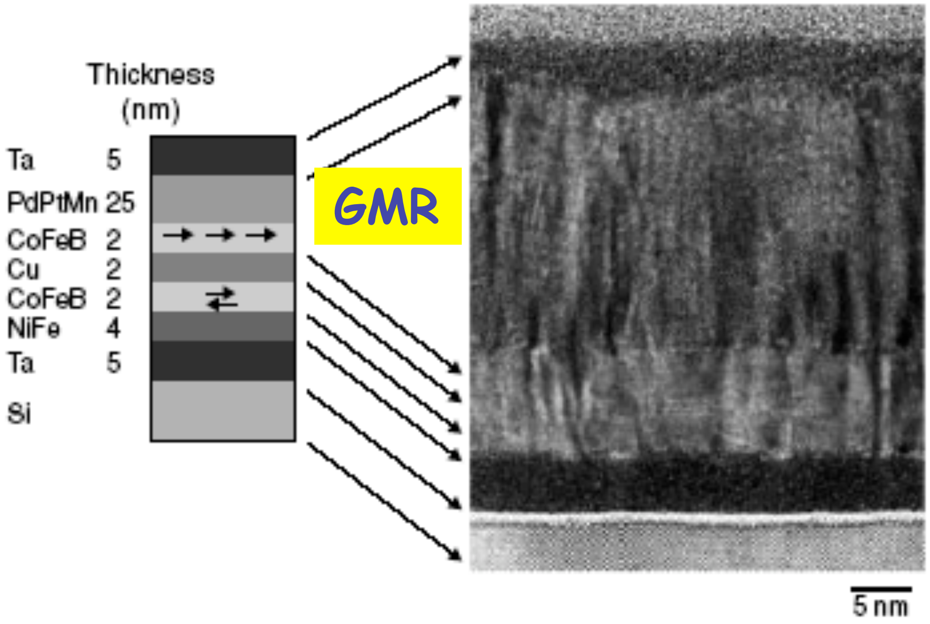
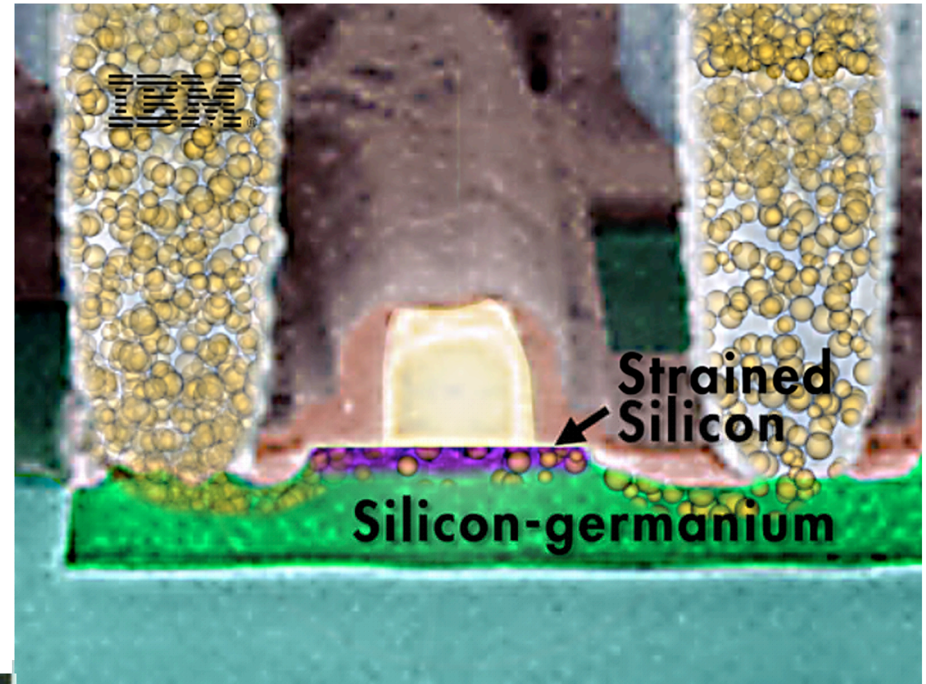
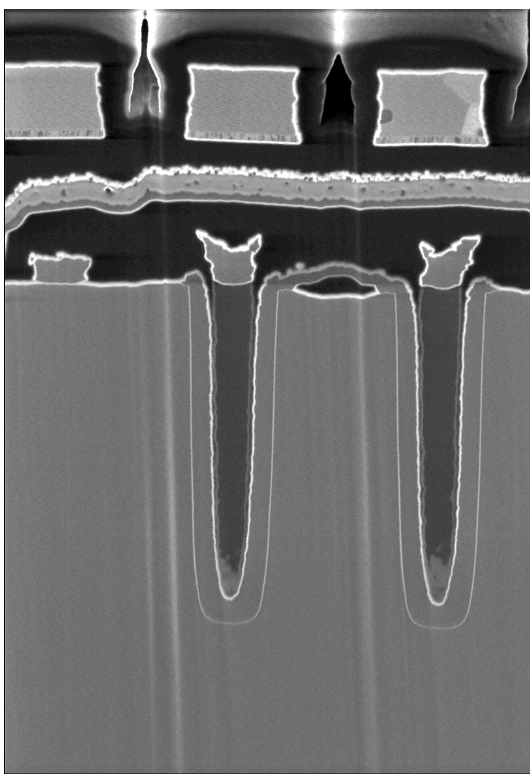
Heat Transport in Nanostructured Materials & Devices

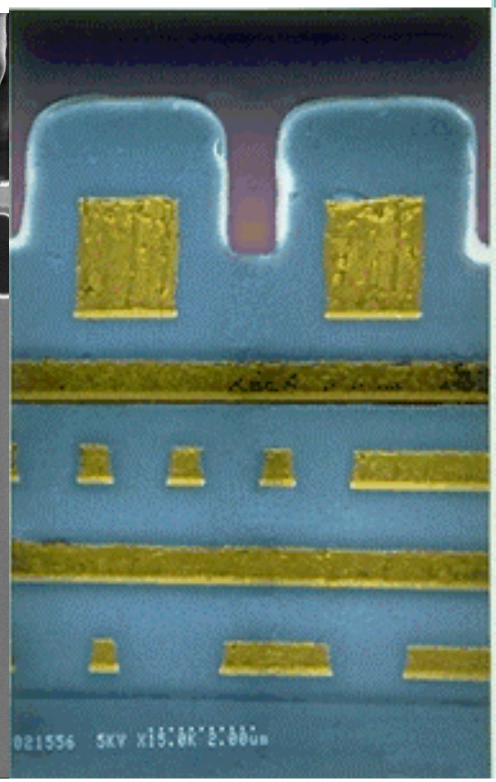
Arun Majumdar
Department of Mechanical Engineering
University of California, Berkeley

