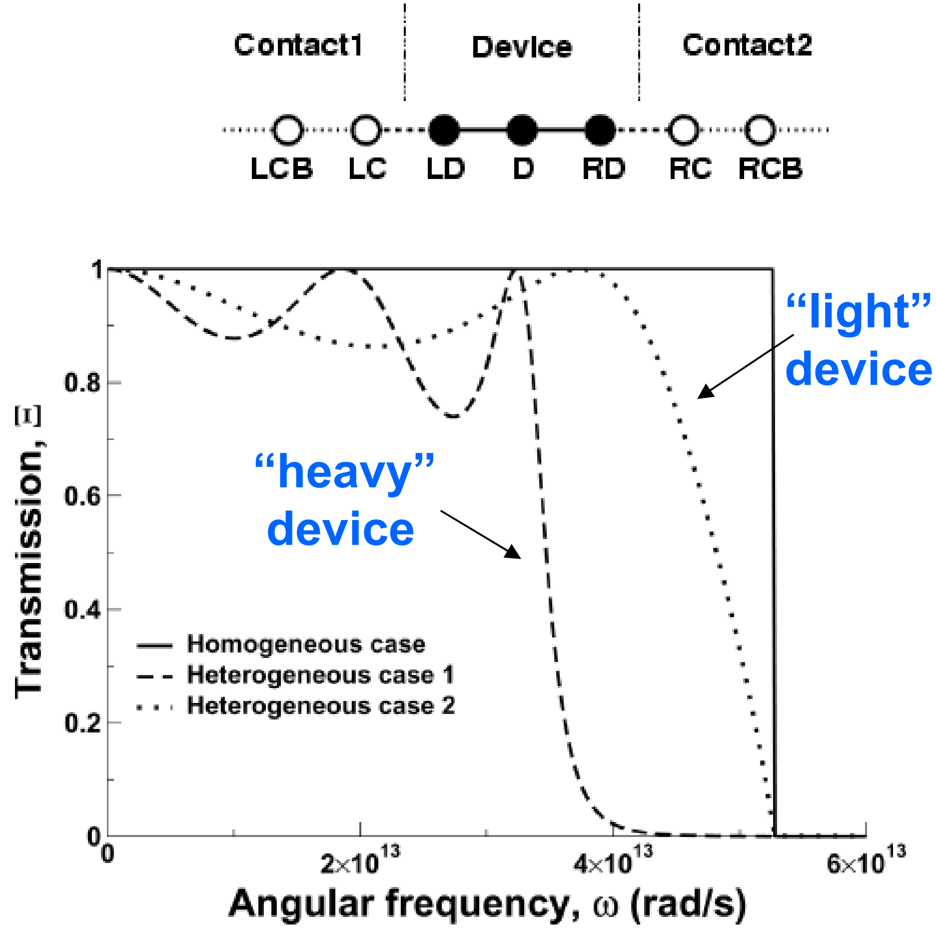
$$\mathbf{D_l}(\omega) = \frac{i\left(\mathbf{G} - \mathbf{G}^{\dagger}\right)\omega}{\pi a}$$

- The local density of states of the ith degree of freedom is the ith diagonal element of $\mathbf{D_l}$
- The global density of states function is the same as the local density of states in homogeneous materials

Results for Simple Atomic Chains



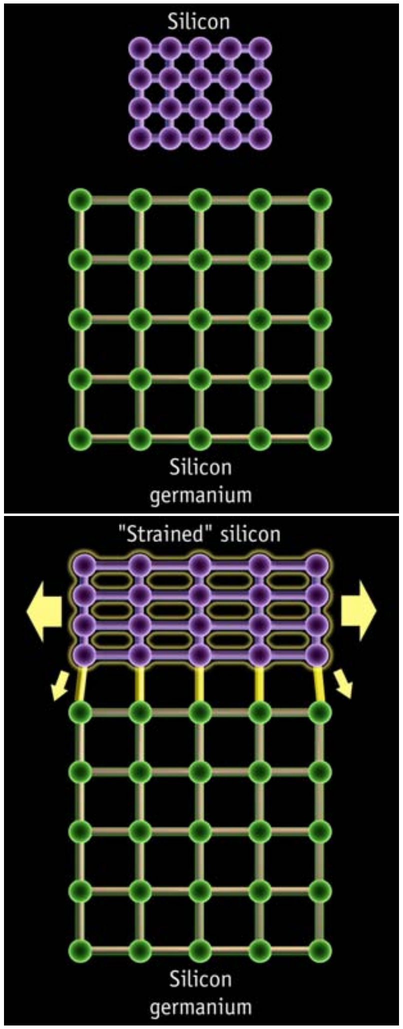
Homogeneous chain density of states



Contact atomic masses = $4.6x10^{-26}$kg
Heavy device masses = $9.2x10^{-26}$kg
Light device masses = $2.3x10^{-26}$kg

