# Thermal transport in group-IV nanostructures and superlattices based on the Boltzmann transport equation

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# Outline

- Thermoelectric conversion
  - Introduction
  - Pros/cons
  - Conversion efficiency
- Nanoscale heat transfer
  - Boundary/interface scattering of phonons
  - Phonon transport at boundaries/interfaces with competing internal scattering mechanisms
- Lattice thermal conductivity of Si-based nanostructures:
  - Ultra-thin Silicon-On-Insulator nanomembranes
  - Si/Ge and $Si_{1-x}Ge_x/Si_{1-y}Ge_y$ superlattices
- Thermal properties of Graphene Nanoribbons (GNRs)
  - Anisotropic thermal conductivity of suspended GNRs
  - Substrate scattering and thermal transport in supported GNRs
- Discussion and Conclusions

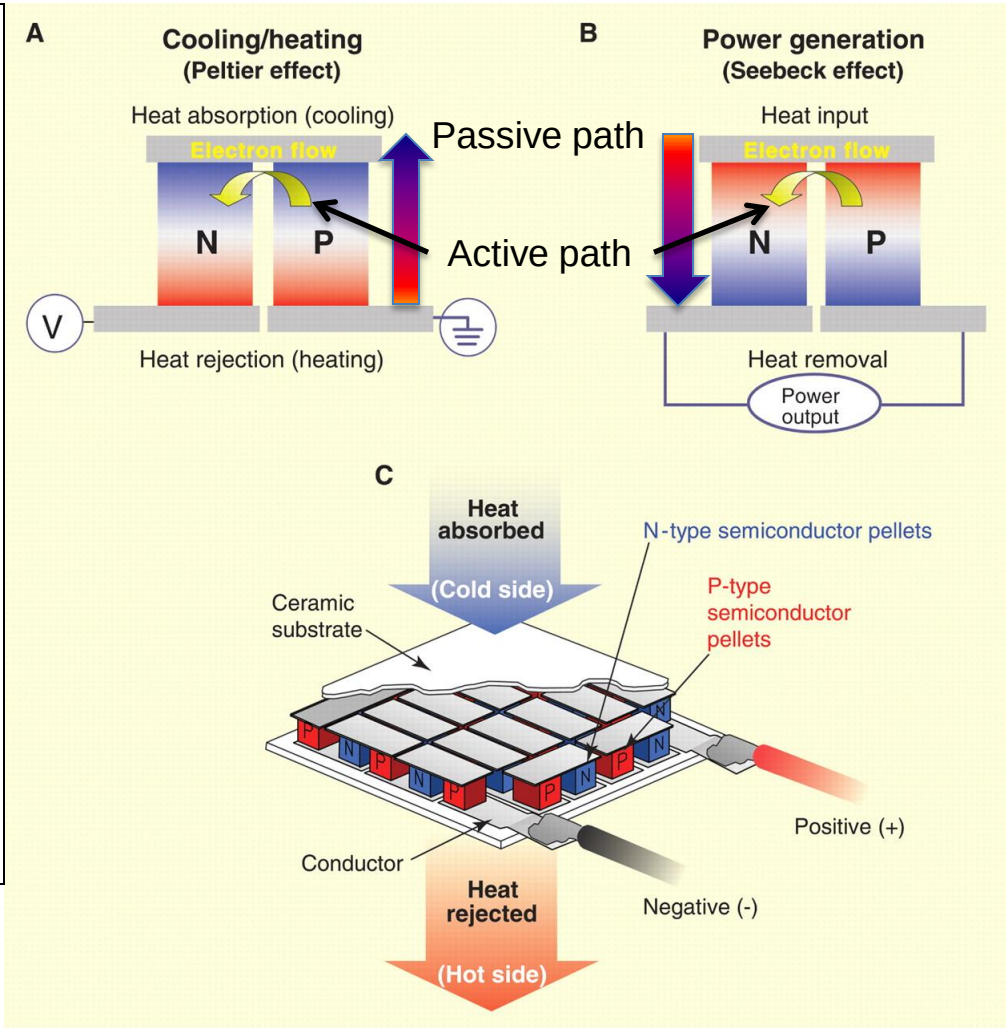
# Thermoelectric Energy Conversion

## Solid State Heat Engines:

(A) When current is run across a TE junction, it heats or cools through the Peltier effect, depending on the direction of the current flow.

(B) When heat flows across the junction, electrical current is generated through the Seebeck effect.

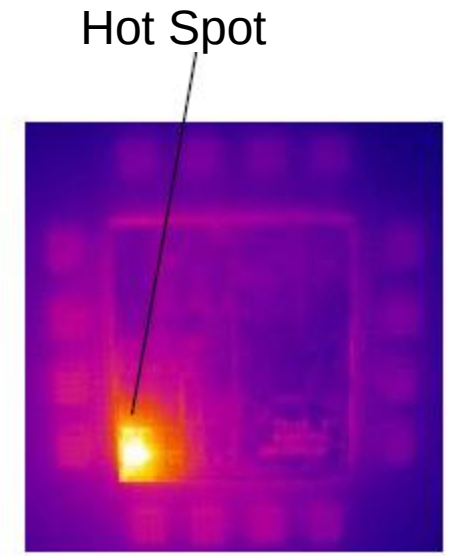
(C) Practical TE generators connect large numbers of junctions in series to increase operating voltage and spread heat flow.




L E Bell Science 2008;321:1457-1461

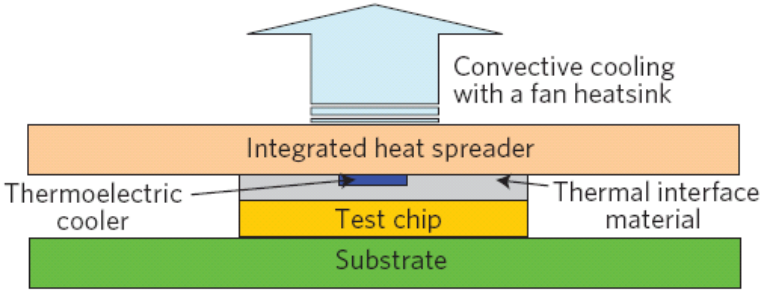
# Pros/Cons of Thermoelectric Devices

- Advantages of thermoelectric (TE) modules:
  - No moving parts (compressors/pipes)
  - Maintenance free, large MTBF
  - No gases or liquids (leakage)
  - Compact and robust (can withstand shock/vibration)
  - Very precise temperature control
  - Can be stacked to reach very low temperatures
  - **Si-based TEs directly integrated with μ-electronic circuits to cool hotspots or recover waste heat**




- Drawbacks:
  - Low efficiency
  - High cost

- Both drawbacks can be addressed by semiconductor nanostructures!




Chowdhury et al., Nature Nano. **4**, 235 (2009)

# Thermoelectric Conversion Efficiency

- Thermoelectric conversion efficiency:
  - measured by the ratio of energy provided to the load to the heat extracted

$$\eta = \frac{\text{Energy Produced}}{\text{Heat Energy Absorbed}} = \left(1 - \frac{T_C}{T_H}\right) \frac{\sqrt{Z\bar{T}+1}-1}{\sqrt{Z\bar{T}+1}+T_C/T_H}$$

- ZT--dimensionless figure of merit:

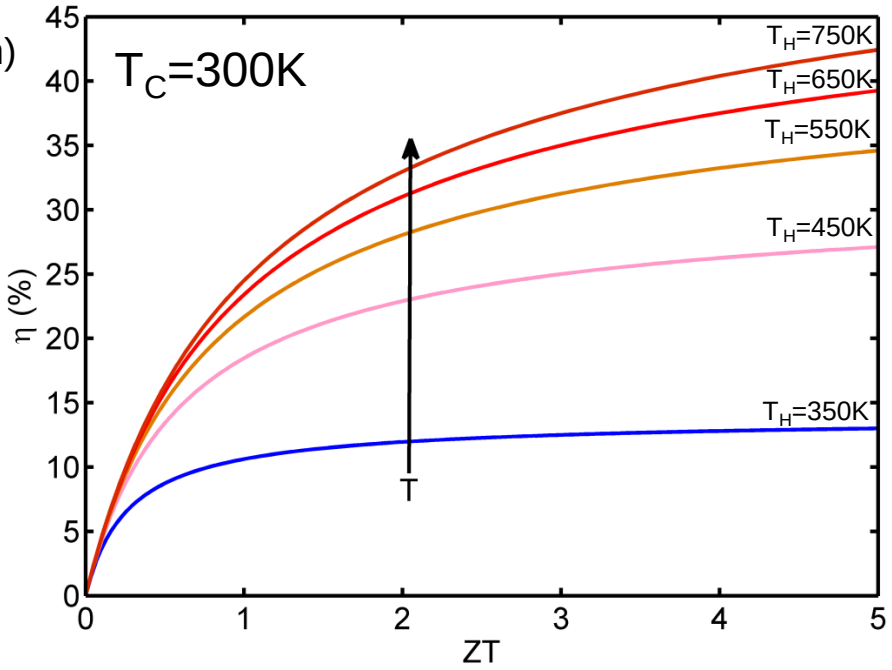
$$ZT = \frac{S^2 \sigma_{el}}{\kappa_{ph} + \kappa_{el}} T$$

Power factor (active path)

Thermal (passive) path

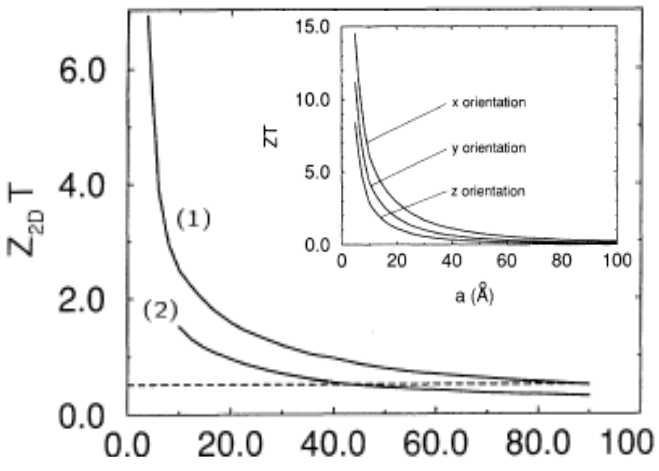
- Increasing ZT causes efficiency to approach the Carnot limit

- Reducing thermal conductivity has tremendous impact on ZT!