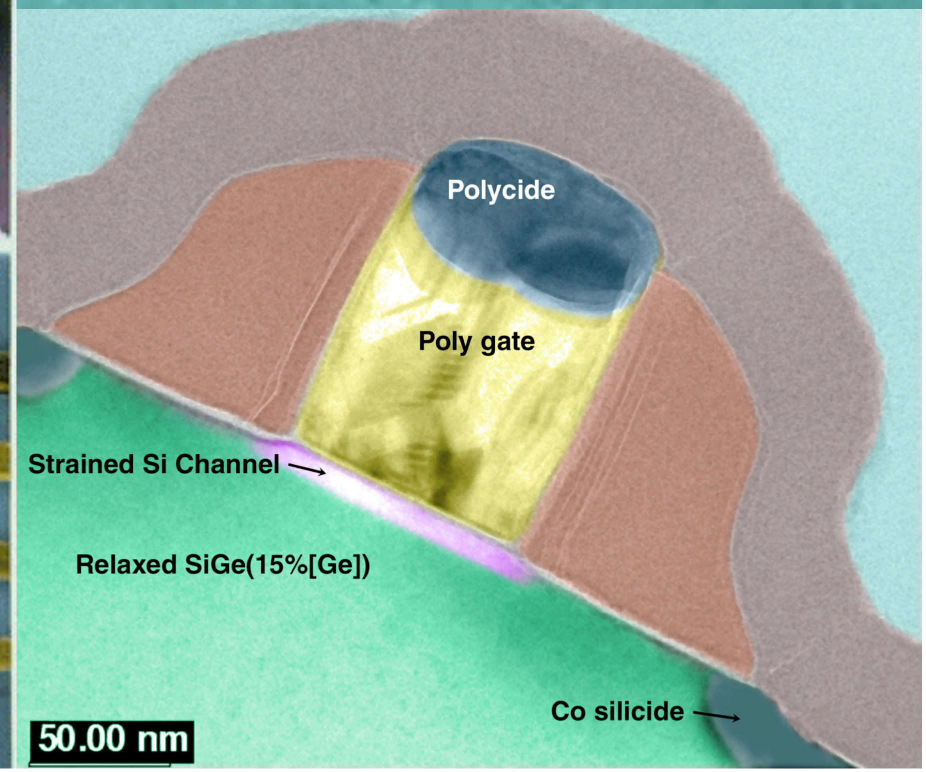
Materials Sciences Division
Lawrence Berkeley National Laboratory


Thickness
(nm)
Ta 5
PdPtMn 25
CoFeB 2
Cu 2
CoFeB 2
NiFe 4
Ta 5
Si
GMR
5 nm


Strained
Silicon
Silicon-germanium



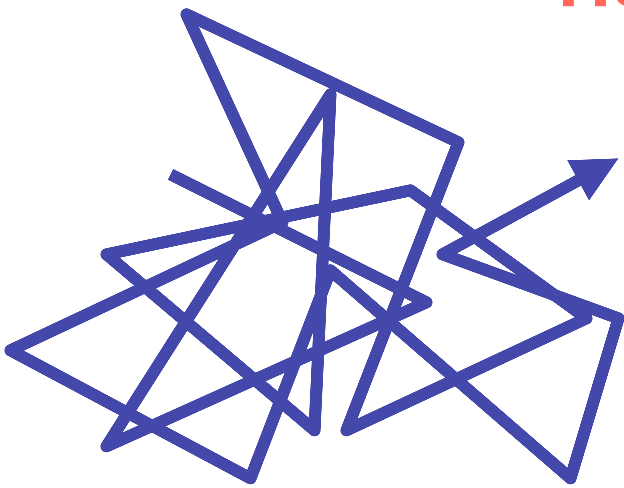



Polycide
Poly gate
Strained Si Channel
Relaxed SiGe(15%[Ge])
Co silicide
50.00 nm

Overview

- Brief history of transport phenomena
- Characteristic length scales of heat transport
- Spectral nature of heat conduction
- Applications
- Summary

Heat Conduction



J. Fourier(1768-1830)

Fourier Law

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

Brownian Motion or Diffusion

Mean Free Path = Λ

Mean Speed of Propagation = v

Kinetic Theory

$k = Cv\Lambda/3$

Specific Heat = C

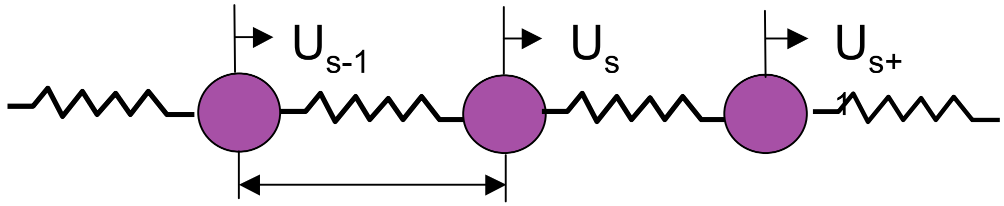
Boltzmann Equation

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = \left(\frac{\partial f}{\partial t} \right)_{col}$$

L. Boltzmann (1844-1906)

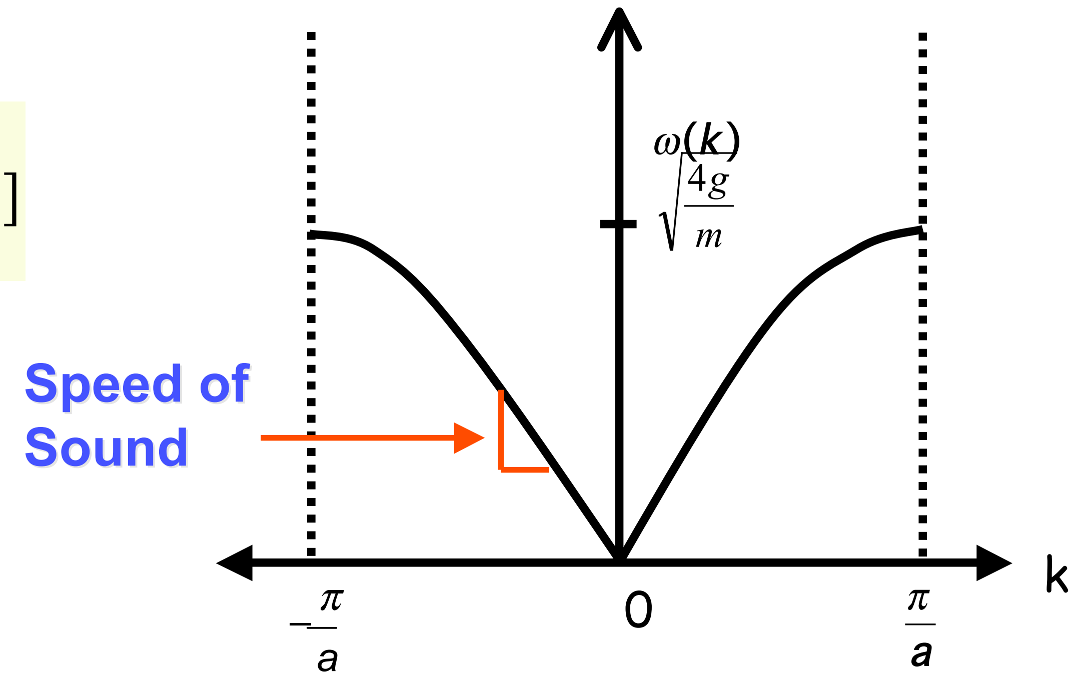
$$k = \frac{1}{3} C v l = \frac{1}{3} \int C(\varepsilon) v(\varepsilon)^2 \tau(\varepsilon) D(\varepsilon) d\varepsilon$$

