Semiclassical Phonon Transport in the Presence of Rough Boundaries

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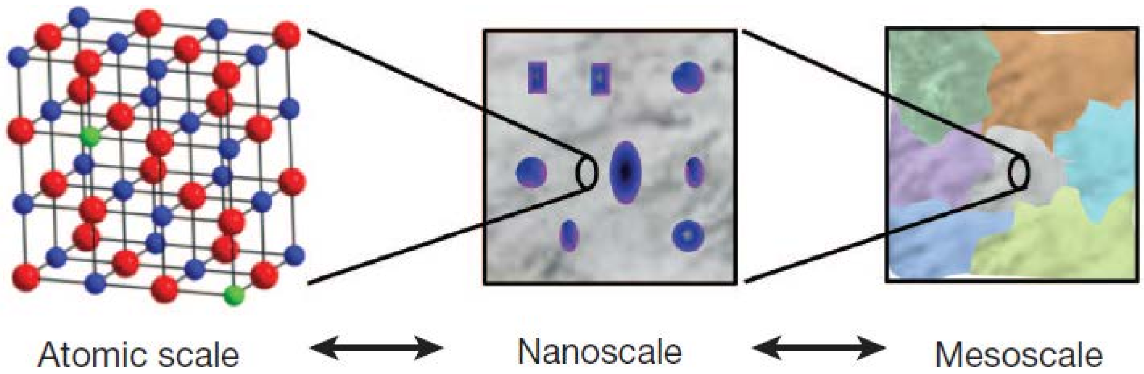
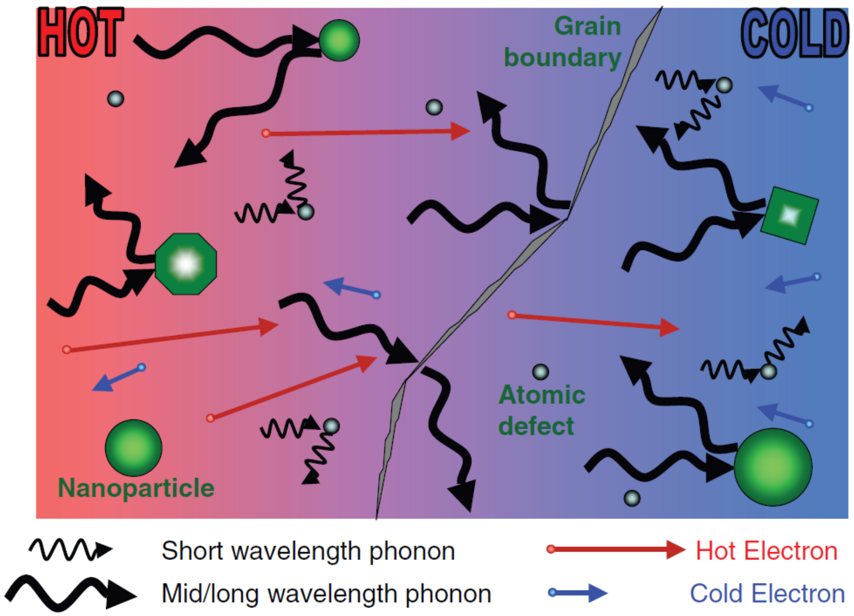
Phonons in Nanostructures

- Phonons scatter with boundaries (mesoscale), imperfections (nanoscale) and isotope/dopant atoms (atomic scale).



Biswas *et al.*, *Nature* **489**, 414 (2012)

- Strong interactions with rough boundaries or interfaces between materials
- Need to understand thermal transport in the presence of both roughness and internal scattering



C. J. Vineis *et al.*, *Adv. Mater.* **22**, 3970 (2010)

Lessons from electronic transport

Time

Semiclassical (electron BTE and derivatives)

Drift-diffusion equations

Hydrodynamic equations

BTE in the relaxation-time approximation (RTA)
Ensemble Monte Carlo

Quantum corrections

Wigner transport equation (Wigner Monte Carlo)

Quantum hydrodynamic equations

Single-particle density matrix formalism

Quantum

Nonequilibrium Green's functions

(NEGF+atomistic tight binding, NEGF+DFT for small systems)

More Accurate

More Complicated

Phonon transport

More Accurate

Semiclassical (phonons BTE and derivatives))

Heat diffusion equation

BTE in the RTA

Ensemble Monte Carlo

Discrete ordinate method

Direct solutions to BTE

Great recent work to extract accurate rates from DFPT to use with Boltzmann transport kernels

Classical (atoms)

Molecular dynamics

Great recent work on applying ab initio to extract accurate potentials for use in MD

Quantum (phonons)

Nonequilibrium Green's functions

Currently not possible to address phonon-phonon scattering

More Complicated

Why semiclassical phonon transport?

Pros:

- ✓ Computationally tractable for experimentally relevant sizes
- ✓ A variety of techniques adaptable to geometry
- ✓ All kinds of scattering mechanisms can be incorporated
- ✓ Intuitive (humans like the distribution function)

Cons:

- ↓ Cannot address coherent transport features
- ↓ Does not account for states being affected by interactions
- ↓ Must a priori decide which mechanisms to account for
- ↓ Only as good as the rates used, rates obtained from elsewhere

Semiclassical transport

From intro-level quantum-mechanics textbooks: The semiclassical (or WKB) approximation holds when the potential vary slowly on the scale of the particle wavelength. The concept of classical trajectories is viable.

When is the semiclassical approximation applicable to transport?

When **relevant length/time scales** on which the single-particle Green's function varies are **much longer than coherence lengths and times**

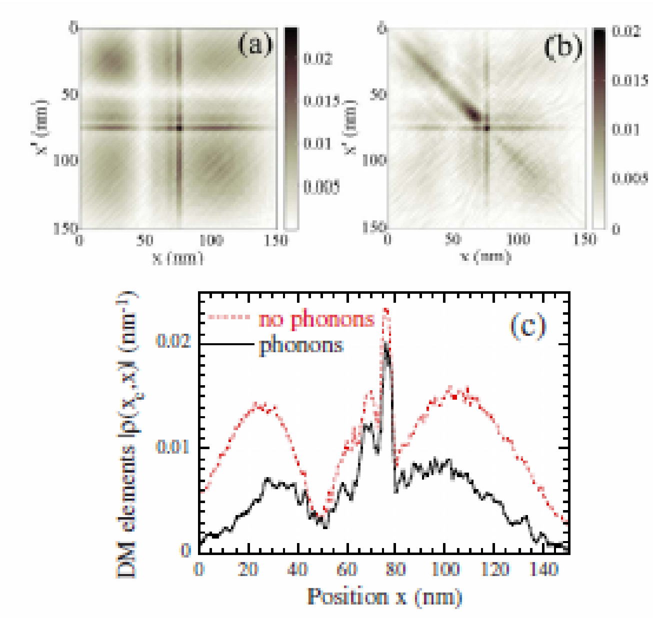
$$
\begin{aligned}
&[\omega - (p^2/2m) - U(\mathbf{R},T) - \mathrm{Re}\, \Sigma(\mathbf{p},\omega;\mathbf{R},T),\ g^<(\mathbf{p},\omega;\mathbf{R},T)] \\
&\quad + [\mathrm{Re}\, g(\mathbf{p},\omega;\mathbf{R},T),\ \Sigma^<(\mathbf{p},\omega;\mathbf{R},T)] \\
&= -\Sigma^>(\mathbf{p},\omega;\mathbf{R},T)\, g^<(\mathbf{p},\omega;\mathbf{R},T) \\
&\quad + \Sigma^<(\mathbf{p},\omega;\mathbf{R},T)\, g^>(\mathbf{p},\omega;\mathbf{R},T)
\end{aligned}
$$

$$
\begin{aligned}
&\int \frac{d\omega}{2\pi} \frac{g^>(\mathbf{p},\omega;\mathbf{R},T) \mp g^<(\mathbf{p},\omega;\mathbf{R},T)}{z-\omega} \\
&= g(\mathbf{p},z;\mathbf{R},T) \\
&= [z - (p^2/2m) - U(\mathbf{R},T) - \Sigma(\mathbf{p},z;\mathbf{R},T)]^{-1}
\end{aligned}
$$

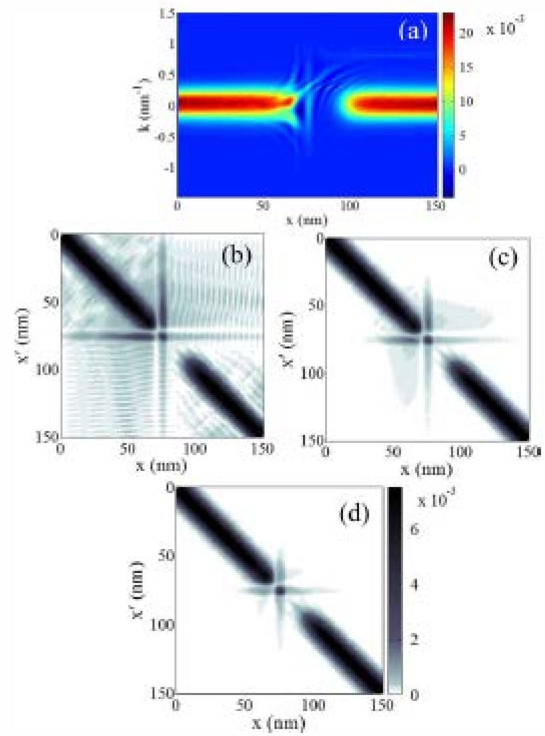
Kadanoff and Baym, Quantum Statistical Mechanics, W.A. Benjamin, New York, 1962

Example from the electronic world

What scattering does to coherences in a double-barrier tunneling structure



Scattering causes transition from resonant to sequential tunneling



Scattering kills off spatial coherences (off-diagonal terms)

PHYSICAL REVIEW B 78, 165306 (2008)

Wigner Monte Carlo simulation of phonon-induced electron decoherence in semiconductor nanodevices

Damien Querlioz,* Jérôme Saint-Martin, Arnaud Bournel, and Philippe Dollfus
Institut d'Electronique Fondamentale, CNRS, University Paris-Sud, 91405 Orsay, France

Semiclassical transport

Semiclassical approximation boils down to **transport being diffusive**:
Length scales longer than the mean free path, timescales longer than relaxation time

Technically, to obtain the Boltzmann equation, two more approximations are needed:

- **The Born approximation** (scattering event completed before the next one)
- **Scattering does little to alter the density of states**

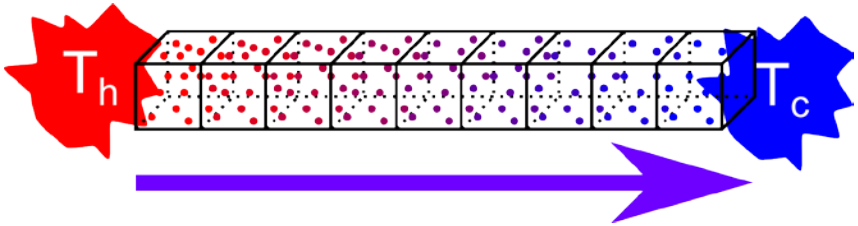
$$
\begin{aligned}
&[\omega - (p^2/2m) - U(\mathbf{R},T) - \mathrm{Re}\,\Sigma(\mathbf{p},\omega;\mathbf{R},T),\ g^<(\mathbf{p},\omega;\mathbf{R},T)] \\
&\qquad + [\mathrm{Re}\, g(\mathbf{p},\omega;\mathbf{R},T),\ \Sigma^<(\mathbf{p},\omega;\mathbf{R},T)] \\
&\quad = -\Sigma^>(\mathbf{p},\omega;\mathbf{R},T)\, g^<(\mathbf{p},\omega;\mathbf{R},T) \\
&\qquad + \Sigma^<(\mathbf{p},\omega;\mathbf{R},T)\, g^>(\mathbf{p},\omega;\mathbf{R},T)
\end{aligned}
$$

$$
\begin{aligned}
&\int \frac{d\omega}{2\pi}\, \frac{g^>(\mathbf{p},\omega;\mathbf{R},T) \mp g^<(\mathbf{p},\omega;\mathbf{R},T)}{z-\omega} \\
&\quad = g(\mathbf{p},z;\mathbf{R},T) \\
&\quad = [z - (p^2/2m) - U(\mathbf{R},T) - \Sigma(\mathbf{p},z;\mathbf{R},T)]^{-1}
\end{aligned}
$$

$$
\begin{aligned}
&\left[\frac{\partial}{\partial T} + \frac{\mathbf{p}\cdot\nabla\mathbf{R}}{m} - \nabla_R U_{\mathrm{eff}}(\mathbf{R},T)\cdot\nabla_p\right] f(\mathbf{p},\mathbf{R},T) \\
&\quad = -\int \frac{d\mathbf{p}'}{(2\pi)^3}\,\frac{d\bar{\mathbf{p}}}{(2\pi)^3}\,\frac{d\bar{\mathbf{p}}'}{(2\pi)^3}\,(2\pi)^4\,\delta(\mathbf{p}+\mathbf{p}'-\bar{\mathbf{p}}-\bar{\mathbf{p}}') \\
&\qquad \times \delta\left(\frac{p^2}{2m} + \frac{p'^2}{2m} - \frac{\bar{p}^2}{2m} - \frac{\bar{p}'^2}{2m}\right)(1/2)\,[v(\mathbf{p}-\bar{\mathbf{p}}) \mp v(\mathbf{p}-\bar{\mathbf{p}}')]^2 \\
&\qquad \times [ff'(1\pm\bar{f})(1\pm\bar{f}') - (1\pm f)(1\pm f')\bar{f}\bar{f}'] \qquad (9\text{-}
\end{aligned}
$$

