Monte Carlo Simulation of Phonon Transport

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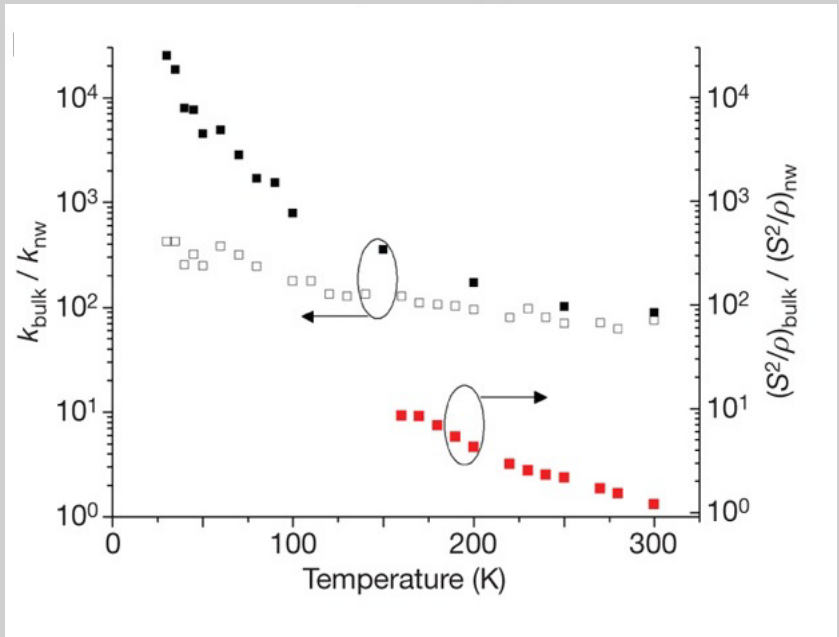
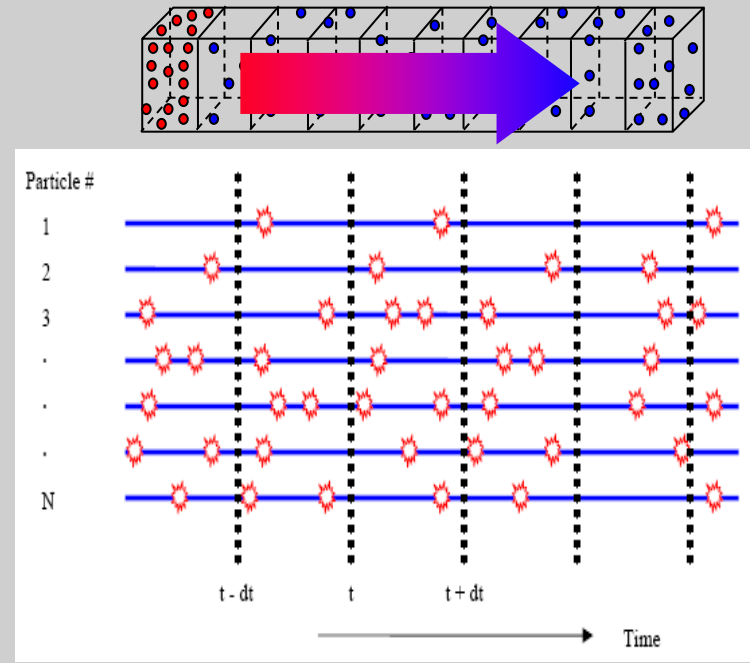
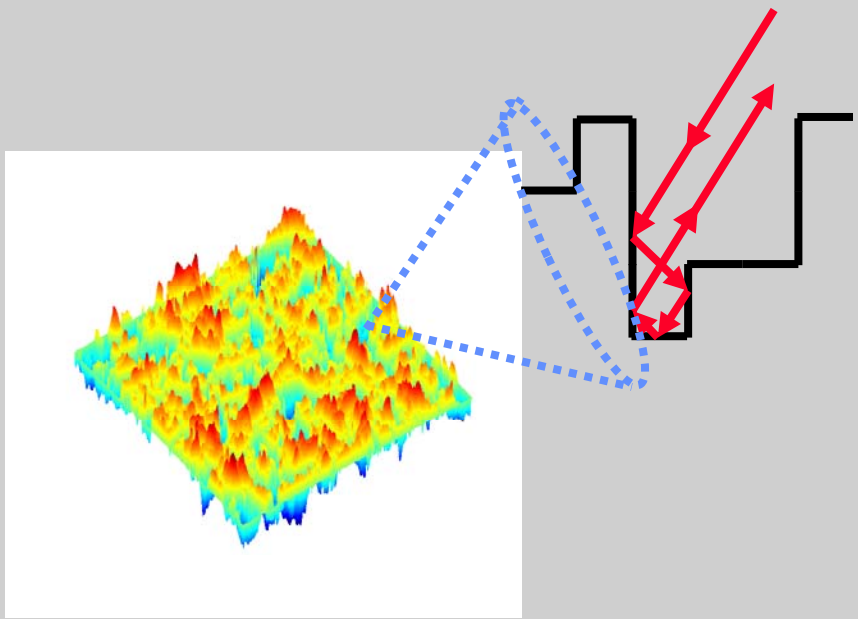
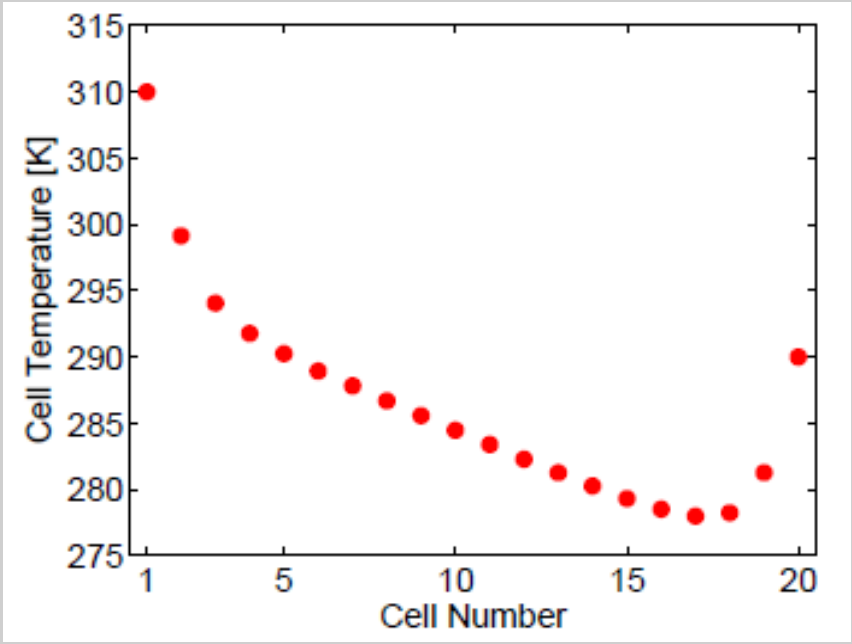
IWCE 2012 Phonon School

Outline

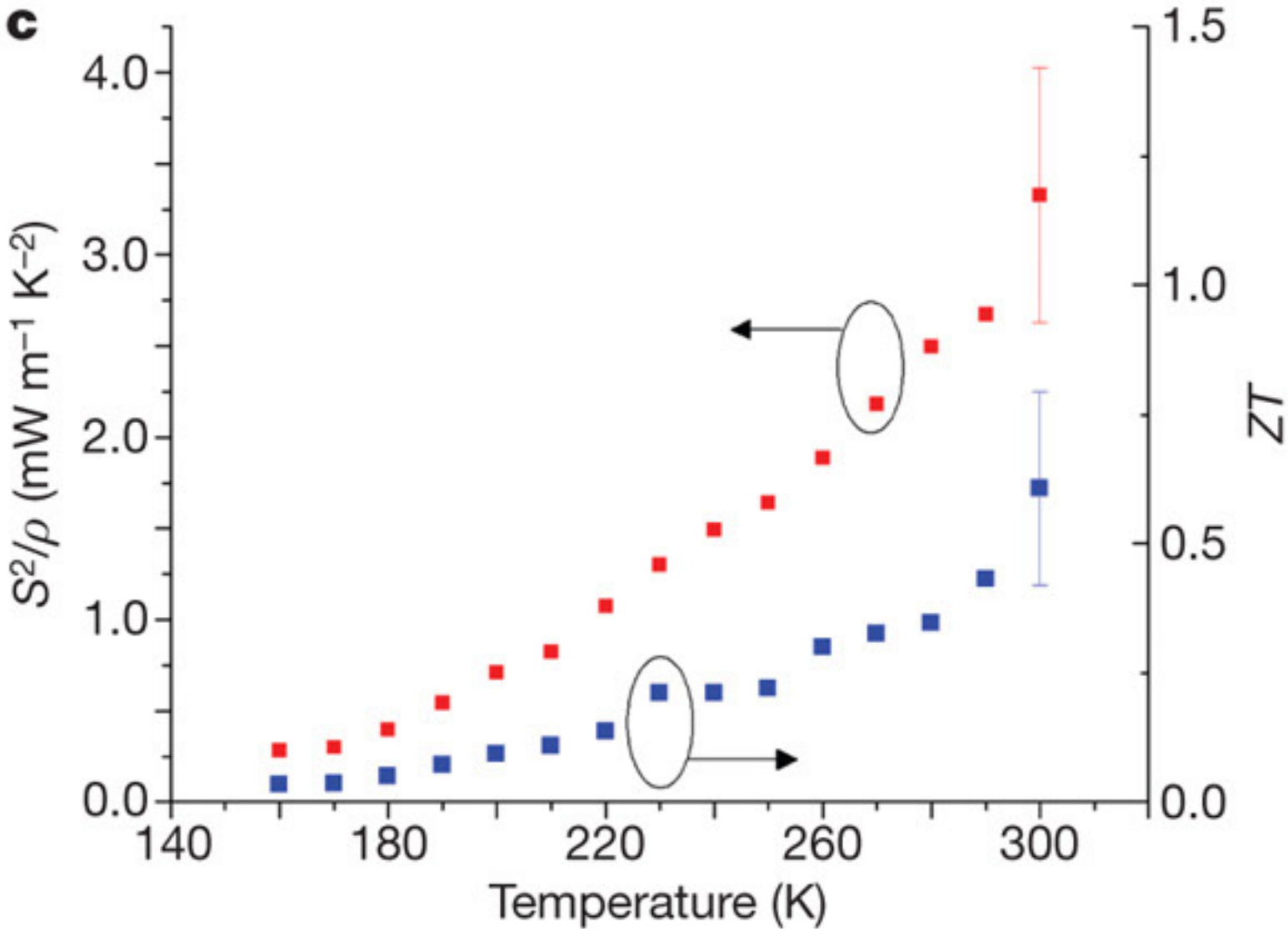

k_{bulk} / k_{nw}
$(S^2/\rho)_{bulk} / (S^2/\rho)_{nw}$
Temperature (K)