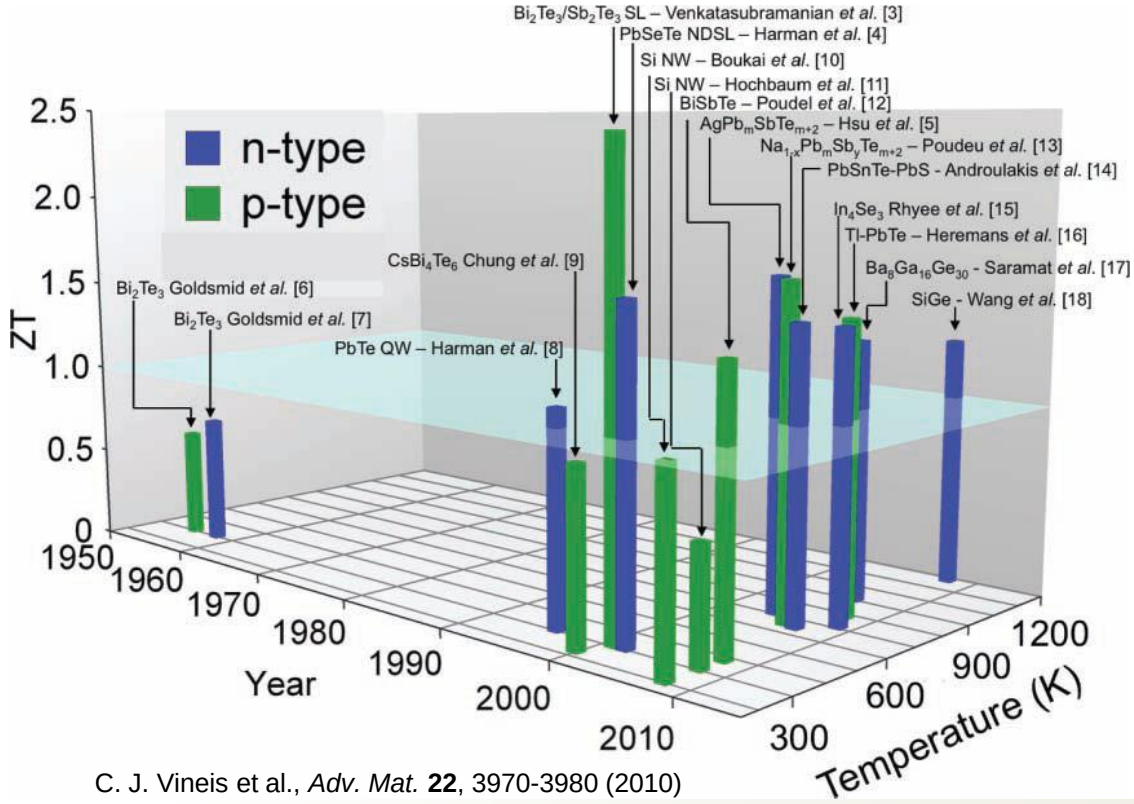


# Thermoelectrics – Historical Perspective

- ZT>1 (~10% efficiency) generally considered very useful
- ZT>3 (~30% efficiency) needed in order to make thermoelectric materials competitive with existing technologies
- Most materials with ZT>1 employ semiconductor nanostructures, most often superlattices




Hicks and Dresselhaus, PRB 47, 12727; PRB 47, 16631 (1993)




C. J. Vineis et al., *Adv. Mat.* **22**, 3970-3980 (2010)

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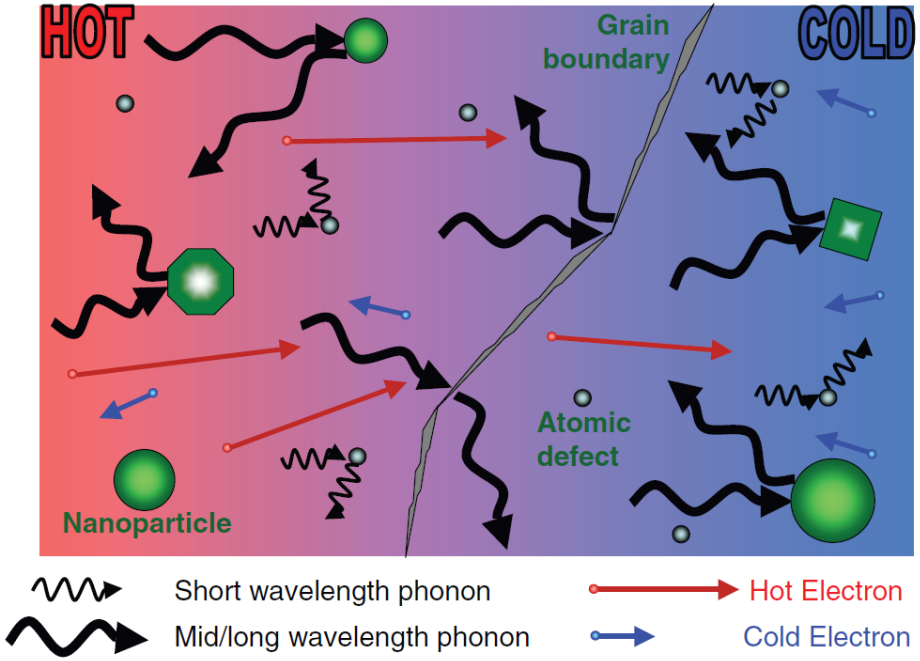
# Nanoscale Heat Transfer

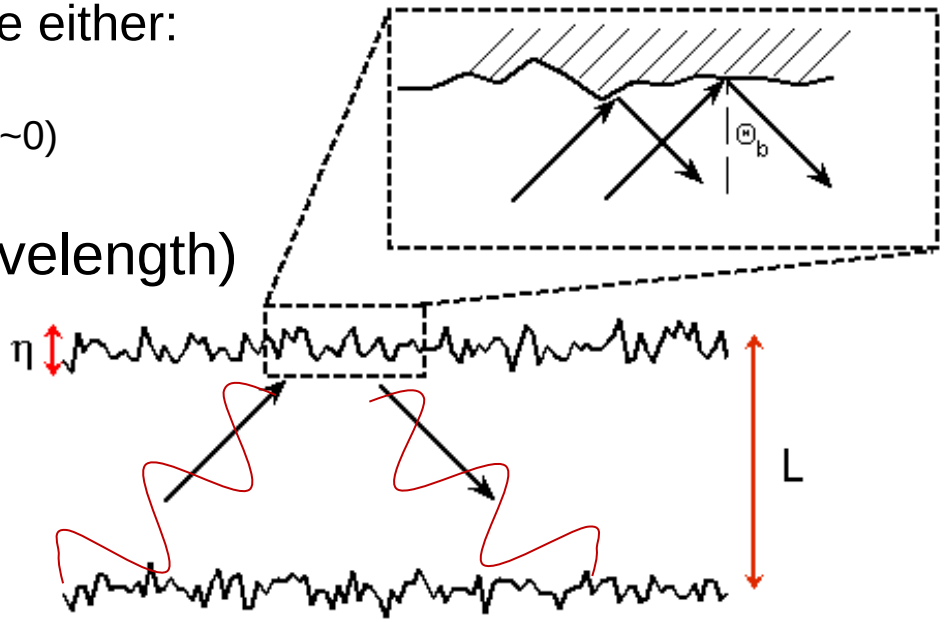
- Heat in semiconductors is carried primarily by lattice vibrations (phonons)
- Phonons scatter with each other (3-phonon anharmonic coupling):
  - Gives rise to finite thermal conductivity
- Phonons scatter with boundaries, imperfections, isotopes and alloys.
- In nanostructures: very strong interactions between phonons and boundaries or interfaces




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

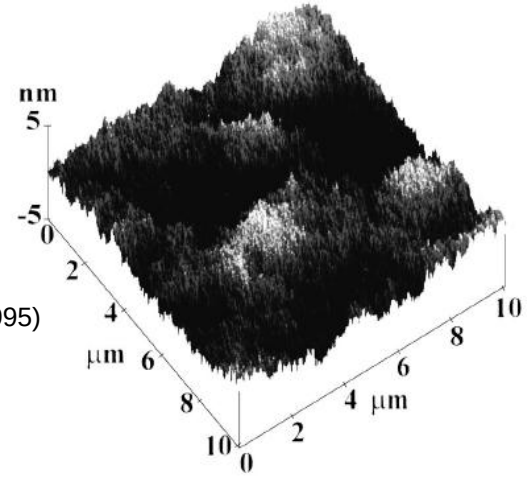
# Boundary Scattering in Nanostructures

- Scattering with interfaces/boundaries dominates transport in nanostructures
- Describe the interaction by a specularity parameter: $0 \le p(\vec{q}) \le 1$
- Specularity represents the probability of the phonon wave undergoing purely specular reflection
  - Specular reflection means no randomization of momentum->no resistance!
- At a rough interface, phonons can be either:
  - reflected (specular, p~1) or
  - scattered in a random direction (diffuse, p~0)
- If the phonon is large (large wavelength)
  - The surface variations look small
  - Results in a mirror-like reflection
  - No change in momentum



# Boundary Scattering in Nanostructures

- If the phonon wavelength is small
  - The surface variation looks big!
  - The phonon is bounced off randomly
  - Alters the momentum->resistance!

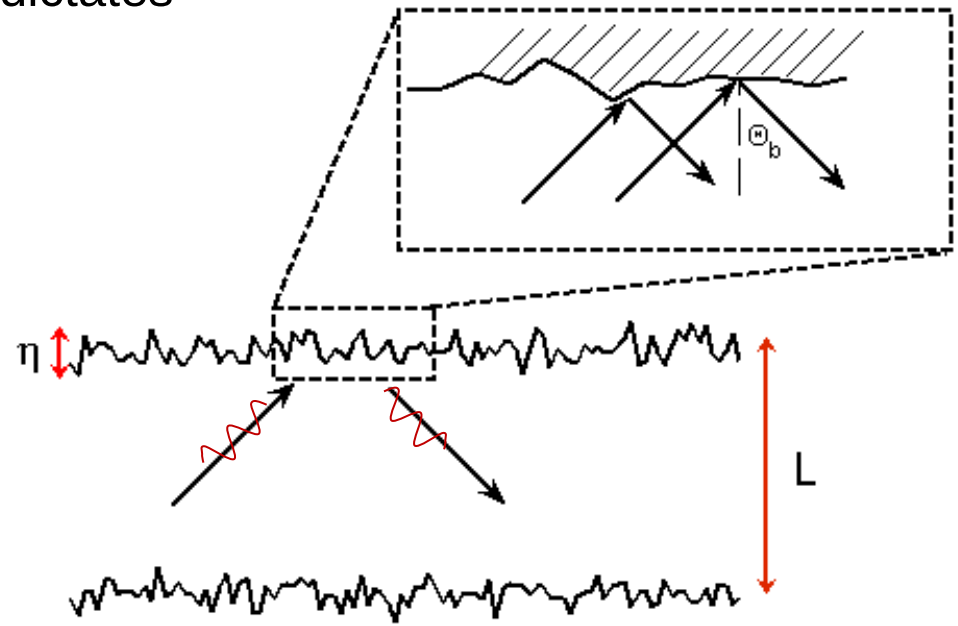



C. Teichert, et al., Appl. Phys. Lett. (1995)

- Momentum-dependent specular-diffuse interface scattering parameter p(q) dictates surface interactions:

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

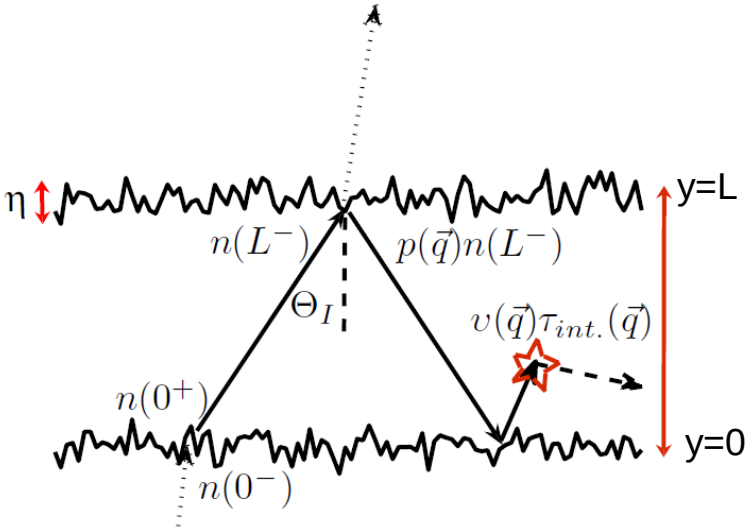
- Allows us to connect specularity parameter to phonon momentum, rms roughness and angle of incidence