Multi-dimensional AGF

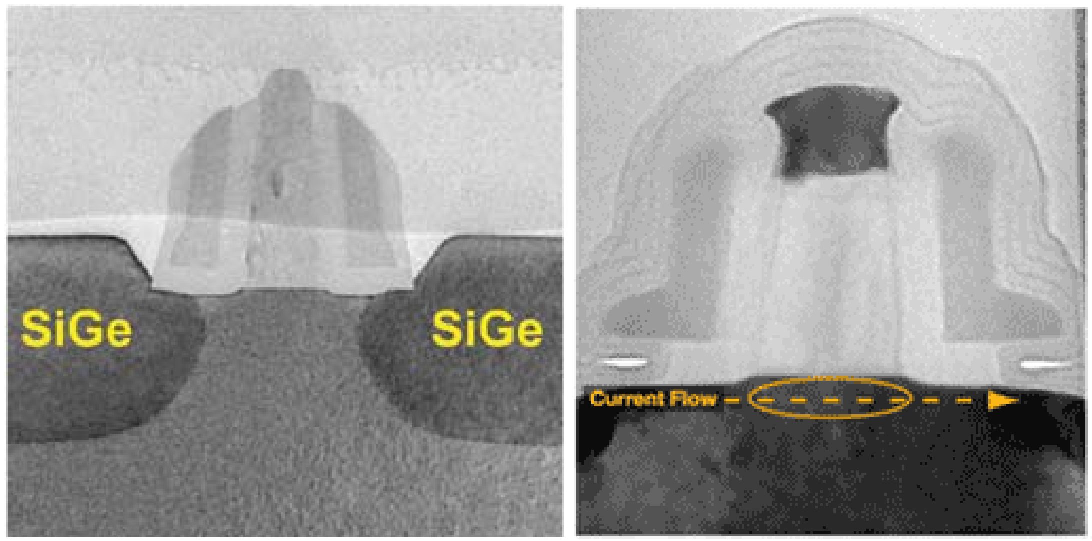
Strained Silicon

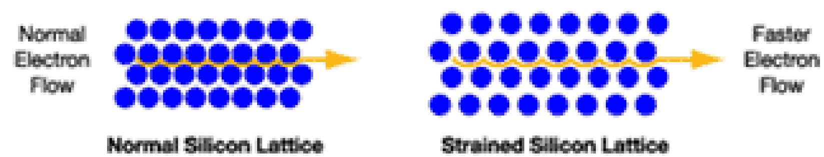


T. Ghani, et al. at IEDM 2003

PMOS

NMOS

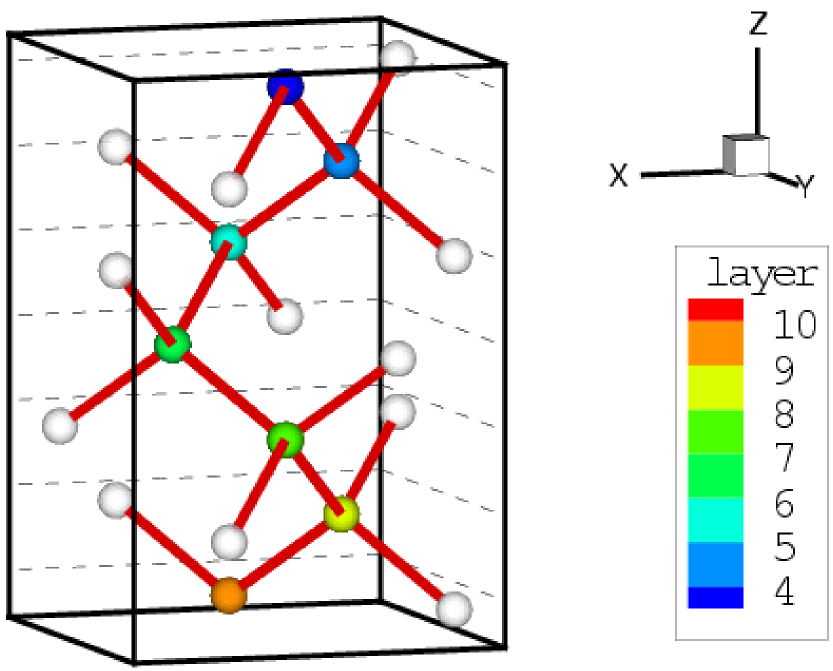


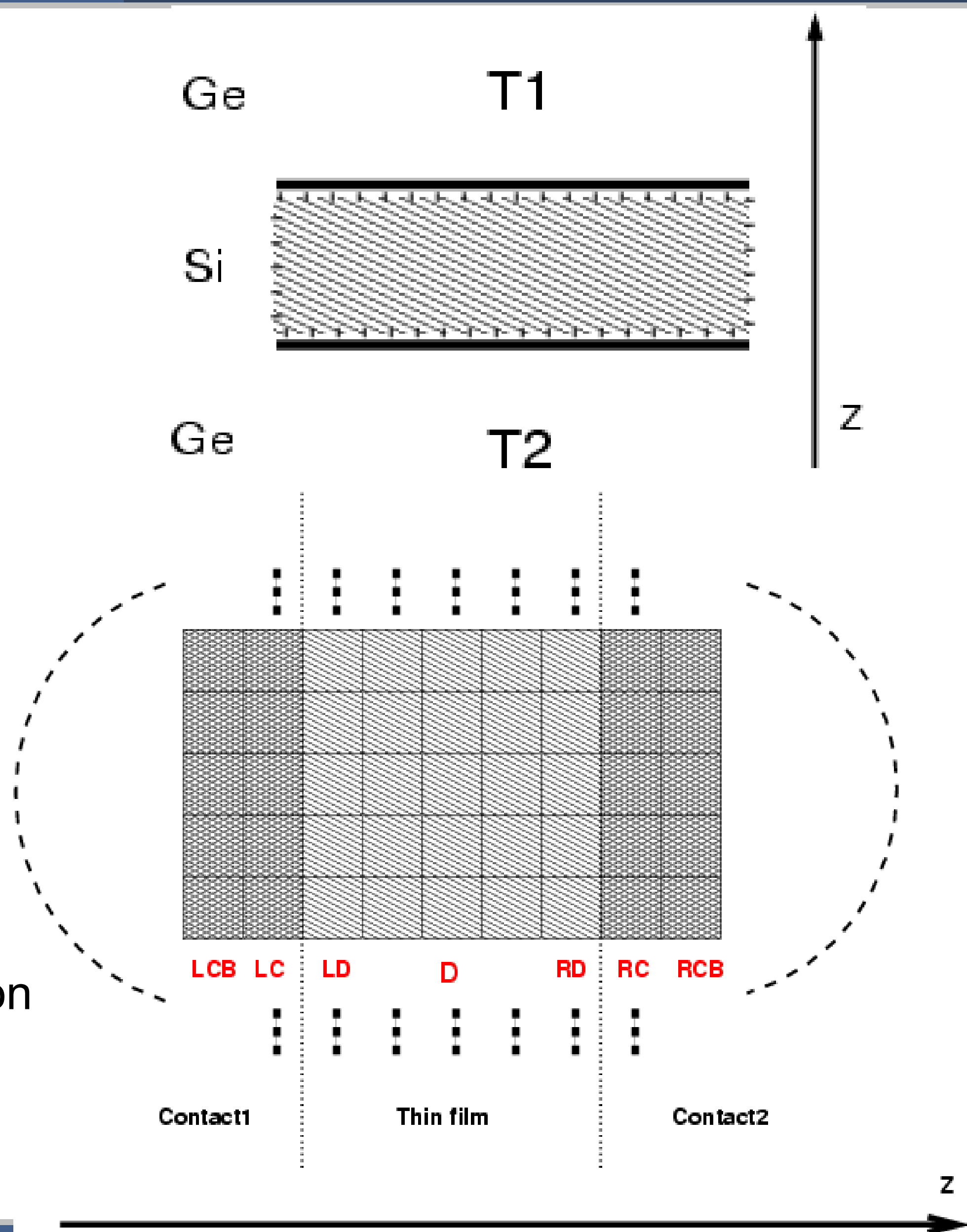


25 % drive current increase in PMOS;
10 % drive current increase in NMOS

http://www.research.ibm.com/resources/press/strainedsilicon/

Thin Films

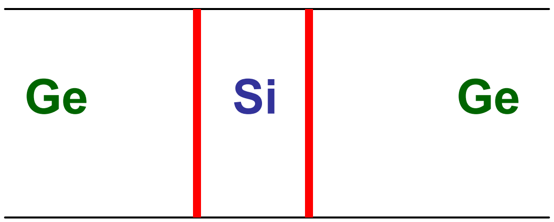




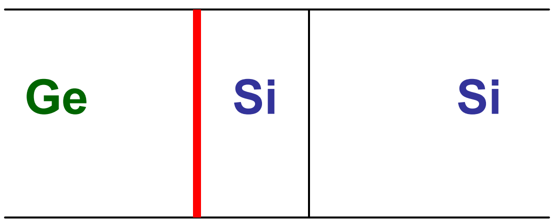
Transport along the (100) direction (i.e., the *z* direction)

Model/Code Validation

Convert Ge/Si/Ge

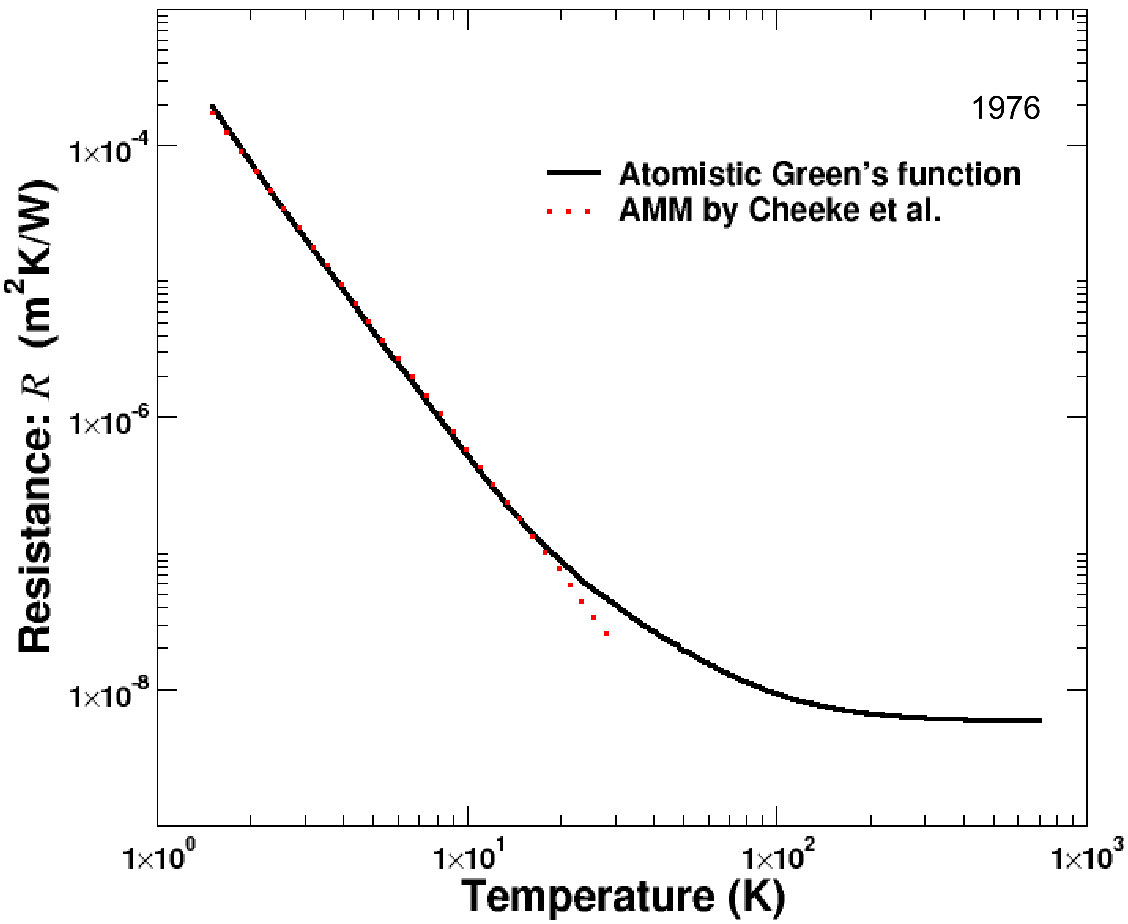


to Ge/Si/Si



to create a single interface.