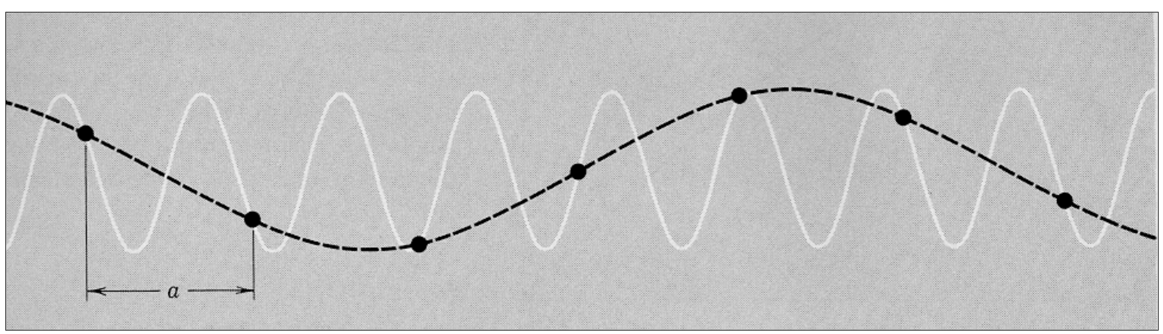
Phonons



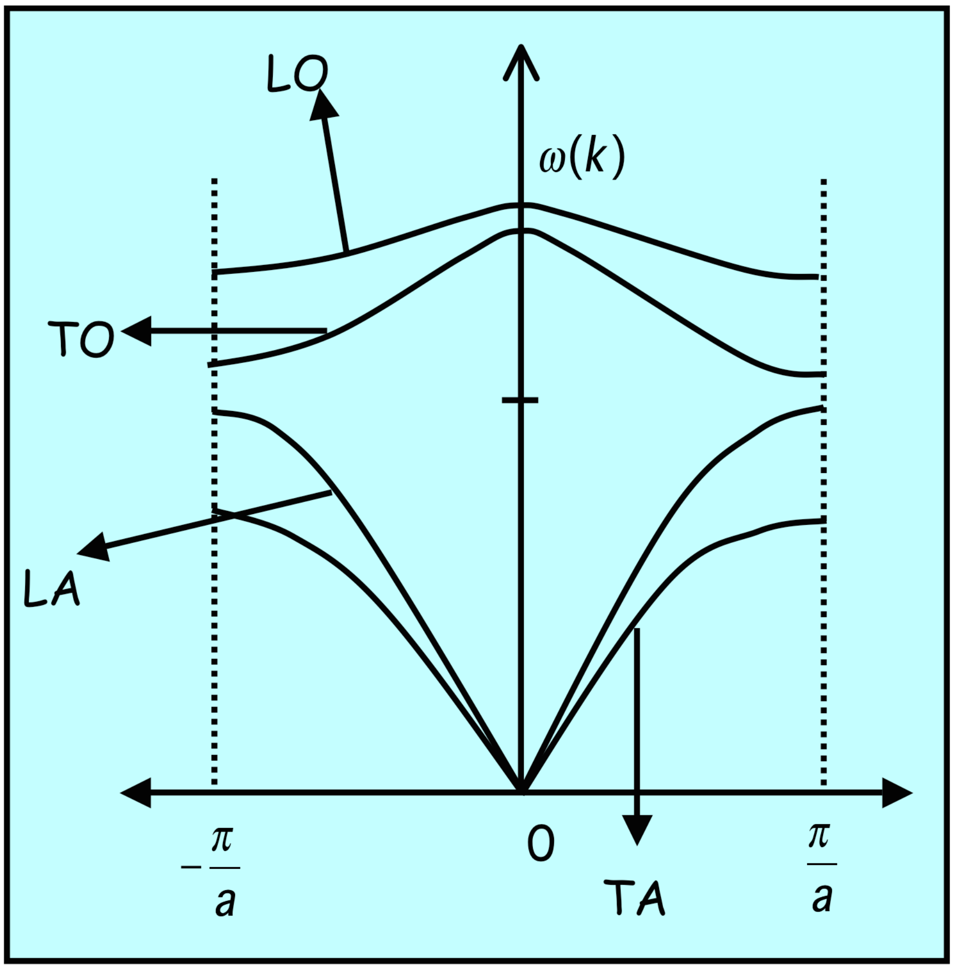
$$\omega(k) = \sqrt{\frac{4g}{m}}[\sin(\frac{ka}{2})]$$