Kadanoff and Baym, *Quantum Statistical Mechanics*, W.A. Benjamin, New York, 1962

Example of semiclassical phonon transport



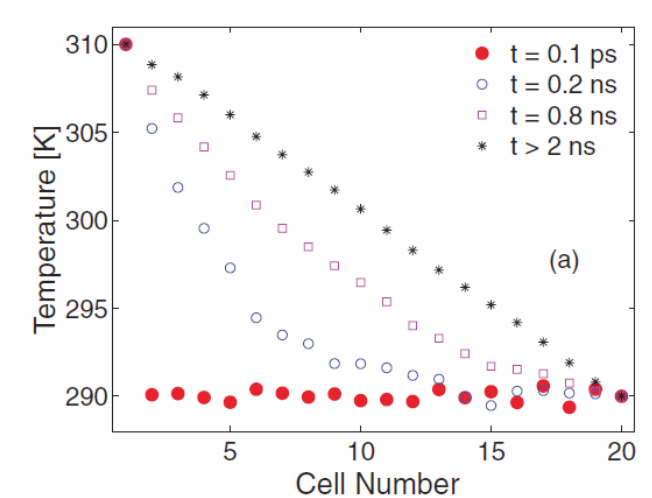
PHYSICAL REVIEW B **86**, 115328 (2012)

Thermoelectric properties of ultrathin silicon nanowires

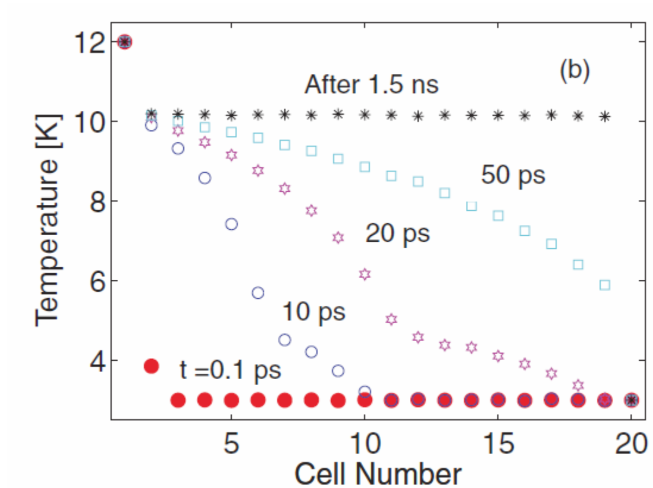
E. B. Ramayya,* L. N. Maurer, A. H. Davoody, and I. Knezevic†
Department of Electrical and Computer Engineering, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

A long smooth nanowire,
room temperature

The same nanowire,
much lower temperature



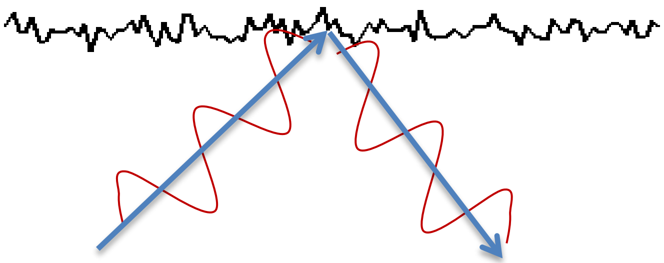
Length > mean free path

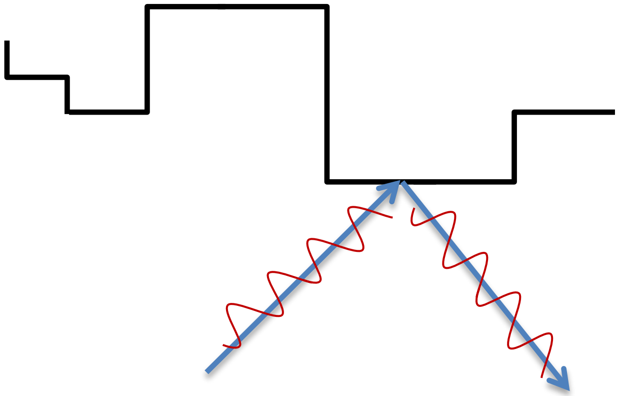


Length < mean free path

Phonons and boundary roughness

Depending on wavelength, they are treated as waves or classical objects when interacting with a rough boundary or rms roughness Δ and correlation length L





$$\lambda >> \Delta, L$$

$$\lambda << \Delta, L$$

Wave limit

Phonons should be treated as waves

Interference effects important

Specularity parameter OK

"Ray phononics" (particle) limit

Semiclassical approximation valid

Treat phonons as little balls

with classical trajectories

The role of correlation length

JOURNAL OF APPLIED PHYSICS VOLUME 38, NUMBER 4 15 MARCH 1967

Statistical Model for the Size Effect in Electrical Conduction*

STEPHEN B. SOFFER

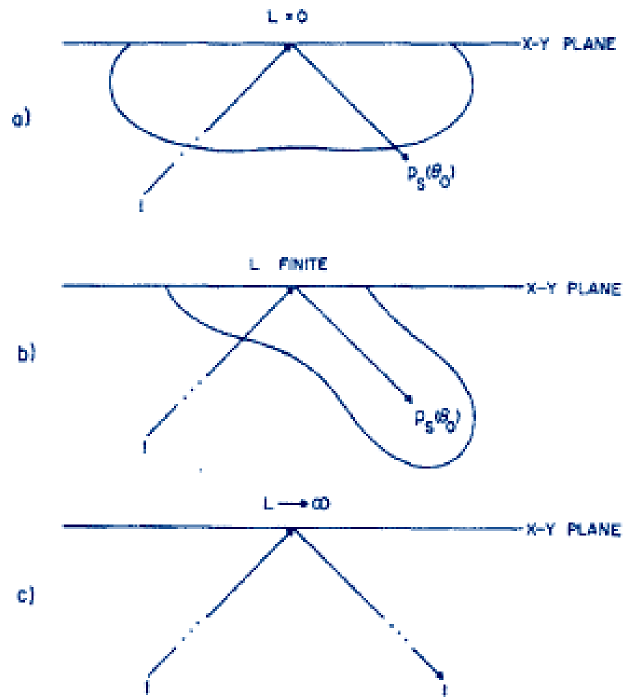


FIG. 2. Schematic diagrams of the incident and emerging average flux densities. The arrows represent beams of indicated magnitudes. The polar plots represent the diffuse intensities in the plane of incidence. The plot in (a) is obtained from the Appendix for $h/\lambda = 0.2.$, $\theta_0 = 45°$. That in (b) is only schematic.

L=0: Nearly isotropic diffuse portion of the scattered wave

L>0: With increasing correlation length, the diffusely scattered wave collimates along the direction obeying Snell's law

L→∞ : Even a rough surface appears completely smooth, as the diffuse and specular reflected waves align

Specularity parameter *p*

Intuitively plausible: *p* – probability of specular reflection

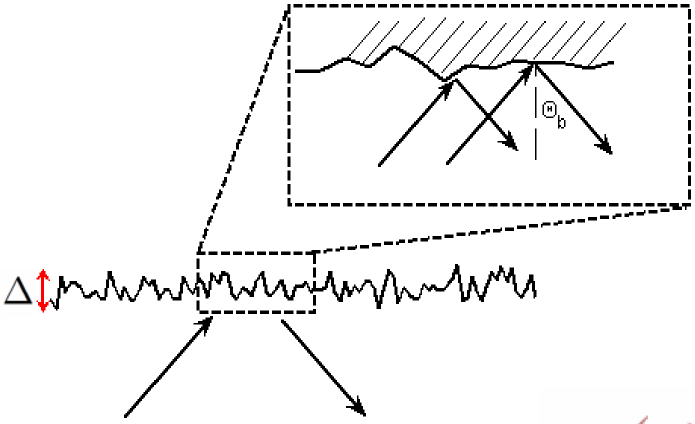
1-*p* – probability of having momentum randomized

Often assumed as a constant, but should be momentum-dependent

Technically valid for OK for $L \rightarrow 0$

OK for for phonons whose wavelengths are considerably larger than the correlation length

$$p(\vec{q}) = \exp(-\langle \phi^2 \rangle)$$



$$\phi(\vec{q}, \vec{r}) = 2\vec{q} \cdot \hat{s} z(\vec{r}) = 2qz(\vec{r}) \cos \Theta_B$$

$$\langle \phi^2 \rangle = (2q \cos \Theta_B)^2 \langle z^2 \rangle$$
$$= 4q^2 \Delta^2 \cos^2 \Theta_B$$

$$p(\vec{q}) = \exp(-4q^2 \Delta^2 \cos^2 \Theta_B)$$

Examples: Partially diffuse interfaces

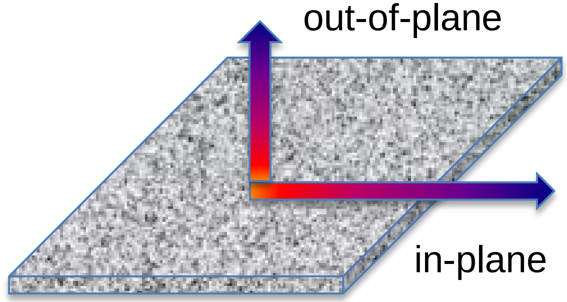
Examples of momentum-dependent specularity parameter $p(\boldsymbol{q})$ used in conjunction with the single-mode RTA and full dispersions on:

1) Thin silicon nanomembranes

2) Graphene nanoribbons

3) SiGe superlattices

Thin Si Nanomembranes

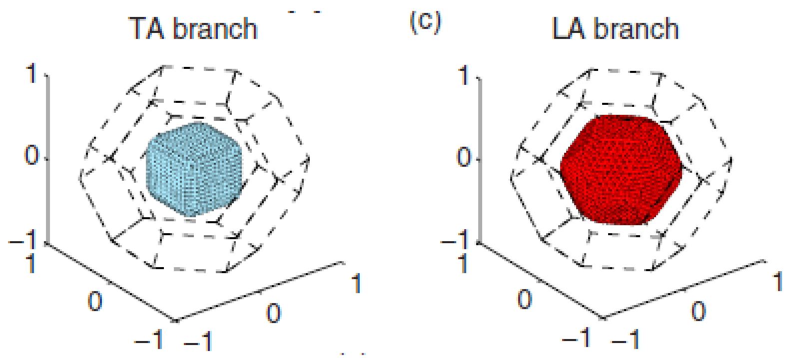


$$K^{\alpha\beta}(T) = k\sum_{j}\sum_{\vec{q}}\left[\frac{\hbar\omega_j(\vec{q})}{kT}\right]^2 \frac{e^{\hbar\omega_j(\vec{q})/kT}}{[e^{\hbar\omega_j(\vec{q})/kT}-1]^2} \times \tau_j(q) v_j^{\alpha}(\vec{q}) v_j^{\beta}(\vec{q}),$$

$$\frac{1}{\tau_j(\vec{q})} = \frac{1}{\tau_{j,N}(\vec{q})} + \frac{1}{\tau_{j,U}(\vec{q})} + \frac{1}{\tau_{j,I}(\vec{q})} + \frac{1}{\tau_{j,B}(\vec{q})}$$

Normal & umklapp 3-phonon processes, isotope, and boundary scattering

$$\tau_{j,B}(\vec{q}) = \left[\frac{1+p(\vec{q})}{1-p(\vec{q})}\right]\frac{L}{v_{j,\perp}(\vec{q})}$$