# Boundary vs. Internal Scattering

- What happens to boundary or interface scattering in the presence of other competing mechanisms?
- Model using the steady-state phonon Boltzmann transport equation in the relaxation time approximation:

$$\vec{v}_{\vec{q}} \cdot \nabla_{\vec{r}} N_{\vec{q}}(\vec{r}) = \frac{N_{\vec{q}}(\vec{r}) - N^0_{\vec{q}}(T)}{\tau_{int.}(\vec{q})}$$




- Using a perturbation solution: $N_{\vec{q}}(\vec{r}) = N^0_{\vec{q}}(T) + n_{\vec{q}}(y)$

- Assume spatial variation is in the y (normal to interface) direction:

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

# Boundary vs. internal scattering

- General solution of the PBTE along the y-axis:

$$n_{\vec{q}}(y) = R_{\vec{q}}\left[1 - \exp\left(-y/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)\right] + n_{\vec{q}}(0)\exp\left(-y/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)$$

- Where R is the (bulk) relaxation-time solution:

$$R_{\vec{q}} = \tau_{int.}(\vec{q})\vec{v}_{\vec{q}} \cdot \nabla_{\vec{r}} T \frac{\partial N^0_{\vec{q}}(T)}{\partial T}$$

- Using the partially specular-diffuse boundary condition at y=0:

$$n_{\vec{q}}(0^+) = p(\vec{q})n_{\vec{q}}(0^-) + \left[1 - p(\vec{q})\right]N^0_{\vec{q}}(T)$$

{does not contribute to heat flux}

- Each interface/boundary contributes one “probability of not scattering” term:

$$p(\vec{q})\exp\left(-L/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)$$

# Boundary vs. Internal Scattering

- We get a series with one term for each interface scattering:

$$n_{\vec{q}}(y) = R_{\vec{q}}\left[1-\exp\left(-y/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)\right] + p(\vec{q})\exp\left(-y/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)\left\{R_{\vec{q}}\left[1-\exp\left(-L/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)\right] + p(\vec{q})\exp\left(-L/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)\left\{R_{\vec{q}}\left[1-\exp\left(-L/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)\right]\ldots\right\}\right\}$$

- Sum the infinite series:

$$n_{\vec{q}}(y) = R_{\vec{q}}\left[1-(1-p(\vec{q}))\exp\left(-y/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)\sum_{k=0}^{\infty}p^{k}(\vec{q})\exp\left(-kL/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)\right]$$

- To get the complete solution:

$$n_{\vec{q}}(y) = R_{\vec{q}}\left[1-\left(\frac{1-p(\vec{q})}{1-p(\vec{q})\exp\left(-L/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)}\right)\exp\left(-y/\tau_{int.}(\vec{q})v_{\perp}(\vec{q})\right)\right]$$

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

# Boundary vs. Internal Scattering

- Using the relaxation-time definition, we extract the “average” solution:

$$R_{\vec{q}} = \left( \frac{1}{\tau_{int.}(\vec{q})} + \frac{1}{\tau_B(\vec{q})} \right) \langle n_{\vec{q}}(y) \rangle$$

- This form gives us the desired definition of boundary scattering rate:

$$\frac{1}{\tau_B(\vec{q})} = \frac{\int_0^L \upsilon_\perp(\vec{q})(\partial n_{\vec{q}}(y)/\partial y)dy}{\int_0^L n_{\vec{q}}(y)dy}$$

- Final boundary scattering rate:

$$\frac{1}{\tau_B(\vec{q})} = \frac{\upsilon_\perp(\vec{q})}{L} \frac{F_p(\vec{q}, L)}{1 - \frac{\tau_{int.}(\vec{q})\upsilon_\perp(\vec{q})}{L} F_p(\vec{q}, L)}$$

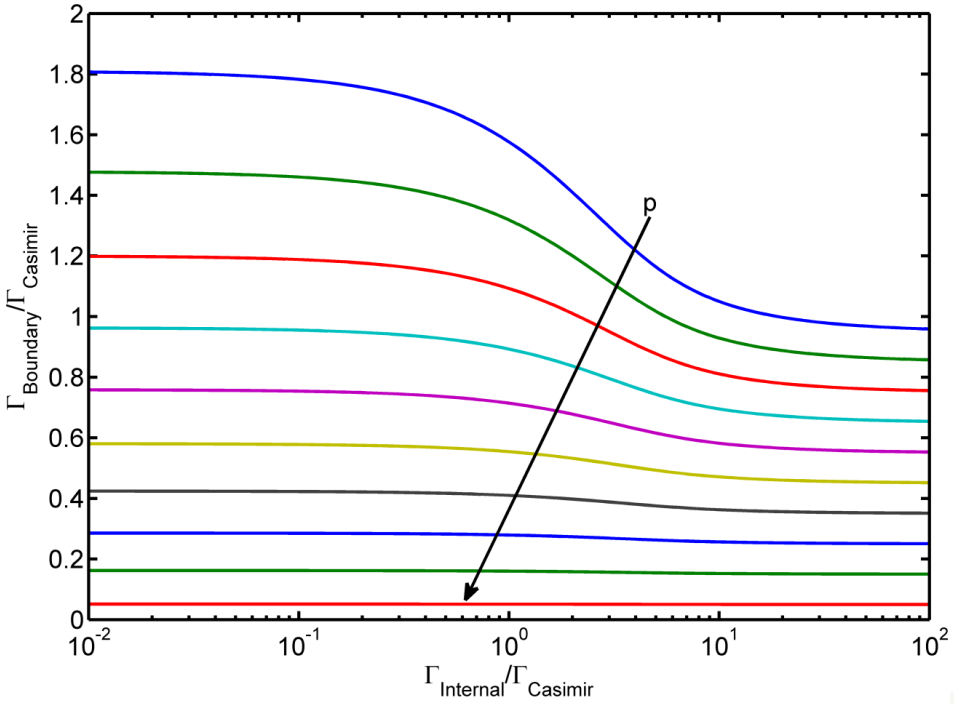
- Where F(q,L) is given by:

$$F_p(\vec{q}, L) = \frac{1 - p(\vec{q}) \left[1 - \exp\left(-L/\tau_{int.}(\vec{q})\upsilon_\perp(\vec{q})\right)\right]}{1 - p(\vec{q}) \exp\left(-L/\tau_{int.}(\vec{q})\upsilon_\perp(\vec{q})\right)}$$

# Boundary scattering rate

- The final result still has the “Casimir” factor of $v_\perp/L$, but now features the complete dependence on the internal scattering lifetime $\tau_{int}$

- Two limits to the solution: strong and weak internal scattering:
  - Weak internal scattering: (1-p)/(1+p)*2*$v_\perp$/L
  - Strong internal scattering: (1-p)*v/L
  - Weaker rate in the case of strong internal scattering due to decoupled interfaces

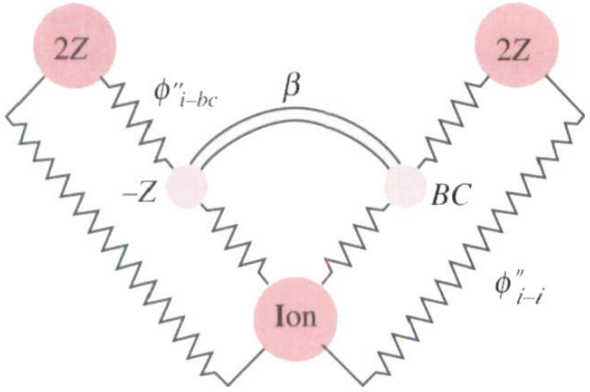


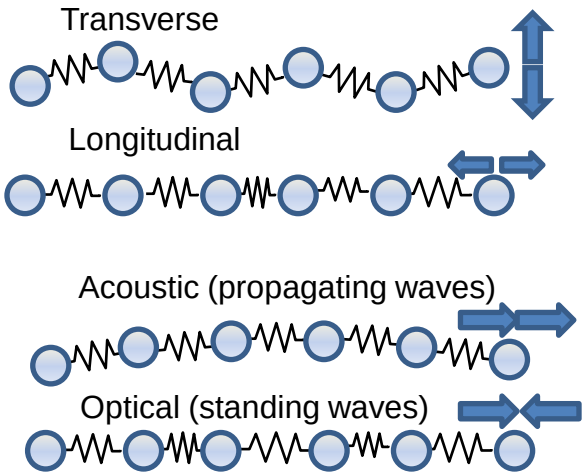
# Model for Thermal Conductivity

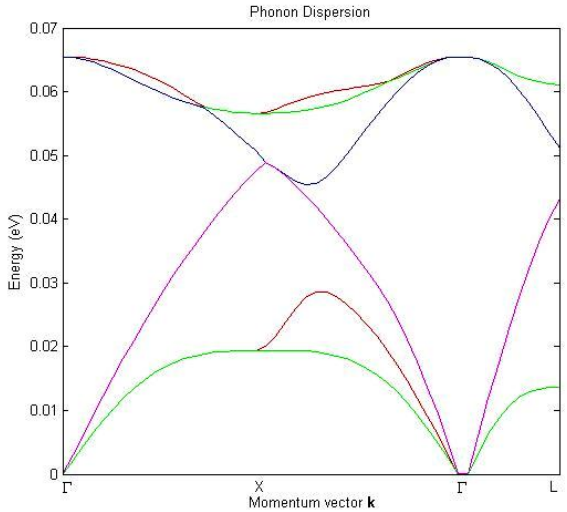
- Compute the full thermal conductivity tensor
- Sum contributions from all phonon branches (b) and modes (q)

$$\kappa^{\alpha\beta}(T) = \sum_{\mathrm{b}} \sum_{\vec{q}} \tau_{\mathrm{b}}(\vec{q}) C_{\mathrm{b}}(\vec{q}, T)\, v_{\mathrm{b}}^{\alpha}(\vec{q}) v_{\mathrm{b}}^{\beta}(\vec{q})$$

- Use the full phonon dispersion for phonon energies and velocities
  - Weber's Adiabatic Bond Charge model is used to calculate the full phonon dispersion throughout the 1st Brillouin zone [W. Weber PRB **15**, 4789–4803 (1977)]
  - Predicts phonon dispersion in silicon with <2% error on the average