Zhang et al., J. Heat Trans. in review

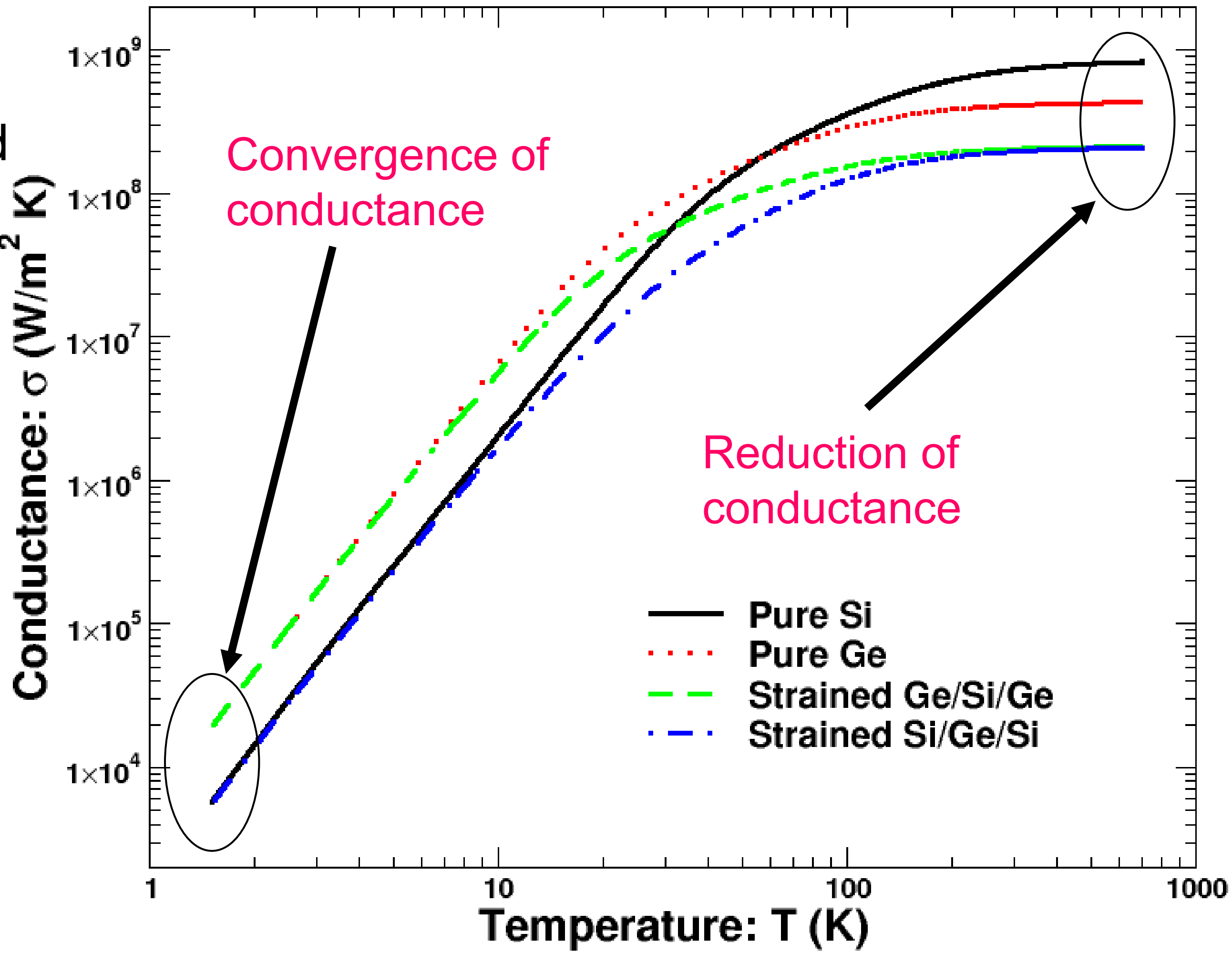


AMM is known to work well at low temperatures

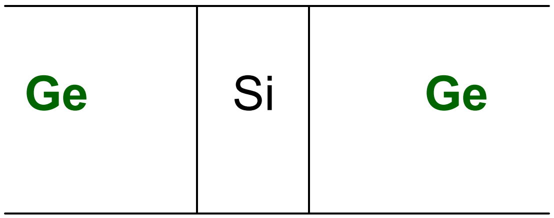
Thermal Conductance

Conductance reduced by 30 to 50% at room temperatures due to heterogeneous interfaces

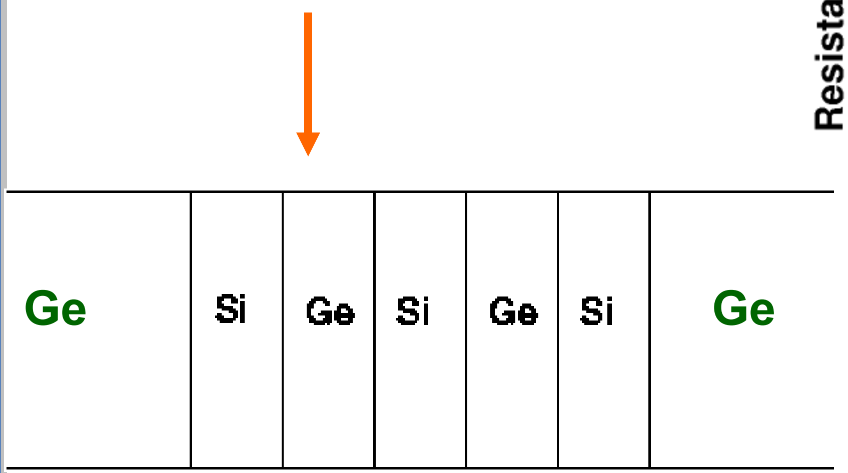
At low temperatures, conductance converges to that of the bulk contacts