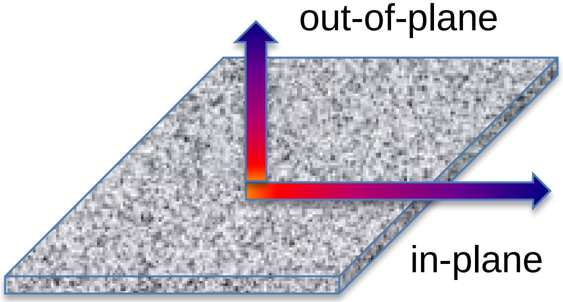
Z. Aksamija* and I. Knezevic†

PHYSICAL REVIEW B **82**, 045319 (2010)

LA phonons scatter strongly from {111} and {100}

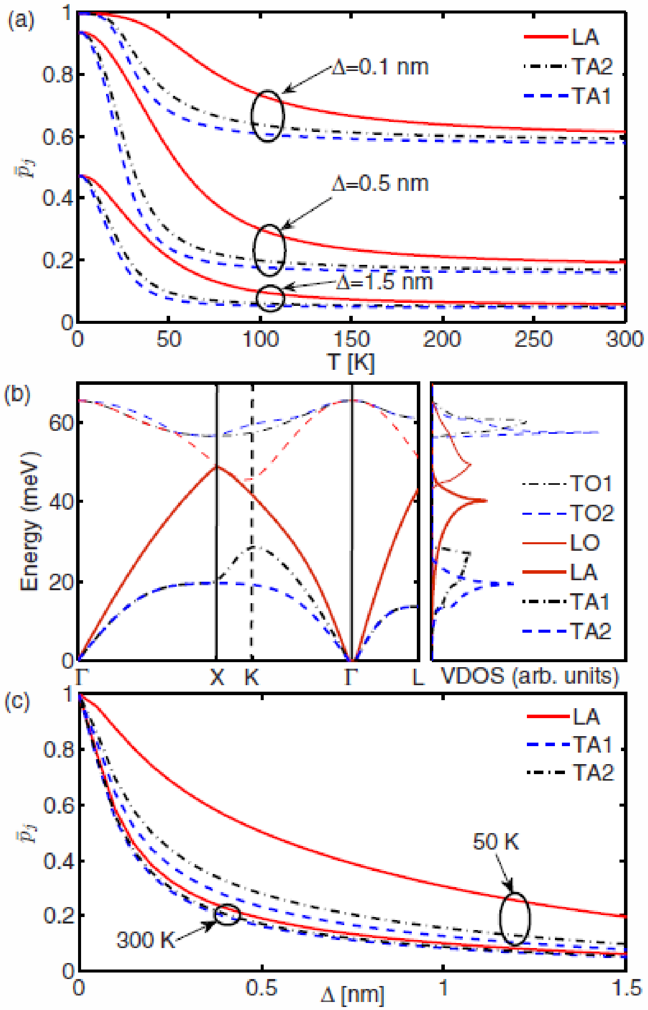
TA phonons scatter strongly from {100}

Thin Si Nanomembranes



$$p(\vec{q}) = \exp(-4q^2\Delta^2 \cos^2 \Theta_B)$$

$$\bar{p}_j = \frac{\int p(\vec{q}) N_0[\omega_j(\vec{q})] d^3\vec{q}}{\int N_0[\omega_j(\vec{q})] d^3\vec{q}}$$



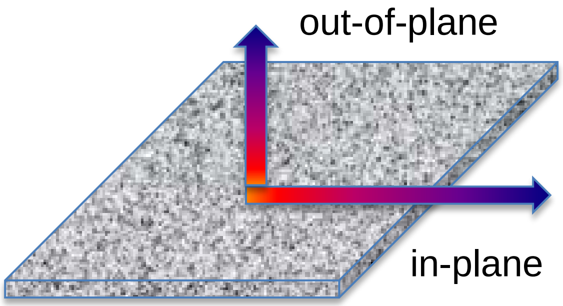
Effective specularity parameter is dependent on branch and temperature

At high roughnesses, here is still a considerable specular component

Z. Aksamija* and I. Knezevic†

PHYSICAL REVIEW B **82**, 045319 (2010)

Thin Si Nanomembranes



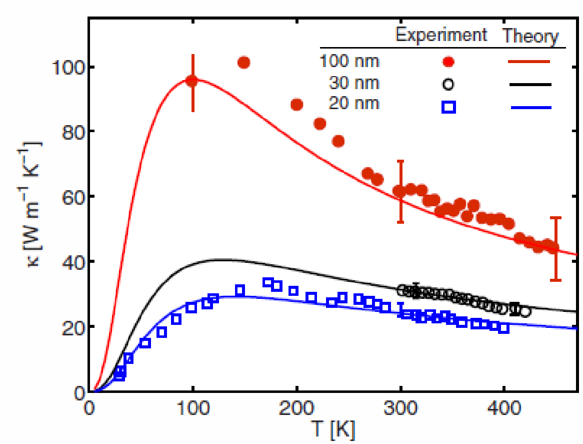
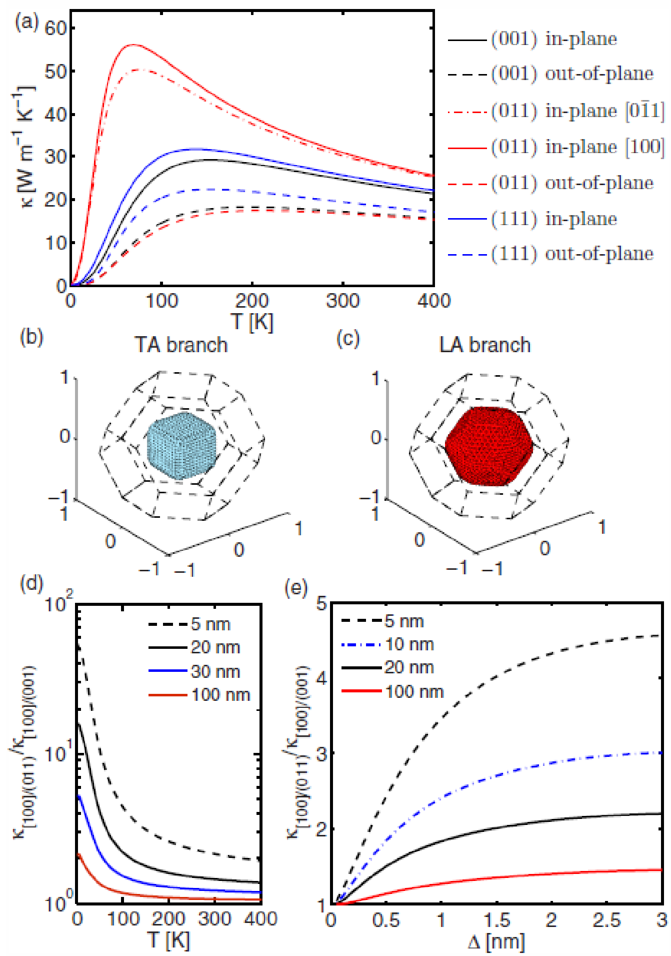


FIG. 3. (Color online) Lattice thermal conductivity of 100 nm (filled circles), 30 nm (open circles), and 20 nm (squares) thick SOI, according to the measurements of Refs. 46 and 47. The curves present our calculations with Δ=0.35 nm for 100 nm SOI, Δ=0.4 nm for 30, and Δ=0.45 nm for 20 nm SOI, in very good agreement with experiment. Thermal conductivity is lower by almost an order of magnitude than the room-temperature bulk value of 148 W/mK, owing primarily to boundary scattering at the rough Si/SiO_2 interfaces.



Z. Aksamija* and I. Knezevic†

PHYSICAL REVIEW B **82**, 045319 (2010)

Casimir limit

When is it OK to treat boundary scattering through an effective scattering rate?

$$\tau_{\mathrm{j,B}}(\vec{q}) = \left[\frac{1+p(\vec{q})}{1-p(\vec{q})}\right]\frac{L}{v_{\mathrm{j},\perp}(\vec{q})}$$

Diffuse (Casimir) limit

$$\lim_{p\to 0} \tau_{\mathrm{j,B}} = \frac{L}{v_{\mathrm{j},\perp}}$$

Specular limit

$$\lim_{p\to 1} \tau_{\mathrm{j,B}} = \infty$$

When the presence of boundaries doesn't affect the solution to the BTE, i.e. when boundaries are farther than the mean free path due to internal scattering, so phonons can thermalize between successive hits.

Casimir rate gives an estimate for how important boundary scattering is

Examples: Partially diffuse interfaces

Examples of momentum-dependent specularity parameter $p(\boldsymbol{q})$ used in conjunction with the single-mode RTA and full dispersions on:

1) Thin silicon nanomembranes

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3) SiGe superlattices

Boundary vs. internal scattering

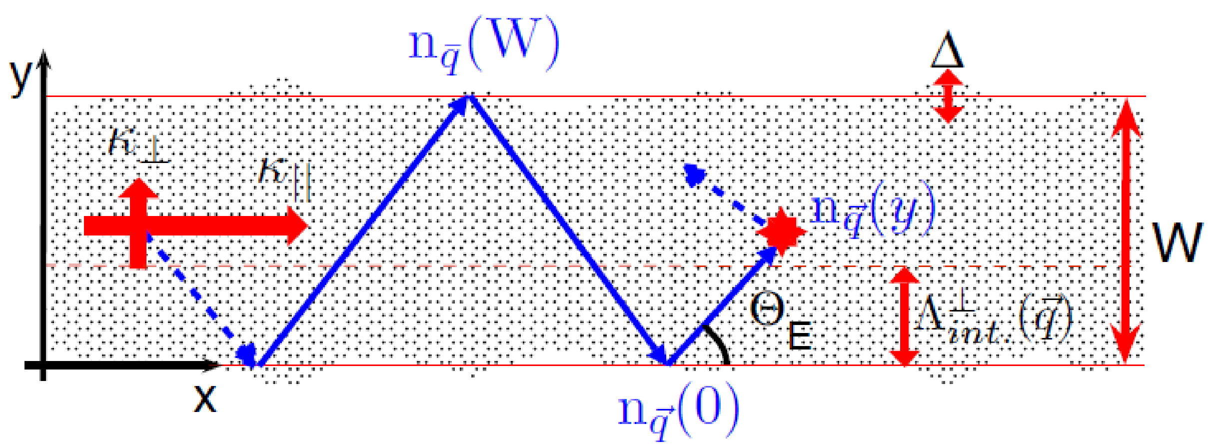
- Model using the steady-state phonon Boltzmann transport equation

$$\vec{v}_{\vec{q}} \cdot \nabla_{\vec{r}} T \frac{\partial N^0_{\vec{q}}(T)}{\partial T} + v_{\perp}(\vec{q}) \frac{\partial n_{\vec{q}}(y)}{\partial y} = \frac{n_{\vec{q}}(y)}{\tau_{int.}(\vec{q})}$$

- In the absence of boundaries, RTA solution: $R_{\vec{q}} = \tau_{int.}(\vec{q}) \vec{v}_{\vec{q}} \cdot \nabla_{\vec{r}} T \frac{\partial N^0_{\vec{q}}(T)}{\partial T}$

- Each boundary contributes one term:

$$p(\vec{q}) \exp\left[-W/\Lambda^{\perp}_{int.}(\vec{q})\right]$$

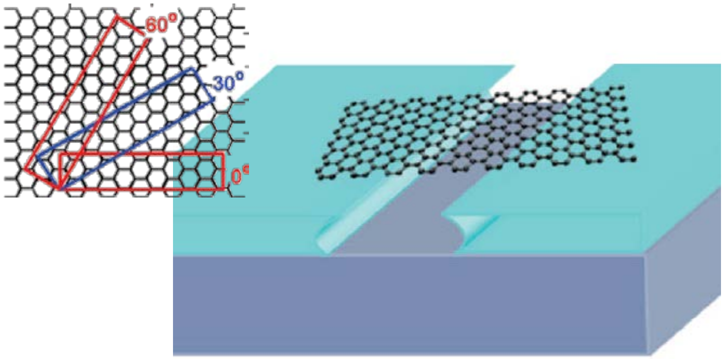


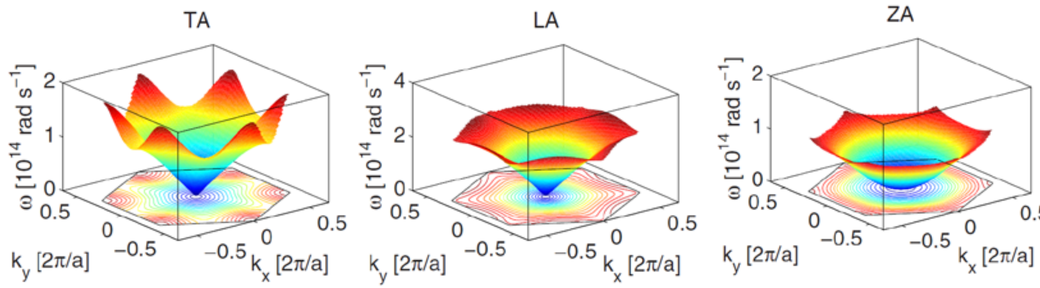
- Sum the infinite series:

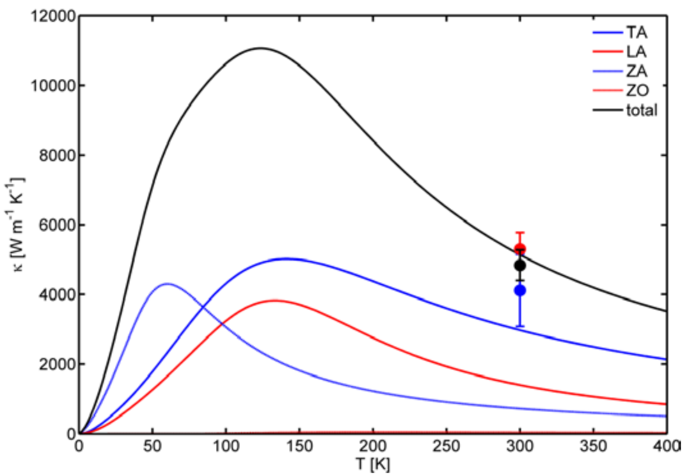
$$n^{+}_{\vec{q}}(y) = R_{\vec{q}} \left\{ 1 - \frac{[1 - p(\vec{q})] \exp\left[-y/\Lambda^{\perp}_{int.}(\vec{q})\right]}{1 - p(\vec{q}) \exp\left[-W/\Lambda^{\perp}_{int.}(\vec{q})\right]} \right\}$$

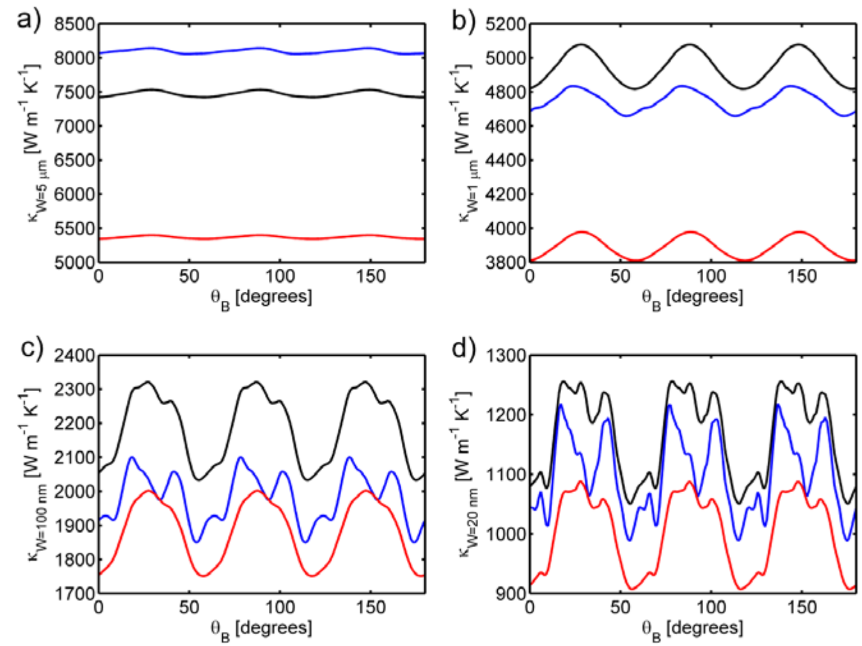
- Heat flux is weaker near boundaries/interfaces due to roughness scattering

Suspended graphene nanoribbons (GNRs)









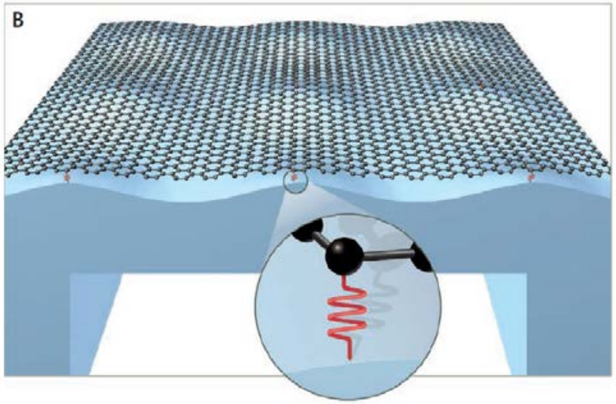
Thermal conductivity very hard to measure
- useful to have theory!

Anisotropy in terms of ribbon orientation

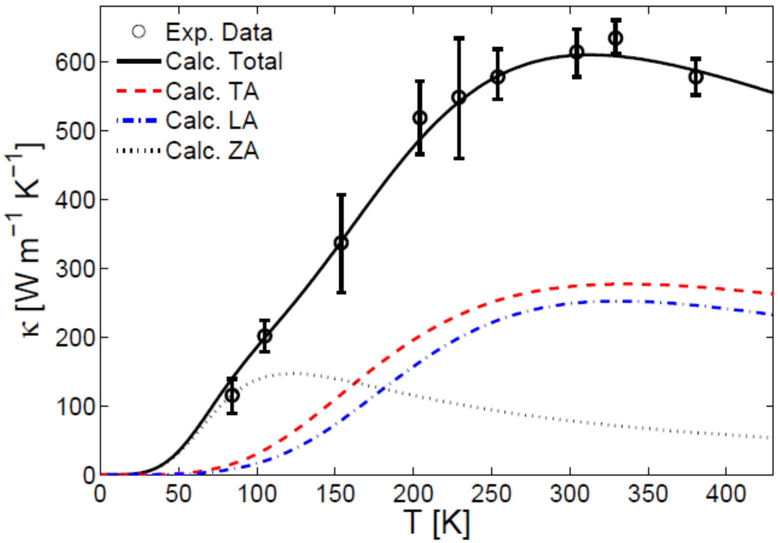
$$\tau_{\mathrm{LER}}^{-1}(\vec{q}) = \frac{v_{\vec{q}}^{\perp}}{W} F_p(\vec{q}) \Bigg/ \left[1 - \frac{\Lambda_{int.}^{\perp}(\vec{q})}{W} F_p(\vec{q})\right]$$

Z. Aksamija and I. Knezevic, *Appl. Phys. Lett.* **98**, 141919 (2011)

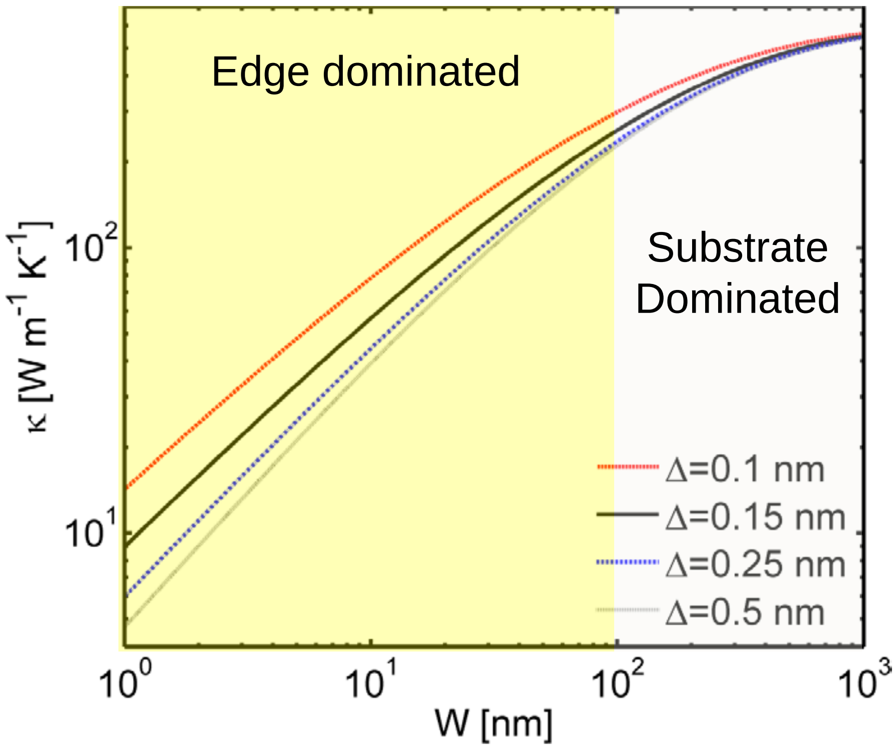
Thermal transport in supported graphene



Seol et al., Science (2010) and R. Prasher, Science (2010)



Z. Aksamija and I. Knezevic, *Phys Rev. B* **86**, 165426 (2012).



M.-H. Bae, Z. Li, Z. Aksamija, P. N. Martin, F. Xiong, Z.-Y. Ong, I. Knezevic, and E. Pop, "Ballistic to diffusive crossover of heat flow in graphene ribbons," *Nature Communications* **4**, 1734 (2013).

Examples: Partially diffuse interfaces

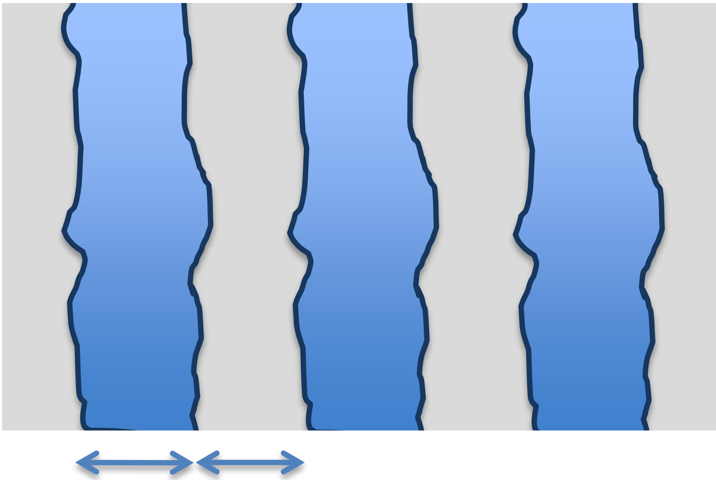
Examples of momentum-dependent specularity parameter $p(\boldsymbol{q})$ used in conjunction with the single-mode RTA and full dispersions on:

1) Thin silicon nanomembranes

2) Graphene nanoribbons

3) SiGe superlattices

SiGe alloy superlattices

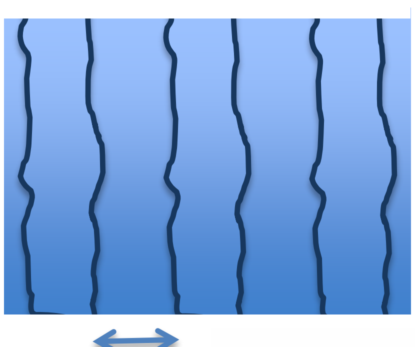


Lattice with reasonably thick layers and partially diffuse interfaces

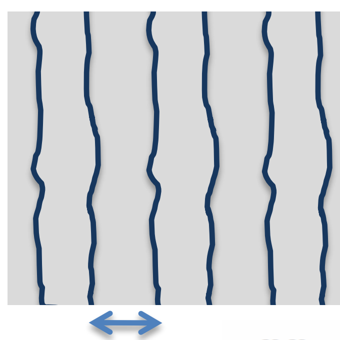
Roughness + mismatch?