Particle #
1
2
3
N
t - dt
t
t + dt
Time



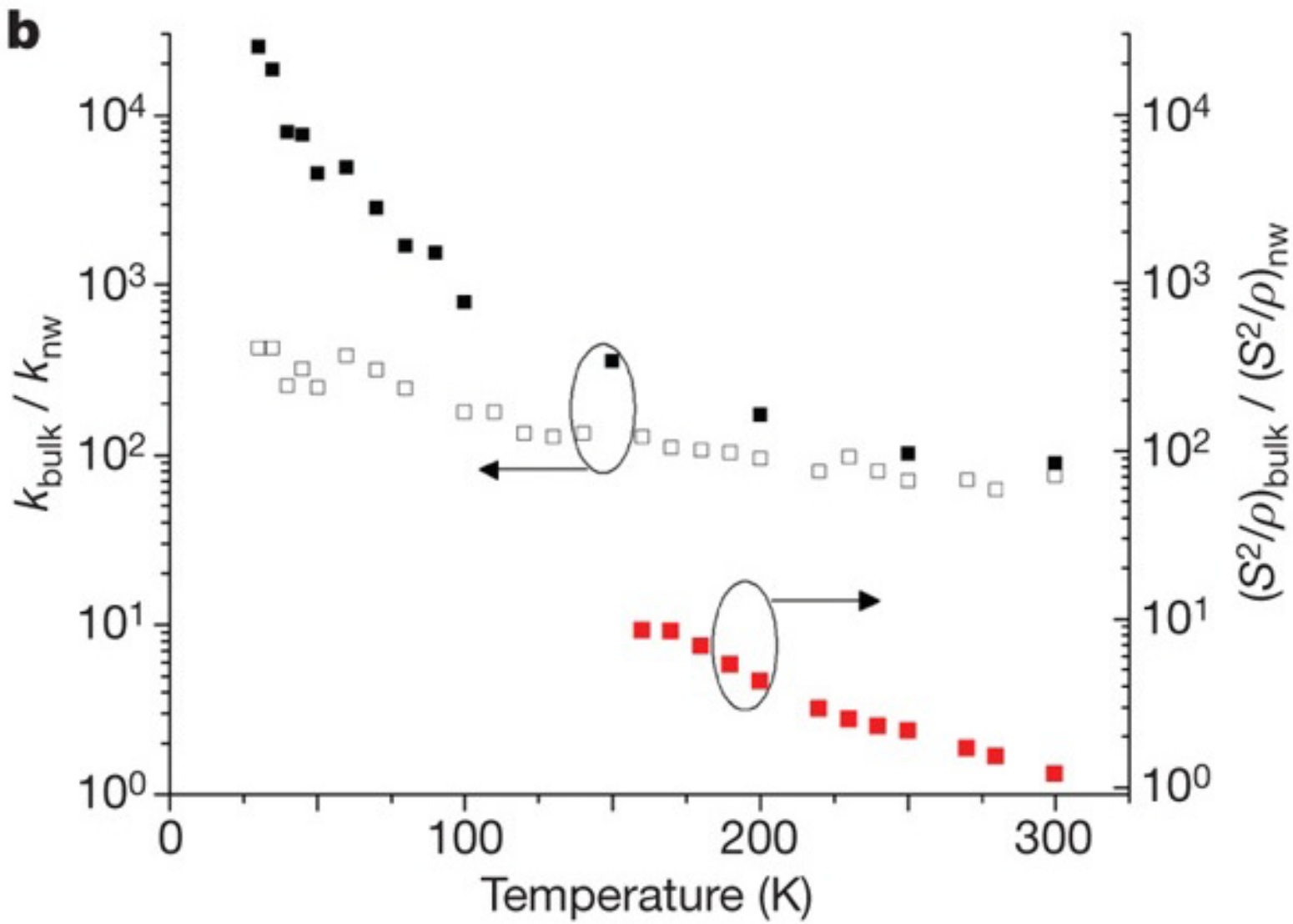

Cell Temperature [K]
Cell Number

Silicon Nanowires – Efficient TE Materials



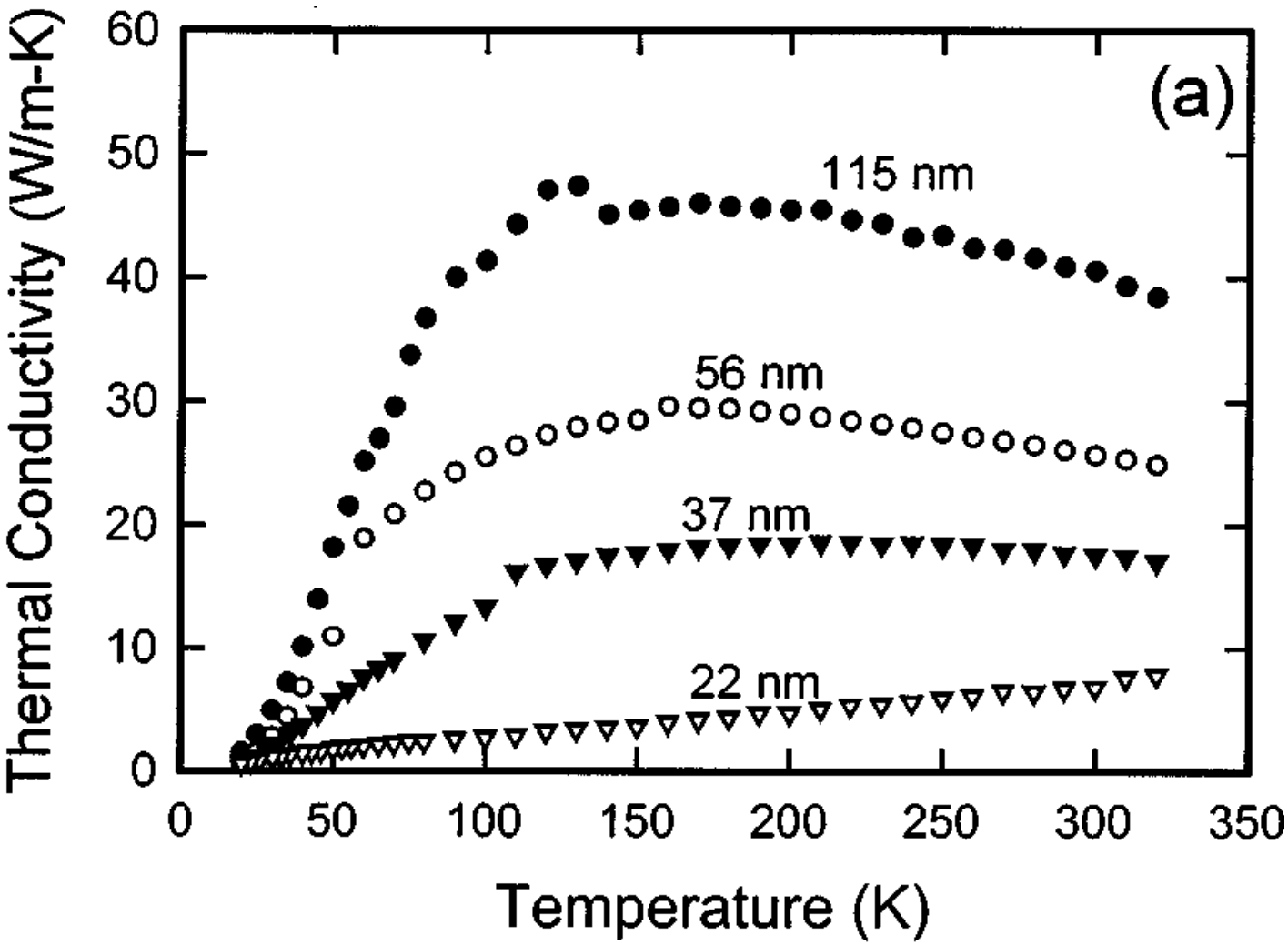
A. I. Hochbaum *et al*., *Nature* **451**, 163 (2008).

Thermal Conductivity in Silicon Nanowires



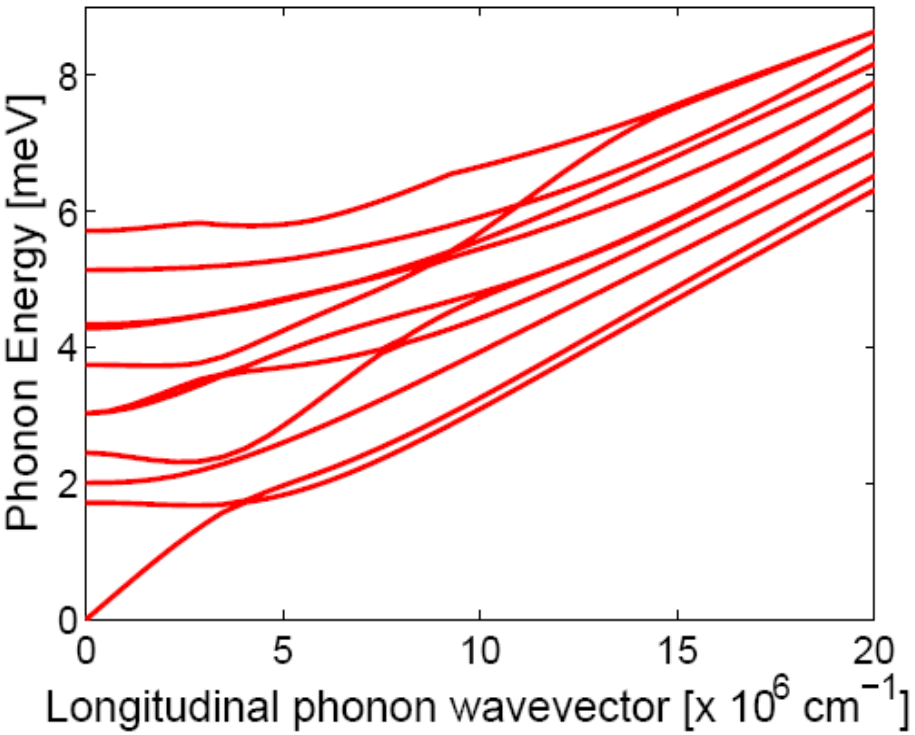
A. I. Hochbaum *et al*., *Nature* **451**, 163 (2008).

Thermal Conductivity in Silicon Nanowires



D. Li *et al*., *Appl. Phys. Lett.* **83**, 2934 (2003).

Confined Acoustic Phonon Spectrum



Why confined ?

Due to acoustic mismatch between Si and SiO_2 – severe when confined more

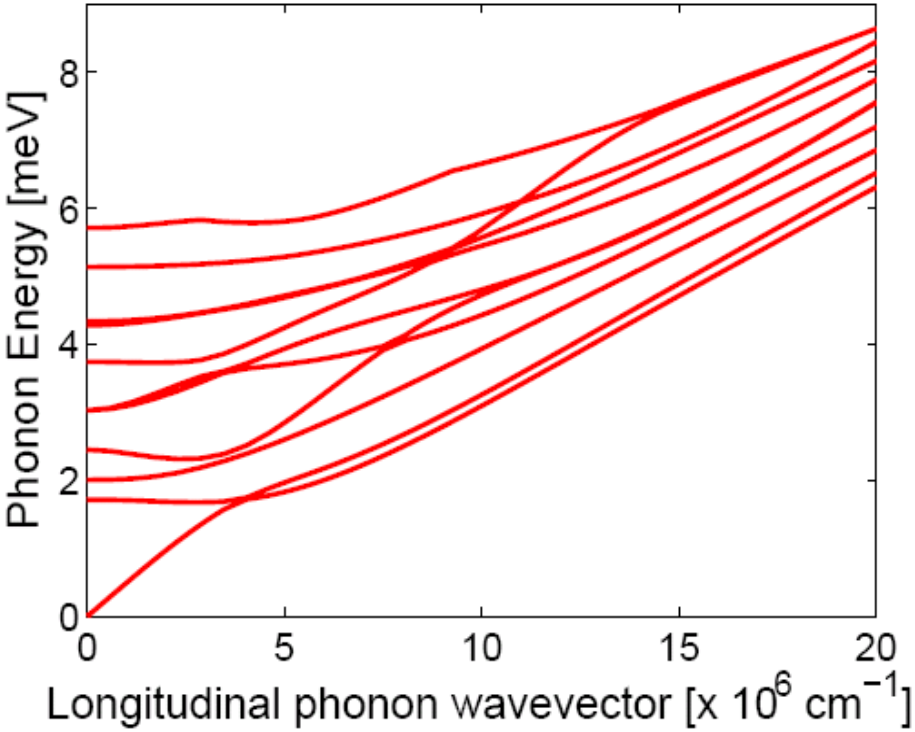
SiO_2 is acoustically soft
Acoustic impedance $\zeta = \rho v_s$ mismatch between Si & SiO_2 is ~40 %

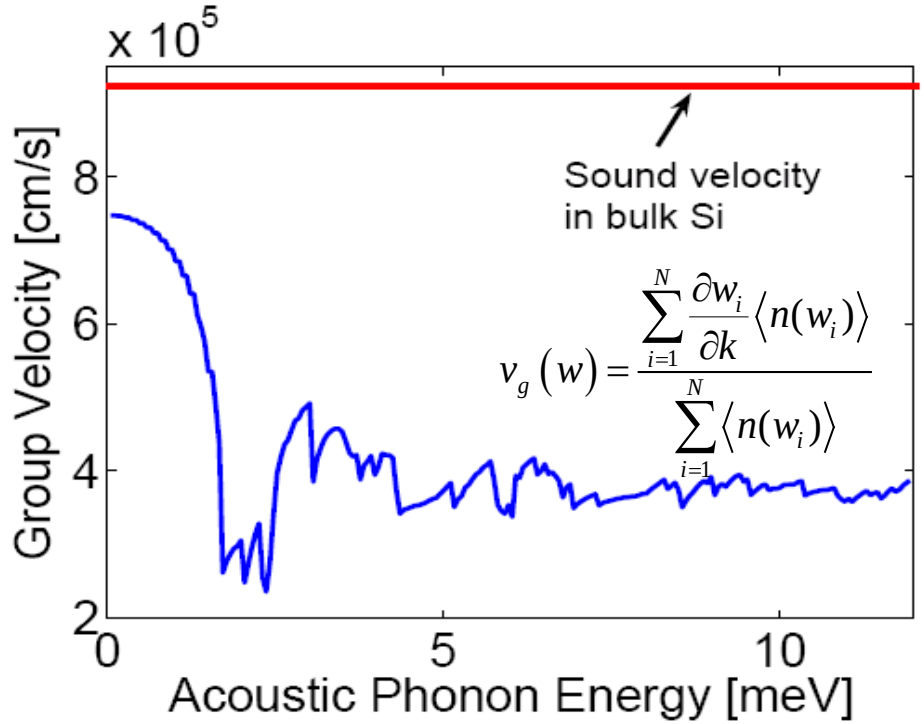
Solve elastic continuum equation with free-standing boundary conditions (**FSBC**):
normal component of stress tensor vanishes at interfaces

$$T_{ij} n_j \Big|_s = 0$$

L.Donetti *et al.*, *J. App. Phys*. **100**, 013701 (2006)
E.P. Pokatilov, *Phys. Rev. B* **72**, 113311 (2005)
M.Dutta *et al.*, *Int. J. High Speed Electronics and Systems* **9**, 1 (1998)
C.M. Sotomayor *et al.*, *Phys. Status Solidi C* **1**, 2609 (2004) (Experimental)

Confined Acoustic Phonons →Slower Phonons

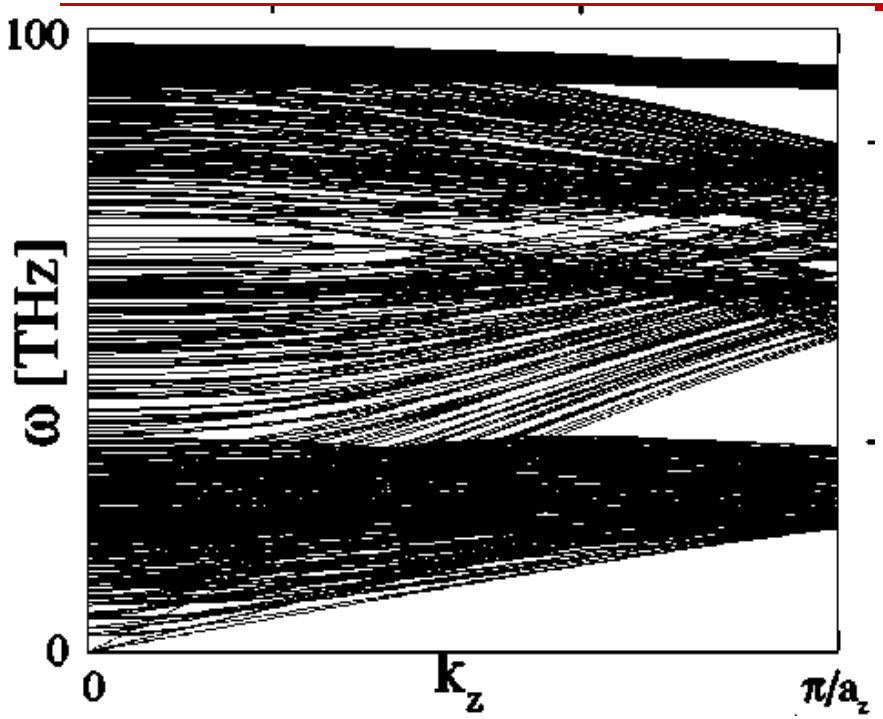


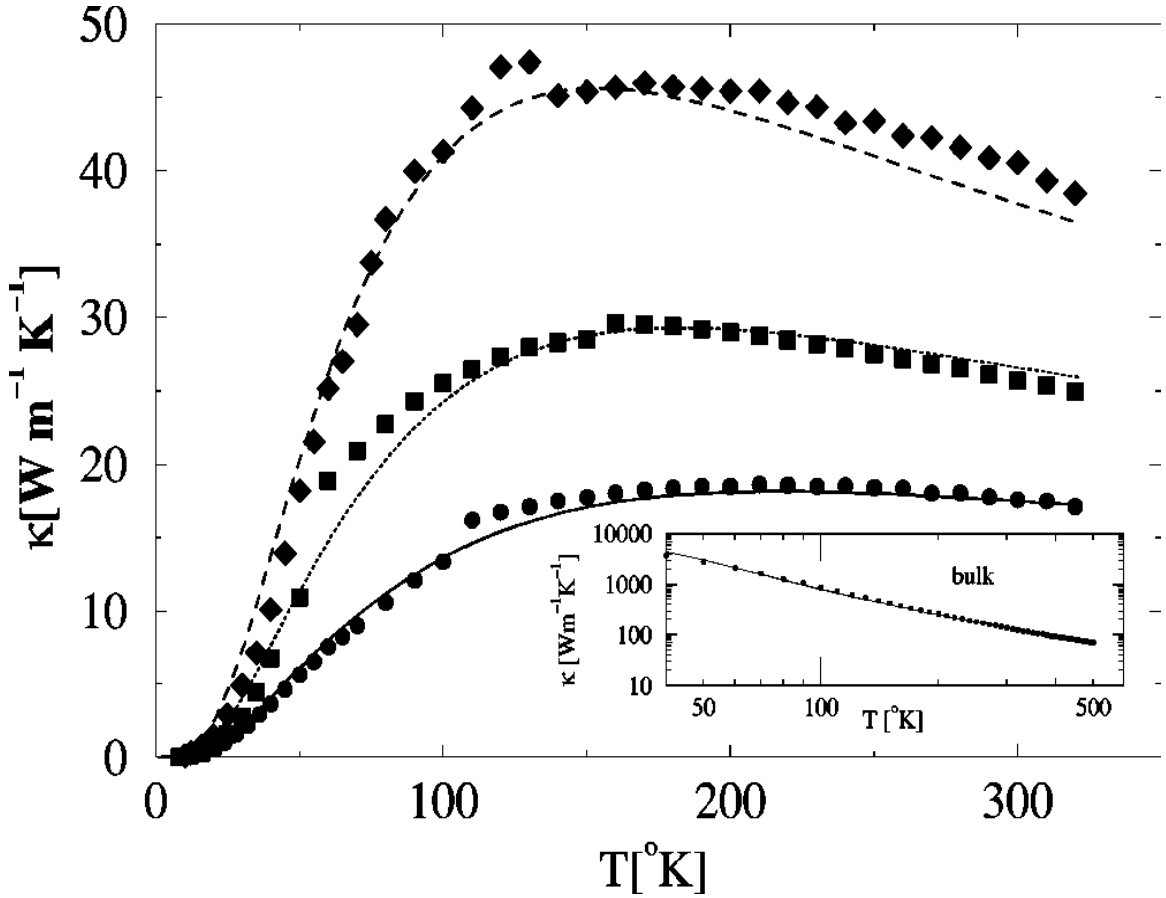


Flattened dispersion → lower group velocity

Edwin B. Ramayya *et al*., *J. Appl. Phys.* 104, 063711 (2008)