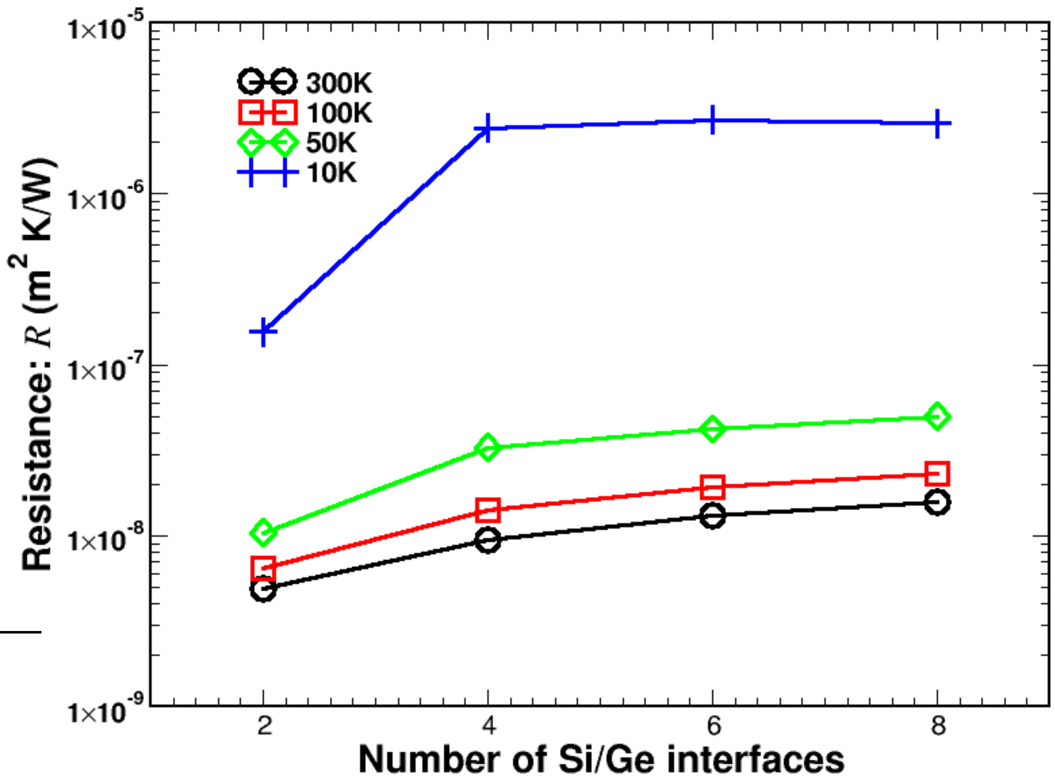


Multilayer Effects



Replace the Si device with a multi-layer structure

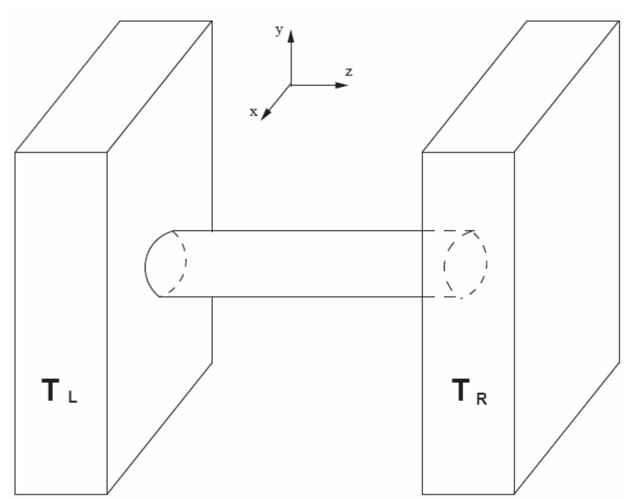


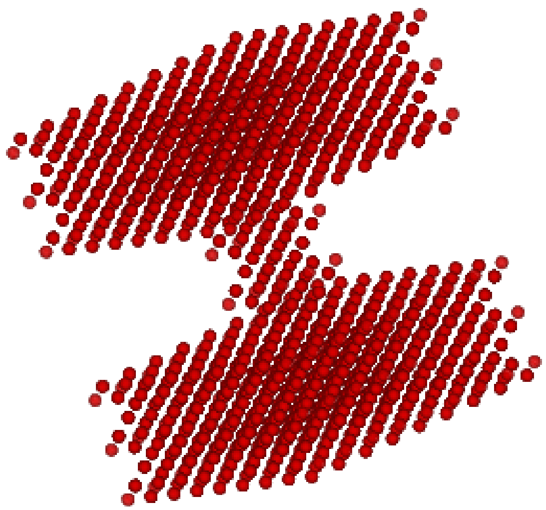


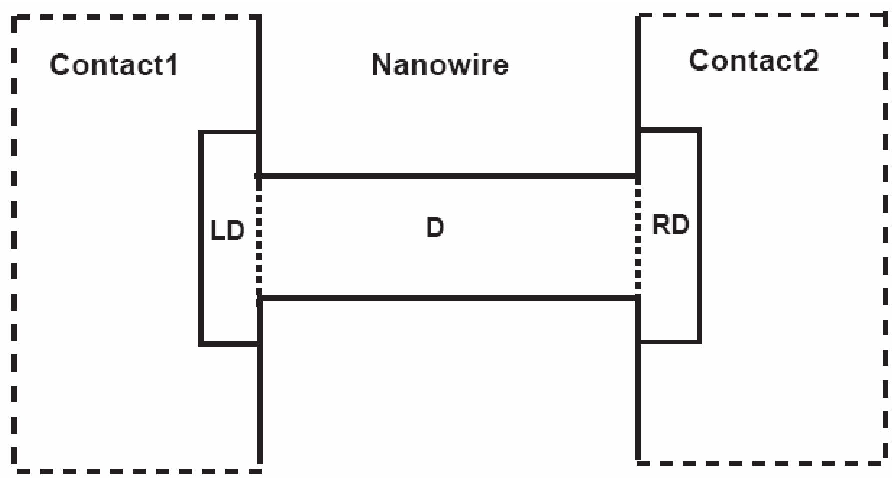
Asymptotic behavior is similar to that of radiation shields

Nanowire-plane Structure

- Nanowires are building blocks for many nanoscale devices and are usually connected to bulk contacts







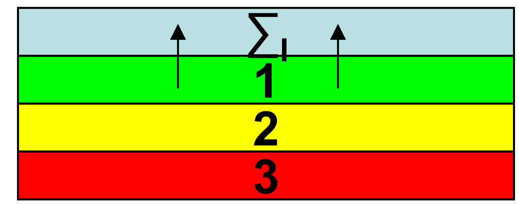
Evaluation of the Self-energy Matrix ∑

- Traditional method (decimation technique) to evaluate the self-energy matrix is difficult to implement at the nanowire-plane interface
  - ♦ Layers have different numbers of atoms as well as shifted atomic locations
  - ♦ Interactions within layers and interactions between layers are difficult to evaluate
- New method is universal for any abruptly changing geometry
  - ♦ Use bare surface g_0 on flat surface

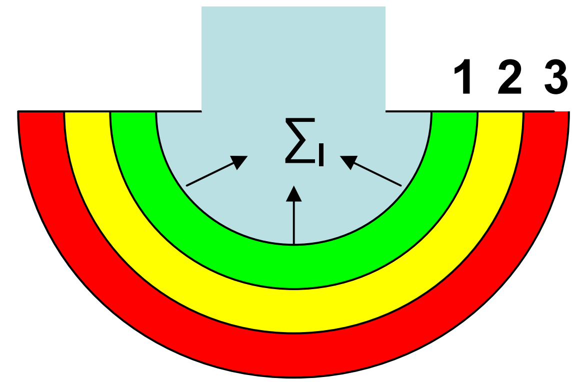
$$\tilde{g}_o = (\omega^2 \mathbf{I} - \mathbf{H}_{LDm} - \Sigma_L)^{-1}$$

  - ♦ $\sum_l$ is the same no matter whether it is attached to nanowire or just a flat bare surface

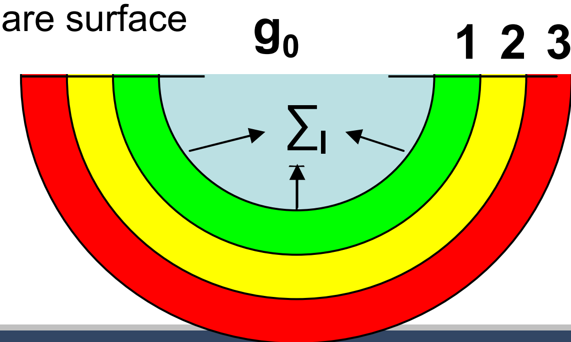
Thin film



Nanowire-plane



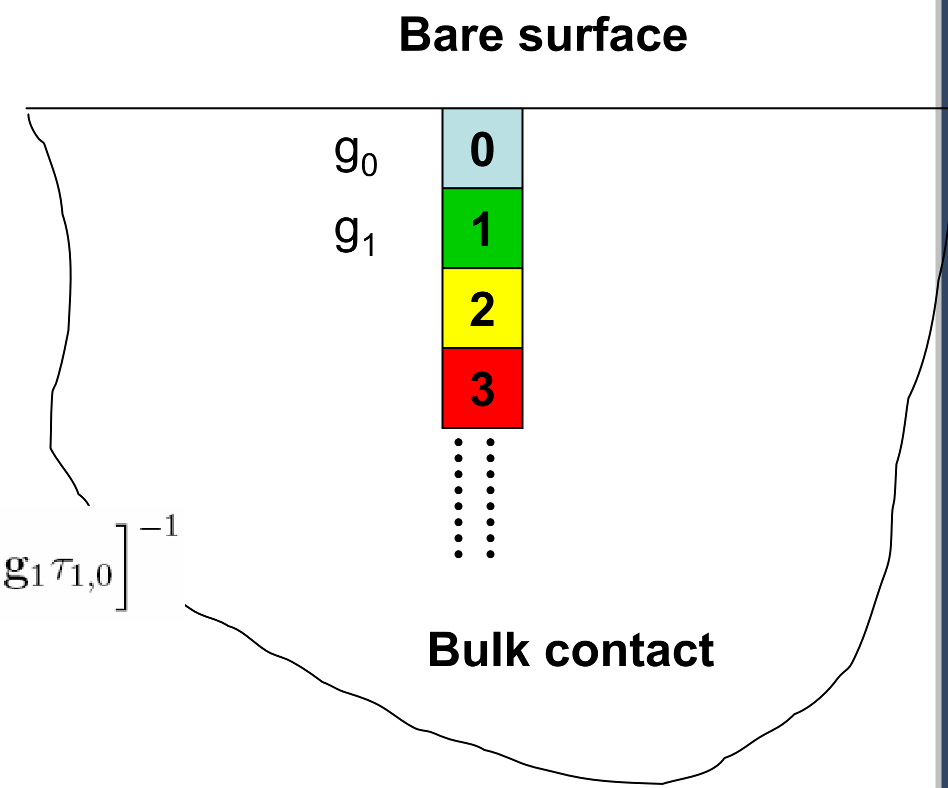
Bare surface



Bare Surface Green's Function

- Each layer is represented by one unit cell with planewave formulation, as in thin-film case
- Use decimation technique (a universal algorithm) to obtain g_1 and then evaluate g_0

$$\mathbf{g}_0(\omega, \vec{\mathbf{k}}_{||}) \equiv \lim_{\delta \to 0} \left[(\omega^2 + \delta i)\mathbf{I} - \mathbf{H}_0(\vec{\mathbf{k}}_{||}) - \tau_{0,1}\mathbf{g}_1\tau_{1,0} \right]^{-1}$$