Experimentally observed:
- **cross-plane/in-plane anisotropy of κ**
- **increasing κ with increasing period**

Separate roughness from mismatch: Calculate $\boldsymbol{\kappa}$ for sublattices with rough interfaces; mismatch figures in $\boldsymbol{\kappa}$, not the BTE itself



$\kappa_1^{xx}, \kappa_1^{yy}$



$\kappa_2^{xx}, \kappa_2^{yy}$

$$\kappa_{\text{in-plane}} = \frac{L_1\kappa_1^{xx} + L_2\kappa_2^{xx}}{L_1 + L_2},$$

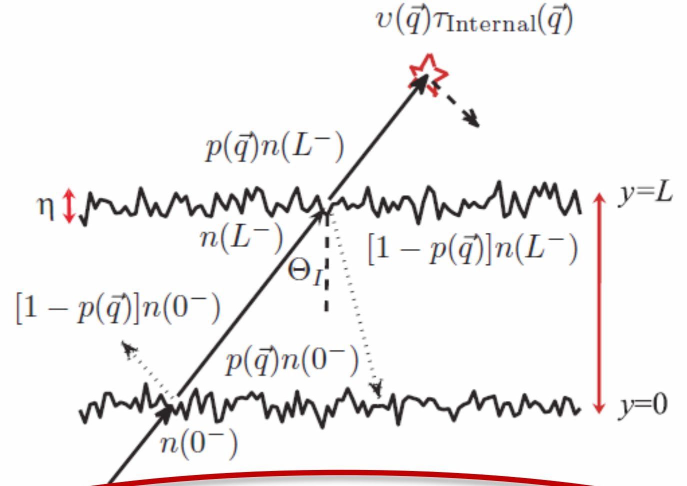
$$\kappa_{\text{cross-plane}} = \frac{L_1 + L_2}{\frac{L_1}{\kappa_1^{yy}} + \frac{L_2}{\kappa_2^{yy}} + \frac{1}{\sigma_1^{\text{AIM}}} + \frac{1}{\sigma_2^{\text{AIM}}}}$$

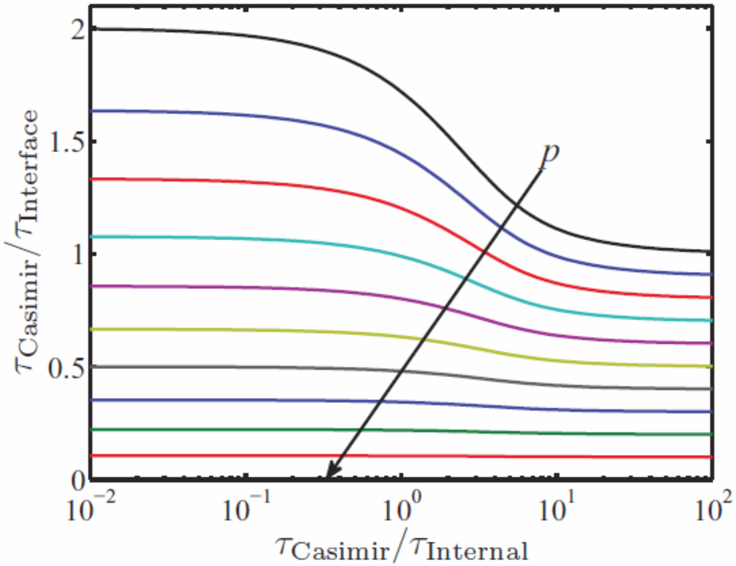
Solving the BTE for superlattices

$$\vec{v}_b(\vec{q}) \cdot \nabla_{\vec{r}} T \frac{\partial N^0_{b,\vec{q}}(T)}{\partial T} + v_{b,\perp}(\vec{q}) \frac{\partial n_b(\vec{q},y)}{\partial y} = \frac{n_b(\vec{q},y)}{\tau_{b,\text{ Internal}}(\vec{q})}$$

A single sublattice with partially diffuse interfaces

$$n_b(\vec{q},y) = R_b(\vec{q})\left\{1 - \left[\frac{1-p(\vec{q})}{1-p(\vec{q})\exp[-L/\tau_{b,\text{ Internal}}(\vec{q})v_{b,\perp}(\vec{q})]}\right]\exp[-y/\tau_{b,\text{ Internal}}(\vec{q})v_{b,\perp}(\vec{q})]\right\}.$$





$$\frac{1}{\tau_{\text{Interface}}(\vec{q})} = \frac{v_{b,\perp}(\vec{q})}{L}\,\frac{F_p(\vec{q},L)}{1-\frac{\tau_{b,\text{ Internal}}(\vec{q})v_{b,\perp}(\vec{q})}{L}F_p(\vec{q},L)}$$

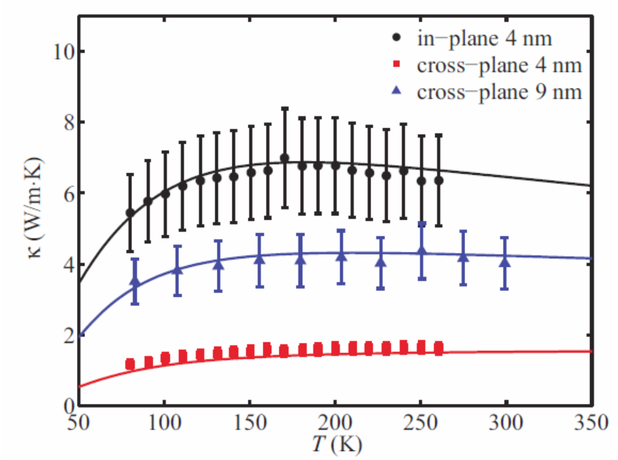
Effective interface scattering rate

$$F_p(\vec{q},L) = \frac{[1-p(\vec{q})]\{1-\exp[-L/\tau_{b,\text{ Internal}}(\vec{q})v_{b,\perp}(\vec{q})]\}}{1-p(\vec{q})\exp[-L/\tau_{b,\text{ Internal}}(\vec{q})v_{b,\perp}(\vec{q})]}$$

Z. Aksamija and I. Knezevic, *Phys. Rev. B* **88**, 155318 (2013)

Si/Ge and SiGe alloy superlattices

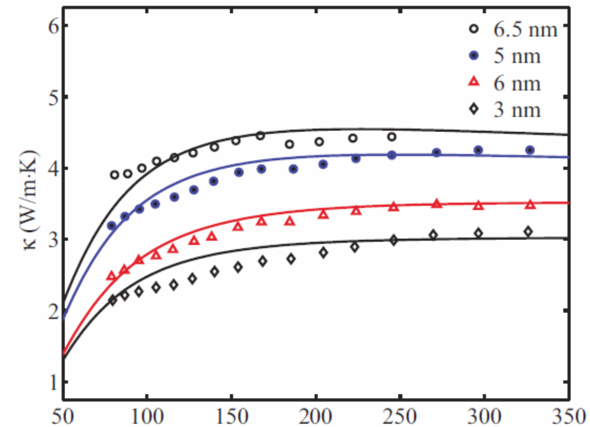
Si/Ge: in-plane vs cross-plane anisotropy



W. Liu, T. Borca-Tasciuc, G. Chen, J. Liu, and K. Wang, J. Nanosci Nanotechnol. **1**, 39 (2001).

T. Borca-Tasciuc, W. Liu, J. Liu, T. Zeng, D. W. Song, C. D. Moore, G. Chen, K. L. Wang, M. S. Goorsky, T. Radetic, R. Gronsky, T. Koga, and M. S. Dresselhaus, Superlattices Microstruct. **28**, 199 (2000).

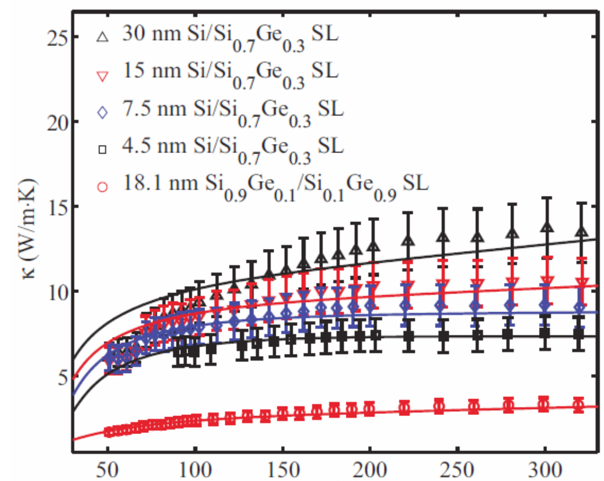
Si/Ge: κ increases w/increasing period



S.-M. Lee, D. G. Cahill, and R. Venkatasubramanian, Appl. Phys. Lett. **70**, 2957 (1997).

Alloy superlattices →

- κ increases w/increasing period
- the role of alloying



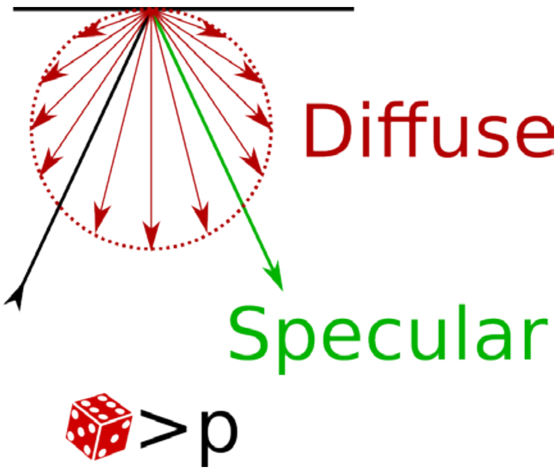
S. T. Huxtable, A. R. Abramson, C.-L. Tien, A. Majumdar, C. LaBounty, X. Fan, G. Zeng, J. E. Bowers, A. Shakouri, and E. T. Croke, Appl. Phys. Lett. **80**, 1737 (2002).

S. T. Huxtable, Ph.D. thesis, University of California, Berkeley, 2002.

Z. Aksamija and I. Knezevic, *Phys. Rev. B* **88**, 155318 (2013)

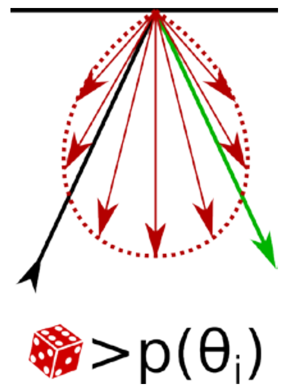
When is *p* not enough?

Wavelength-independent:



- Diffuse scattering angle from $\cos\theta\, d\Omega$ probability distribution
- 100% diffuse scattering called the Casimir Limit
- Thermal conductivities below this limit have been measured in Si nanowires
- H. B. G. Casimir, *Physica* **5**, 459 (1938)
- R. Berman, F. E. Simon, and J. M. Ziman, *Proc. Roy. Soc. A* **220**, 171 (1953)

Wavelength-dependent:



- For zero correlation length, and large wavelength:

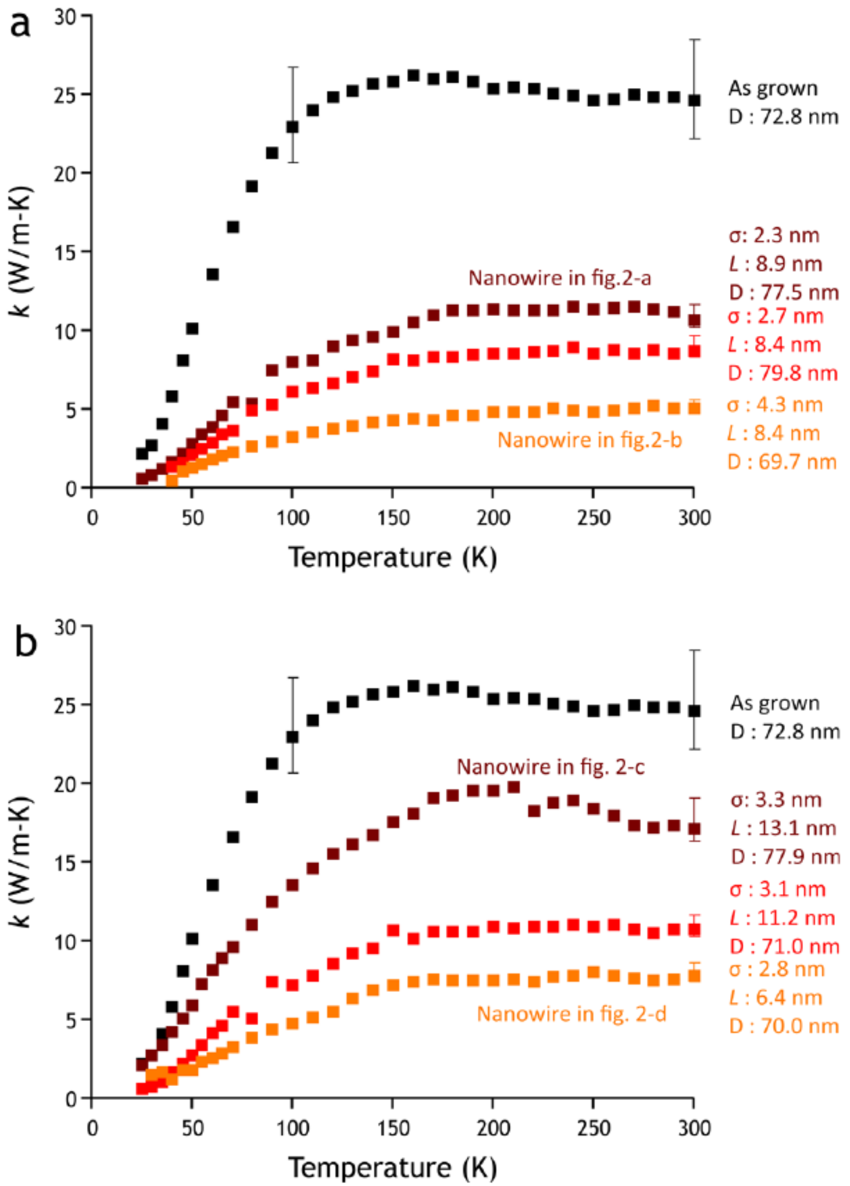
$$p(\theta_i) = e^{-(2q\sigma\cos\theta_i)^2}$$

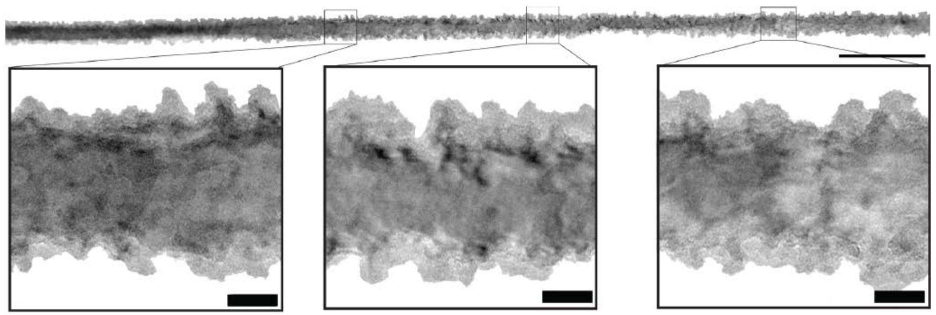
- Diffuse scattering angle from

$$\left[1 - e^{-(2q\sigma\cos\theta)^2}\right]\cos\theta\, d\Omega$$

- Same limit of 100% diffuse scattering as previous model
- Z. Aksamija and I. Knezevic, *Phys. Rev. B*. **82**, 45319 (2010)
- S. Soffer, *J. Appl. Phys.* **38**, 1710 (1967)
- H. Davies, *Proc. IEEE part IV* **101**, 209 (1954)

When things get really really rough….