Confined Acoustic Phonons



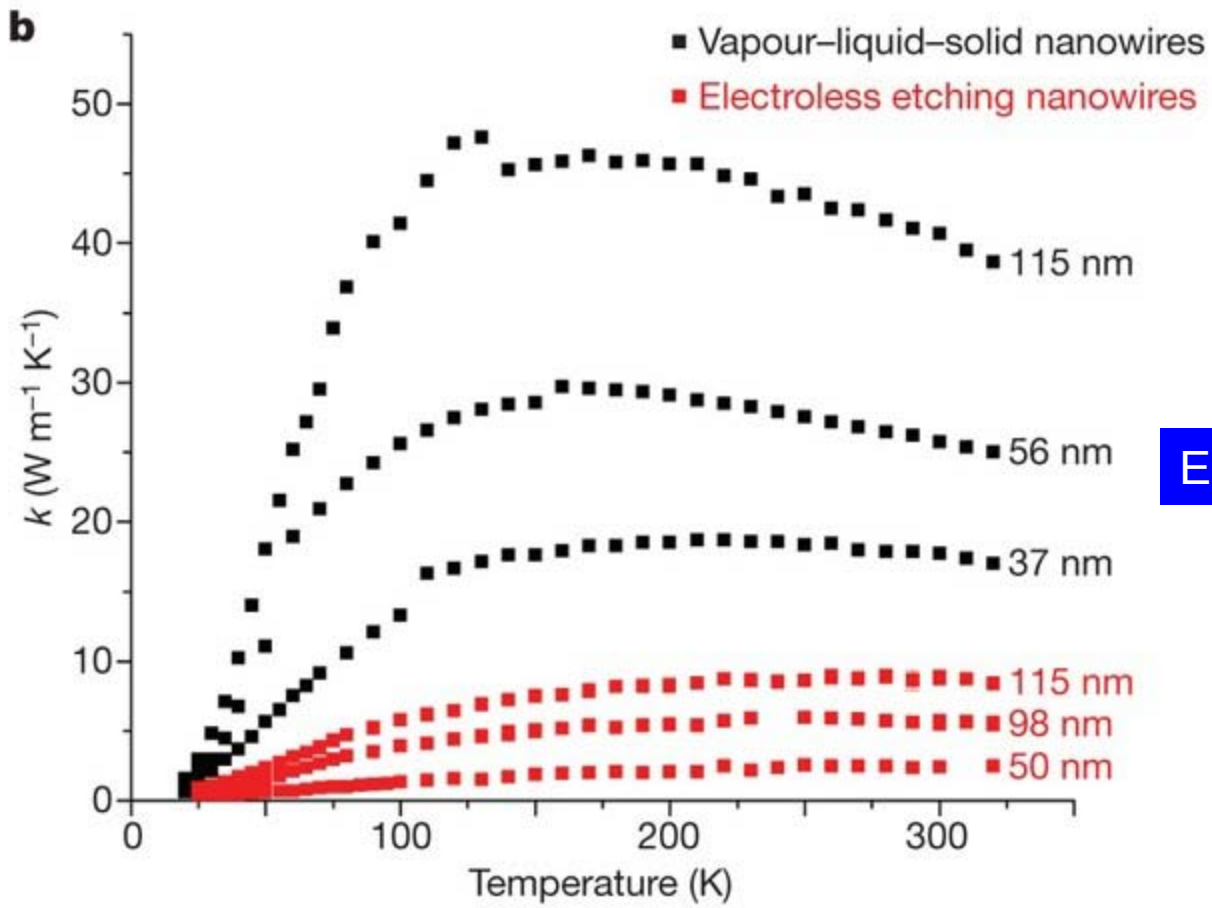


N. Mingo, Phys. Rev. B **68**, 113308 (2003)

D. Li *et al*., *Appl. Phys. Lett.* **83**, 2934 (2003)

Phonon confinement insufficient to explain two orders of magnitude reduction in thermal conductivity

Thermal Conductivity – Roughness Dependence

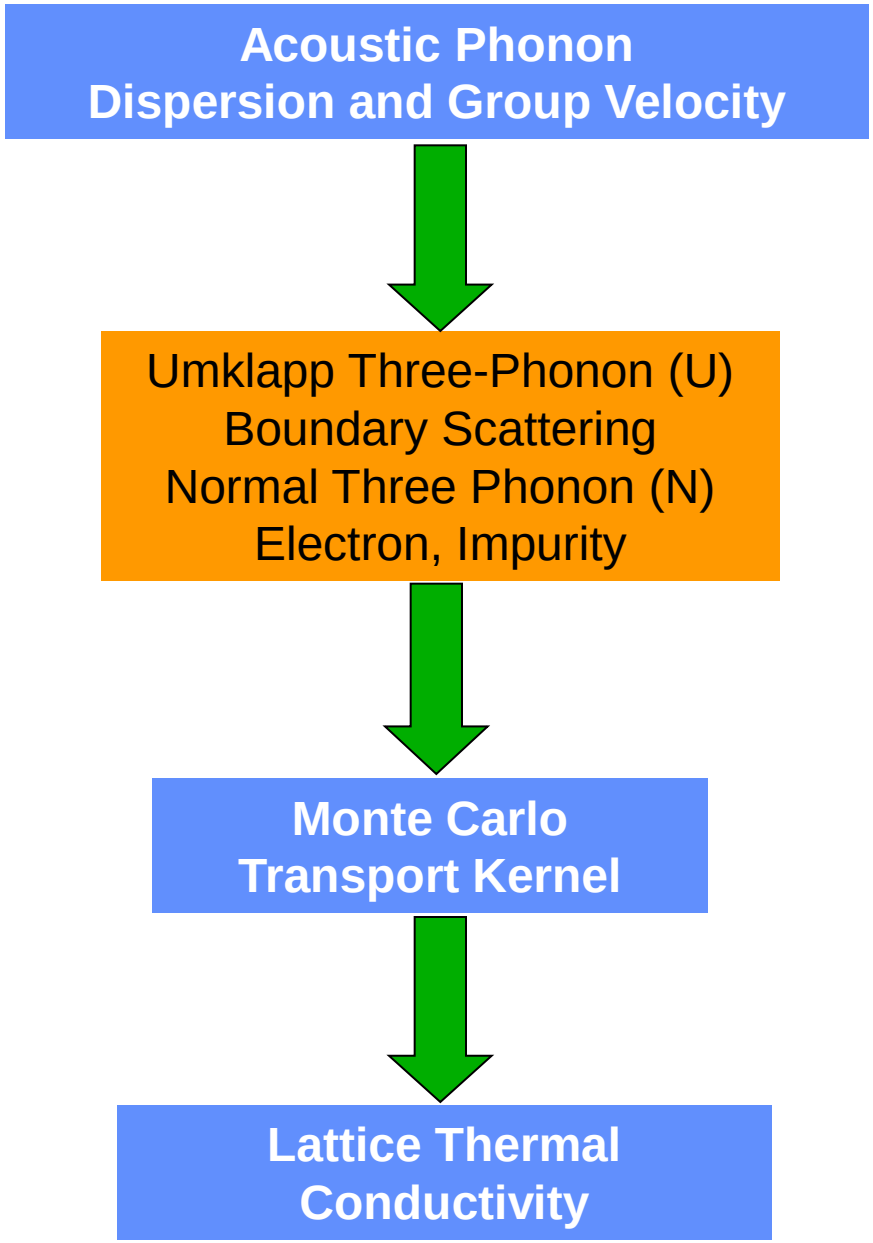


EE wires roughness RMS ~ 3 nm

Bulk Si → SiNWs : Two orders of magnitude reduction in thermal conductivity

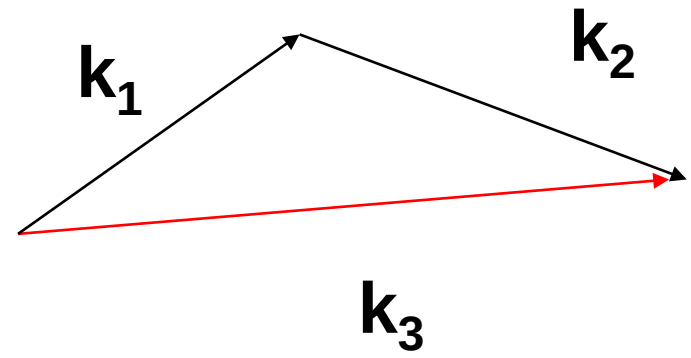
A. I. Hochbaum *et al*., *Nature* **451**, 163 (2008).

Simulator Flowchart – Thermal Conductivity



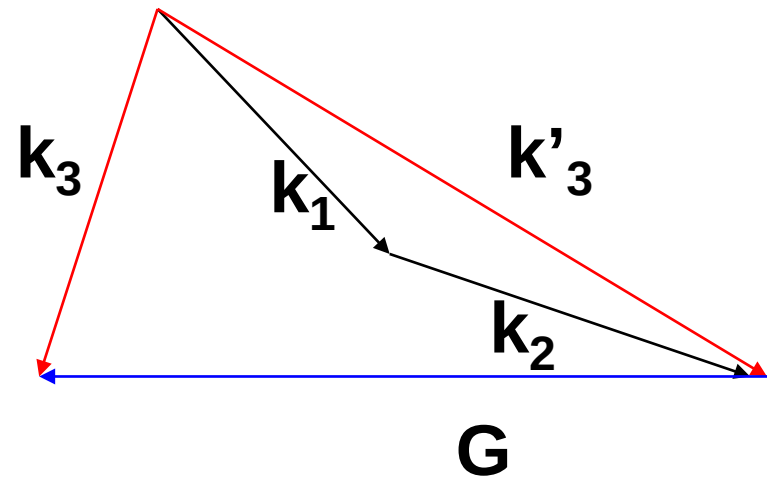
Why Monte Carlo for Phonons

- **Normal (N) processes do not offer resistance because there is no change in direction**



$$\vec{k}_1 + \vec{k}_2 \Leftrightarrow \vec{k}_3$$

- **Umklapp (U) processes offer resistance to phonons because they turn phonons around**



Reciprocal lattice vector

$$\vec{k}_1 + \vec{k}_2 \Leftrightarrow \vec{k}_3{}' \pm \vec{G}$$

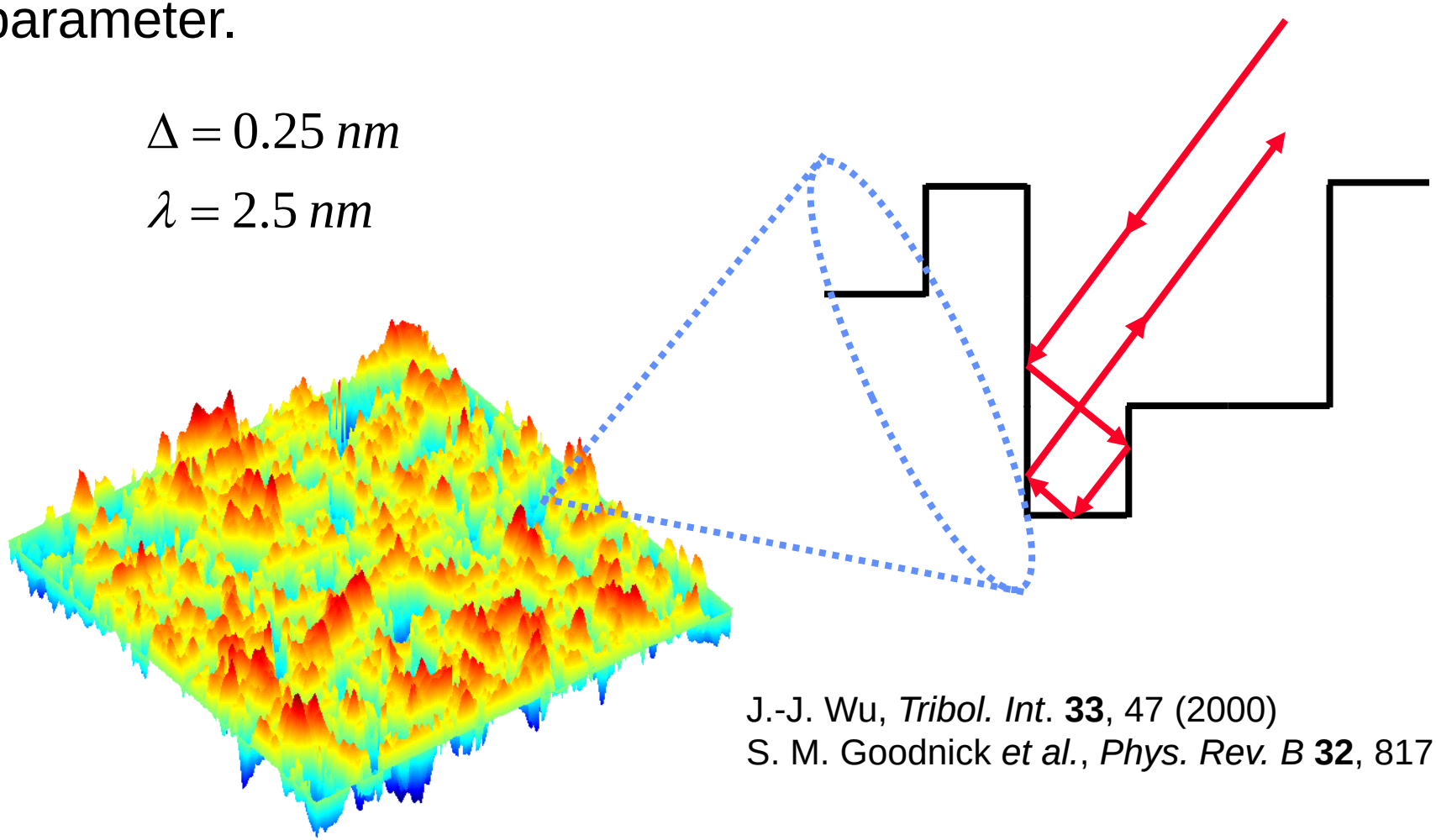
N processes change the phonon distribution → indirectly affect the thermal conductivity

Why Monte Carlo for Phonons

Can treat the actual surface without using a specularity parameter.