- With g_0 known, we can find Σ_l

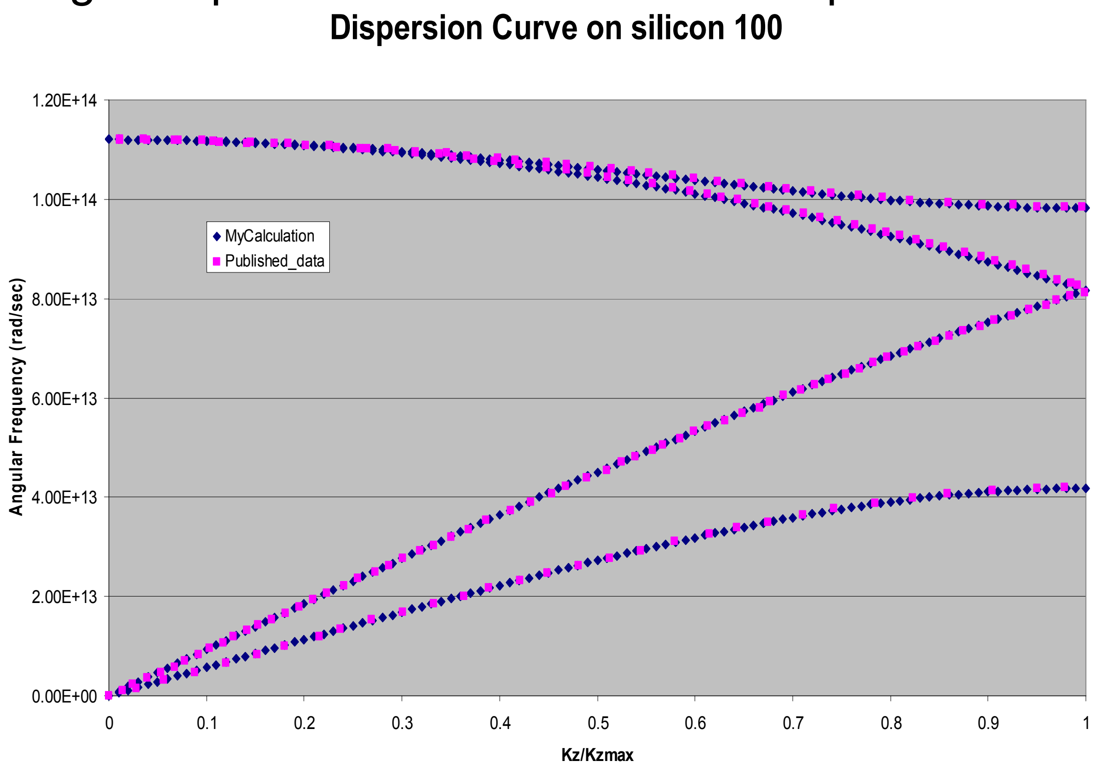
$$\Sigma_L = \omega^2\mathbf{I} - \mathbf{H}_{LDm} - \tilde{g}_o^{-1}$$

Harmonic Matrix and Dispersion

- Requirements:
  - Atom locations
  - Force between two atoms in

$$\mathbf{H} = \{H_{ij}\} = \frac{1}{\sqrt{M_i M_j}} \begin{cases} \frac{\partial^2 U}{\partial u_i \partial u_j}, & \text{if i} \neq \text{j} \\ -\sum_{m \neq j} \frac{\partial^2 U}{\partial u_j \partial u_m}, & \text{if i} = \text{j} \end{cases}$$

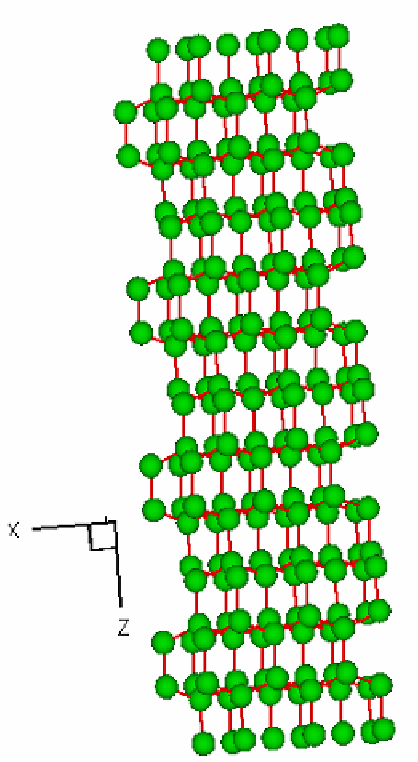
- Benchmark against published theoretical bulk dispersion curves

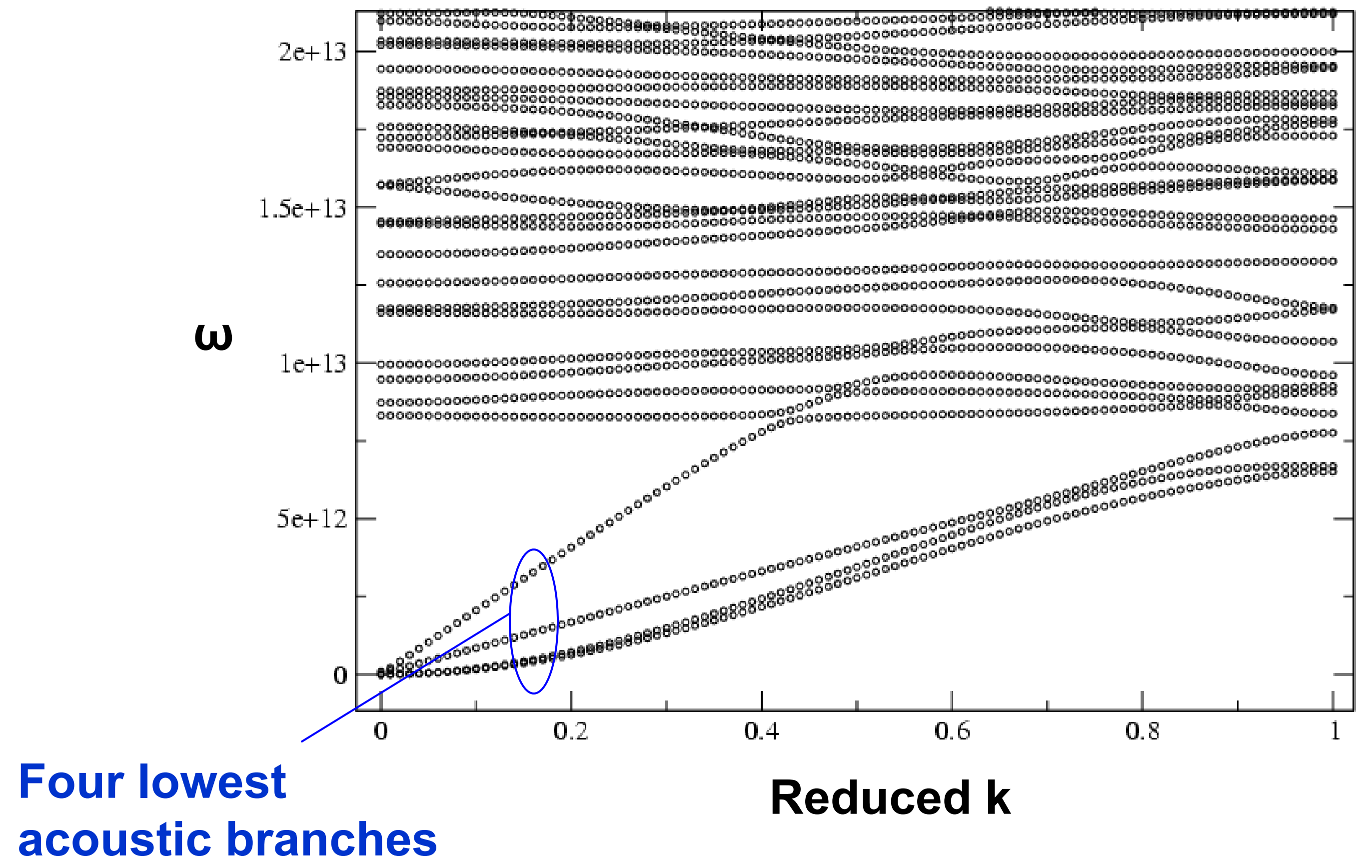


L.J. Porter, *et.al*. J Appl Phys 82(5378), 1997

Dispersion of Infinite Nanowires

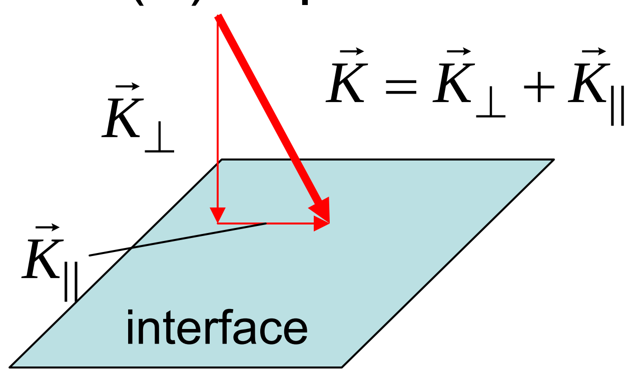
Orientation: (111)