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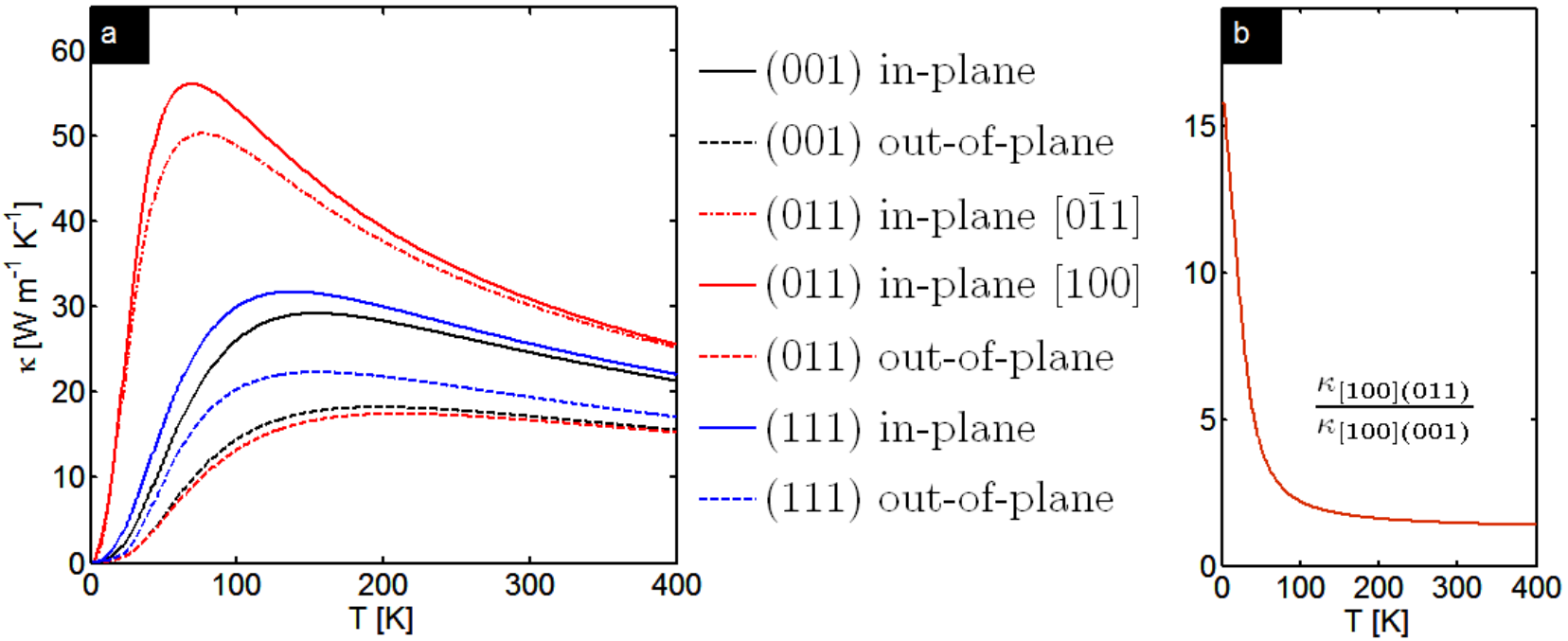
# Anisotropic Thermal Transport in Ultrathin SOI

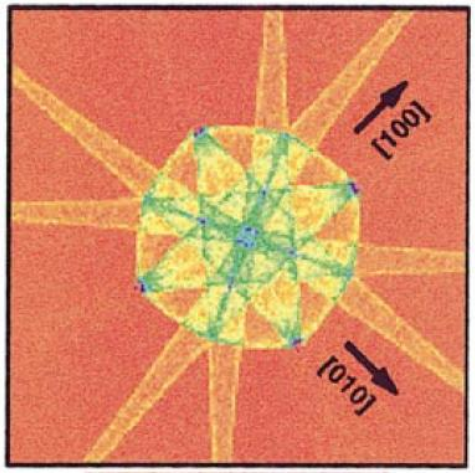
- Computed thermal conductivity in 20nm SOI shows strong anisotropy
- Lowest thermal conductivity is on a (001) surface
- Highest thermal conductivity achieved on (011) surface
- Overall ratio of highest and lowest in-plane thermal conductivity is roughly a factor of 2 at room temp. and higher at low temperature
- Allows additional control over thermal conductivity



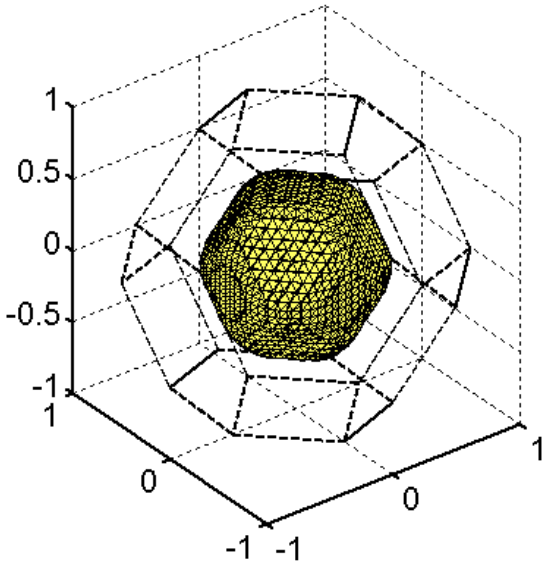

Z. Aksamija and I. Knezevic, Phys. Rev. B **82**, 045319 (2010)

# Anisotropy of Phonon Dispersion

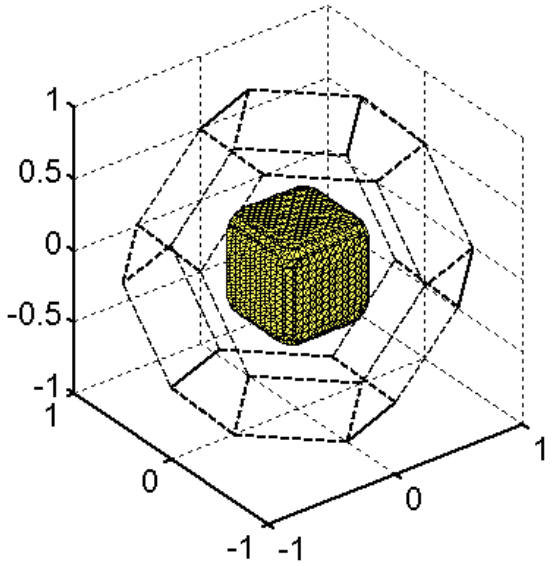
- Phonon isosurfaces show strong anisotropy and phonon focusing [Cahill et al., JAP 93, 793 (2003)]
- LA branch (left) has very flat faces with phonons propagating mainly in the [111] direction
- TA branch (middle) has flat isosurfaces with normal vectors (phonon velocities) in the [100] direction



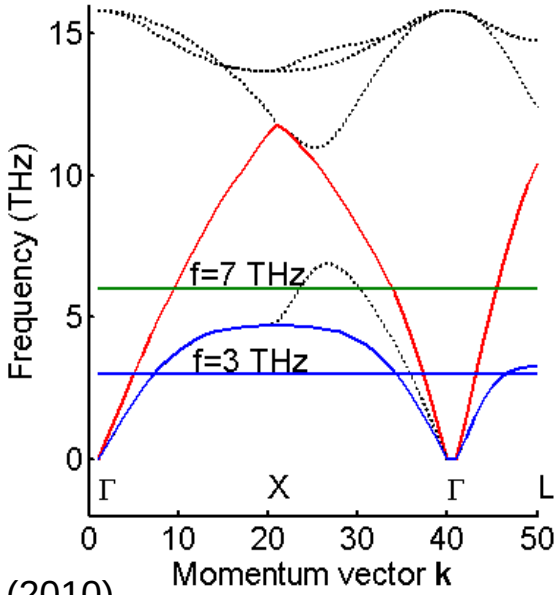

Longitudinal Acoustic (LA) branch




Transverse Acoustic (TA) branch



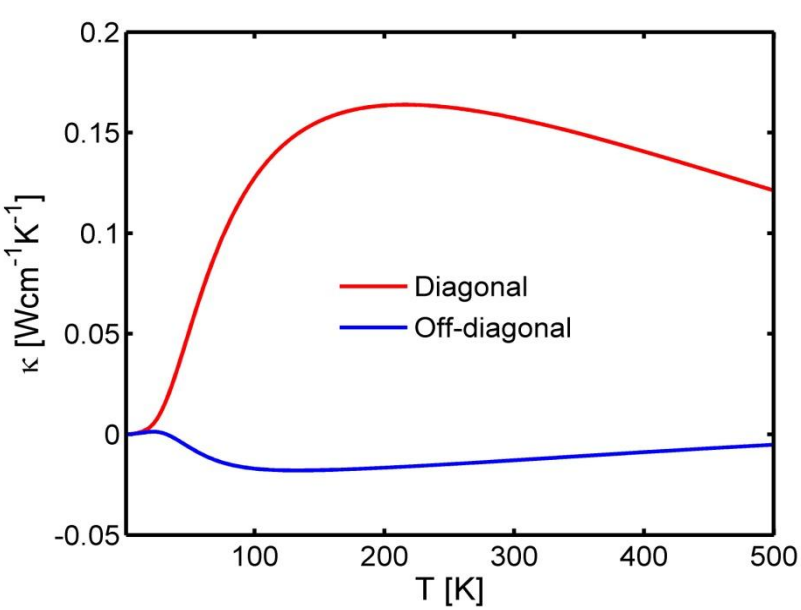

Phonon Dispersion

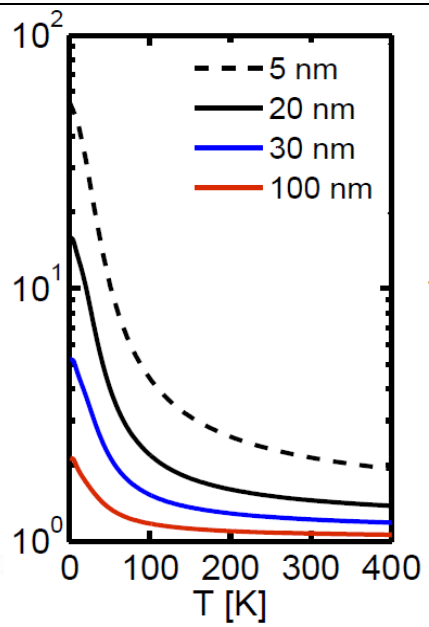


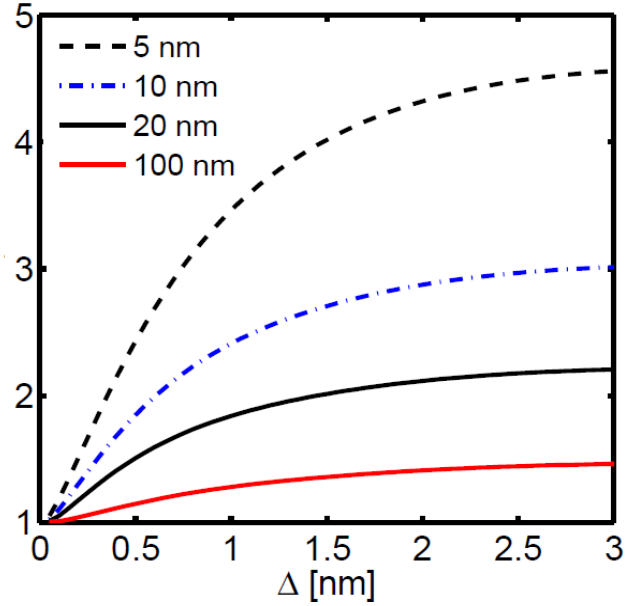

Z. Aksamija and I. Knezevic, Phys. Rev. B **82**, 045319 (2010)

# Thermal Conductivity Tensor in Ultrathin SOI

- 3x3 thermal conductivity tensor has distinct diagonal and off-diagonal components at each temperature
- 3 eigenvalue/eigenvector pairs:
  - 1 eigenvector in the direction of the surface and 2 in-plane
- Eigenvectors independent of temperature, only depend on surface orientation
- In/out-of-plane and highest/lowest in-plane ratios both depend on thickness and rms surface roughness