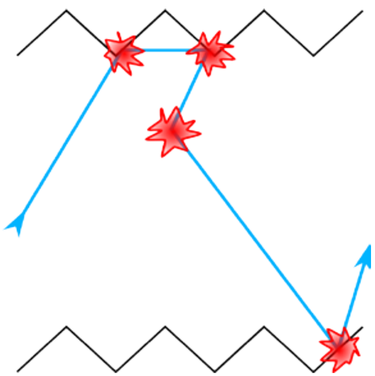


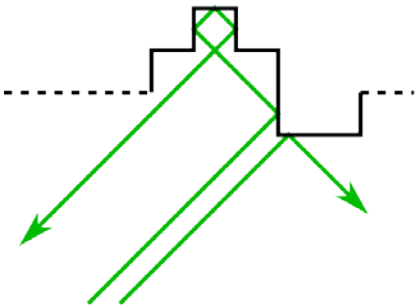


- Rough Si nanowires show greatly reduced κ vs bulk
- Potential thermoelectric applications
- Lower than the Casimir limit, showing limitation of the specularity model
- Depends on σ and L

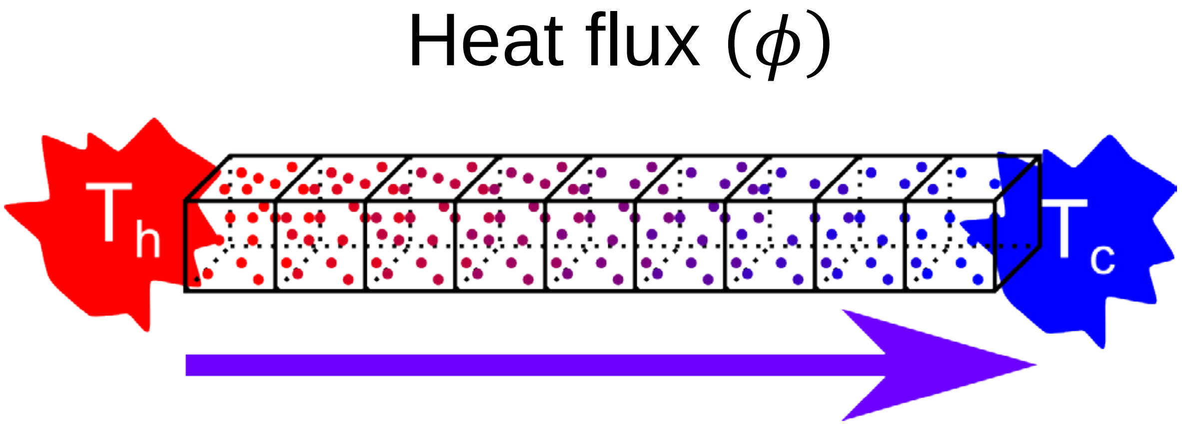
J. Lim, K. Hippalgaonkar, S. C. Andrews, A. Majumdar, and P. Yang, *Nano Lett.* **12**, 2475 (2012)

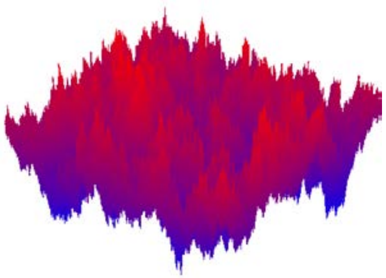
Phonon EMC

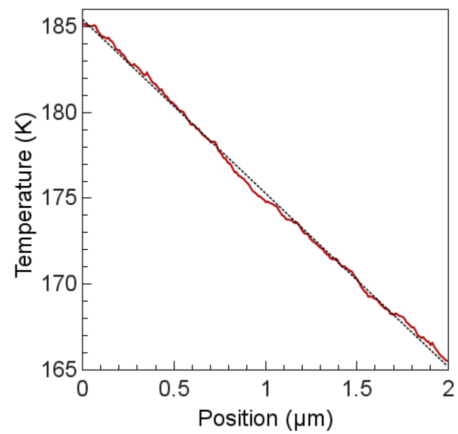




surface



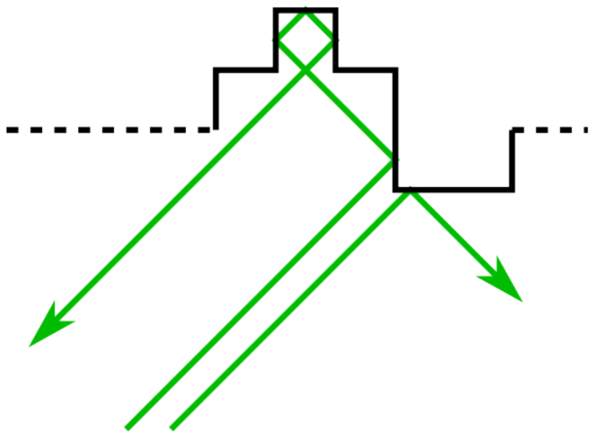


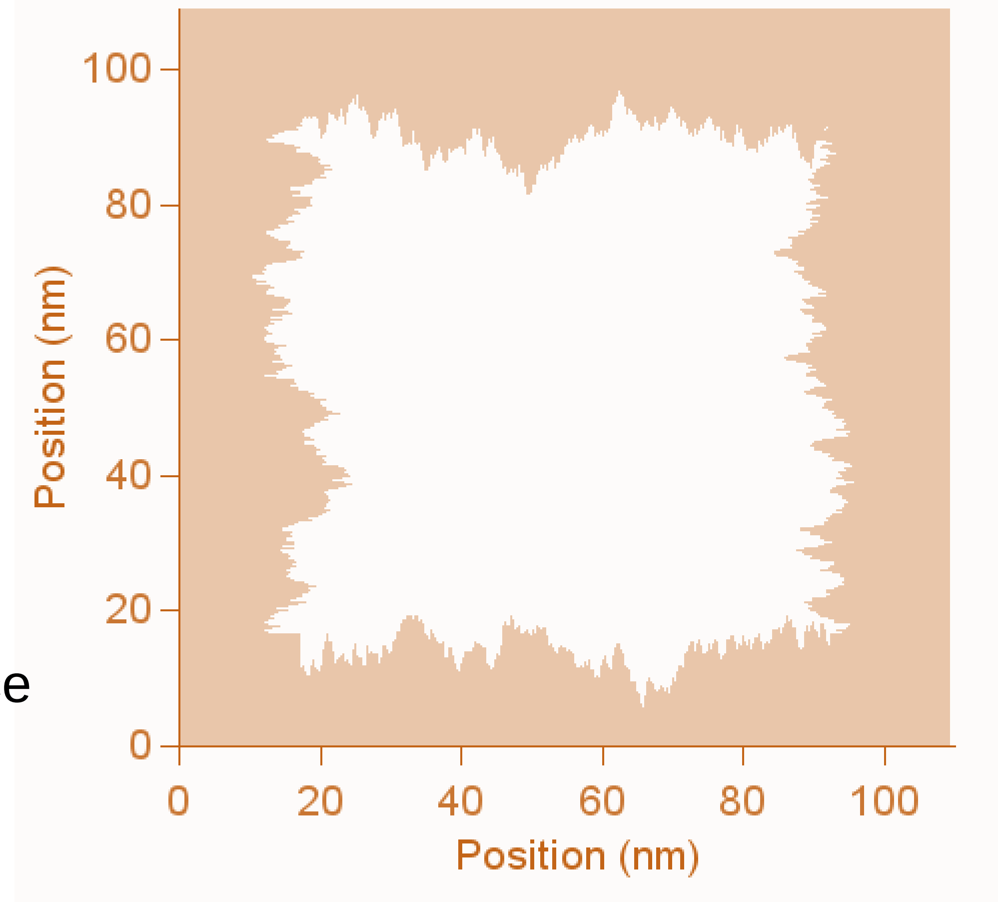


E. B. Ramayya, L. N. Maurer, A. H. Davoody, and I. Knezevic, *Phys. Rev. B* **86**, 115328 (2012)
R. B. Peterson, *J. Heat Transfer* **116**, 815 (1994)
S. Mazumder, and A. Majumdar, *J. Heat Transfer* **123**, 749 (2001)
D. Lacroix, K. Joulain, and D. Lemonnier, *Phys. Rev. B* **72**, 064305 (2005)

$$\phi = -\kappa \frac{dT}{dx}$$

Real-space rough surfaces



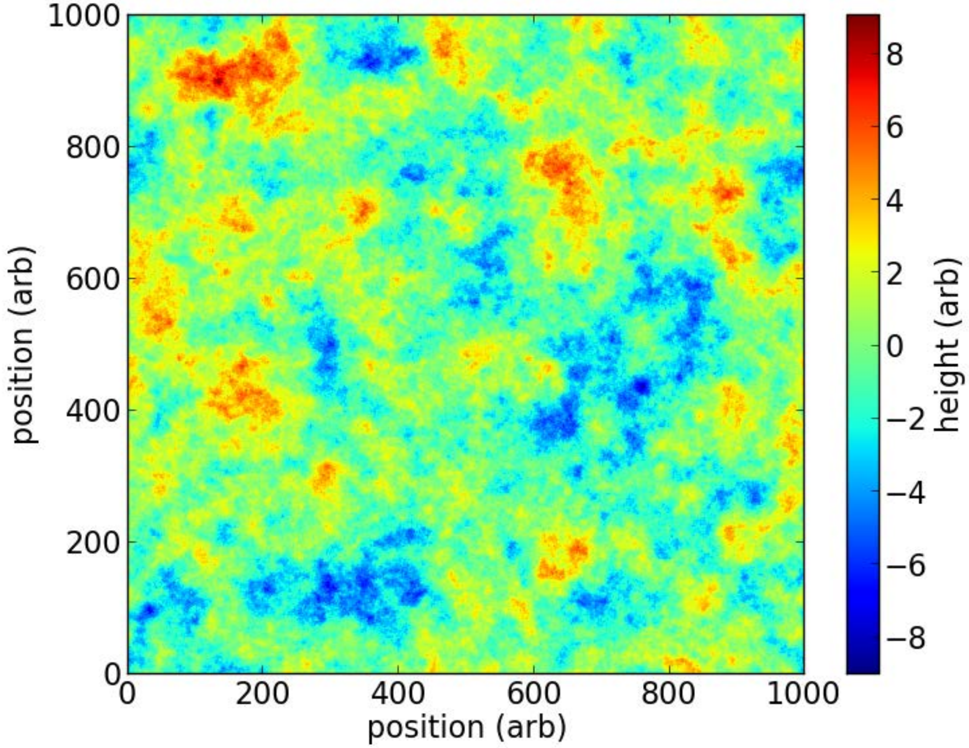


- Generates a random rough surface from an autocorrelation function
- Captures important features, **like multiple scattering**
- Allows lower thermal conductivities