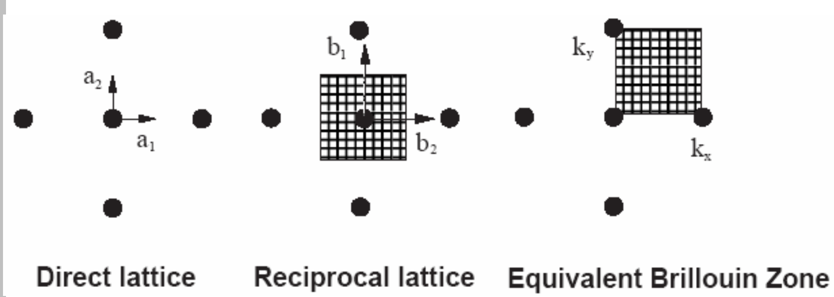
Integration over K-parallel Space

- Phonon transmission (Ξ) depends on frequency **and** direction

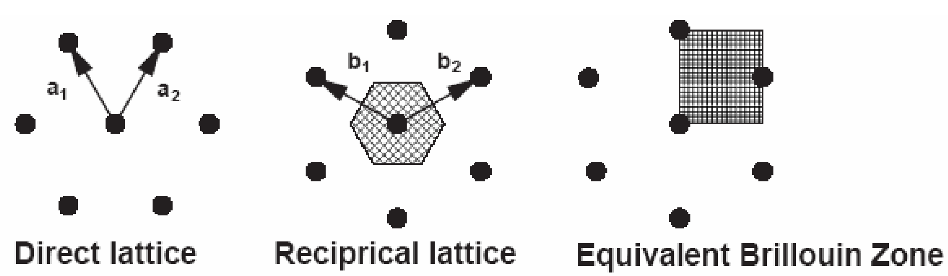


- $K_{||}$ mesh is chosen so that doubling mesh density changes thermal conductance within 3%

(100) direction



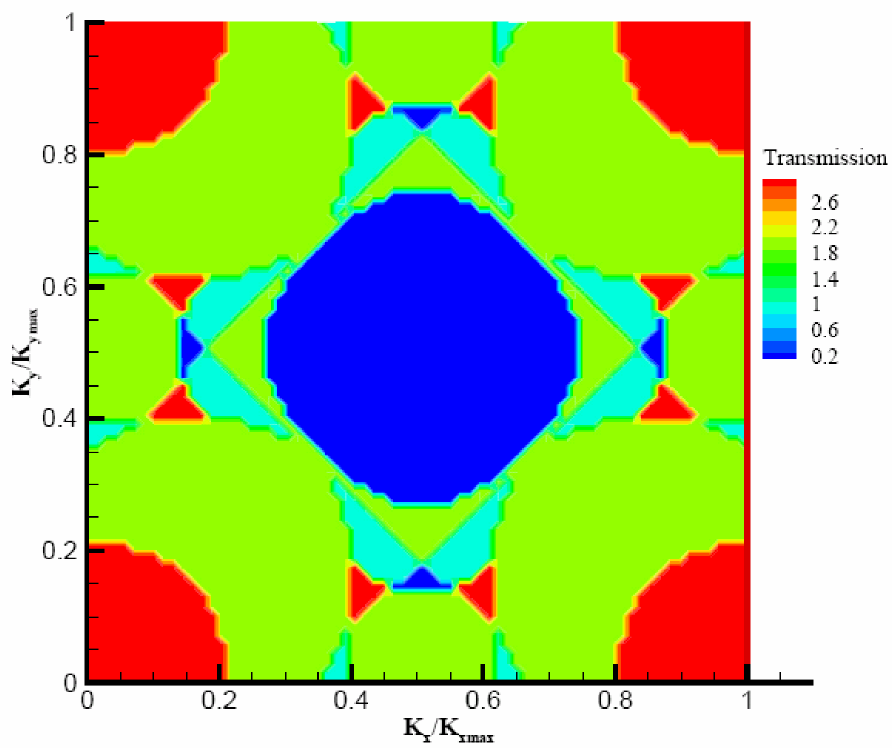
(111) direction



Transmission Distribution

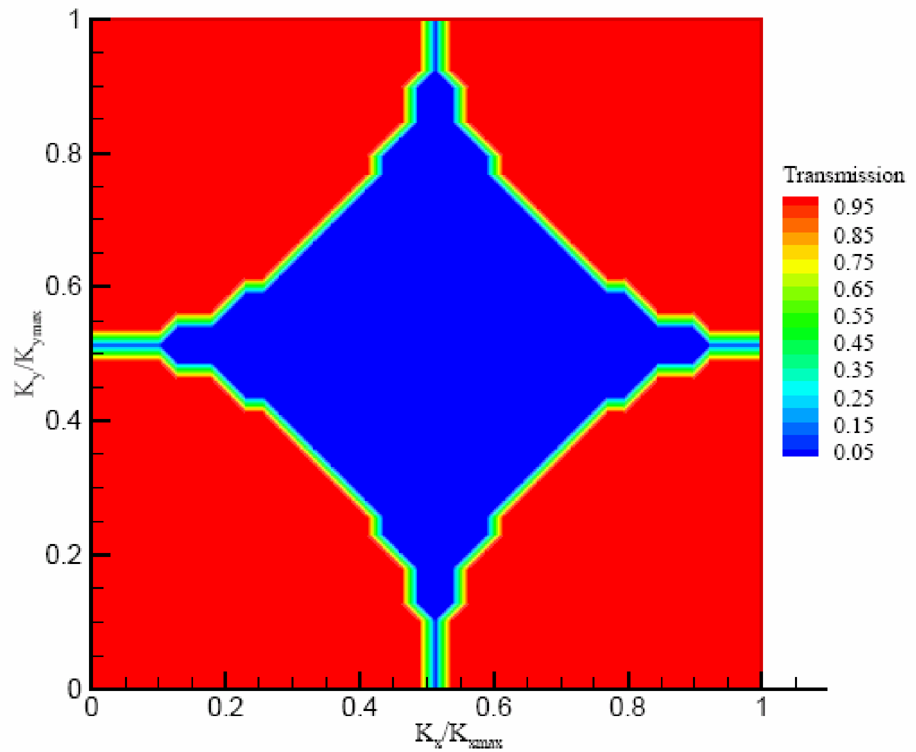
Low-frequency Phonons (2.4×10^{13} rad/sec)

High transmission confined to corners of K-space



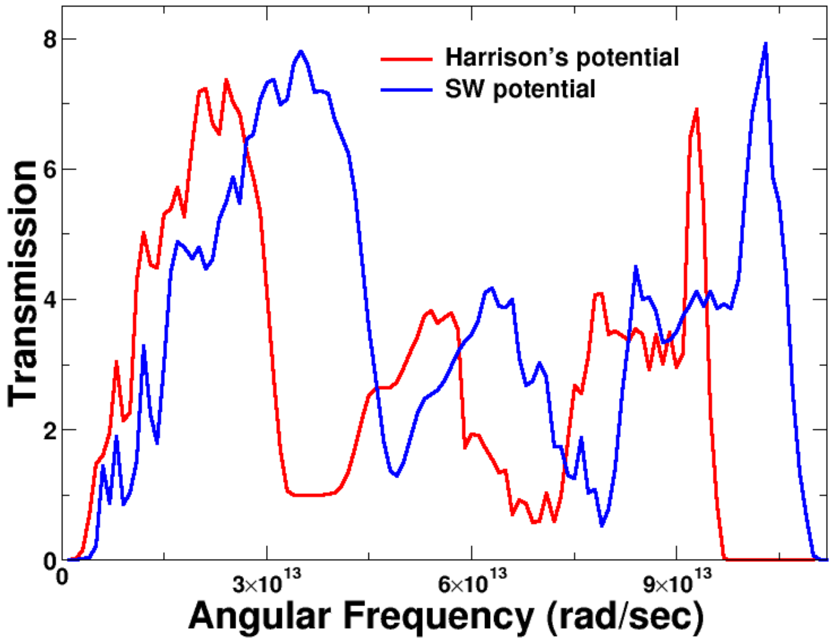
Higher-frequency Phonons (5.0×10^{13} rad/sec)