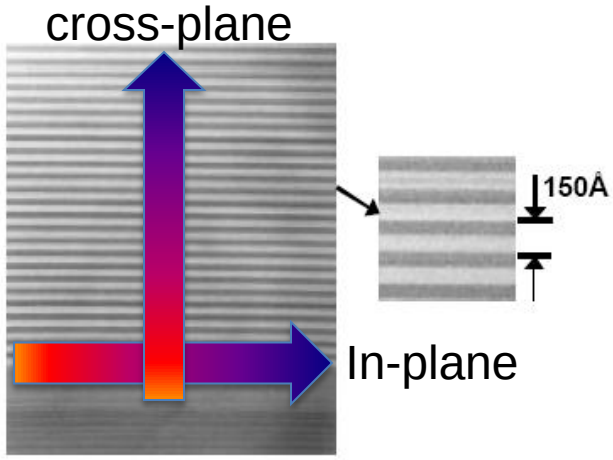

Z. Aksamija and I. Knezevic, Phys. Rev. B **82**, 045319 (2010)

# Thermal Transport in Superlattices

- Superlattices are made up from many thin (new nm) layers of alternating semiconductor materials
- Layers separated by a rough interface with an rms roughness Δ
- Thermal conductivity of the two alternating layers is combined in series for cross-plane transport and in parallel for in-plane transport

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

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



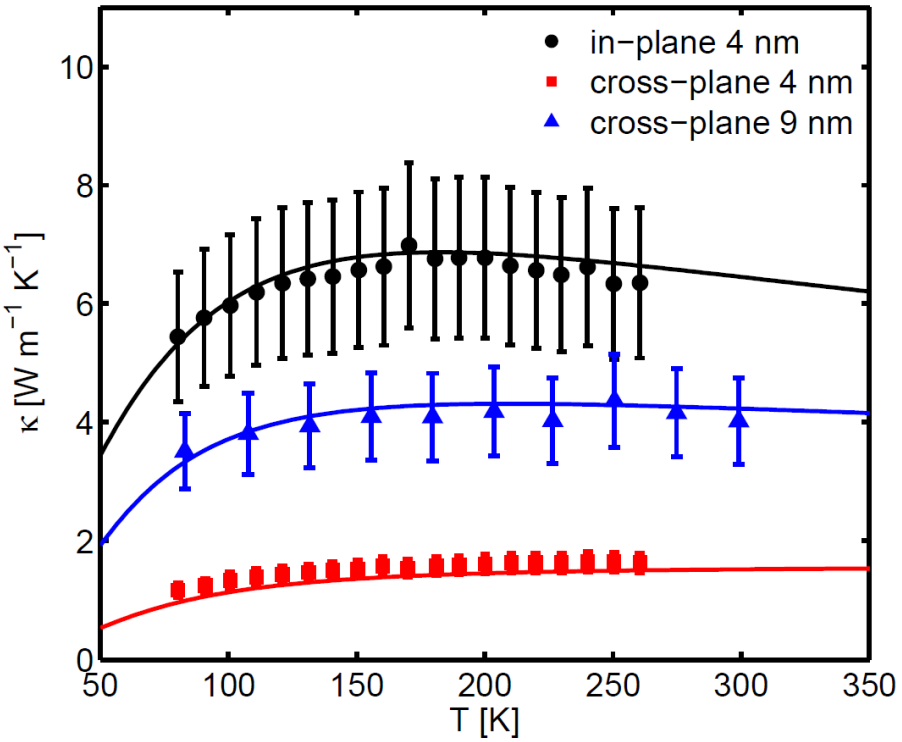

SEM image from S. T. Huxtable, Ph.D. Thesis

- Additional interface resistance due to acoustic mismatch between dissimilar materials

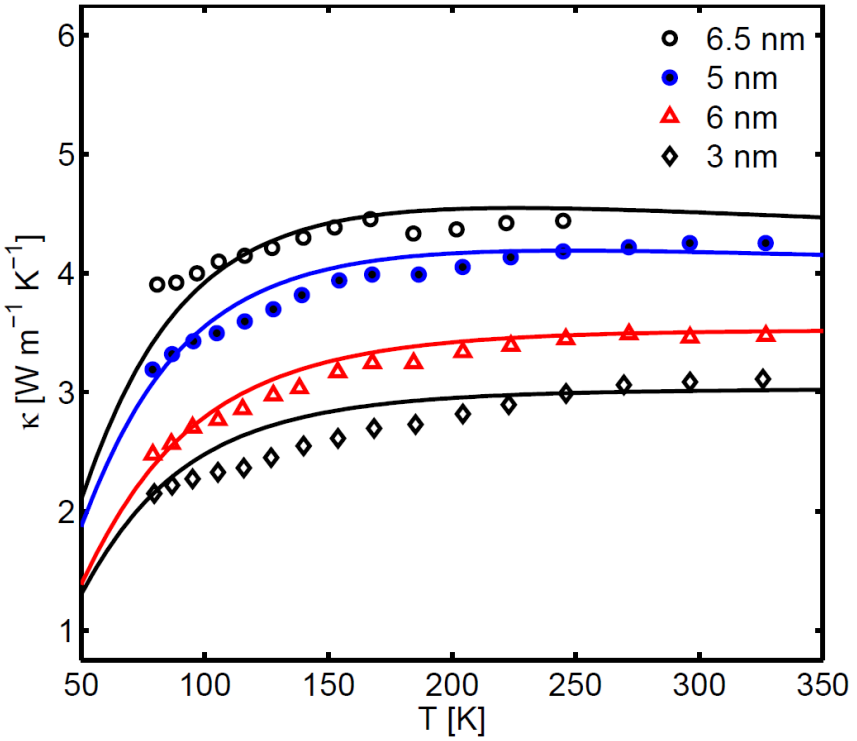
$$\sigma_i^{AIM}(T) = \frac{1}{2}\sum_{\text{b}} \frac{\sum_{\vec{q}} C\left(\omega_{\text{b,i}}(\vec{q}), T\right) v_{\text{b,i}}^{\perp}(\vec{q}) t_{\text{b}}^{AIM}(\vec{q})}{1 - \langle t_{\text{b}}^{AIM}(\vec{q})\rangle}$$

# Anisotropy in Si/Ge Superlattices

- Strong in-plane/cross-plane anisotropy in 4 nm period Si/Ge superlattice (left)
- Very low (1~5 W/m/K) cross-plane (through the SL) lattice thermal conductivity in Si/Ge SLs with a wide range of period thickensses (right)



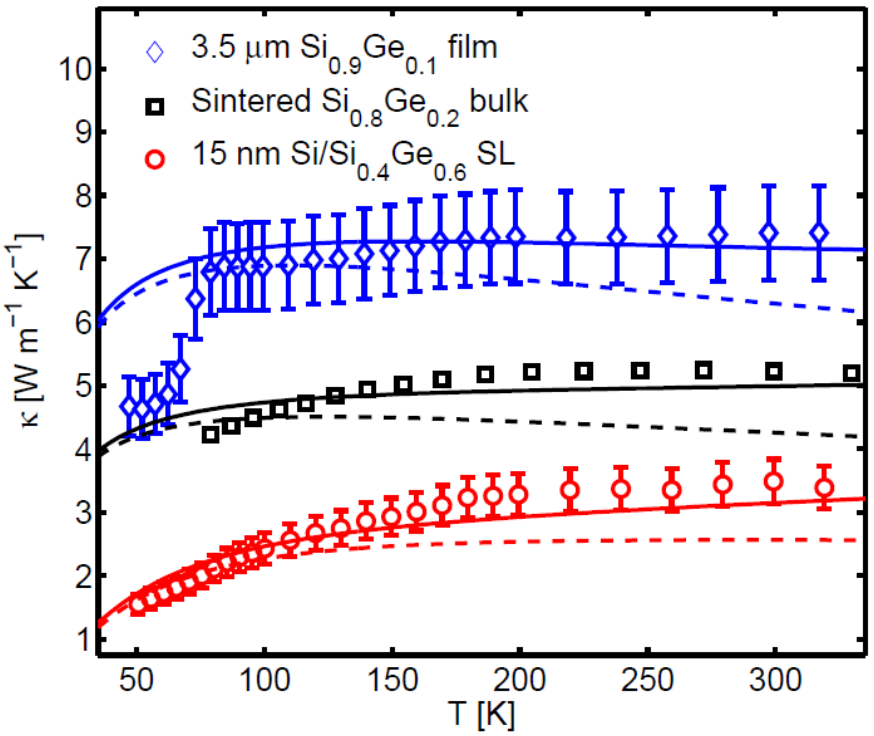

Data points from: Liu et al., J. Nanosci. Nanotech. **1**, 39 (2001)

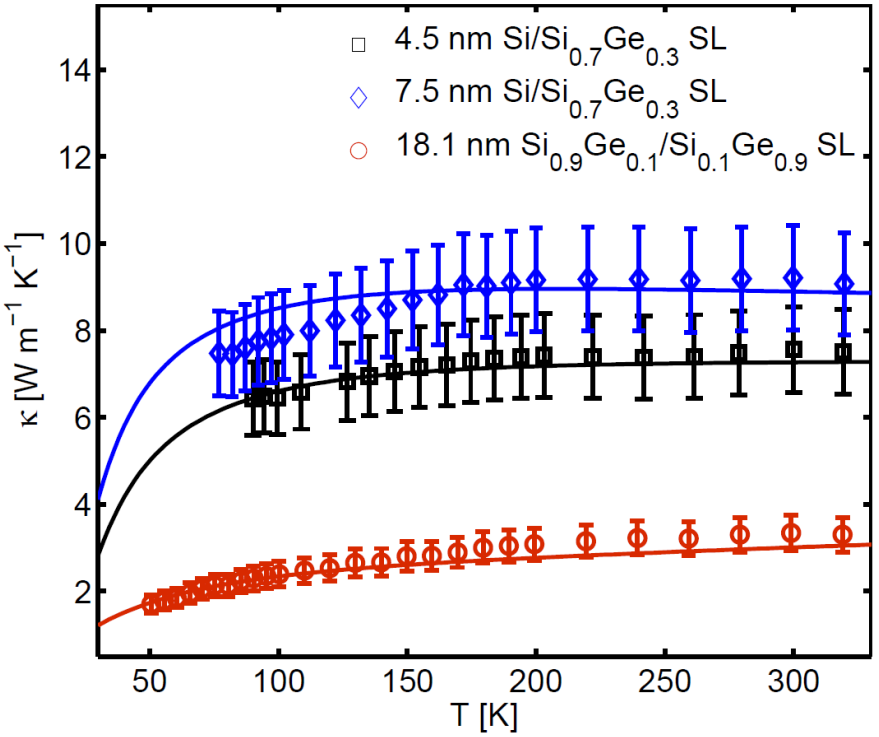



Data points from: Lee et al., Appl. Phys. Lett. **70**, 2957 (1997)