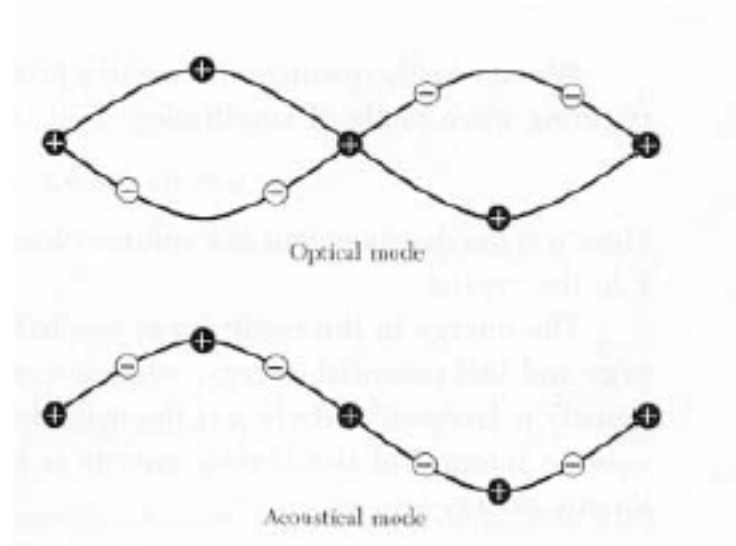
$$\upsilon_g = \frac{d\omega}{dk}$$



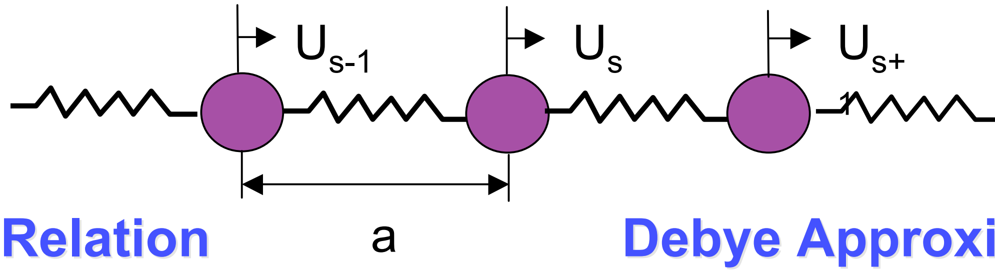


Phonon Dispersion in a General Lattice

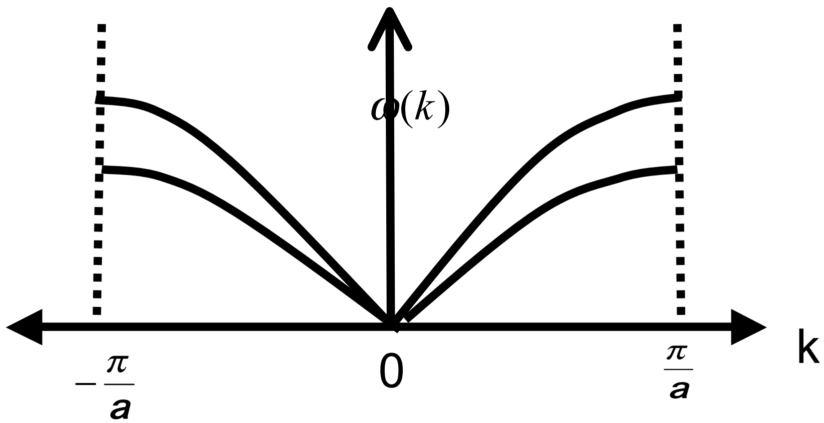


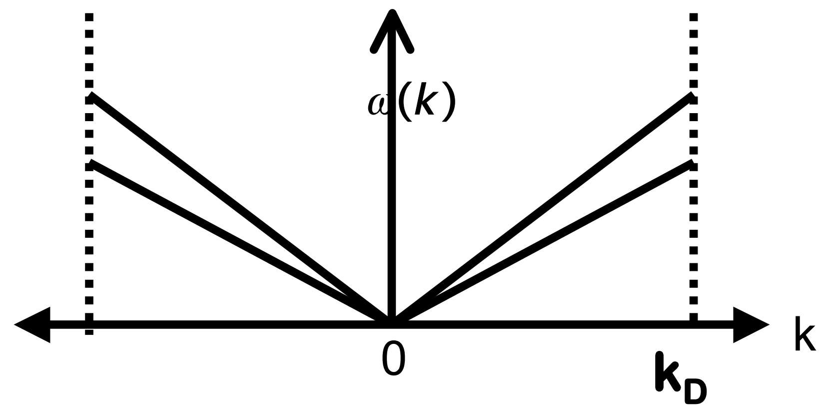


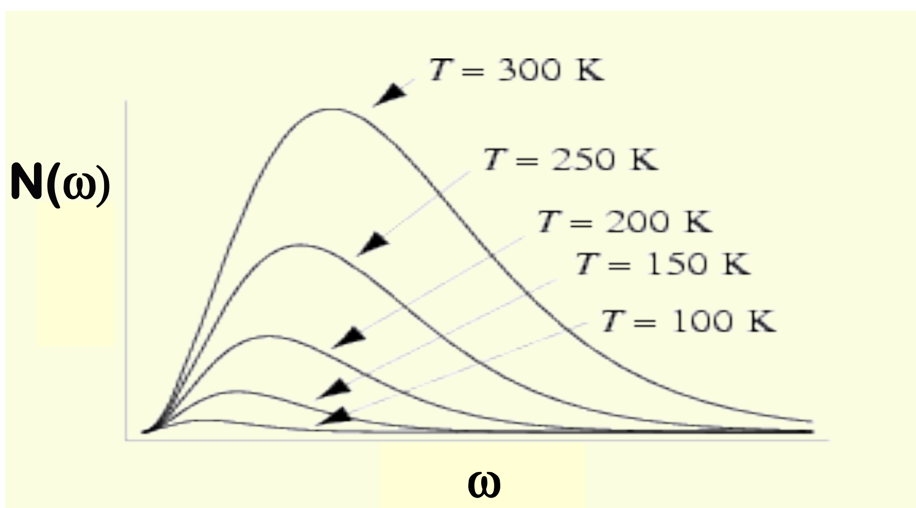
Phonons



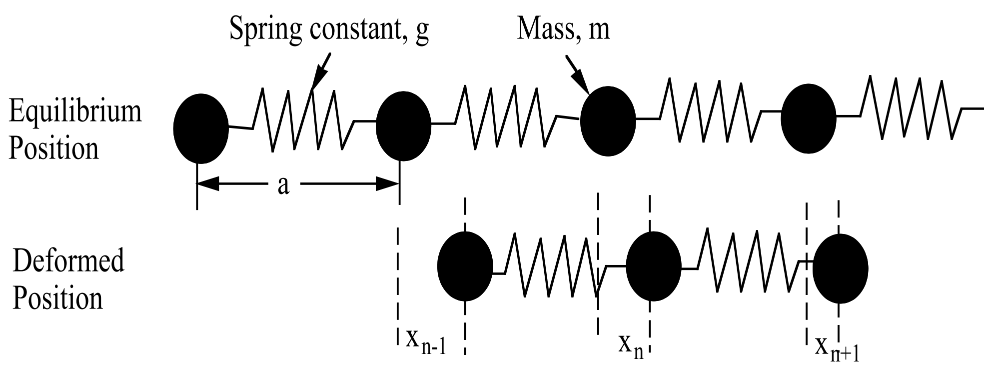
Dispersion Relation **Debye Approximation**