$$\Delta = 0.25\,nm$$

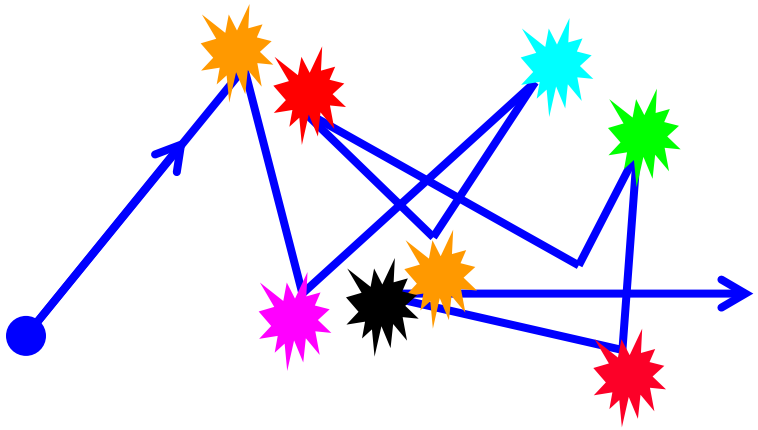
$$\lambda = 2.5\,nm$$

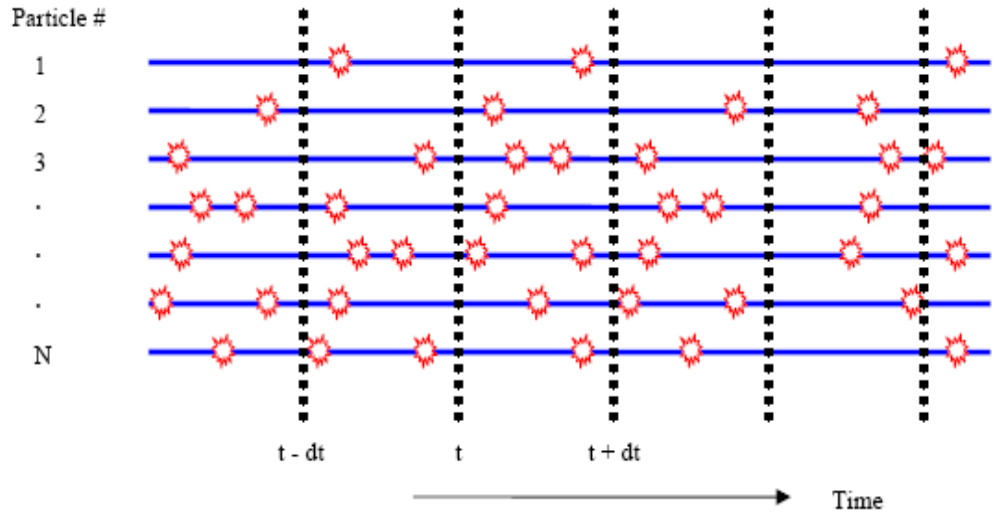


J.-J. Wu, *Tribol. Int*. **33**, 47 (2000)
S. M. Goodnick *et al.*, *Phys. Rev. B* **32**, 8171 (1985)

A good way to capture phonon localization and the particular features of a given surface ← better than specularity parameter

Ensemble Monte Carlo Simulation



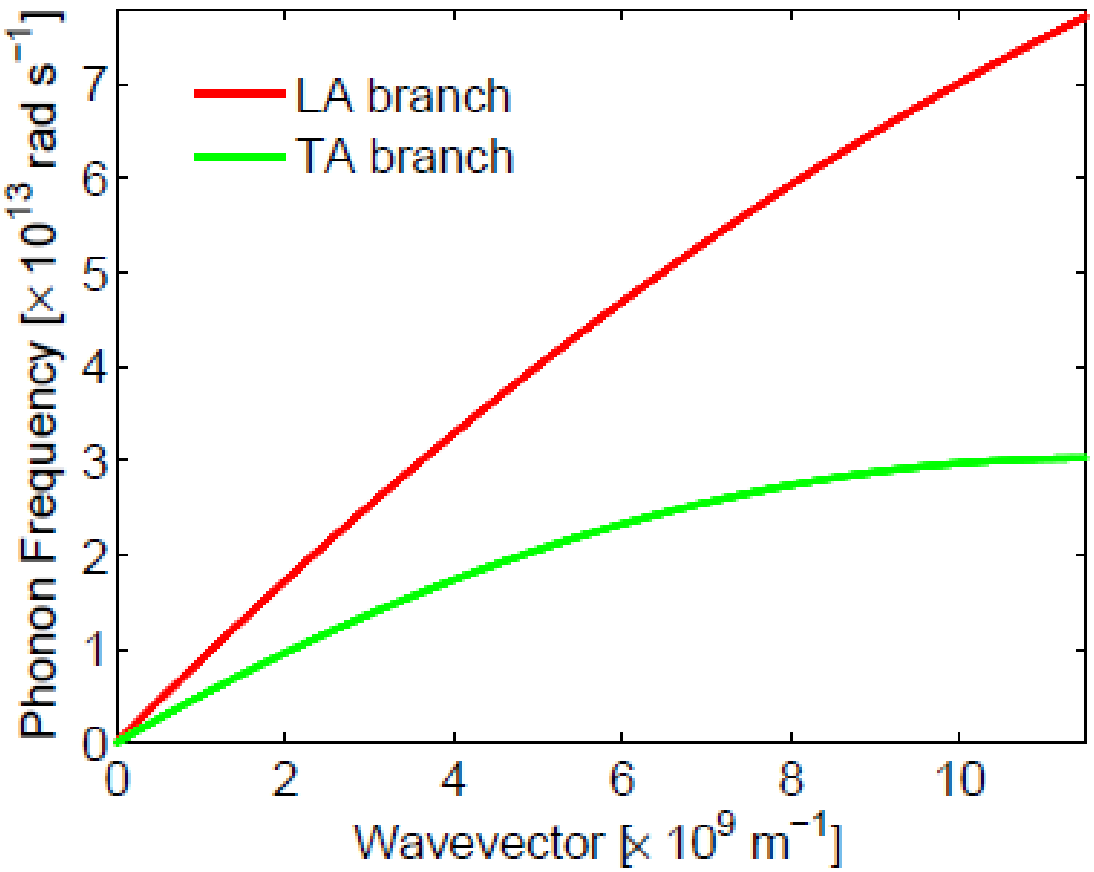


When solving the BTE –
ensemble Monte Carlo (EMC) technique is the state-of-the-art

Utilizing random numbers to determine
- how long does a particle fly between scattering events
- what scattering mechanism to choose
- how to update momentum afterwards

Very robust and versatile

Dispersion Approximation

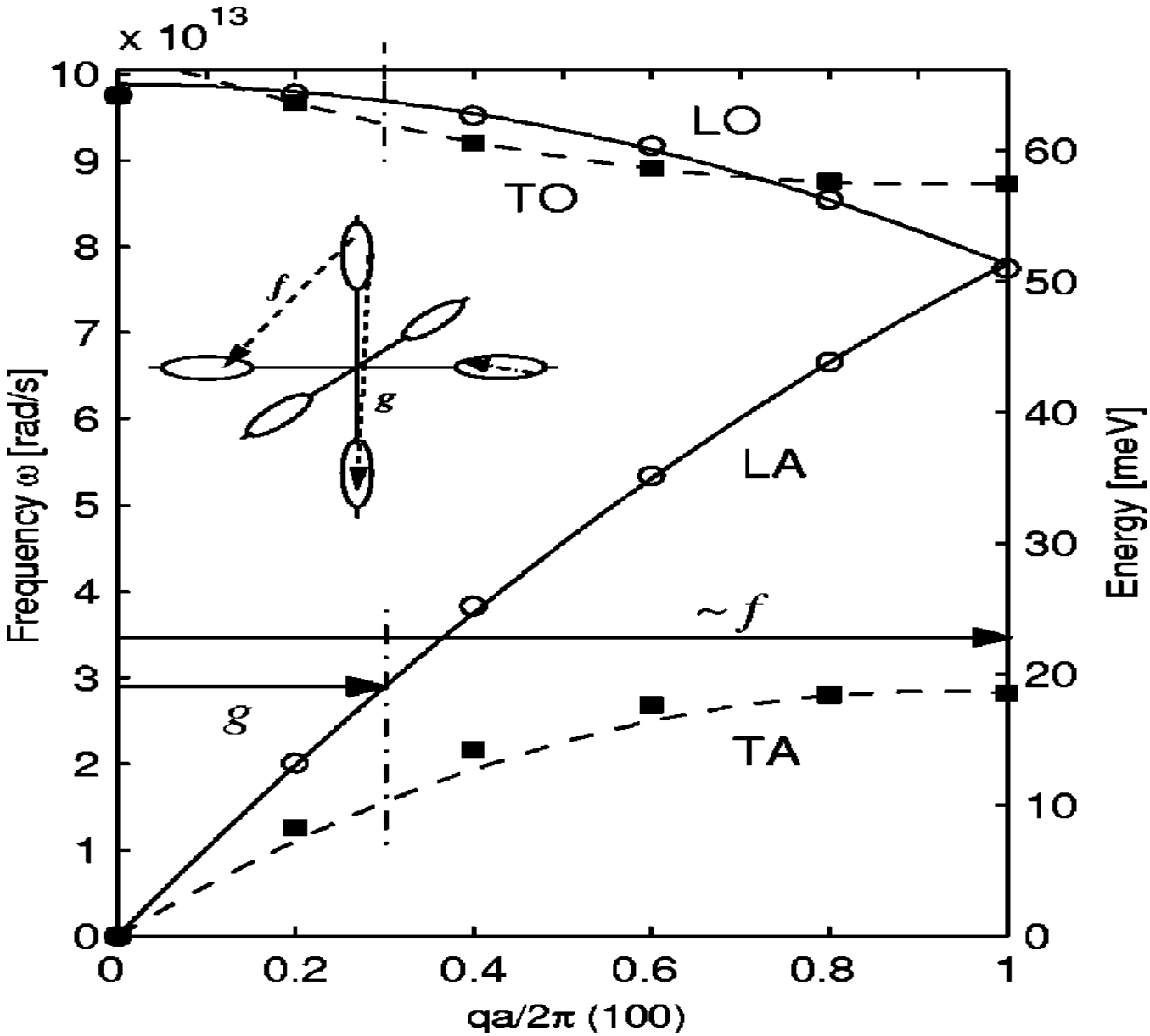


$$\omega_q = \omega_o + v_s q + c q^2$$

E. Pop *et al.*, *J Appl. Phys*. **96**, 4998 (2004)

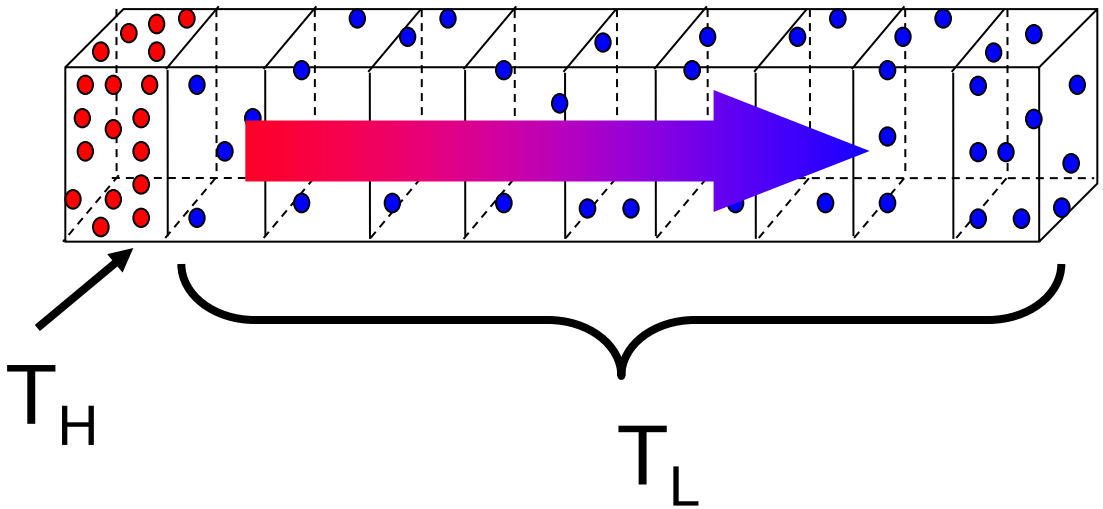
	ω_o 10^{13} rad/s	v_s 10^5 cm/s	c 10^{-3} cm^2/s
LA	0.00	9.01	−2.00
TA	0.00	5.23	−2.26
LO	9.88	0.00	−1.60
TO	10.20	−2.57	1.11

Dispersion Approximation



E. Pop *et al*., *J Appl. Phys.* **96**, 4998 (2004)

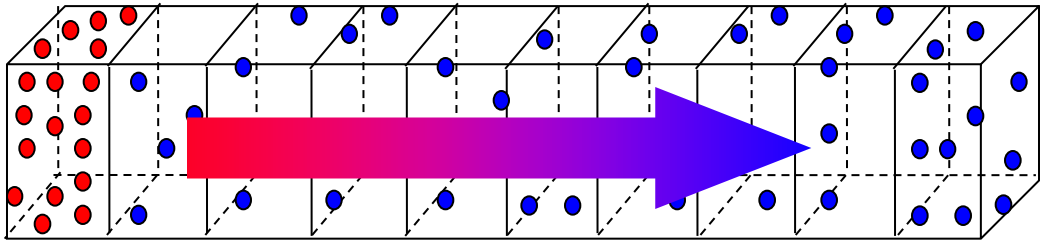
Thermal Transport EMC



Heat one end, let phonons diffuse, wait for steady state temperature gradient to be established, and from Fourier's law determine the thermal conductivity

R. B. Peterson, *J. Heat Transfer* **116**, 815 (1994)
S. Mazumder and A. Majumdar, *J. Heat Transfer* **123**, 749 (2001)
Lacroix *et al*. *Phys. Rev. B* **72**, 064305 (2005)

Phonon Initialization: Number of Phonons



$$N = V \sum_{p=LA,TA} \sum_{\mathbf{q}} (\langle n_{\mathbf{q},p,T} + \frac{1}{2} \rangle),$$

$$\langle n(\mathbf{q},p,T) \rangle = \frac{1}{exp(\frac{\hbar\omega p,\mathbf{q}}{k_B T}) - 1}$$

N_w spectral intervals

$$N = V \sum_{p=LA,TA} \sum_{i=1}^{N_w} \left[\frac{1}{exp(\frac{\hbar\omega_i}{K_B T}) - 1} \right] \frac{q_{i,p}^2}{2\pi^2 \upsilon_{i,p}} g_p \Delta\omega$$

10 x 10 x 10 nm^3 cell has ~ 10^5 phonons

$$\tilde{N} = N/W_t.$$

E. B. Ramayya and I. Knezevic, *Phys. Rev. B*, submitted (2012)

Phonon Initialization: Phonon Attributes

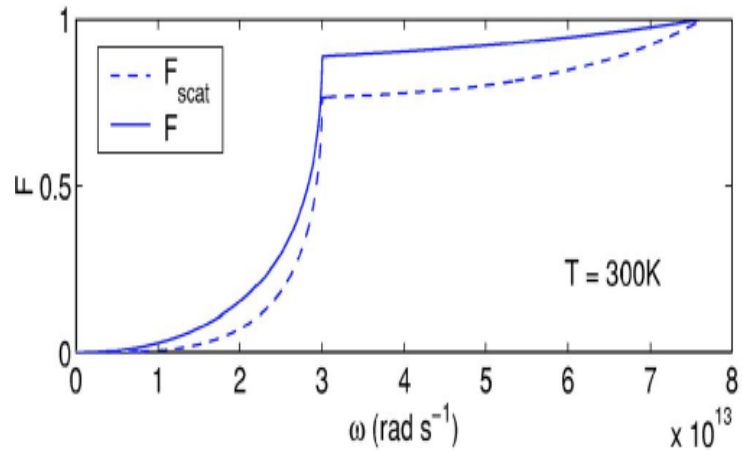
$$N = V \sum_{p=LA,TA} \sum_{i=1}^{N_w} \left[\frac{1}{exp(\frac{\hbar\omega_i}{K_B T}) - 1} \right] \frac{q_{i,p}^2}{2\pi^2 \upsilon_{i,p}} g_p \Delta\omega$$

- Frequency
- Polarization
- Group Velocity
- Direction (q_x,q_y,q_z)
- Position (x,yz)