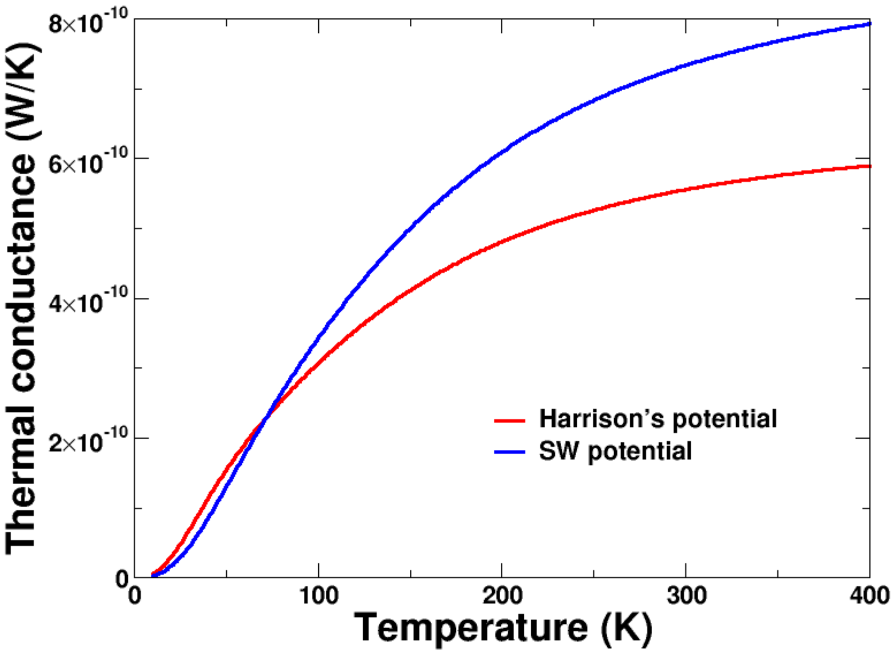
High transmission extends into middle of K-space



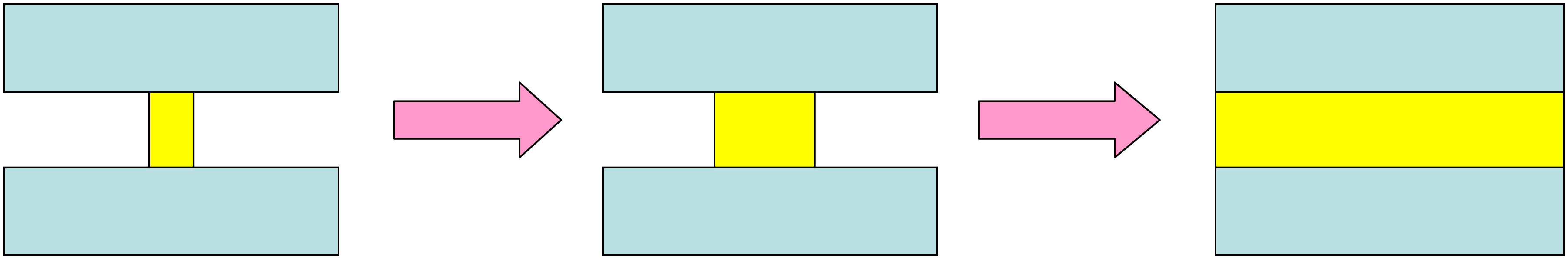
Choice of Potential Function

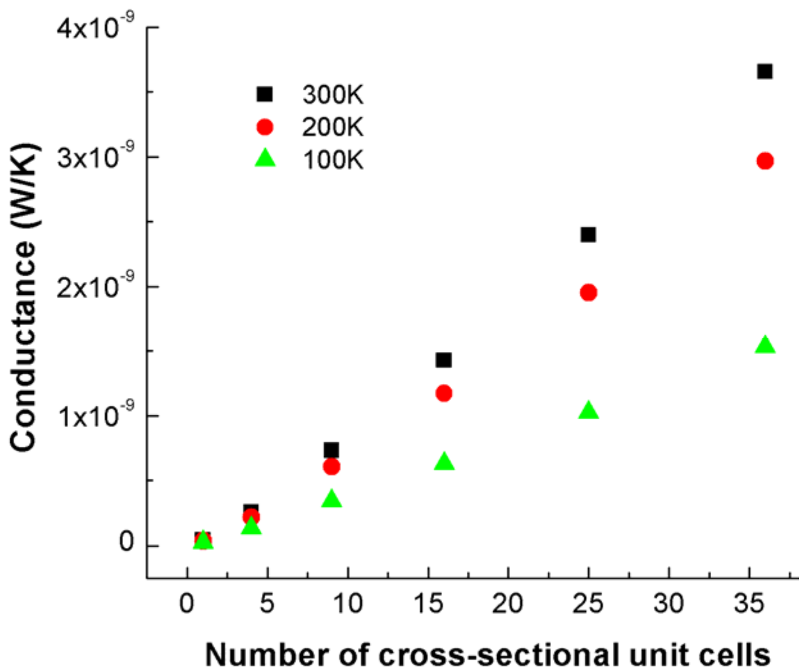
- 3 unit cells per layer; 3 unit cells long nanowire-plane structure
- Use Harrison's and Stillinger-Weber potentials