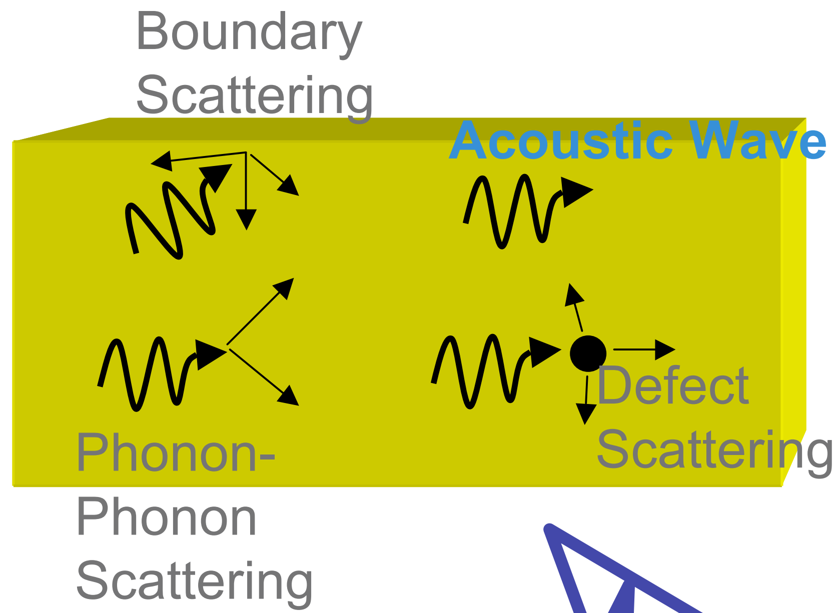


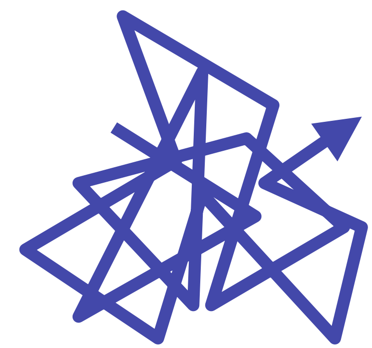




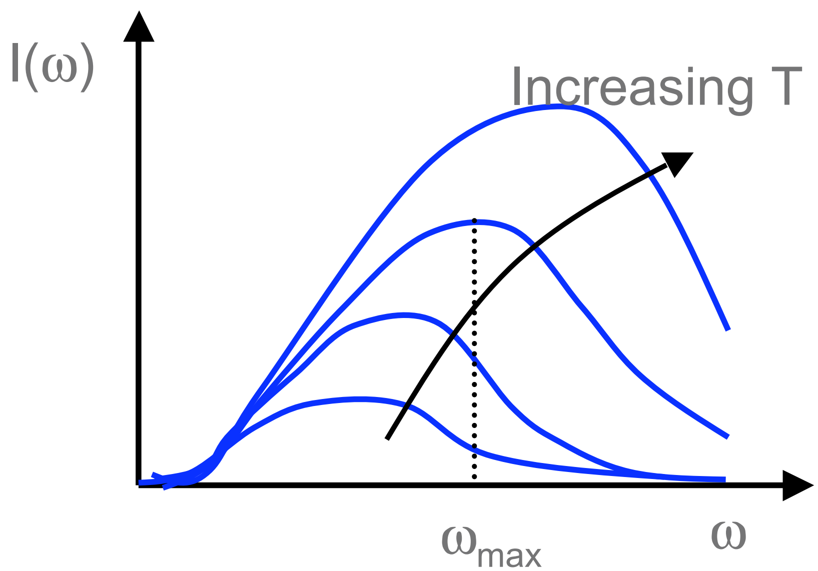
Physics of Heat Conduction in Nonmetals







Blackbody Phonon Radiation

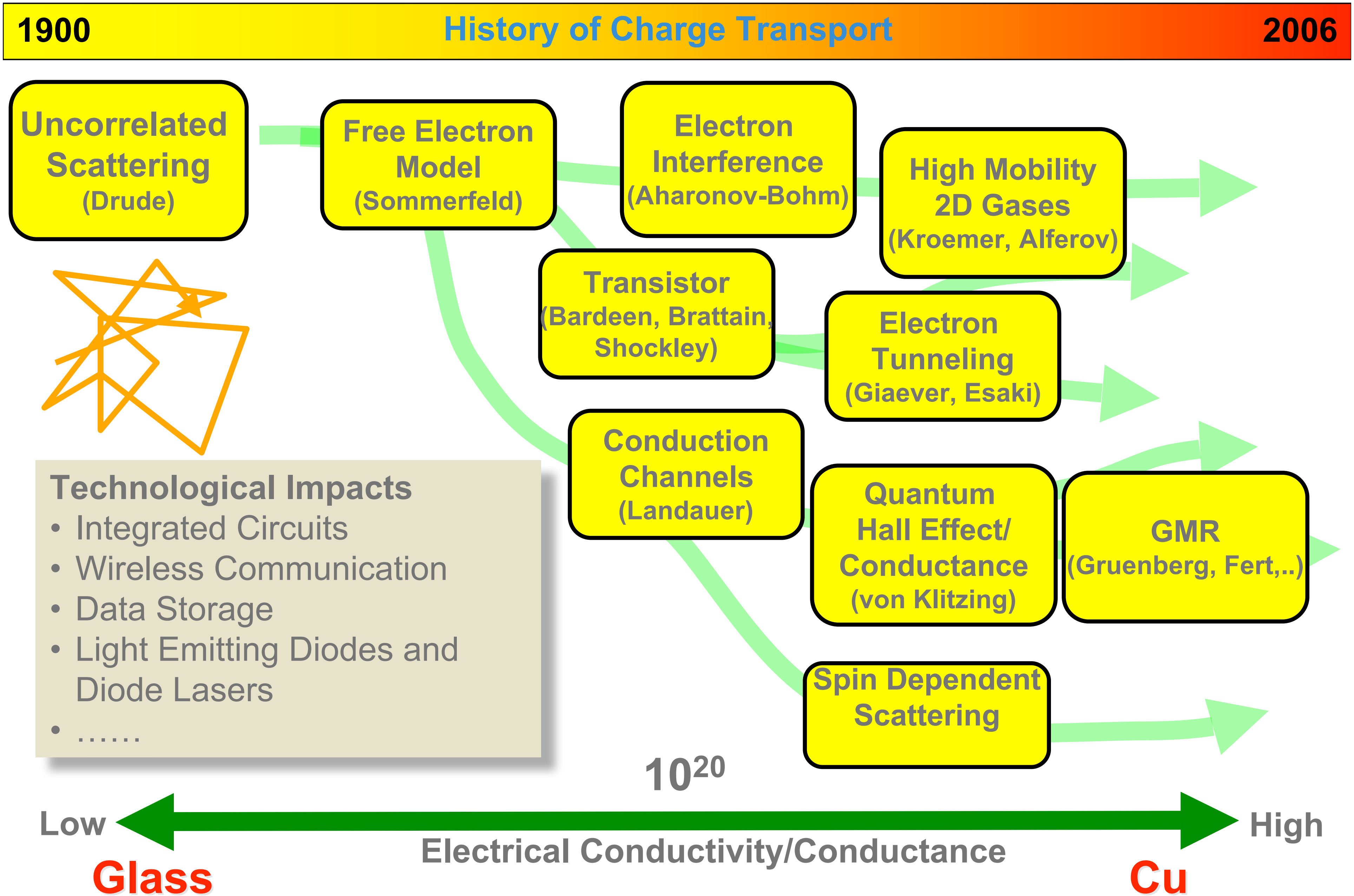


$$\omega_{max} \approx \frac{3k_B}{\hbar} T$$

$$\lambda_{max} T \approx \frac{hc}{3k_B}$$

$$c_{light} = 3\times10^8 \, m/s$$

$$c_{sound} \approx 3-10\times10^3 \, m/s$$



1900
History of Charge Transport
2006
Uncorrelated Scattering (Drude)
Free Electron Model (Sommerfeld)
Electron Interference (Aharonov-Bohm)
High Mobility 2D Gases (Kroemer, Alferov)
Transistor (Bardeen, Brattain, Shockley)
Electron Tunneling (Giaever, Esaki)
Conduction Channels (Landauer)
Quantum Hall Effect/ Conductance (von Klitzing)
GMR (Gruenberg, Fert,..)
Spin Dependent Scattering
Technological Impacts
• Integrated Circuits
• Wireless Communication
• Data Storage
• Light Emitting Diodes and Diode Lasers
• ……
10^20
Low
High
Electrical Conductivity/Conductance
Glass
Cu

Phonon Optics at Low Temperature (1970s--.)
(Narayanamurti, Dynes, et al; Wolfe et al.)

Quantum Phonon Conductance
(Schwab,Roukes, 2000)

Molecular Heterostructures | **Nanowires & Arrays** | **Nanotubes**

Phonon Filtering | Correlated scattering & diffusion | Uncorrelated scattering & diffusion | Waveguiding & ballistic transport