Phonon Initialization: Frequency

Frequency is found from the cumulative number density function

$$F_i = \sum_{k=1}^{i} N_k / \sum_{k=1}^{N_w} N_k$$



- Pick a random number *R*

$$F_{i-1} \leq R \leq F_i$$

- Select ω from the ith spectral interval

Phonon Initialization: Polarization

Polarization is found from the ratio of LA to TA phonons in a particular spectral interval

$$P_i(LA/TA) = \frac{N_i(LA)}{N_i(LA) + N_i(TA)}$$

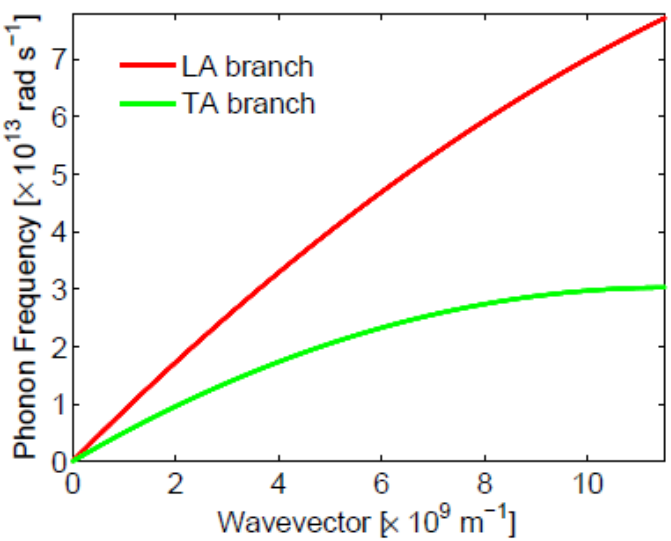
- Pick a random number *R*

$$R < P_i(LA/TA)$$

polarization p = LA else p = TA

Phonon Initialization: Group Velocity and Wavevector

Group velocity and magnitude of wavevector can be found from the dispersion



$$\omega_q = \omega_o + v_s q + c q^2$$

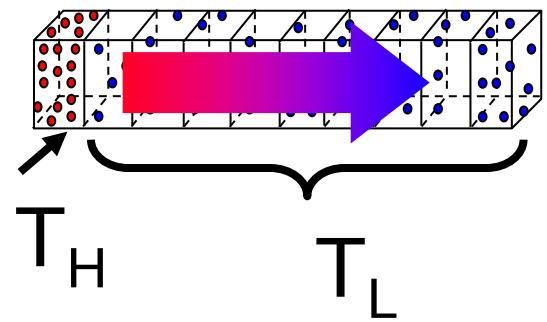
Direction of wavevector - isotropic

$$\hat{\mathbf{s}} = \begin{pmatrix} \sin\theta \cdot \cos\psi \\ \sin\theta \cdot \sin\psi \\ \cos\theta \end{pmatrix} \qquad \psi = 2\pi R_2, \ \cos\theta = 2R_1 - 1$$

Phonon Initialization: Position

Phonons in a cell are distributed isotropically

Position of nth phonon in c^{th} cell



$$\mathbf{r}_{n,c} = \mathbf{r}_c + L_x R_1 \mathbf{i} + L_y R_2 \mathbf{j} + \frac{L_z}{n_z} R_3 \mathbf{k}$$

R_1, R_2, and R_3 are random numbers
L_x, L_y, and L_z are dimensions of the device
n_z is the number of cells

Phonon Initialization: Energy of Cell

Energy of the cell should automatically be in accordance to the cell temperature

$$E = V \sum_{p=LA,TA} \sum_{i=1}^{N_w} \left[\frac{\hbar\omega_i}{exp(\frac{\hbar\omega_i}{K_B T}) - 1} \right] \frac{q_{i,p}^2}{2\pi^2 v_{i,p}} g_p \Delta\omega$$

- Check for consistency between *N*, *E*, and *T*
- Find *T* from *numerical inversion of E* (of each cell) and check if it corresponds to the initialization temperature

Phonon Diffusion

- Let the phonons diffuse with the their initial velocities and track the position

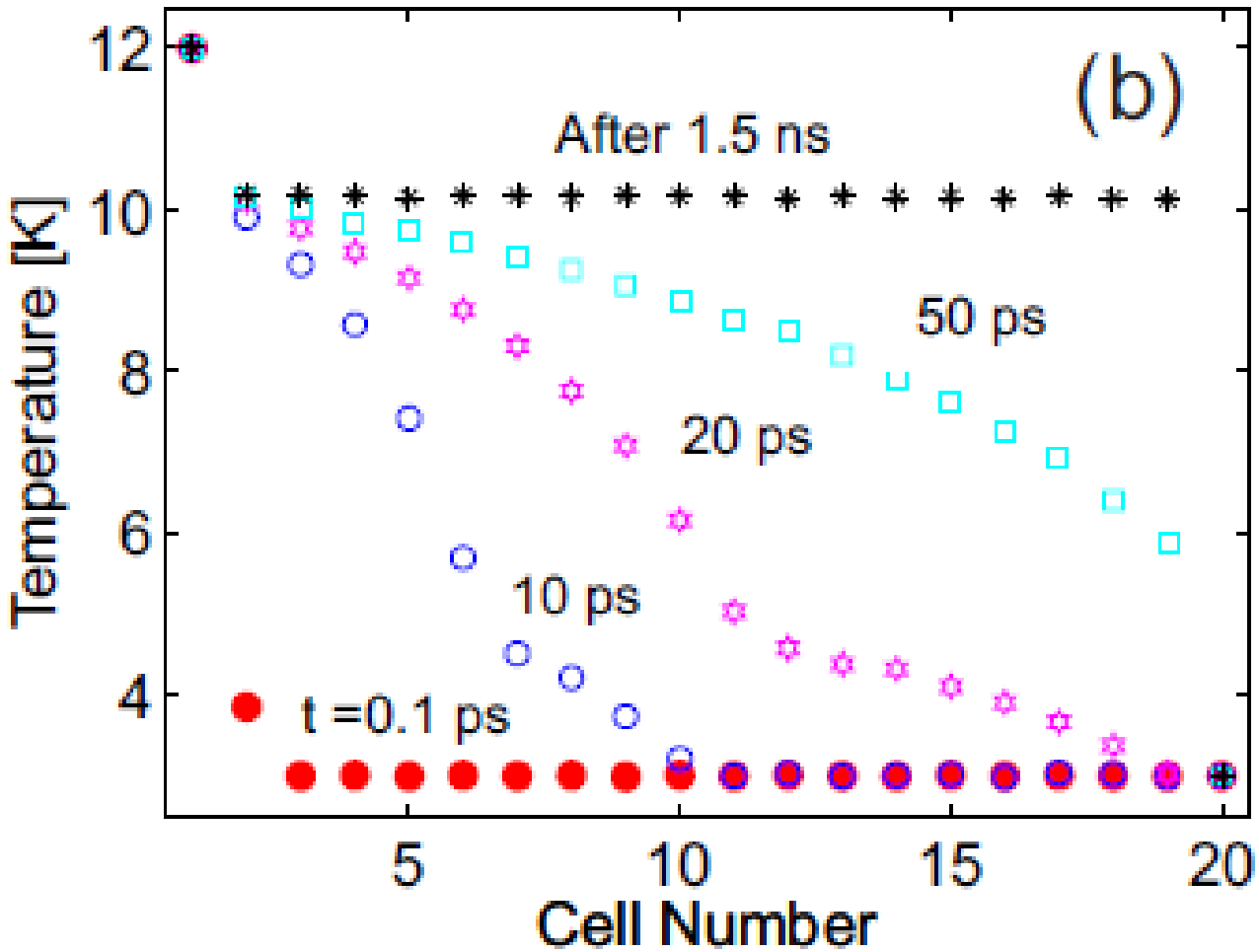
- If the phonon crosses a cell delete it from that cell and assign the new cell number

- After each time step calculate the temperature from the net new energy of each cell

- If a phonon reaches an end cell delete it from the simulation domain

- Reinitialize the phonons in the end cells after each *dt*

Thermal Transport Ballistic Phonons



Ballistic steady state temperature is given by the Stefan-Boltzmann law of blackbody radiation

$$T_{ss}^{B} = [(T_H^4 + T_L^4)/2]^{1/4}$$

Phonon Monte Carlo Transient Simulation

Phonon-Boundary Diffuse Scattering

- Phonon that underwent a scattering at the boundary is deleted and a new phonon is emitted from the boundary

Direction of wavevector – isotropic (normal to the surface)

$$\hat{s} = \begin{pmatrix} \sin\theta \cdot \cos\psi \\ \sin\theta \cdot \sin\psi \\ \cos\theta \end{pmatrix} \qquad \begin{aligned} \theta &= \sin^{-1}(R_1) \\ \psi &= 2\pi R_2 \end{aligned}$$

M. Modest, Radiative Heat Transfer p.654 (Academic Press, New York 2003)

Phonon Scattering

- Phonon that underwent scattering is deleted and a new phonon is created from new distribution function weighted by the scattering rate

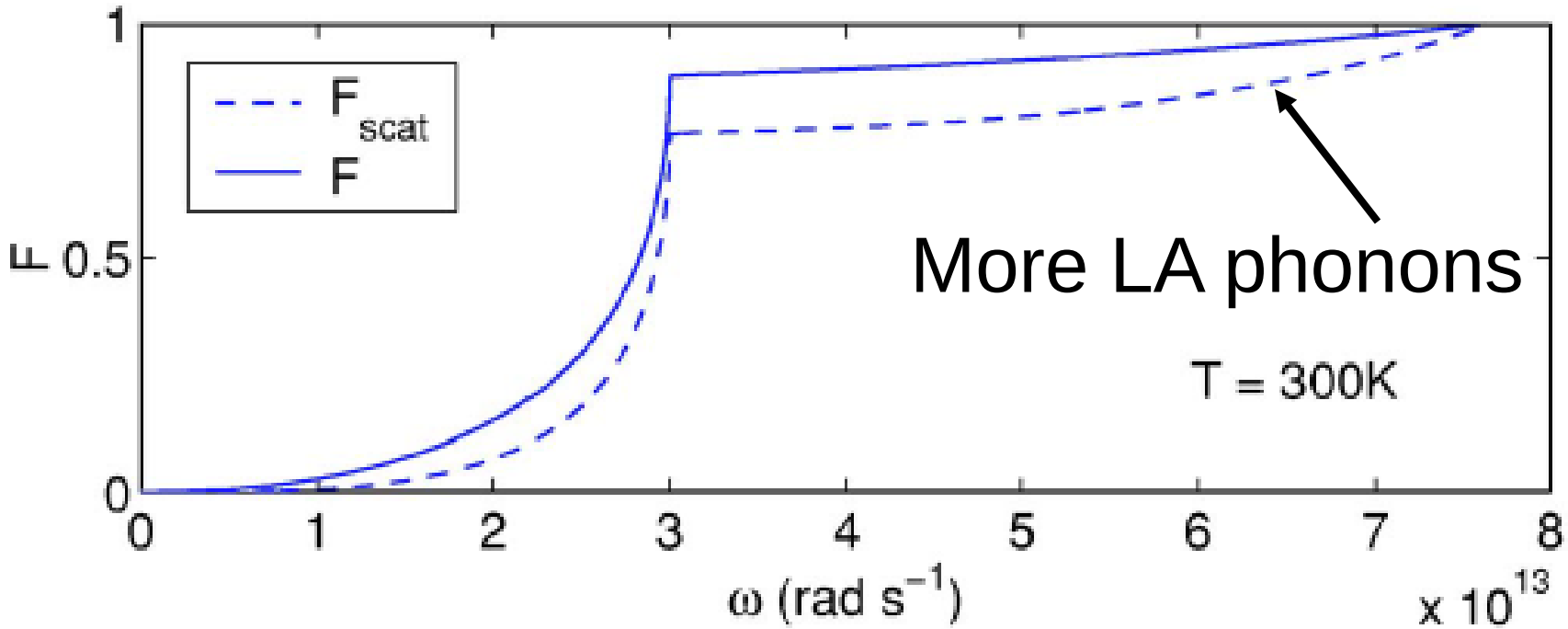
- Phonons that underwent a U scattering are replaced by phonons which have a new direction

- Phonons that underwent a N scattering are replaced by phonons with same direction but different magnitude.

- Phonon-impurity/isotope scattering is treated as isotropic

Phonon Reinitialization

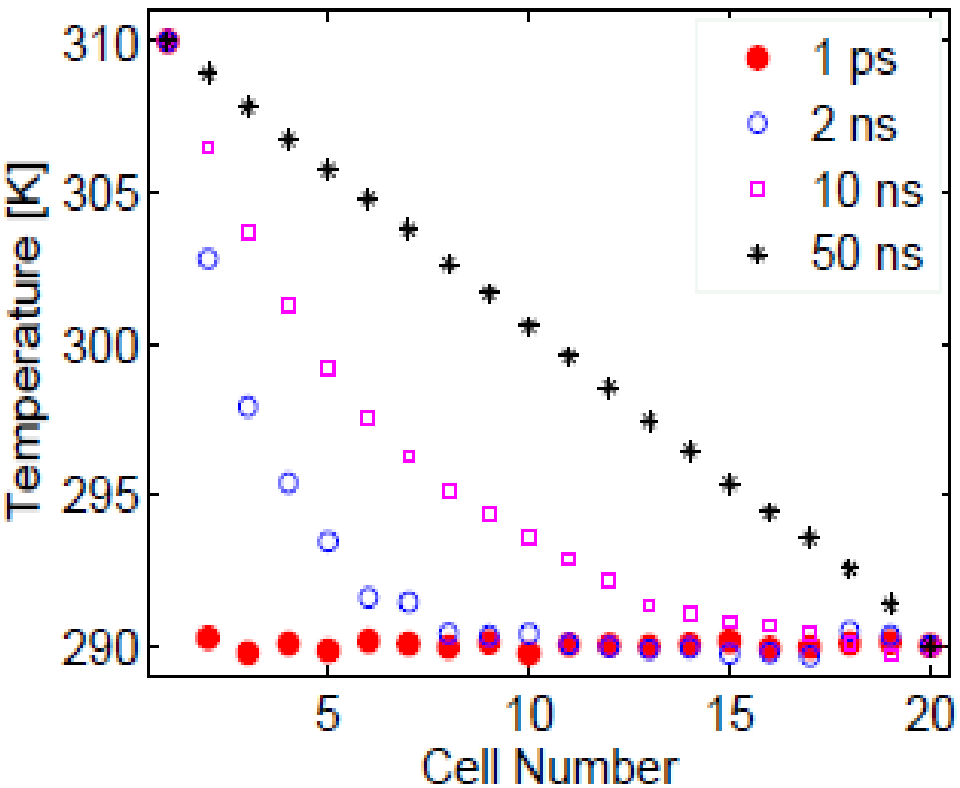
Frequency is found from the cumulative number density function weighted by scattering probability

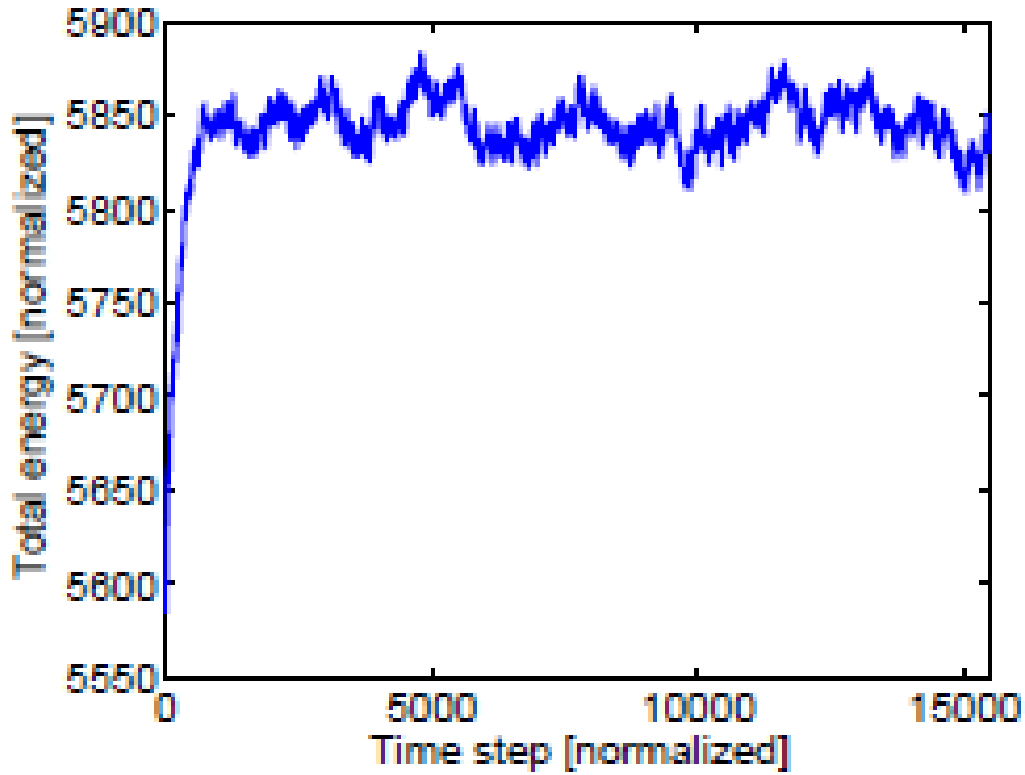


Lacroix *et al*. Appl. Phys. Lett. **89**, 103104 (2006)