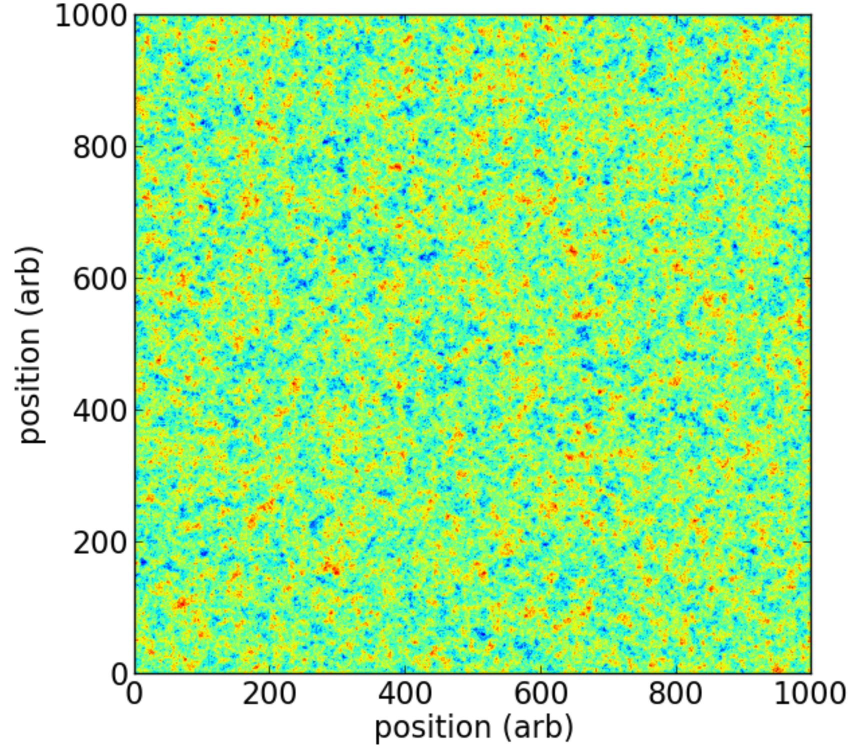
E. B. Ramayya, L. N. Maurer, A. H. Davoody, and I. Knezevic, *Phys. Rev. B* **86**, 115328 (2012)

Autocorrelation functions

$L = 50, \sigma = 2$



$L = 5, \sigma = 2$

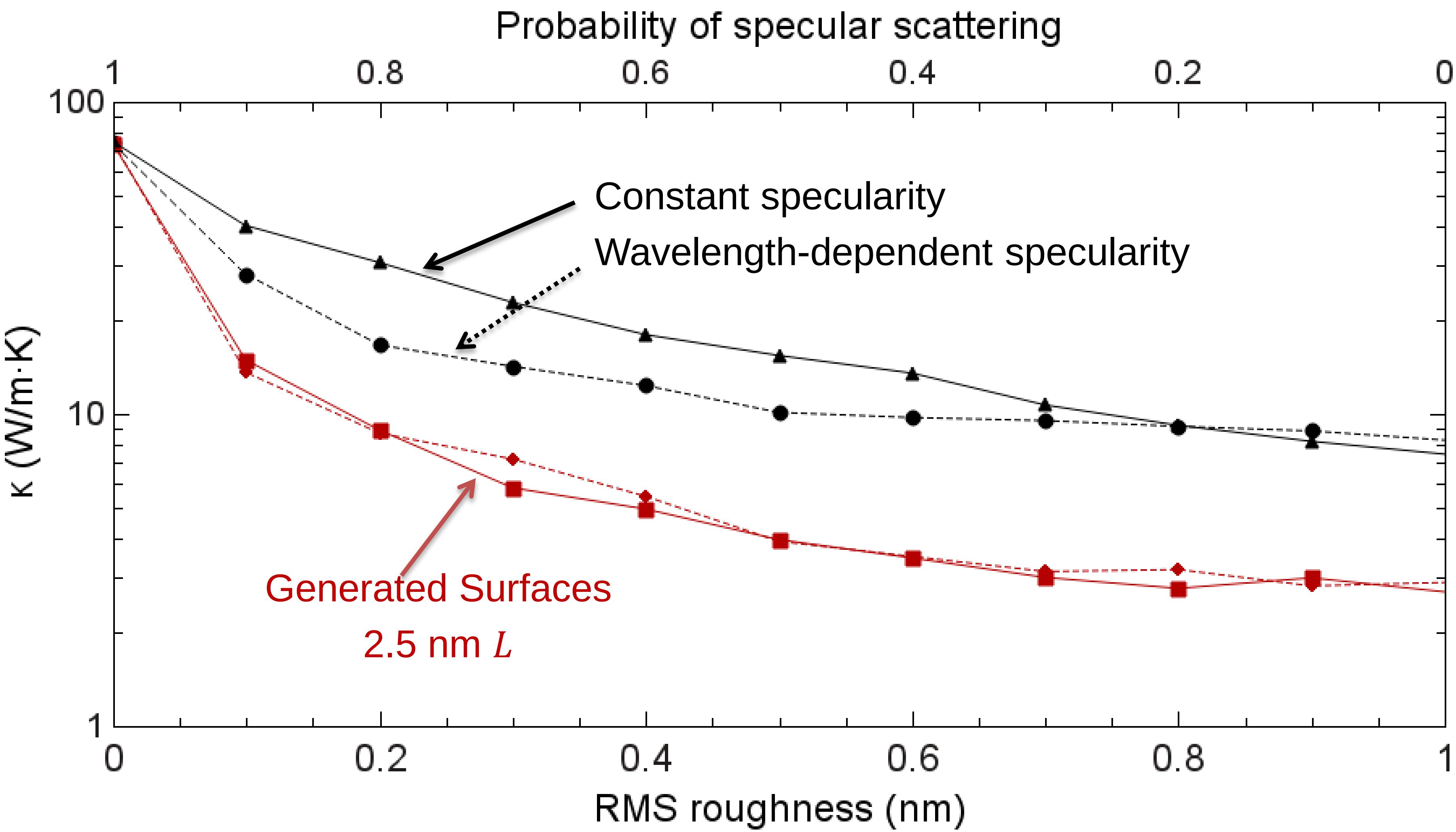


We can make a surface to match any ACF.

$$ACF(\vec{r}) = \sigma^2 e^{-|\vec{r}|/L}$$

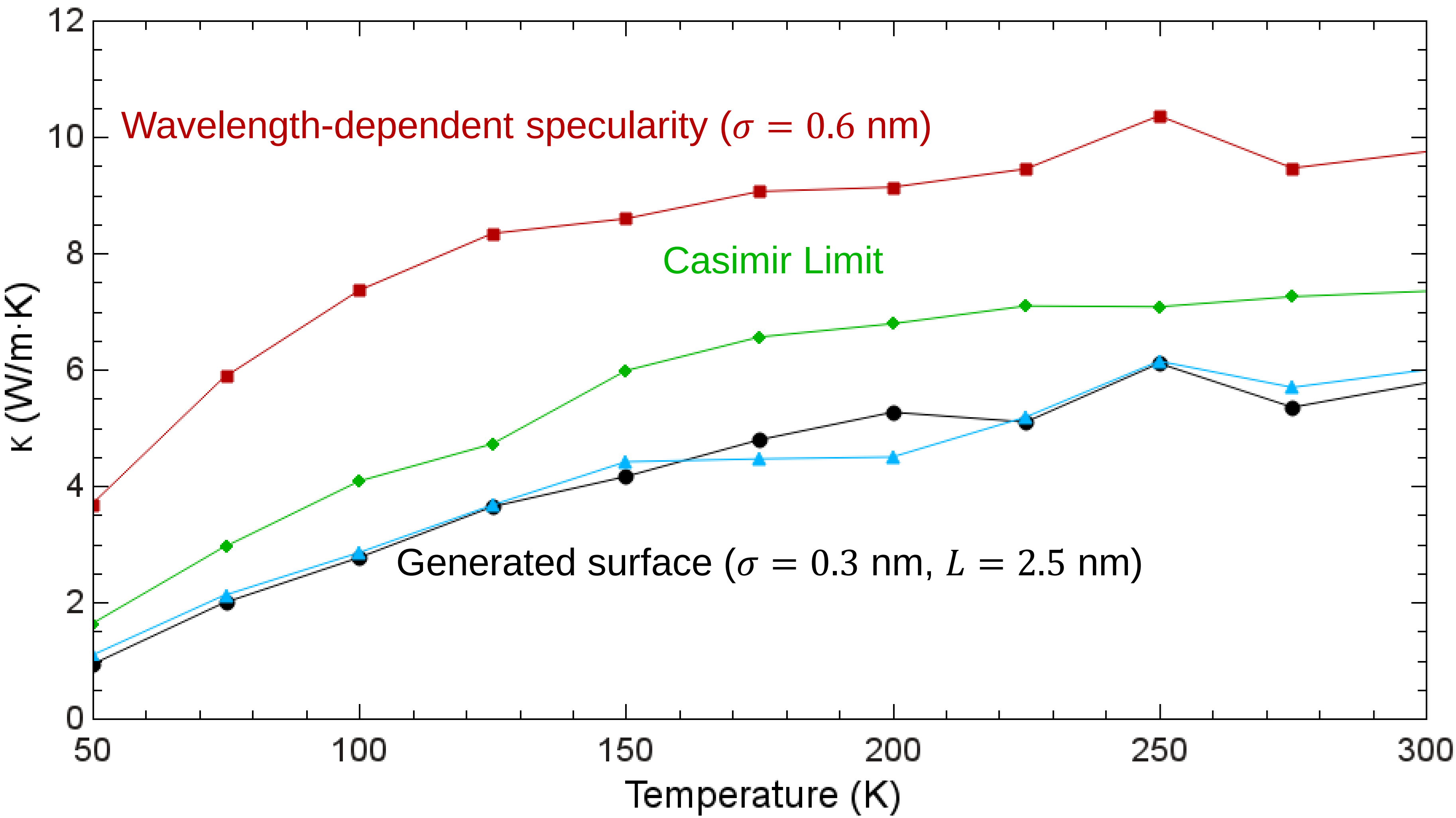
C. Buran, M. G. Pala, M. Bescond, M. Dubois, and M. Mouis, *IEEE Trans. Electron Devices* **56**, 2186 (2009)