Ultralow — Polymers ↔ Diamond — Ultrahigh

10^4 @300K

Phonon Length Scales (300K)
Wavelength = 1-10 nm
Mean Free Paths = 10-100 nm

Thermal Conductivity
$k = Cvl/3$

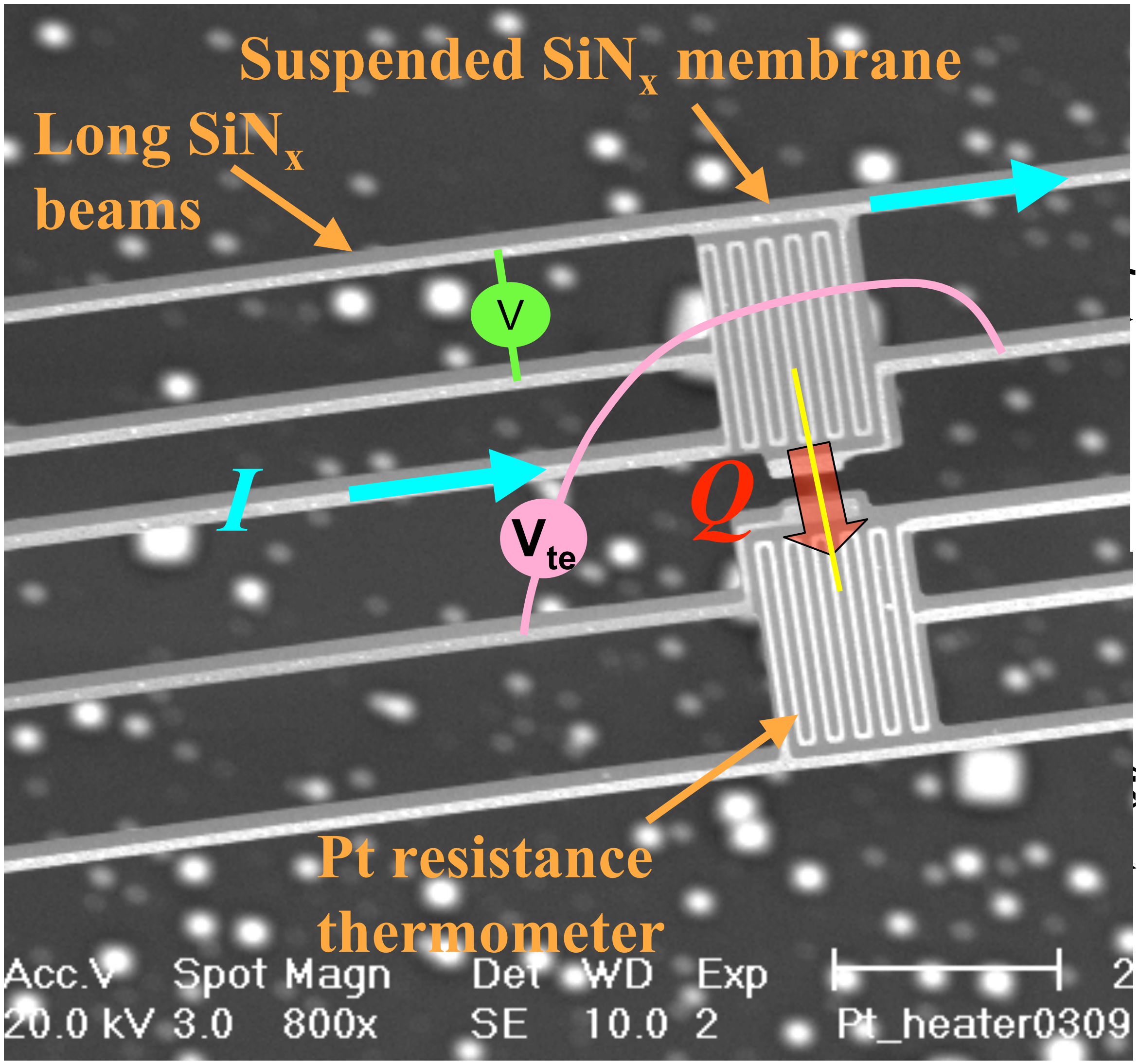
Information Technology

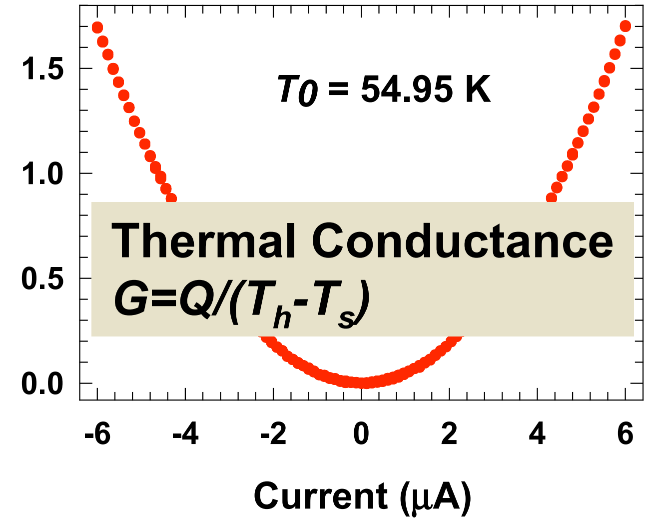
- Microelectronics
- Data Storage (> 1 TBits/in^2)
- Wireless (>100 GHz)

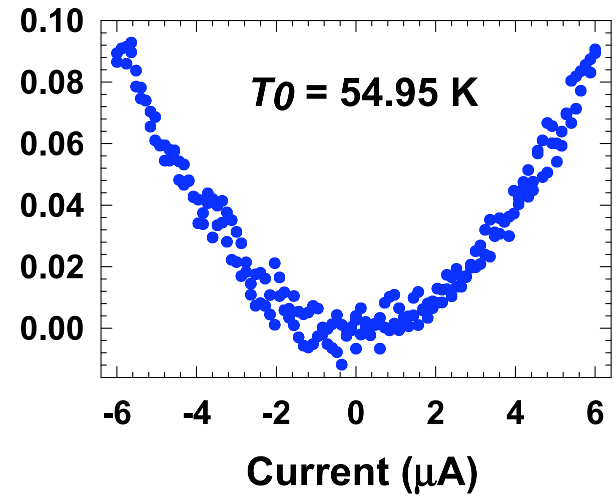
Energy Technology

- Insulation (k < 1 mW/m-K)
- High Cond (k > 5000 W/m-K)
- Thermoelectricity (ZT > 3)

Transport in Individual Nanotubes and Nanowires

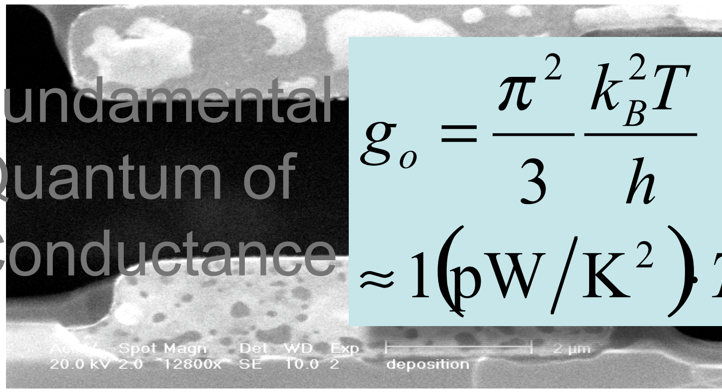






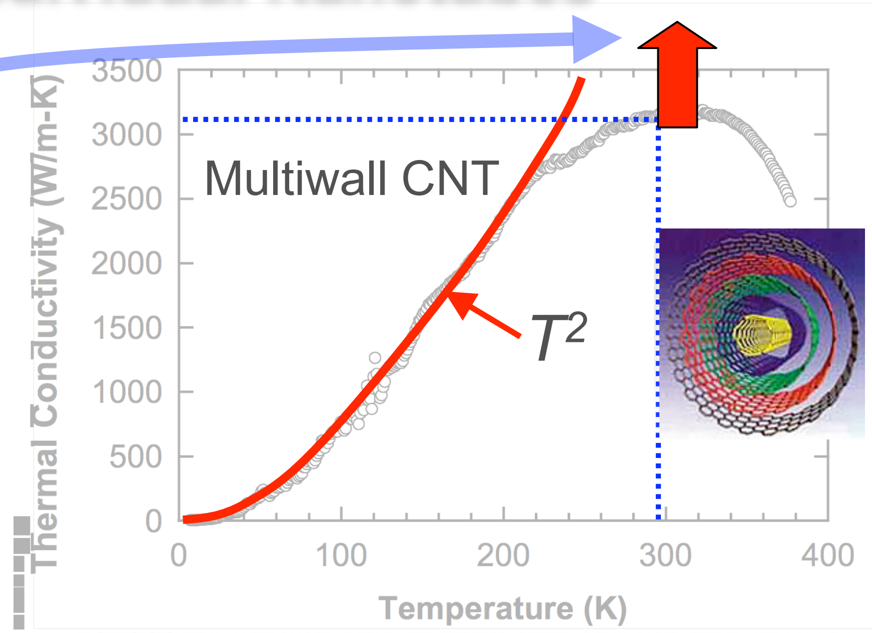
Kim, Shi, Majumdar, McEuen, *PRL* **87**, 215502 (2001); Shi, Li, Yu, Jang, Kim, Yao, Kim, Majumdar, *JHT* **125**, 881 (2003)