Important for conserving the energy

Phonon Monte Carlo Transient Simulation





E. B. Ramayya and I. Knezevic, *Phys. Rev. B*, submitted (2012)

Thermal Conductivity

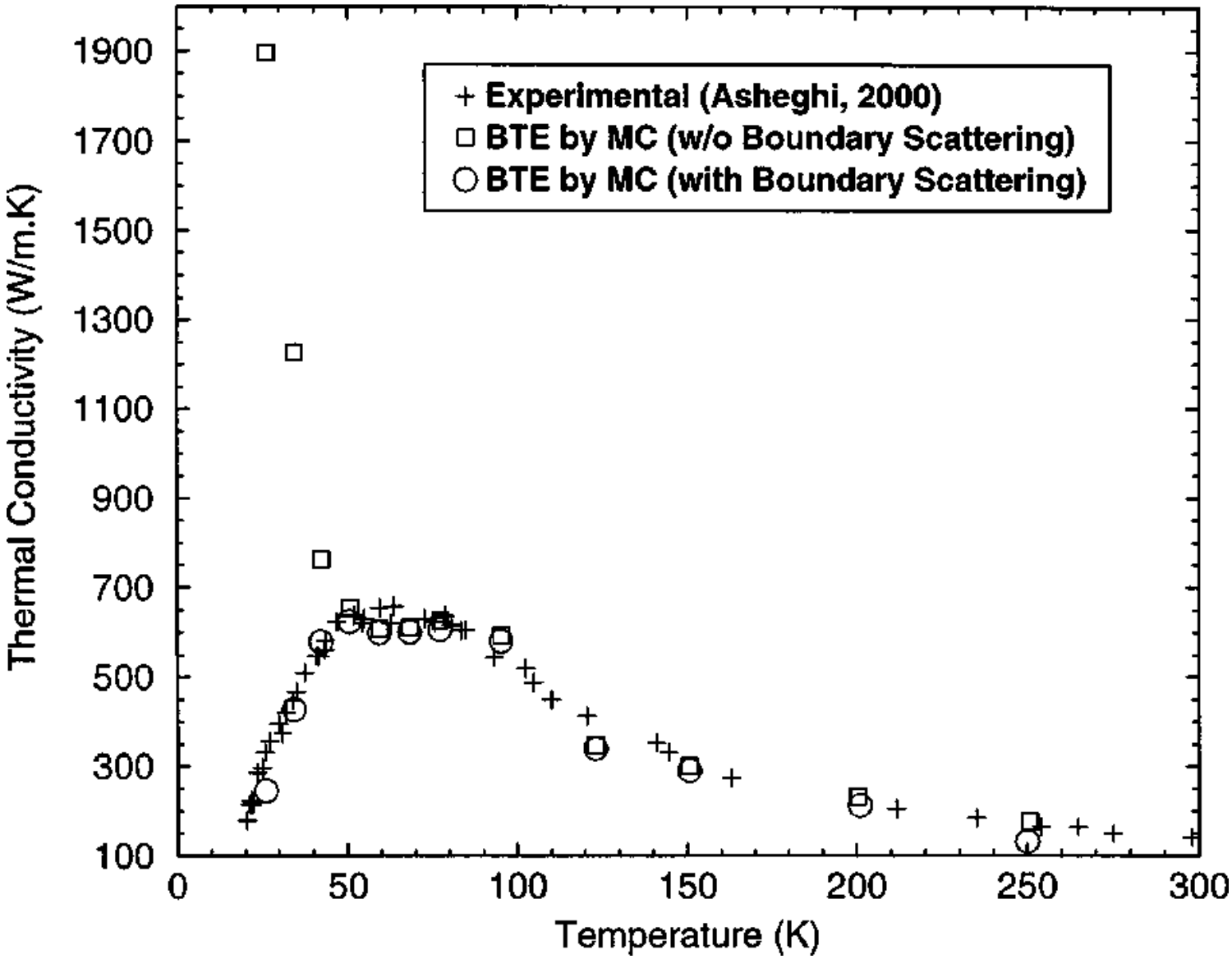
Flux crossing two adjacent cells in steady state

$$\Phi = \frac{W_t}{dt} \sum_{i=1}^{N_c} \hbar\omega \frac{\mathbf{q}_z}{|q|}$$

Thermal conductivity is calculated from Fourier's law

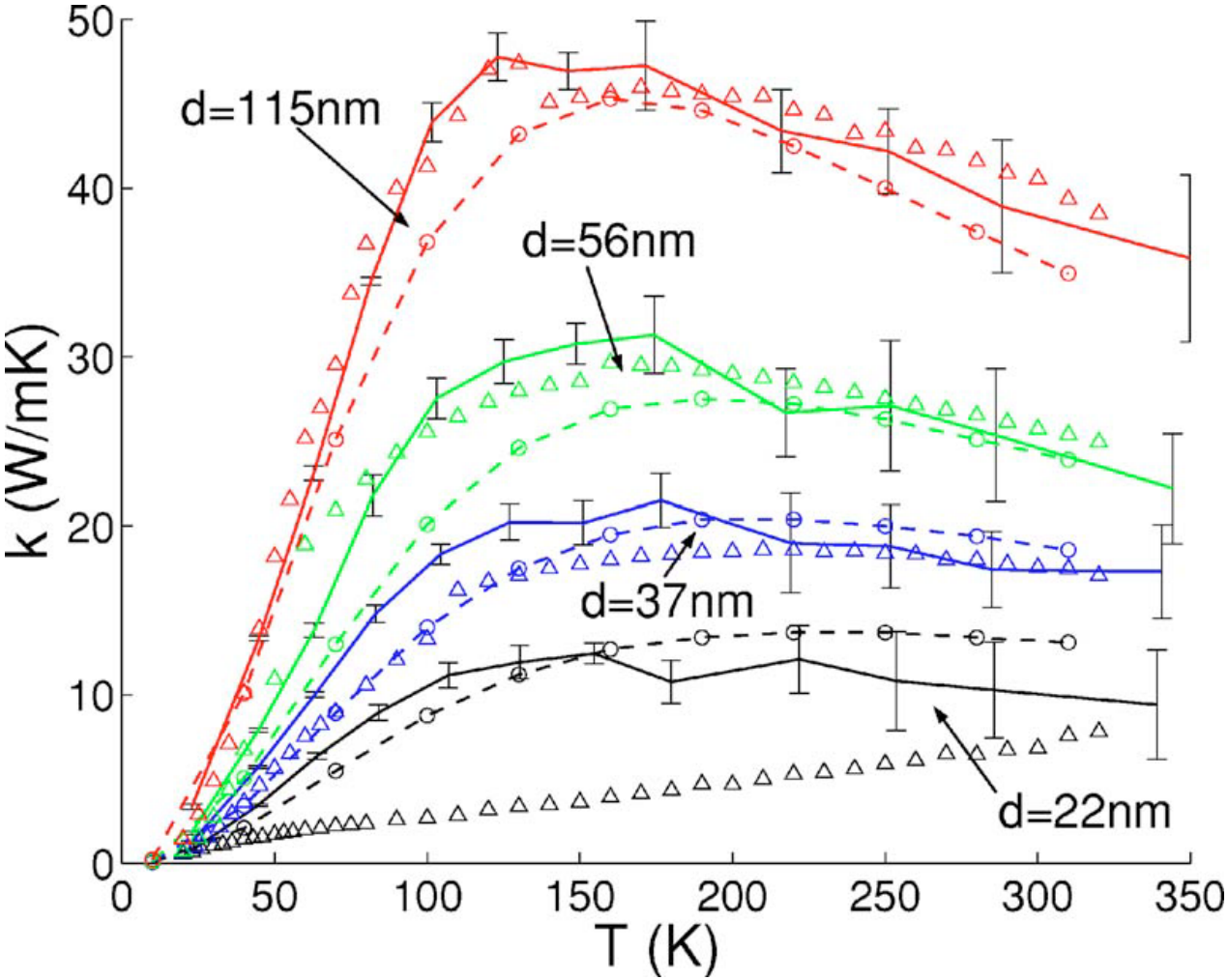
$$\kappa = \frac{1}{A} \frac{\Delta L}{\Delta T} \Phi$$

Bulk Silicon Thermal Conductivity



S. Mazumder and A. Majumdar, *J. Heat Transfer* **123**, 749 (2001)

Limitation of Diffuse Boundary Scattering



Lacroix *et al*. Appl. Phys. Lett. **89**, 103104 (2006)

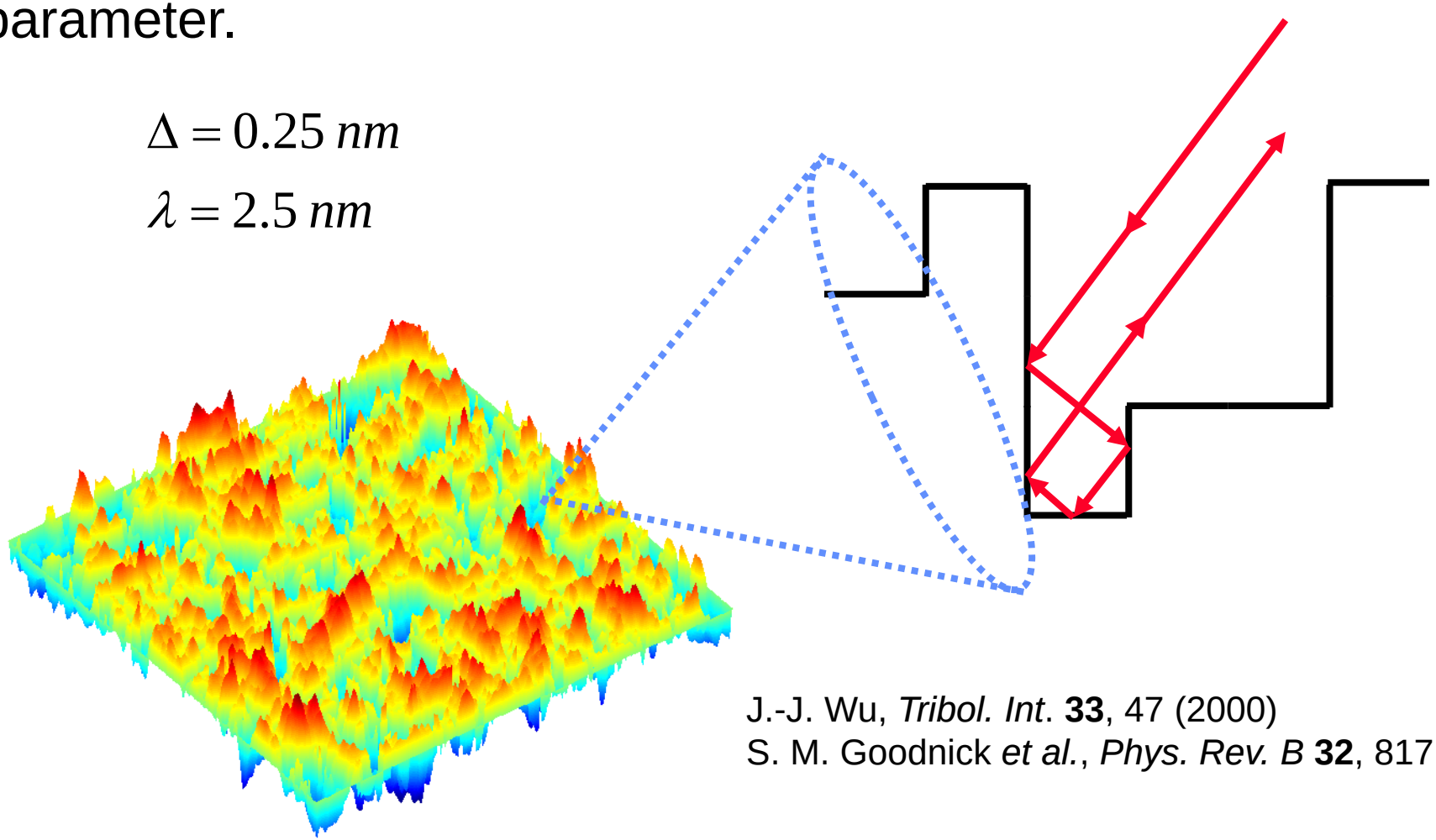
D. Li *et al*., *Appl. Phys. Lett.* **83**, 2934 (2003)

Surface Roughness Inclusion in Monte Carlo

Can treat the actual surface without using a specularity parameter.

$$\Delta = 0.25\,nm$$

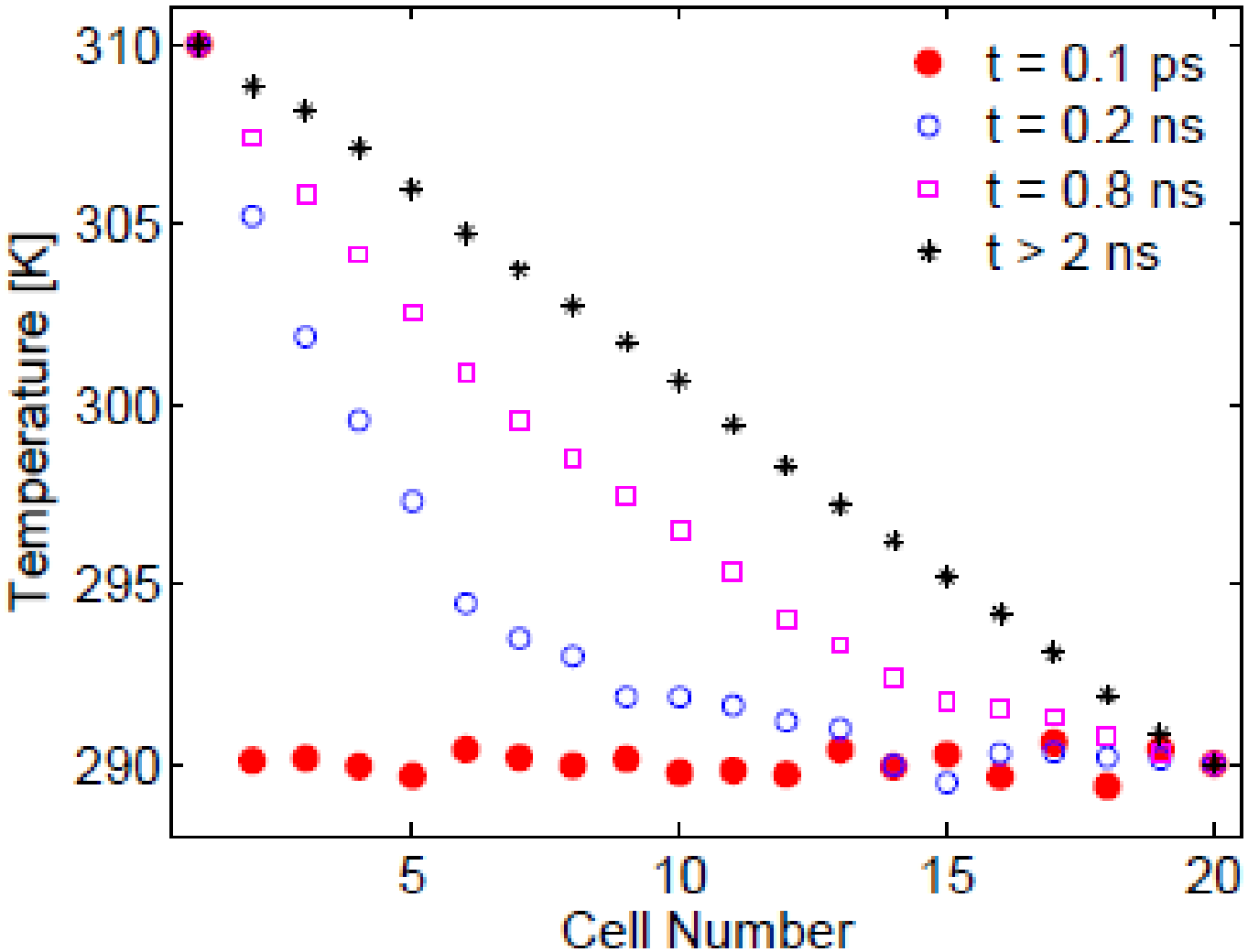
$$\lambda = 2.5\,nm$$



J.-J. Wu, *Tribol. Int*. **33**, 47 (2000)
S. M. Goodnick *et al.*, *Phys. Rev. B* **32**, 8171 (1985)