# $Si_{1-x}Ge_x$ Alloy Film and $Si/Si_{1-x}Ge_x$ SLs

- Black: 3.5um $Si_{0.3}Ge_{0.7}$ alloy film, Red: 15nm $Si/Si_{0.4}Ge_{0.6}$ SL (left)
- Superlattice thermal conductivity below "alloy limit"
- Explained by scattering of phonons from rough interfaces
  - Dashed line: lattice only, solid line: lattice+electron constribution
- Alloying both layers reduces thermal conductivity even further (right)




Data points from: Huxtable et al. Appl. Phys. Lett. **80**, 1737 (2001)

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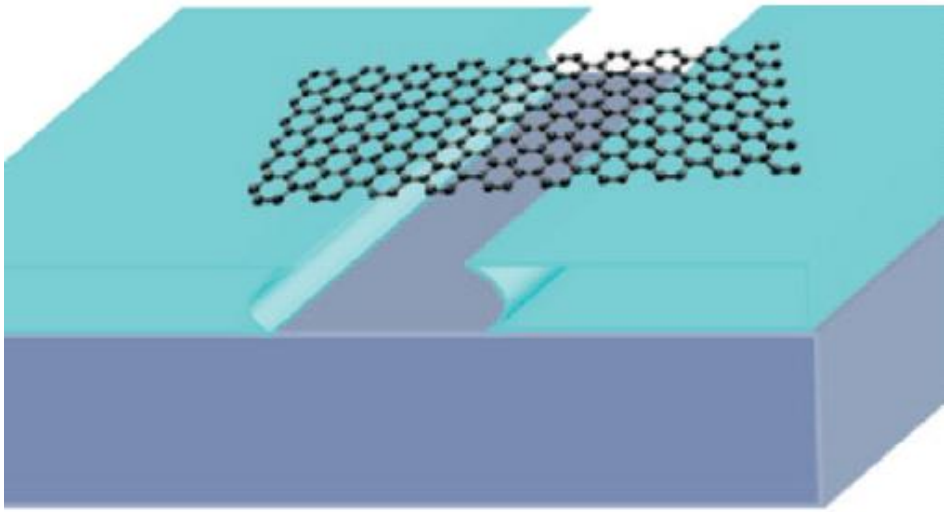
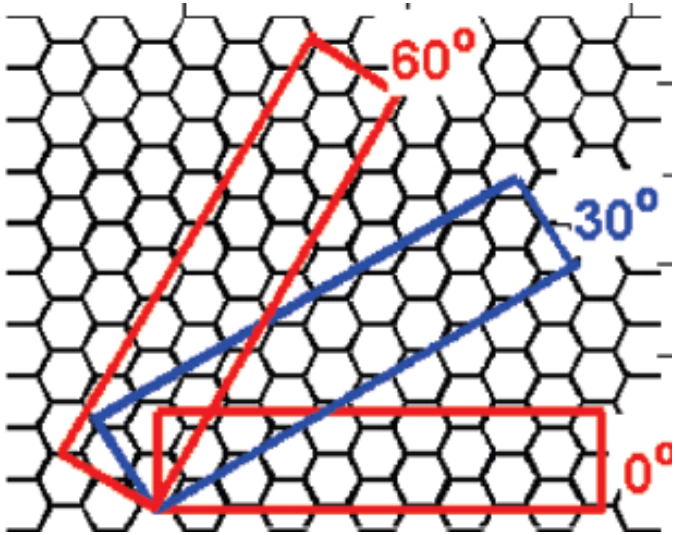
  - Boundary/interface scattering of phonons
  - Phonon transport at boundaries/interfaces with competing internal scattering mechanisms
- Lattice thermal conductivity of Si-based nanostructures:
  - Ultra-thin Silicon-On-Insulator nanomembranes
  - Si/Ge and $Si_{1-x}Ge_x/Si_{1-y}Ge_y$ superlattices
- Thermal properties of Graphene Nanoribbons (GNRs)
  - Anisotropic thermal conductivity of suspended GNRs
  - Substrate scattering and thermal transport in supported GNRs
- Discussion and Conclusions

# SLG and GNR geometry

- SLG (single-layer graphene) is a 2D honeycomb lattice of carbon atoms (left)
- Electronic properties of SLG earned Geim and Novoselov Nobel Prize
- GNRs (graphene nano-ribbons) are typically narrrow strips of SLG (right) cut along different angles
- SLG and GNR samples can be either suspended over a trench or supported by a substrate



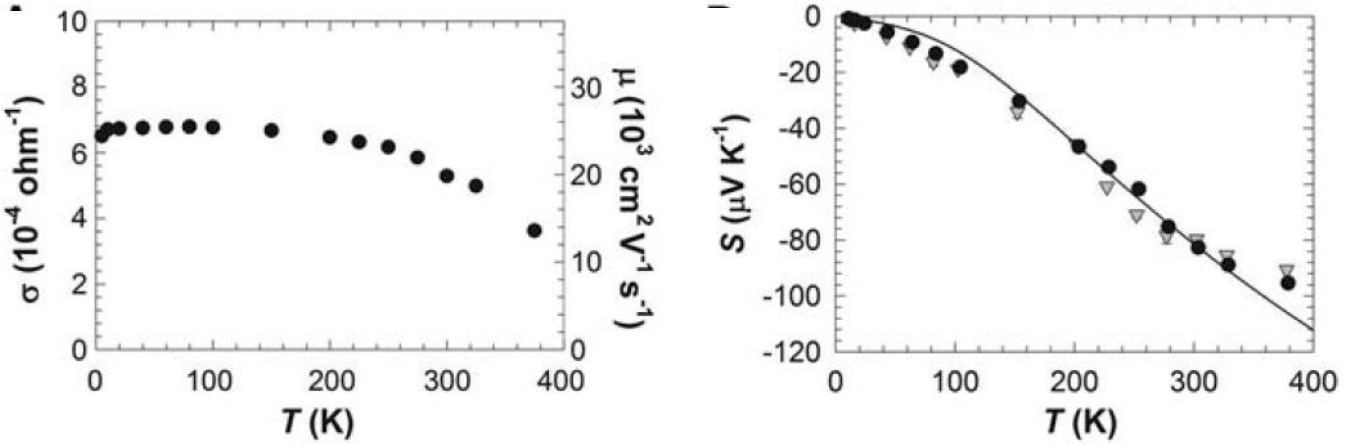


# Comparison of Experimental Results

- Suspended SLG is shown to have superior thermal conductivity

| sample type | $K$ (W/mK) | method | comments | ref |
|---|---|---|---|---|
| SLG | ~4840–5300 | optical | individual; suspended | this work |
| MW-CNT | >3000 | electrical | individual; suspended | Kim et al.[15] |
| SW-CNT | ~3500 | electrical | individual; suspended | Pop et al.[16] |
| SW-CNT | 1750–5800 | thermocouples | bundles | Hone et al.[17] |

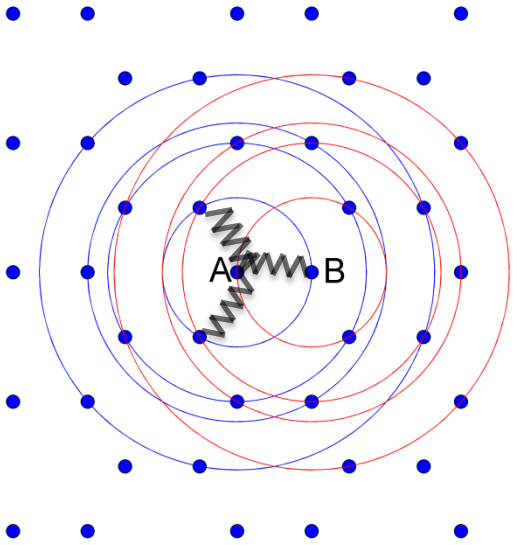
- This opens up the possibility of using SLG and GNRs for cooling applications in future microelectronic circuits
- Question: what happens to thermal conductivity when the physical dimensions of graphene are reduced?

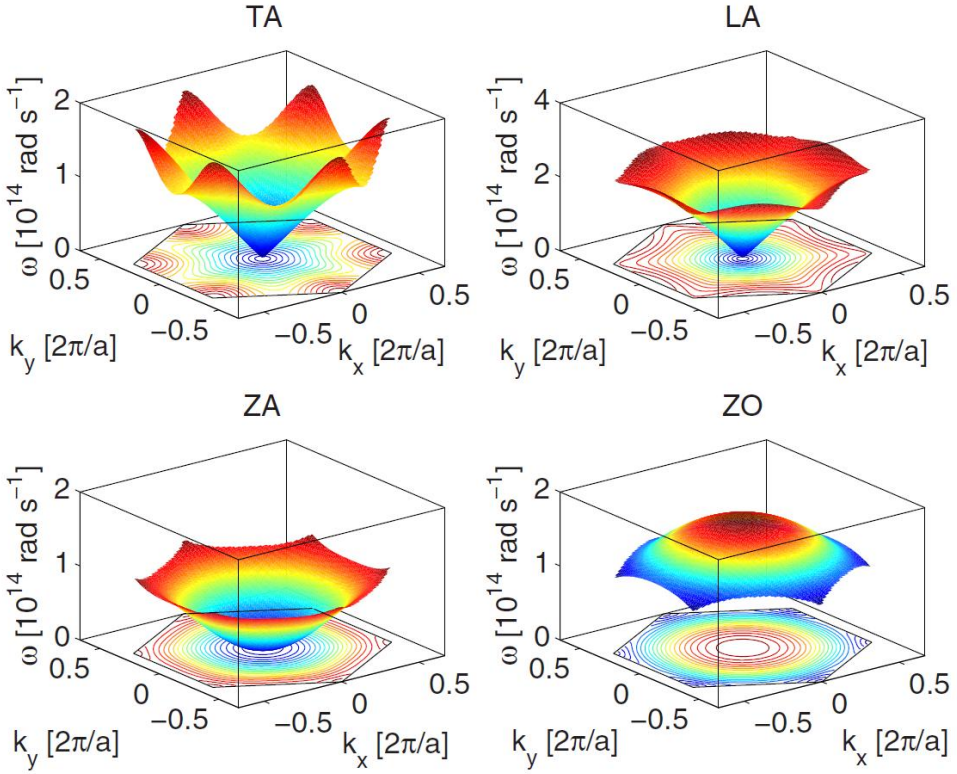



- Superior electrical + reduced thermal conductivity = great thermoelectric!