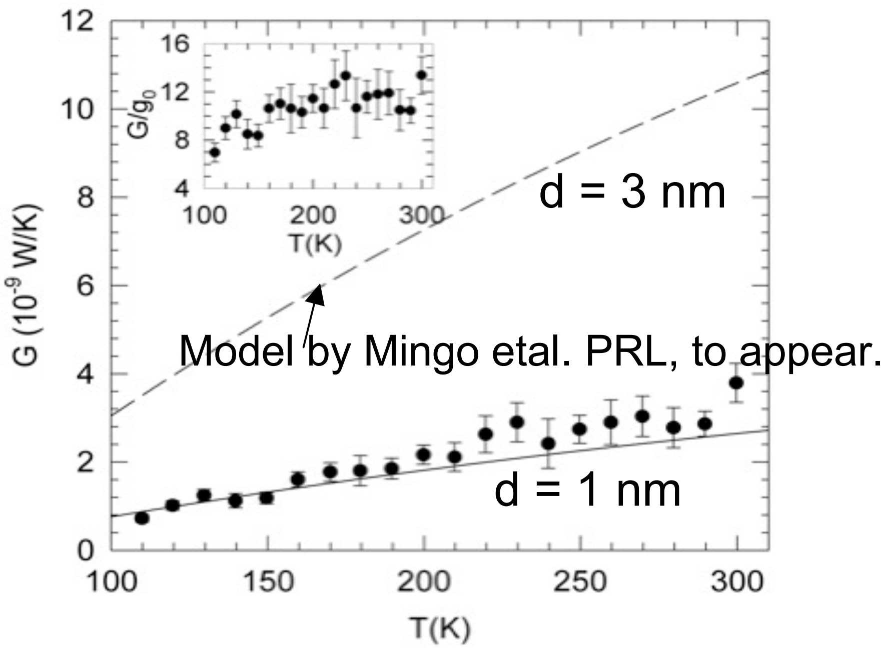
Transport in Individual Nanotubes



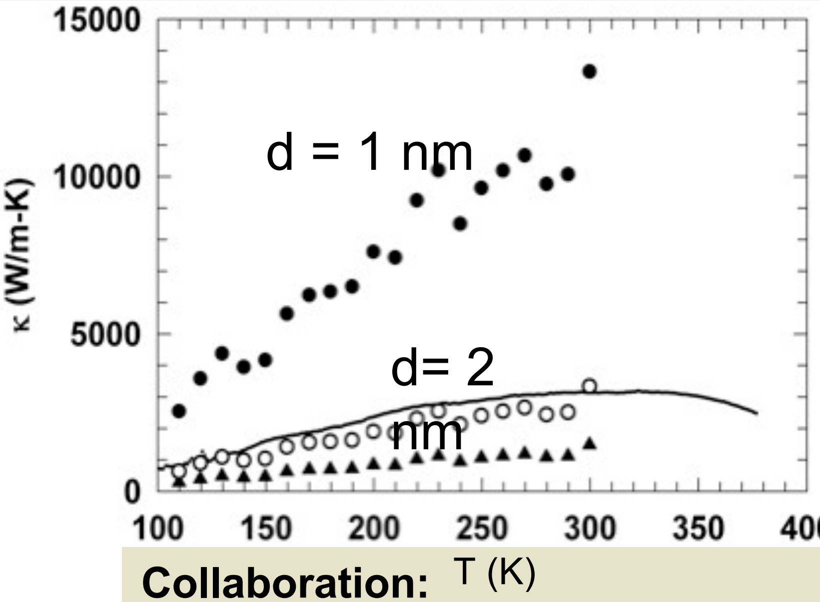
Fundamental Quantum of Conductance

$$g_o = \frac{\pi^2}{3}\frac{k_B^2 T}{h} \approx 1\left(\mathrm{pW/K^2}\right) T$$



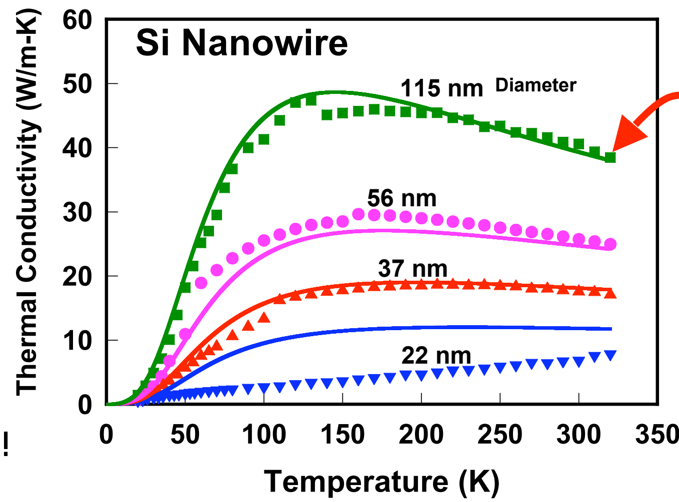


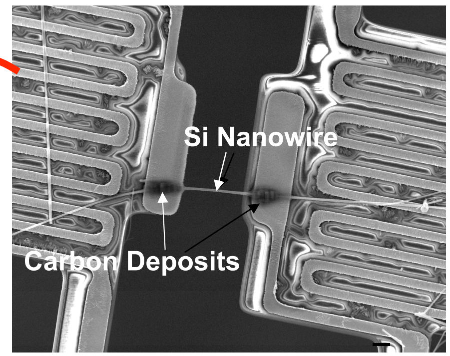
Yu et al., *Nanoletters* (2005)



Collaboration:
Li Shi (UT-Austin); P. McEuen (Cornell)
Philip Kim (Columbia); Alex Zettl (UCB)

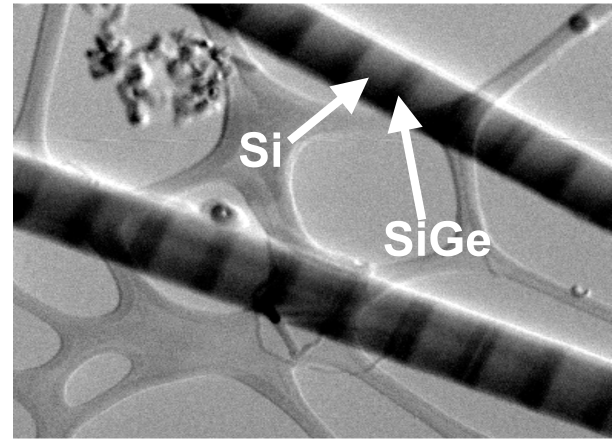
Transport in Nanowires

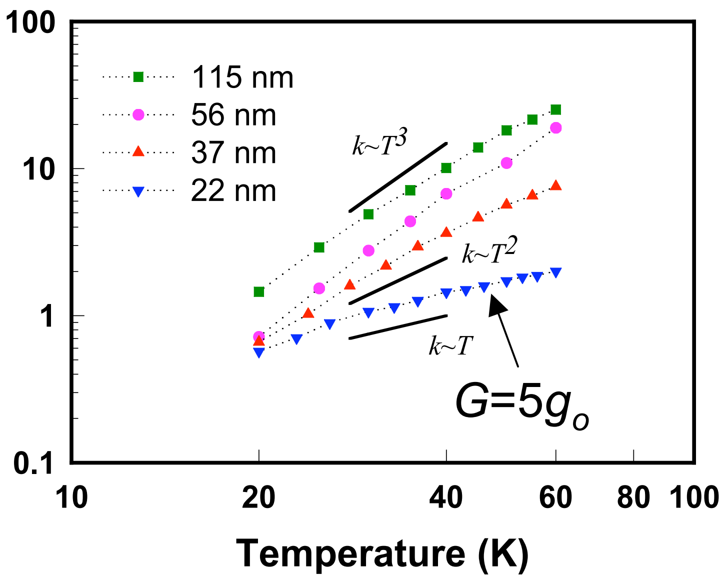




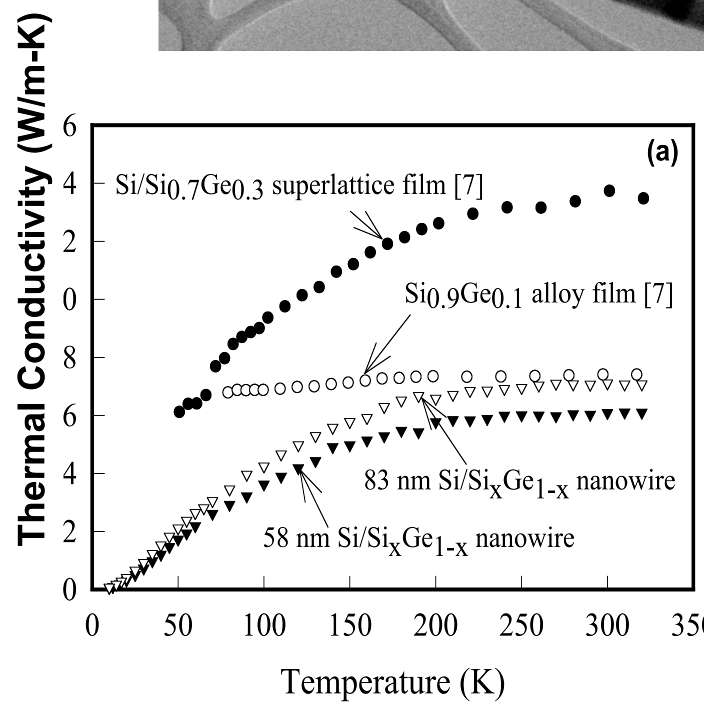
Li, …, Yang, Majumdar, APL (2003a,b)