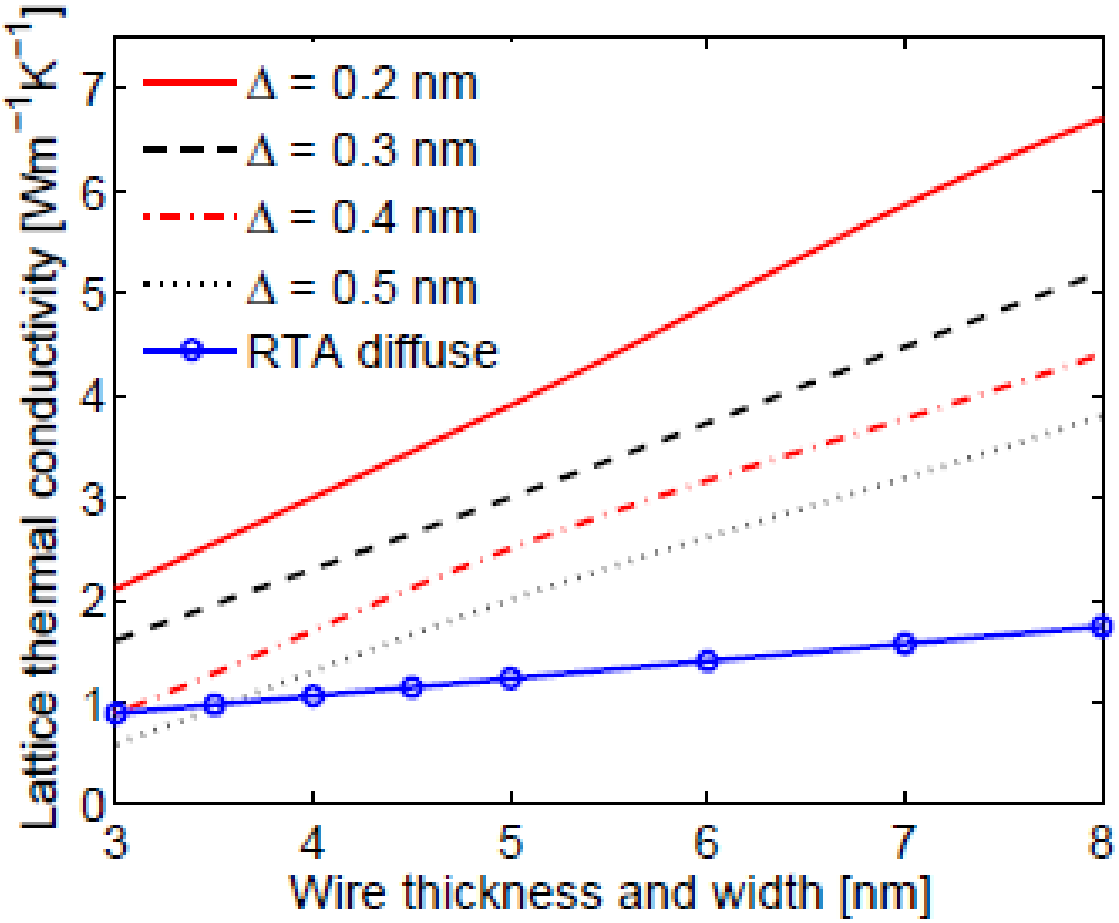
A good way to capture phonon localization and the particular features of a given surface ← better than specularity parameter

Transient Results



E. B. Ramayya and I. Knezevic, *Phys. Rev. B*, submitted (2012)

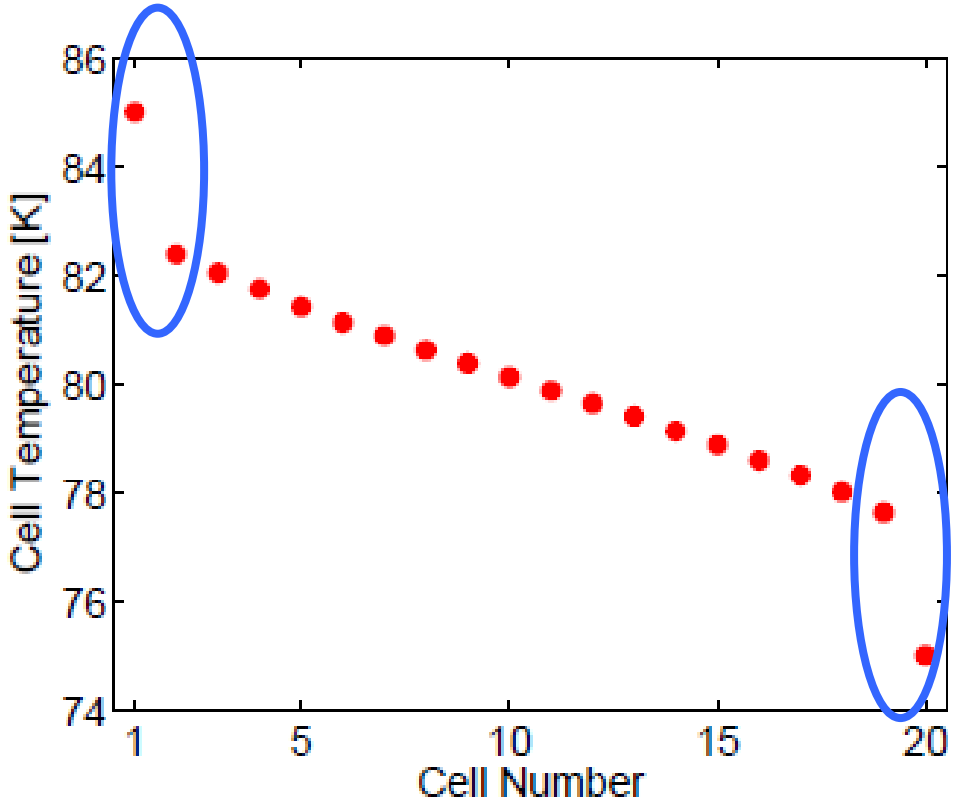
Thermal Conductivity: Roughness Dependence

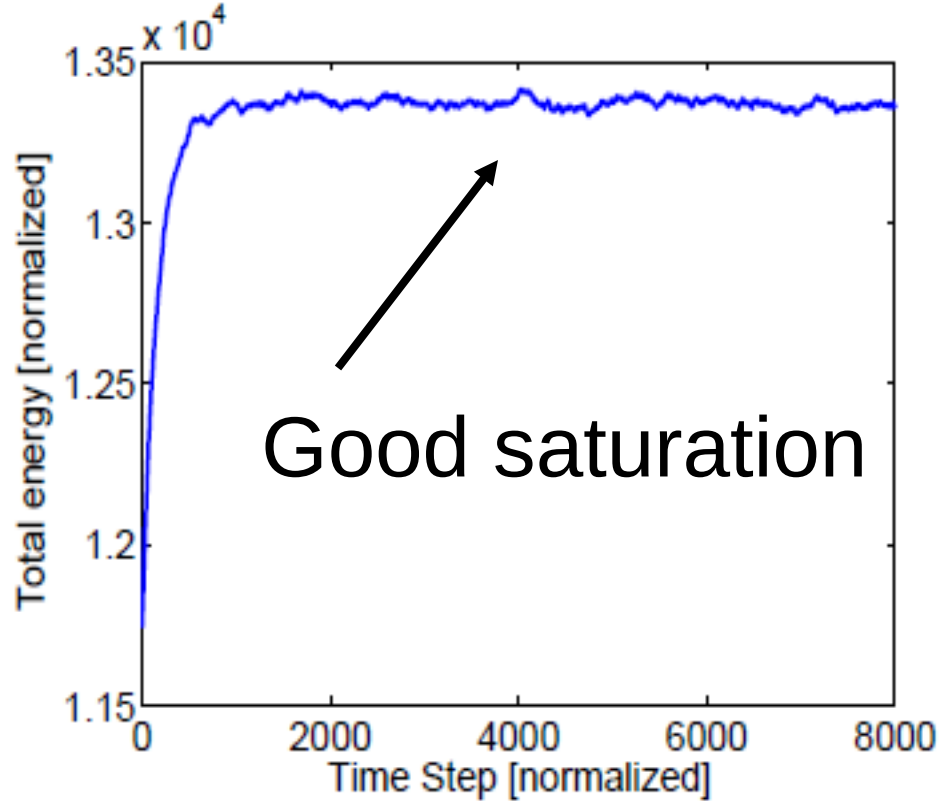


$\kappa_{l\ bulk}$ = 148 Wm^{-1}K^{-1}

- κ_l is more than an order of magnitude lower than that in bulk due to strong boundary scattering of phonons
- Decreases with increase in rms.

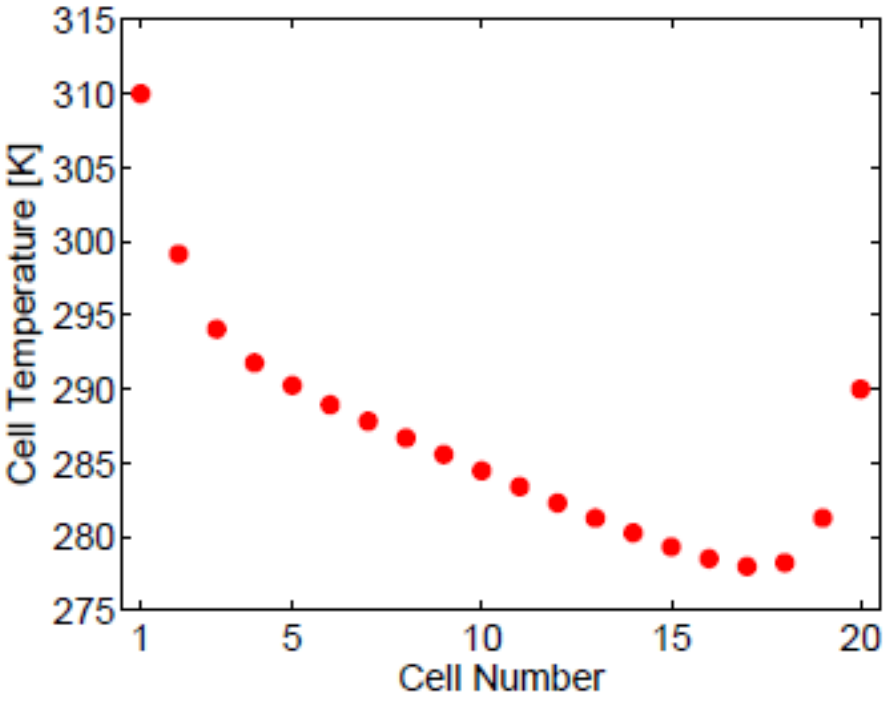
Thermal Transport Quasi-Balistic Phonons