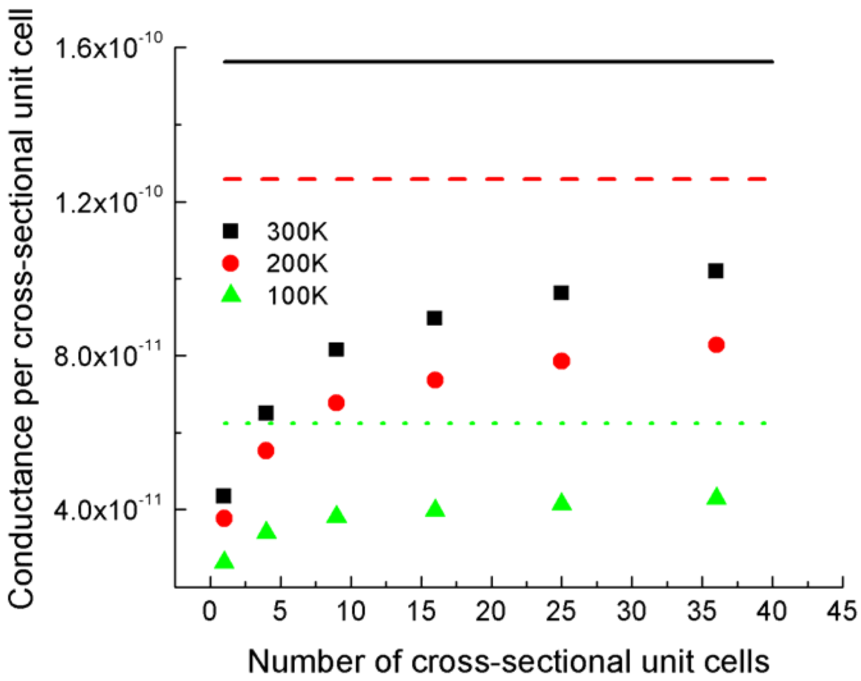




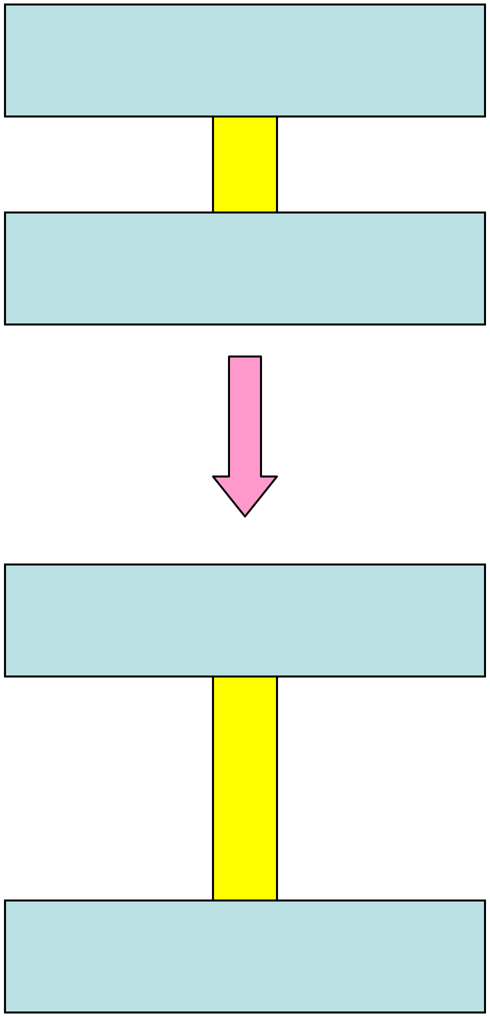
Diameter Dependence

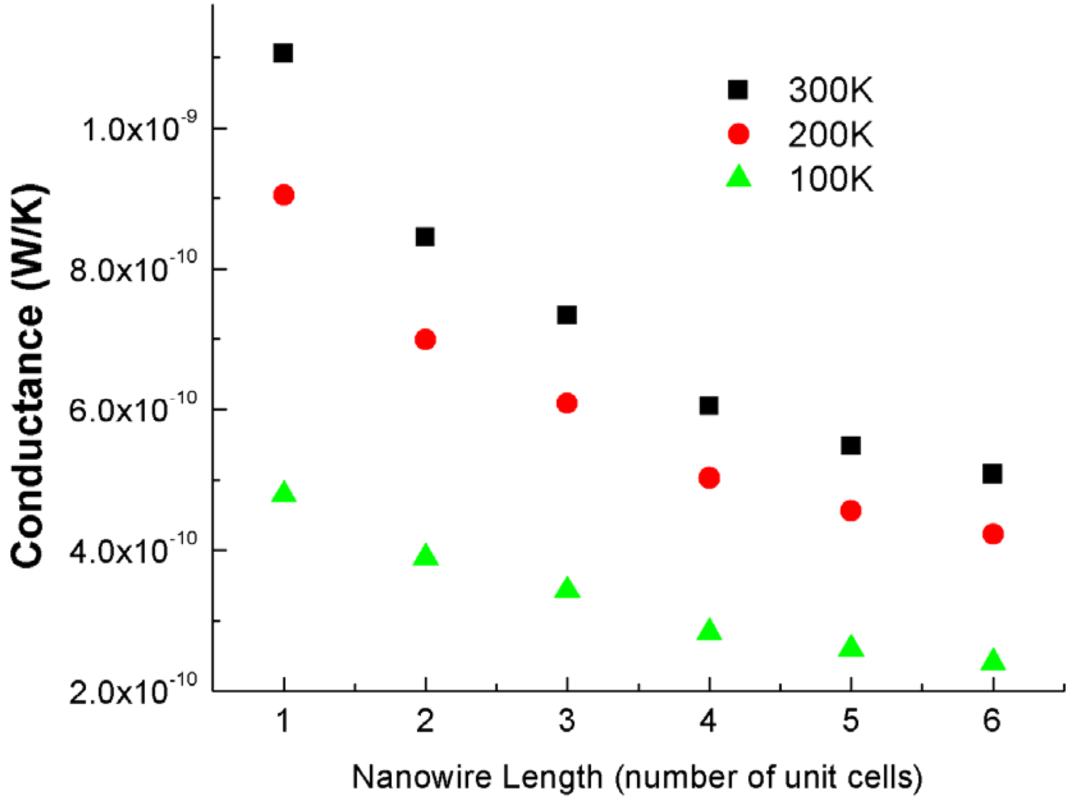






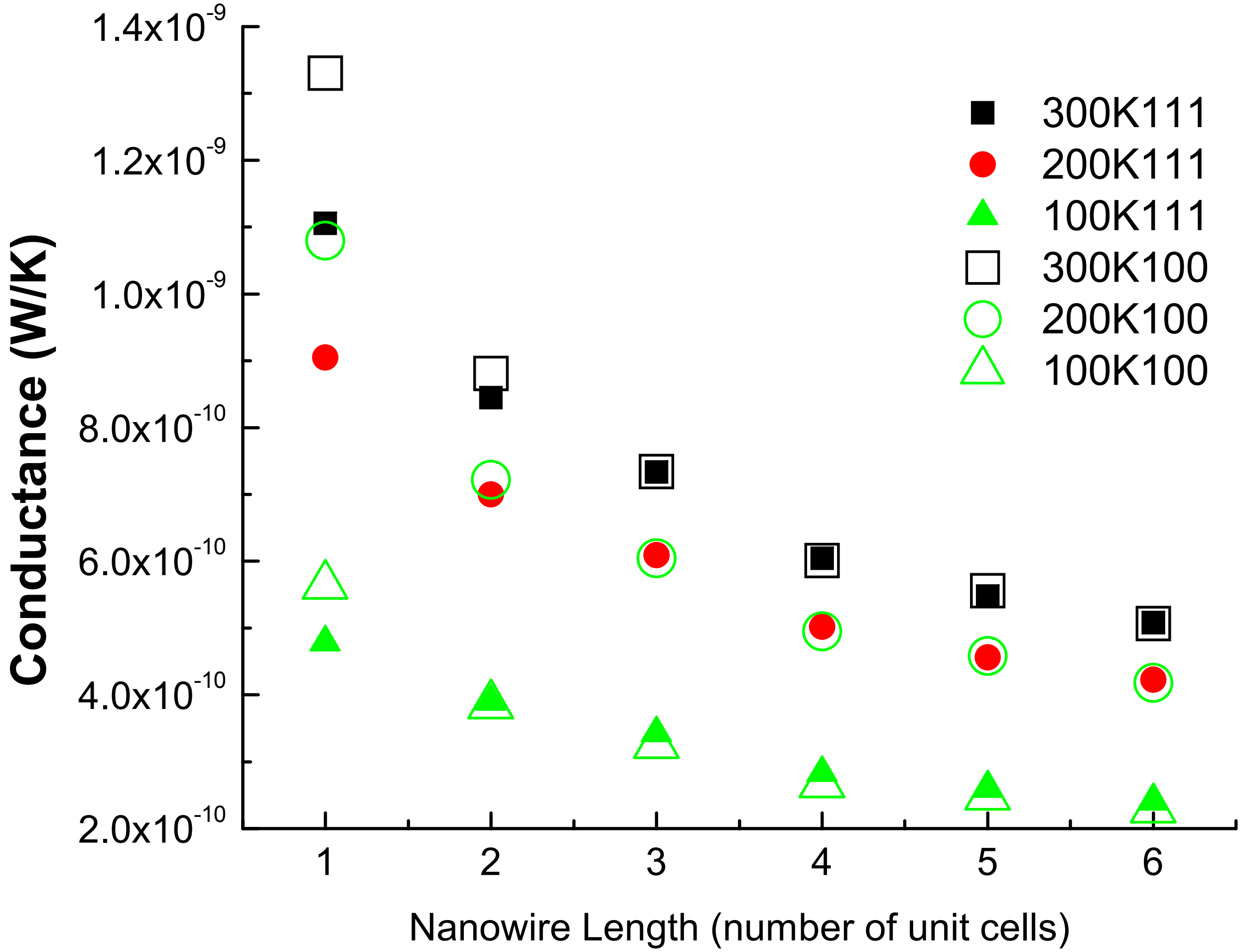
Length Dependence





Orientation Dependence

- Comparison of (111) and (100) orientations



Conclusions

- The AGF method is an effective tool in simulating ballistic phonon transport through relevant interfaces involving bulk and nanoscale materials
- Strain effects are small compared to heterogeneous-material effects
- A heterogeneous device layer reduces thermal conductance significantly at room temperature
- Increasing film thickness decreases thermal conductance
- The first few heterogeneous interfaces are most responsible for decreasing thermal conductance

Acknowledgements

- Wei Zhang, PhD (August 2006)
- Zhen Huang (PhD student)
- Dr. Natalio Mingo, NASA AMES
- Prof. Jayathi Murthy, Purdue
- Funding from the Purdue NASA Institute of Nanoelectronics and Computing

References

- Cahill et al., Journal of Applied Physics **93**, 793 (2003)
- Mingo, Physical Review B **68**, 245406 (2003)
- Cheeke, Canadian Journal of Physics **54**, 1749 (1976)
- C. Kittel, Introduction to Solid State Physics, Wiley, 1996.
- Zhang et al., Num Heat Trans-B **51**, 333 (2007).
- S. Datta, Electronic Transport in Mesoscopic Systems. Cambridge University Press, 1st ed., 1995.
- Zhang et al., J Heat Transfer **129** 483 (2007).