Models at room temperature



10x10x1000nm Si wires

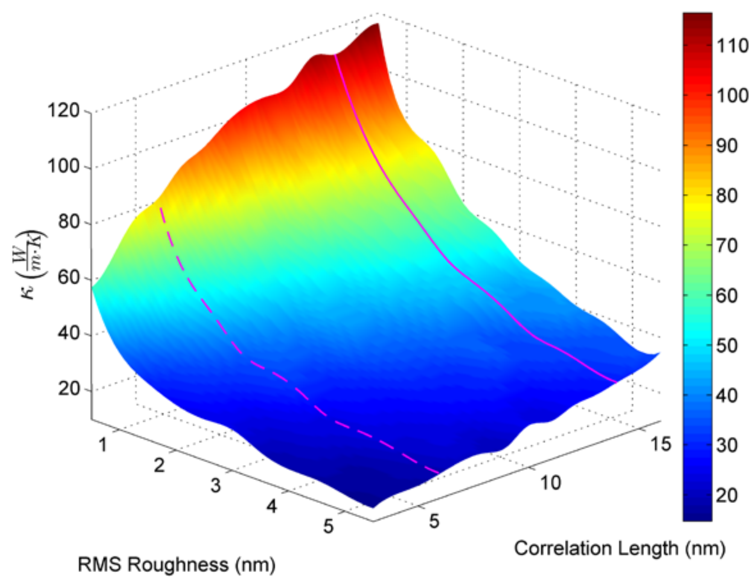
Temperature dependence



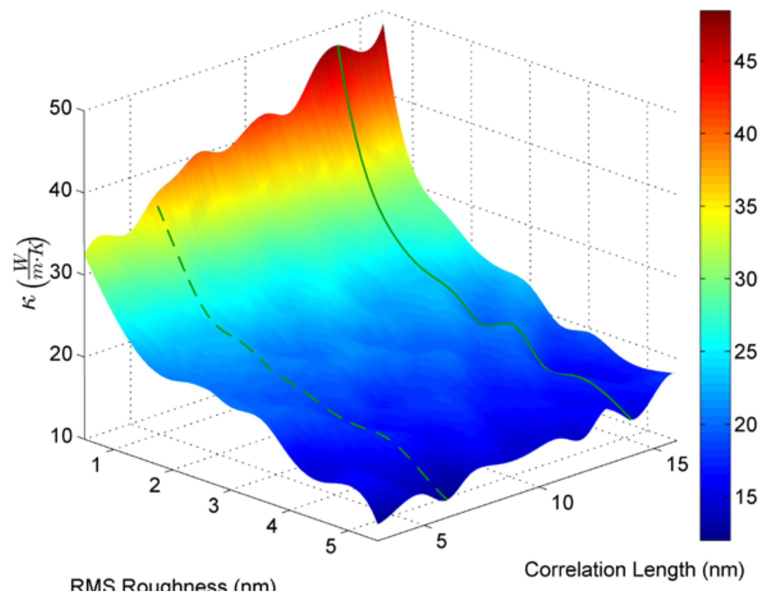
10x10x2000 nm Si wires

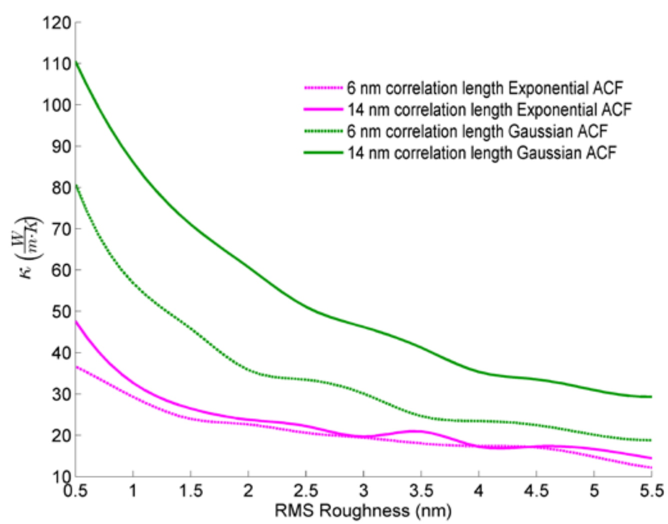
Dependence on rms roughness

Exponential autocorrelation



Gaussian autocorrelation

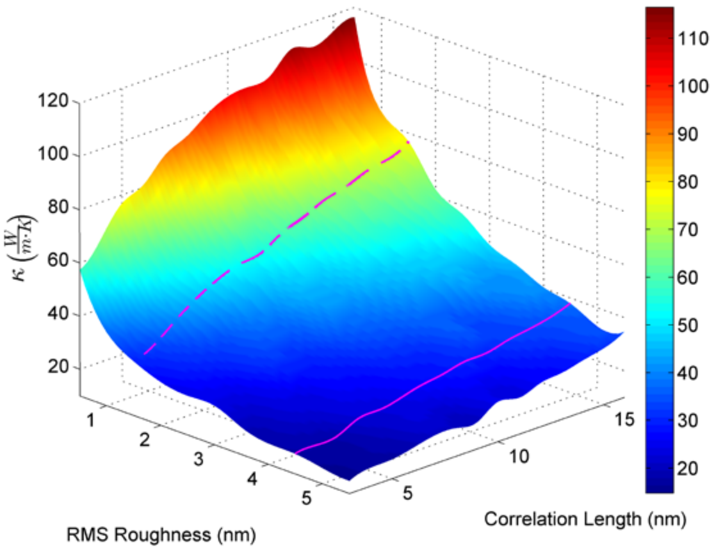




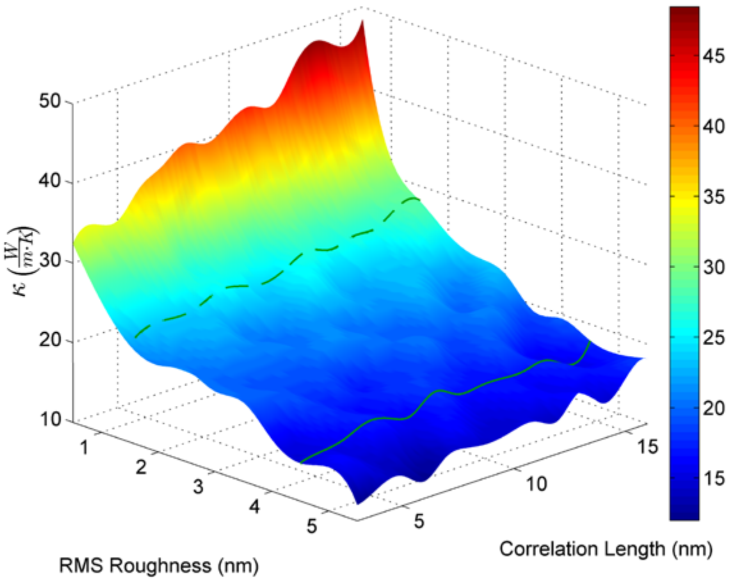
L.N. Maurer and I. Knezevic,
in prep (2013).

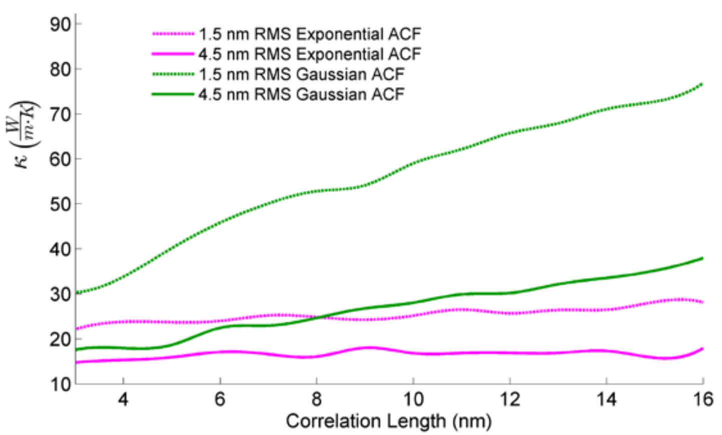
Dependence on correlation length

Exponential autocorrelation



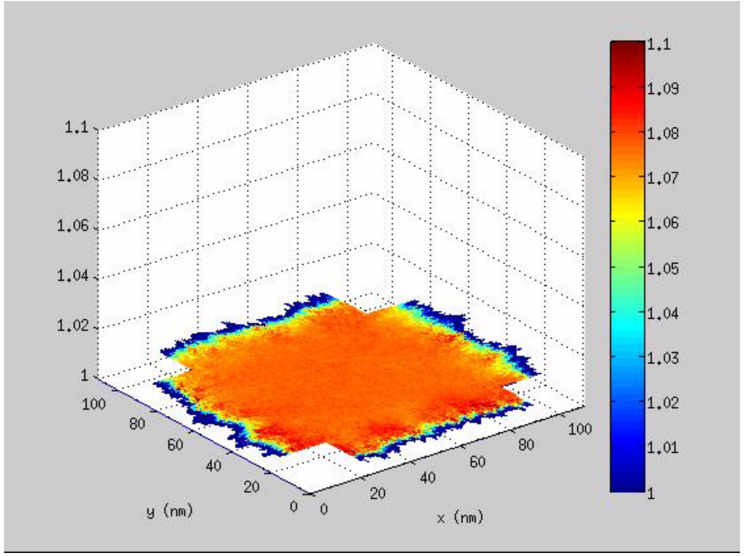
Gaussian autocorrelation



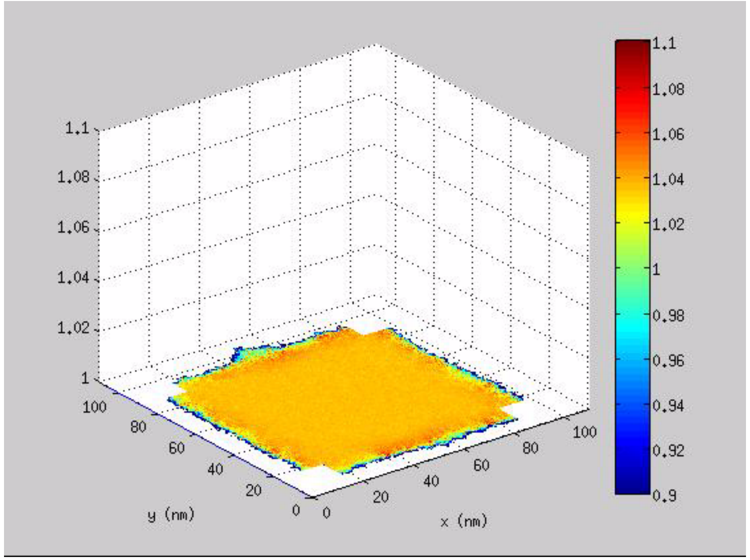


L.N. Maurer and I. Knezevic,
in prep (2013).

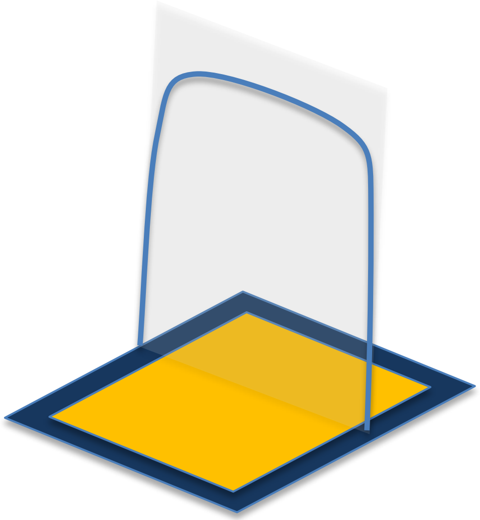
Phonon trapping

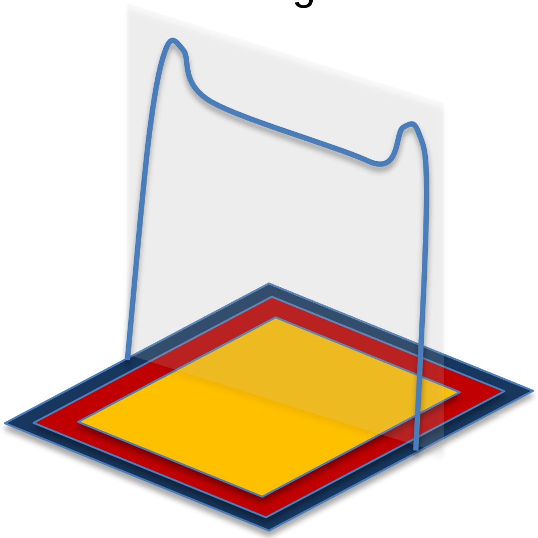


70 nm thick, **3 nm rms roughness**,
10 nm correlation length



70 nm thick, **6 nm rms roughness**,
10 nm correlation length

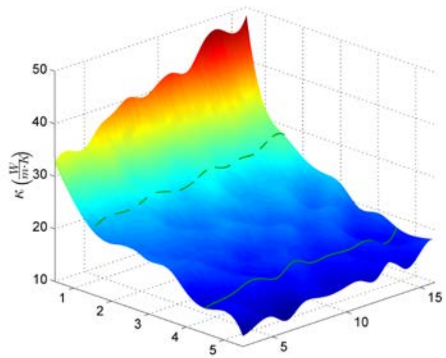


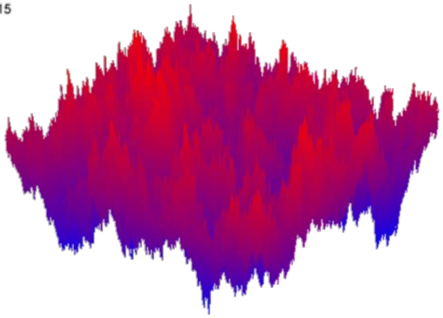


L.N. Maurer and I. Knezevic,
in prep (2013).

Conclusions

- Semiclassical transport simulations of great practical utility
- Specularity parameter limited to moderately rough interfaces with very low correlation
- Very rough or correlated surfaces require a different approach
- High roughness – phonon trapping



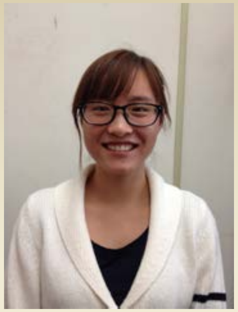


Thanks to

Thermal transport gang

Leon

Amirhossein



Song

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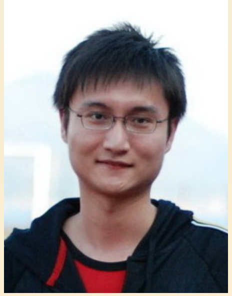
Dr. Edwin Ramayya (Intel, OR)

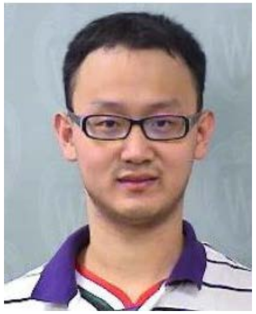


Yanbing

Nishant

Farhad

Olafur



Gordon

DOE BES, Award No. DE-SC0008712

NSF ECCS, Award No. 1201311