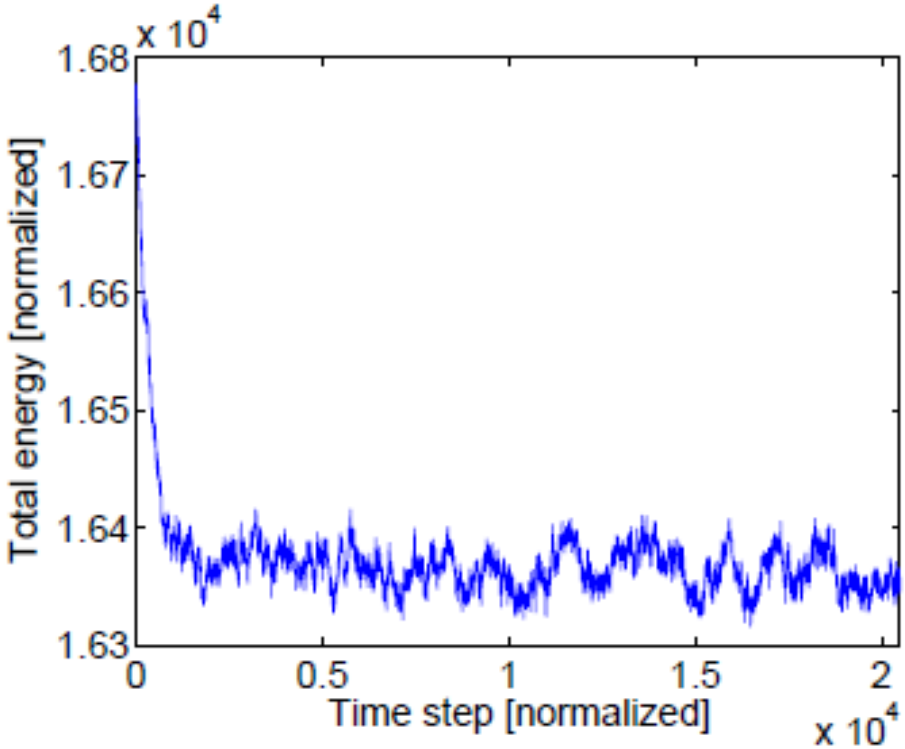




Increase the length

Thermal Transport: Things to Look For

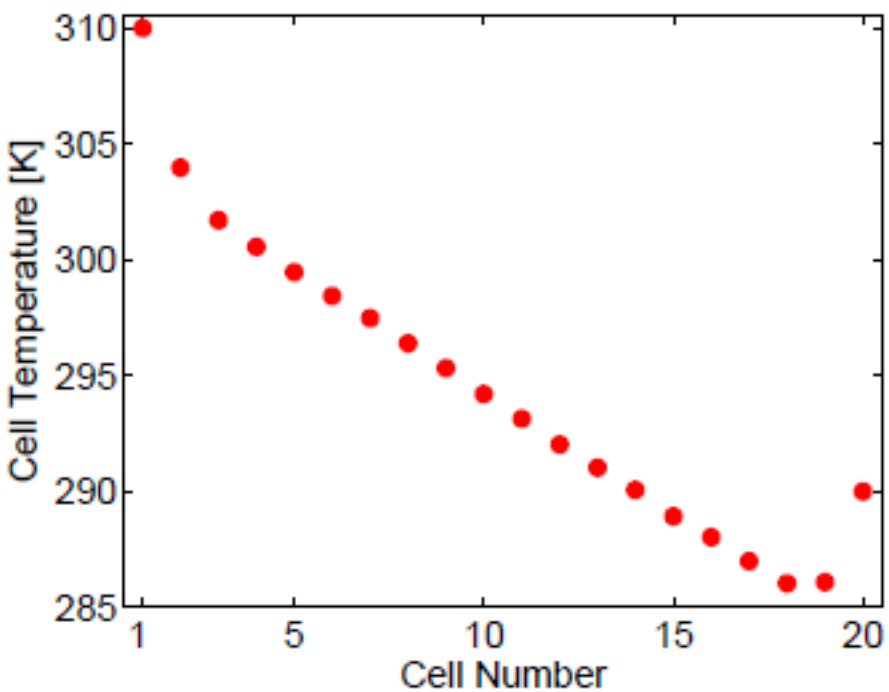


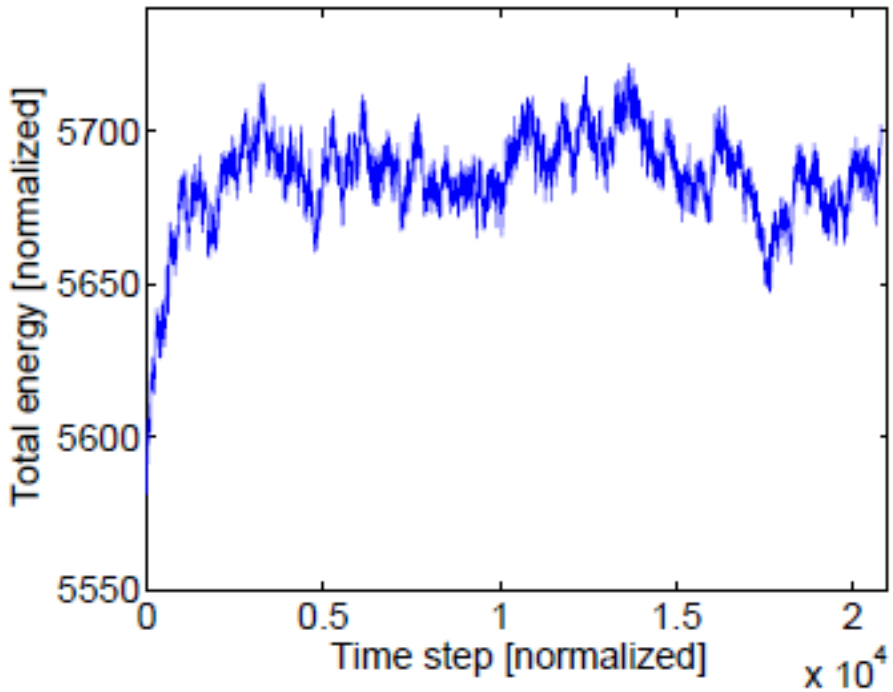


Losing phonons

Bug in the code

Thermal Transport: Things to Look For



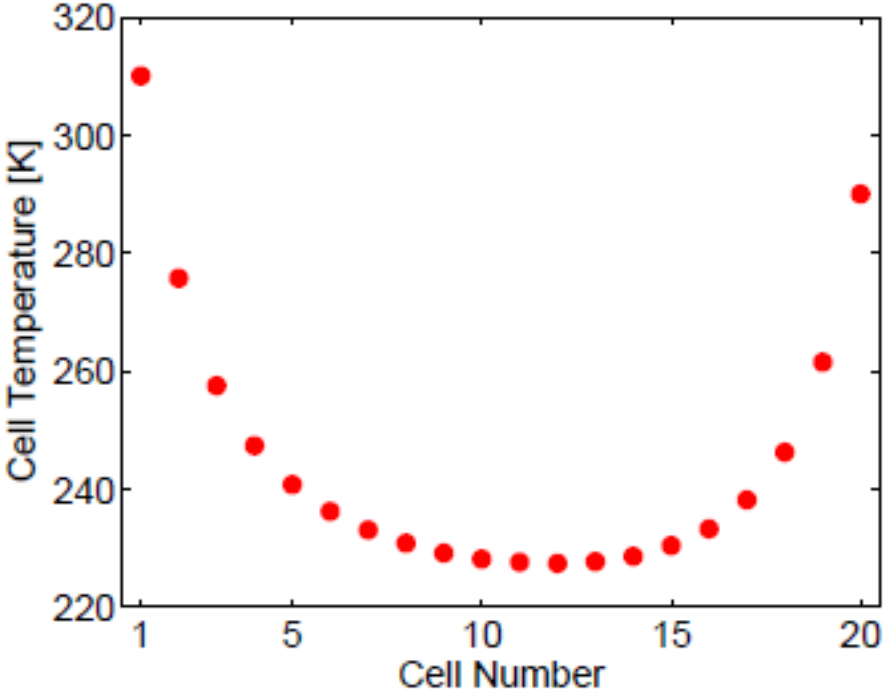


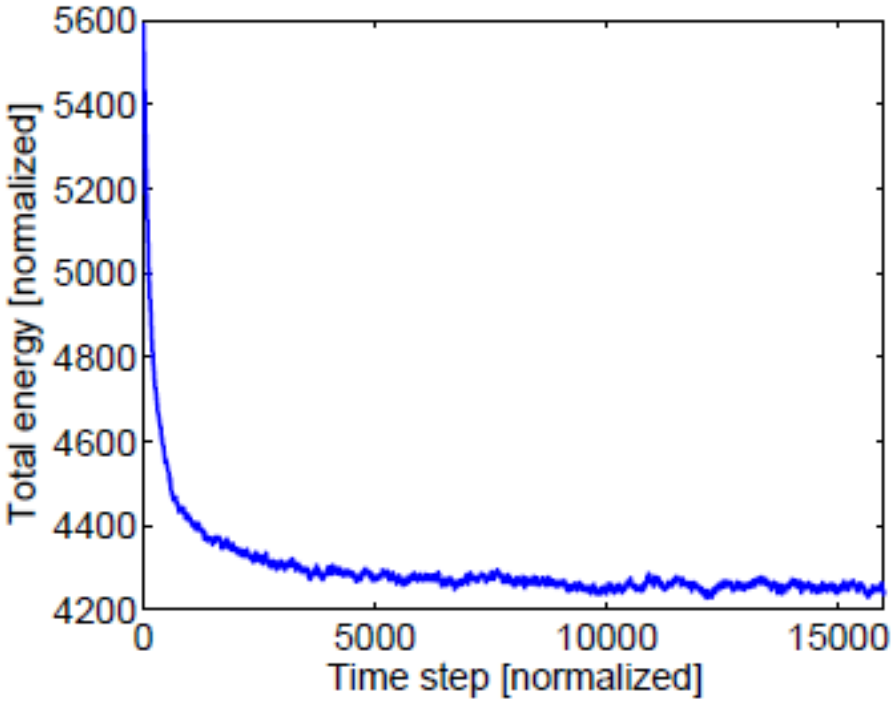
10x phonon-phonon scattering

Losing phonons but not as much as before

Bug in the code

Thermal Transport: Things to Look For





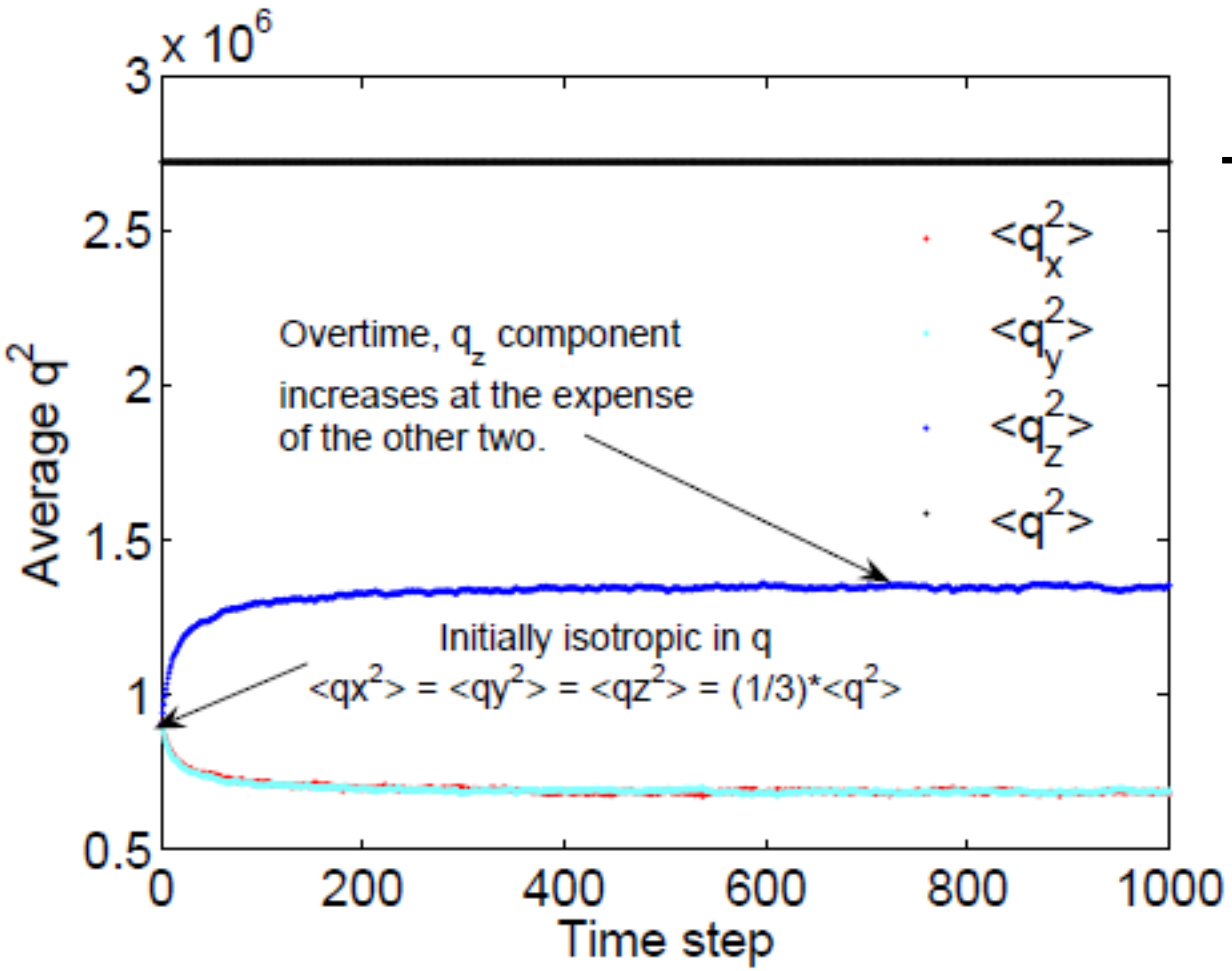
Worse than before

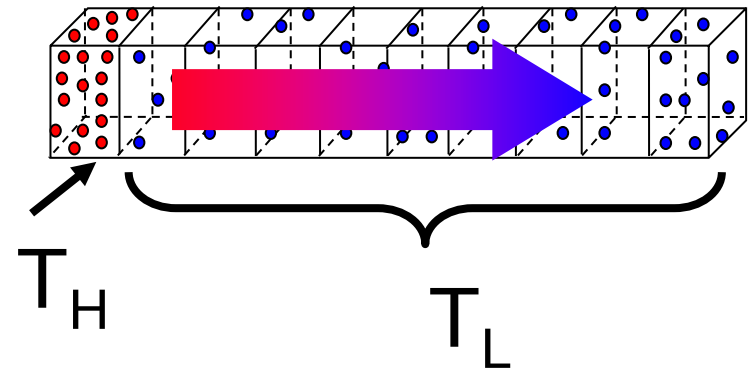
Losing phonons

Only boundary scattering

Bug in the randomization after boundary scattering

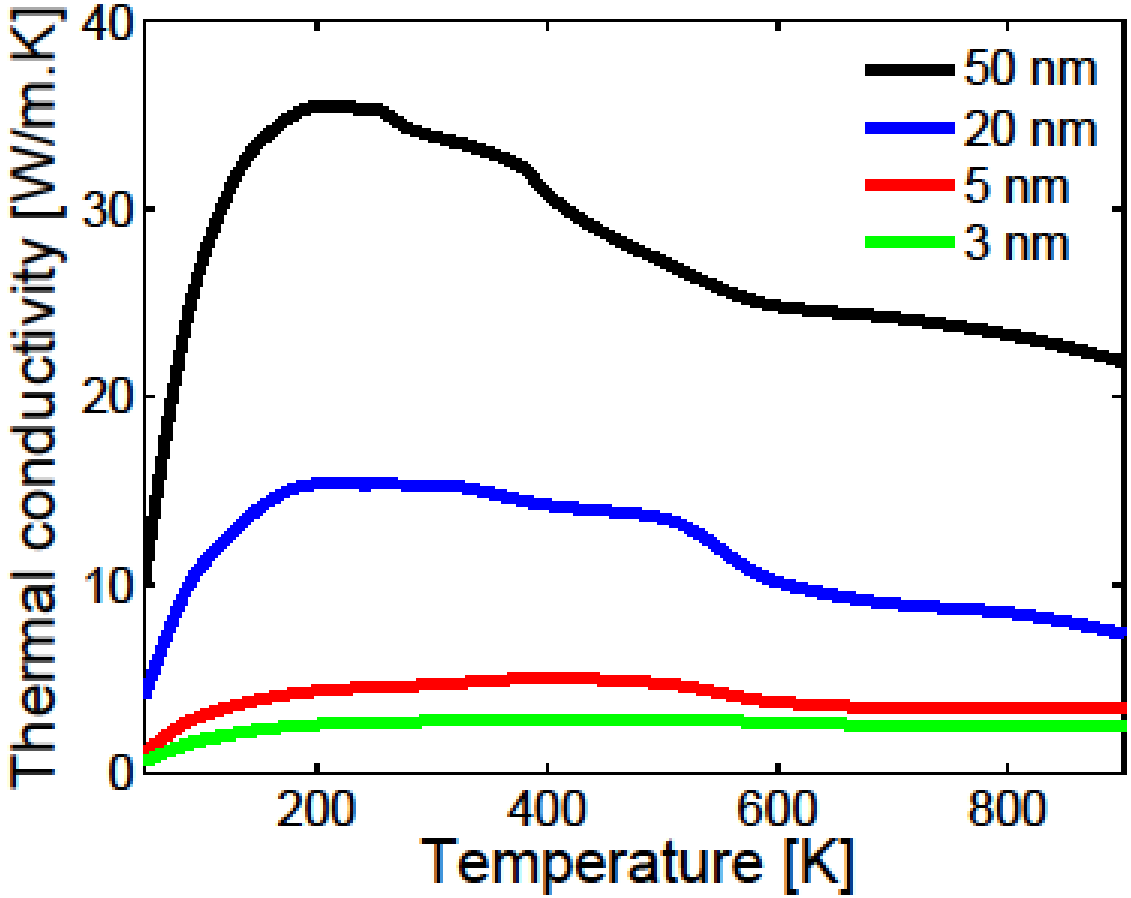
Thermal Transport: Things to Look For





Losing more phonons than that are injected

Thermal Conductivity: GaN



GaN Nanowires for Thermoelectric Applications
A. Davoody 3:30 Thursday

By changing the dispersion, the algorithm can be easily adapted to calculate the thermal conductivity of different semiconductors

Summary

Monte Carlo simulation of phonon transport can be used to account for the large reduction in thermal conductivity in silicon nanowires

- Roughness inclusion as in electron transport
- Can be adapted to other semiconductors

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