# Phonon Dispersion of Graphene

- Phonon dispersion calculated in Saito's fourth-nearest-neighbor force-constant approach (4NNR) with new parameters from Zimmermann et al. PRB **78**, 045410 (2008).
- Dispersion highly anisotropic, especially the transverse acoustic (TA) mode



# Line Edge Roughness Scattering of Phonons

- Phonon lifetime due to scattering with the rough edges
  - proportional the ratio of the width of the nanoribbon (W) and the phonon velocity in the direction of edge normal ($v_\perp$):

$$\frac{1}{\tau_E(\vec{q})} = \frac{\upsilon_\perp(\vec{q})}{W} \frac{F_p(\vec{q},W)\left[1-\exp\left(-W/\tau_{int.}(\vec{q})\upsilon_\perp(\vec{q})\right)\right]}{1-\frac{\tau_{int.}(\vec{q})\upsilon_\perp(\vec{q})}{W}F_p(\vec{q},W)\left[1-\exp\left(-W/\tau_{int.}(\vec{q})\upsilon_\perp(\vec{q})\right)\right]}$$

- Edge scattering rate also depends on the competing internal processes (such as substrate scattering) through the parameter F:

$$F_p(\vec{q},W) = \frac{1-p(\vec{q})}{1-p(\vec{q})\exp\left(-W/\tau_{int.}(\vec{q})\upsilon_\perp(\vec{q})\right)}$$

- Phonon lifetime depends on rms edge roughness, angle, and temperature because of the specularity parameter p(q)

# Model for Thermal Conductivity of GNRs

- Use the full phonon dispersion for phonon energies and velocities
- Include Umklapp, isotope, and edge scattering:

$$\tau_{\lambda,U}^{-1}(\vec{q}) = \frac{\hbar\gamma_\lambda^2}{\bar{M}\Theta_\lambda \bar{v}_\lambda^2}\omega_\lambda^2(\vec{q})Te^{-\Theta_\lambda/3T} \qquad \tau_I^{-1}(\omega) = \Gamma\Omega_0/12\omega^2 g(\omega)$$

- Compute the full thermal conductivity tensor

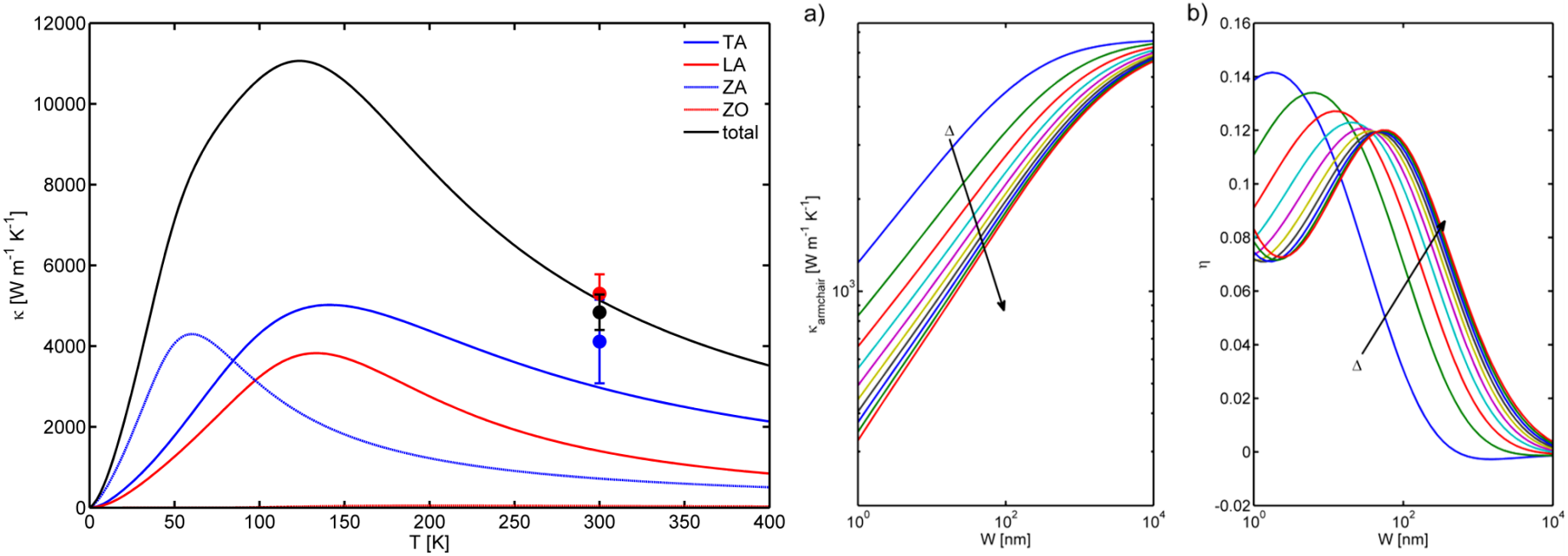
- Sum contributions from all phonon branches (b) and all modes (q):

$$\kappa^{\alpha\beta}(T) = \frac{1}{\delta}\sum_{\lambda,\vec{q}} v_\lambda^\alpha(\vec{q})v_\lambda^\beta(\vec{q})\tau_\lambda\ (\vec{q})\hbar\omega_\lambda(\vec{q})\frac{\partial N_0(T)}{\partial T}$$

- Capture temperature, orientation, and rms edge roughness dependence

# Thermal Conductivity of Graphene

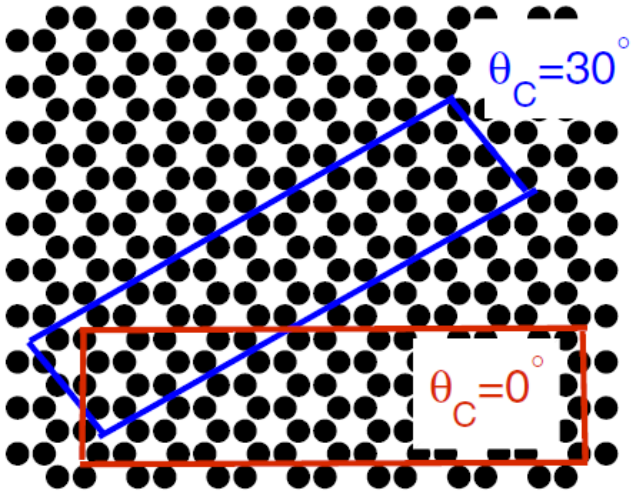
- Calculated thermal conductivity agrees well with measurements
  - Balandin et al., Nano Lett. **8**, 902 (2008) and Ghosh et al., Appl. Phys. Lett., **92**, 115 (dots/error bars)
- Thermal conductivity has a strong contribution from ZA mode at low temperatures and from TA mode at high temperatures (left)
- Strong dependence of thermal conductivity (a) and armchair/zig-zag anisotropy (b) on both width and edge roughness

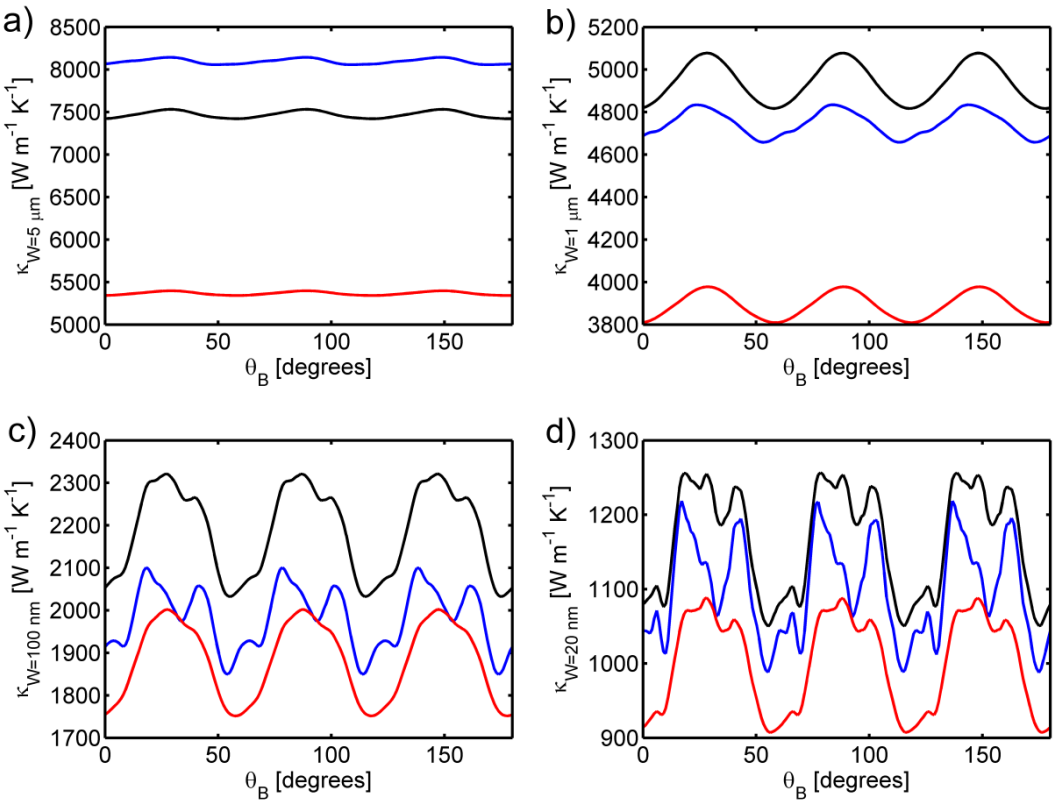



Z. Aksamija and I. Knezevic, Appl. Phys. Lett. v.98, 141919 (2011)

# Angular Dependence of Thermal Conductivity

- Angular depence of thermal conductivity reveals rich and complex behavior, especially in narrow and rough ribbons
- Zig-zag edge ribbons have up to 20% higher thermal conductivity than their armchair counterparts

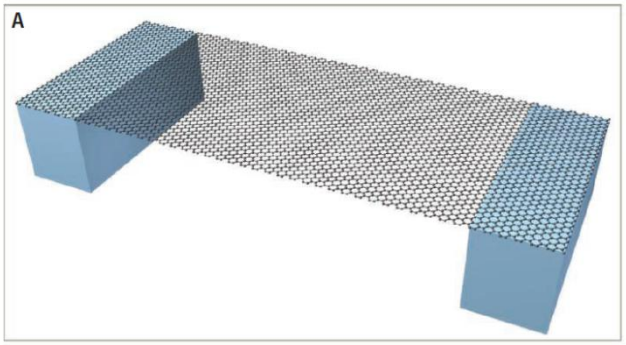



Z. Aksamija and I. Knezevic, Appl. Phys. Lett. v.98, 141919 (2011)

# Thermal Transport in Supported Graphene

- In most applications, graphene is placed on a SiO2 substrate instead of being freely suspended (A)
- Graphene forms point contacts with the substrate (B)

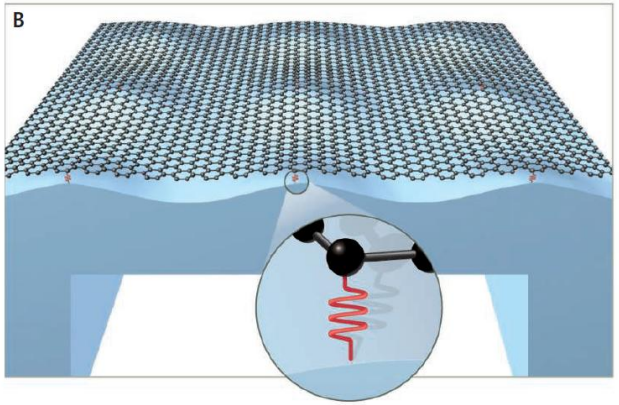



- Model the interaction with substrate as clusters of point contacts:

$$\lambda = \left( \frac{p}{N_c 4c\omega^2} 2\pi \left\{ N_c \left| K_{fi} / \sqrt{M_C M_X} \right|^2 \rho_{SiO2}(\omega) + F(N_c, \omega) \left| K_{fi} / M_C \right|^2 \rho_{graphene}(\omega) \right\} \right)^{-1}$$

where F is the form function of the contact region:

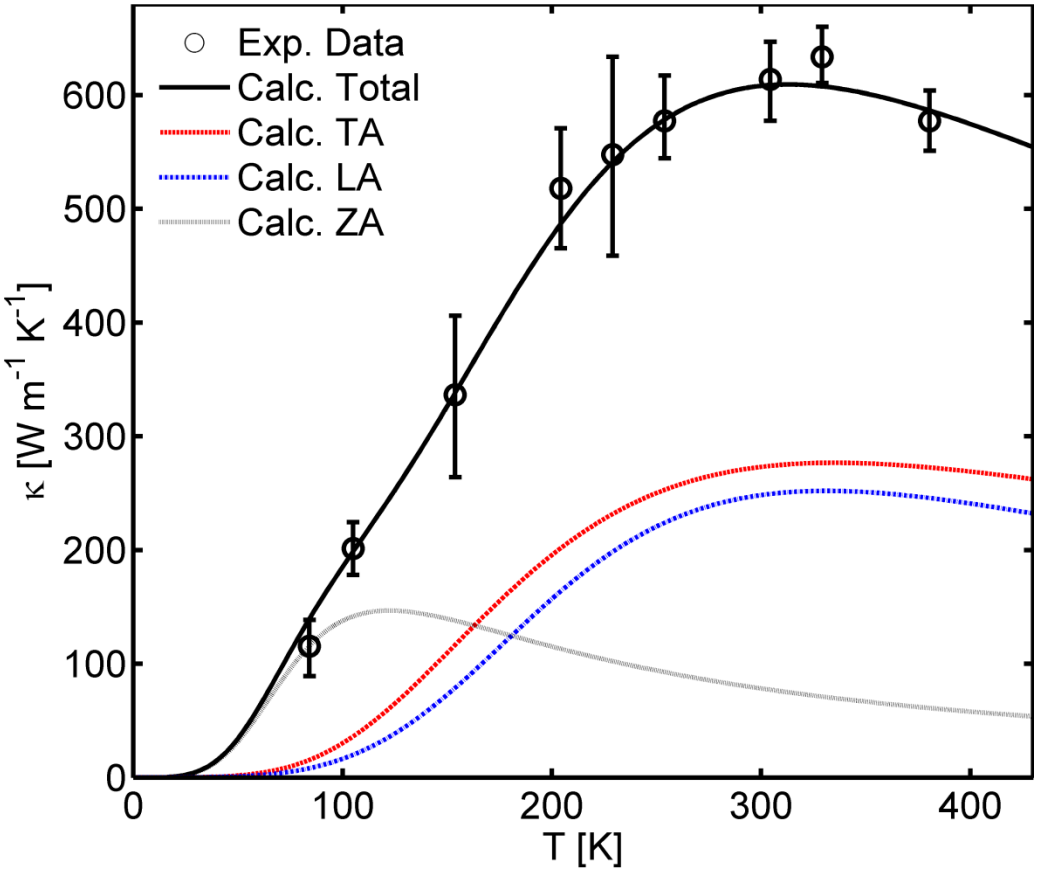
$$F = \frac{\pi a^2}{S_{atom}^2} \frac{1}{\pi} \int_0^\pi I^2(q) d\theta = N_c \frac{1}{\pi} \int_0^\pi I^2(q) d\theta$$

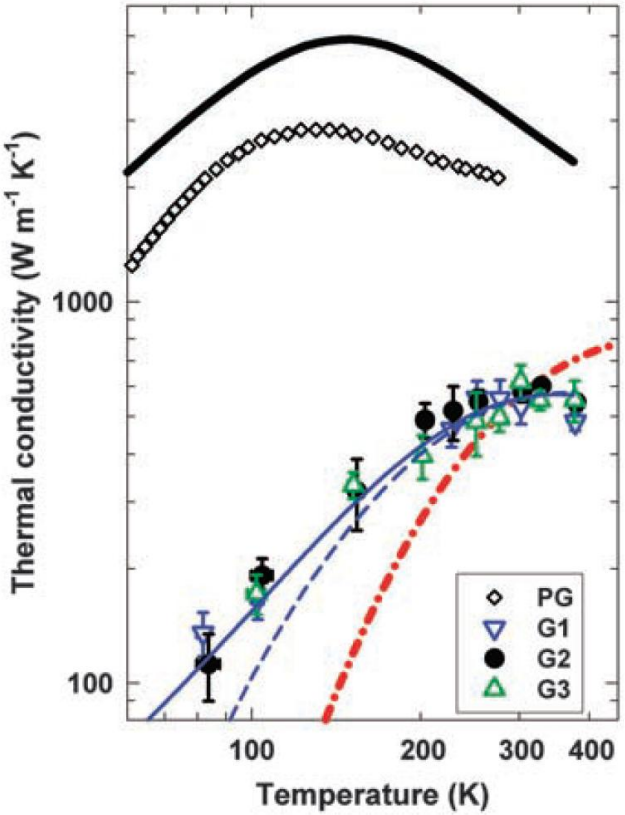



Seol et al., Science (2010) and R. Prasher, Science (2010)

# Thermal Conductivity of Graphene on $SiO_2$

- Excellent agreement with data from Seol et al., Science (2010)
- ZA mode dominates at low T, LA/TA (in-plane) modes at high T

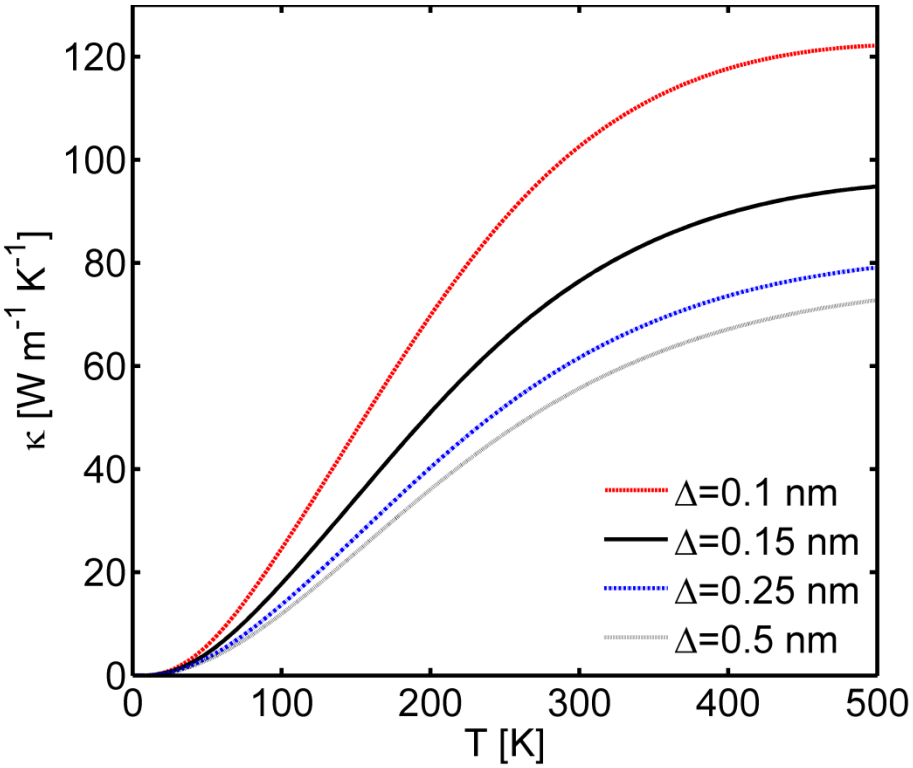


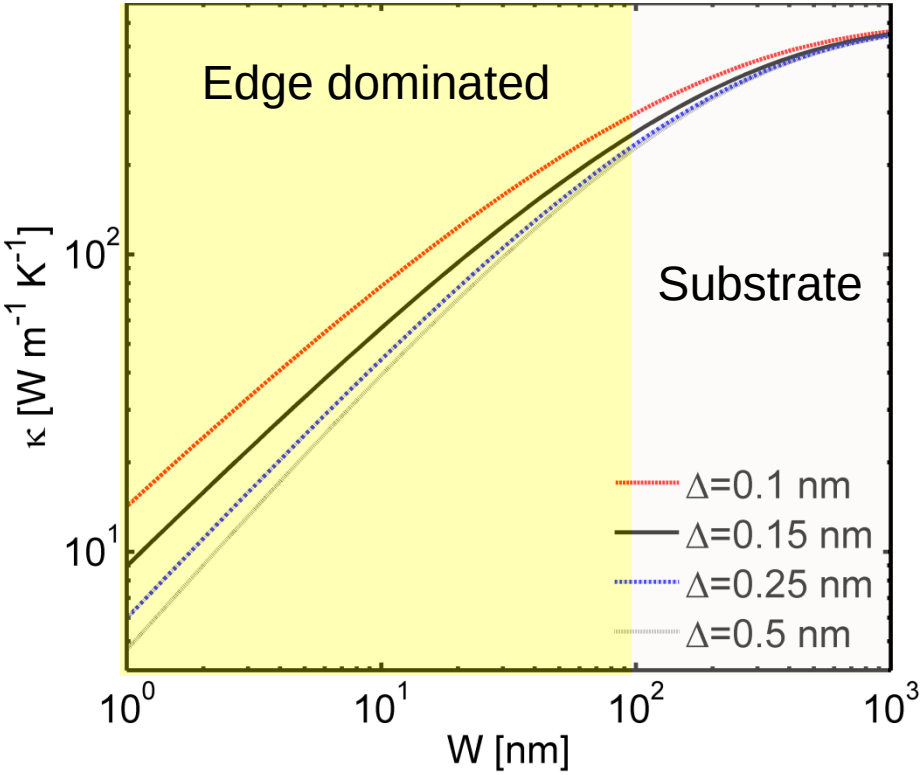




Data points taken from Seol et al., Science (2010)

# Thermal Conductivity in Supported GNRs

- Thermal conductivity in 15 nm wide supported ribbon shows a dramatic reduction and strong edge roughness dependence (left)
- Thermal conductivity for W<100 nm scales with ribbon width (right) down >2 orders of magnitude from suspended SLG



# Discussion and Conclusions

- Boundary/interface scattering depends on competing internal scattering
  - Internal scattering from umklapp phonon, isotope, mass difference (alloy), and impurity interactions
- General Goal: Maximize the influence of boundaries/interfaces by:
  - minimizing competing internal scattering (pure crystals)
  - maximizing roughness/diffuse scattering (make p small by using roughness or QDs)
- Si Nanomembranes have controllable thermal properties
  - tailored by the choice of thickness, roughness, and crystalline orientation
- Si/Ge and $Si_{1-x}Ge_x/Si_{1-y}Ge_y$ SLs thermal conductivity below alloy limit
  - explained by addition of boundary scattering to alloy scattering
- Thermal conductivity in GNRs is also anisotropic
  - strongly dependent on the properties (roughness and crystalline orientation) of edges
- Drastic reduction in thermal conductivity with reducing width of the ribbon
- Applications of graphene nanostructures in thermoelectric conversion
  - High electron mobility and reduced thermal conductivity

# Acknowledgement


- This work has been supported by:
  - The Computing Research Association and by the National Science Foundation through the Computing Innovation Fellowship (CIFellows) program
  - The National Science Foundation through the “Transformative Computational Science” Fellowship (CI TraCS) program
  - The AFOSR (YIP program, award No. FA9550-09-1-0230)


- Questions?