SiGe Superlattice NW



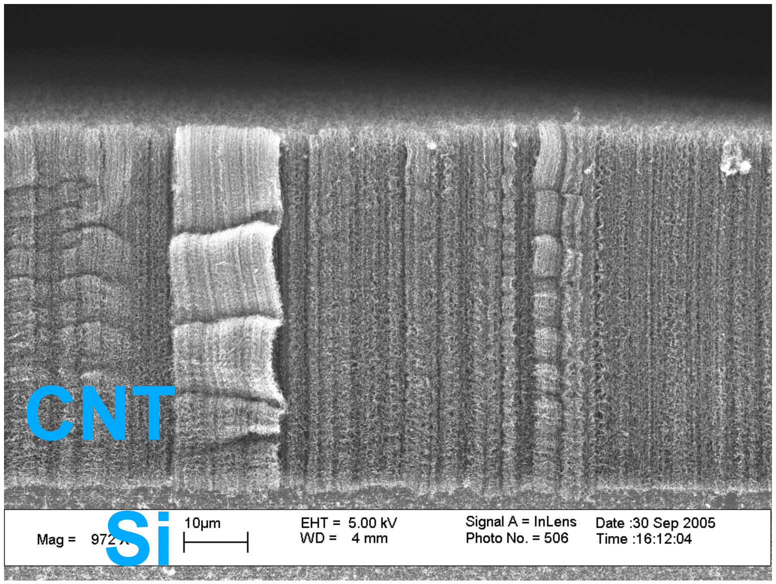


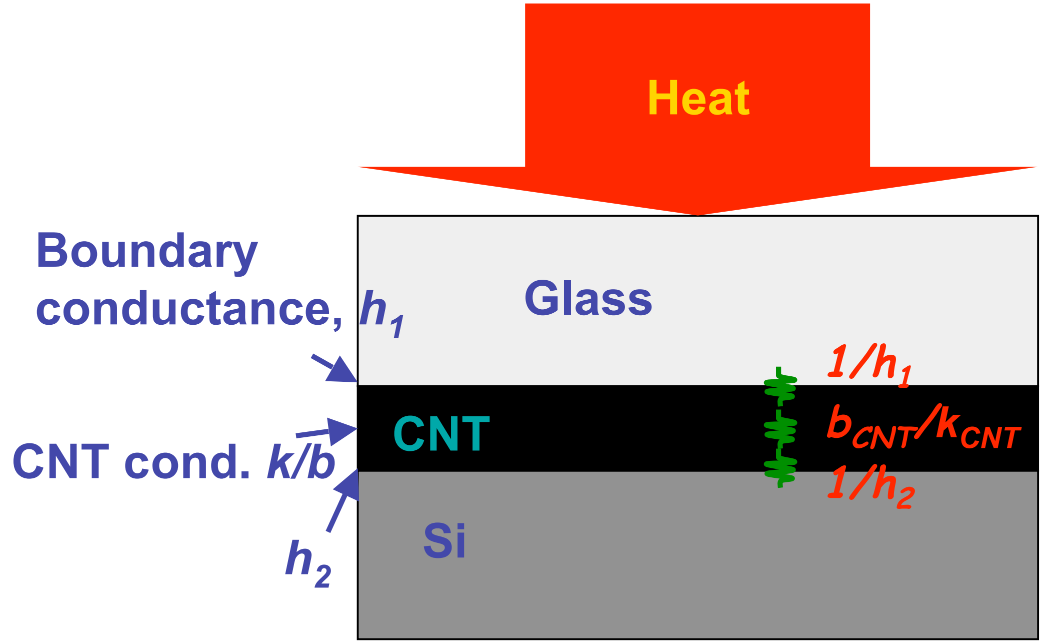
$$g_o = \frac{\pi^2}{3}\frac{k_B^2 T}{h}$$
$$\approx 1\left(\mathrm{pW/K^2}\right)T$$



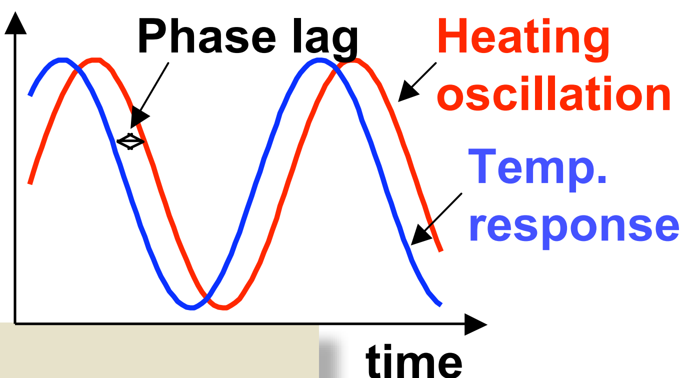
Collaboration:
Deyu Li (ME, Vanderbilt)
Peidong Yang (Chem, UCB); Joel Moore (Phys, UCB)

CNT as Thermal Interface Materials





- Harmonically modulated CW laser heating
- Phase detection to determine thermal properties



CVD MWNT

- Catalyst:10nm Al / 10nm Fe
- 750 °C, ethylene
- Si or Mo substrate

Tube Φ 20~30 nm
Height 5 ~ >100 µm
Density 10^{10}~10^{11} cm^{-2}

Collaboration:
Lance Delzeit, M. Meyyappan (NASA-Ames); Yang Zhao, Ali Kashani (Atlas Sci.)

Two Types of Interface Resistance

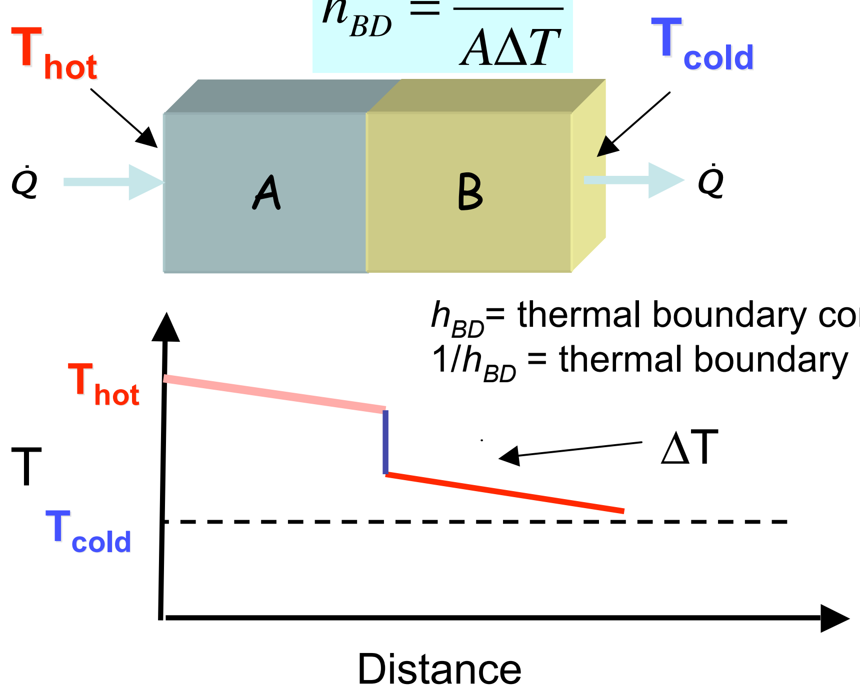
Thermal Boundary Resistance

- Due to difference in the acoustic properties: Phonon reflection at the interface
- Electron-phonon interaction
- Present even in the case of perfect contact with no roughness
- Microscopic quantity

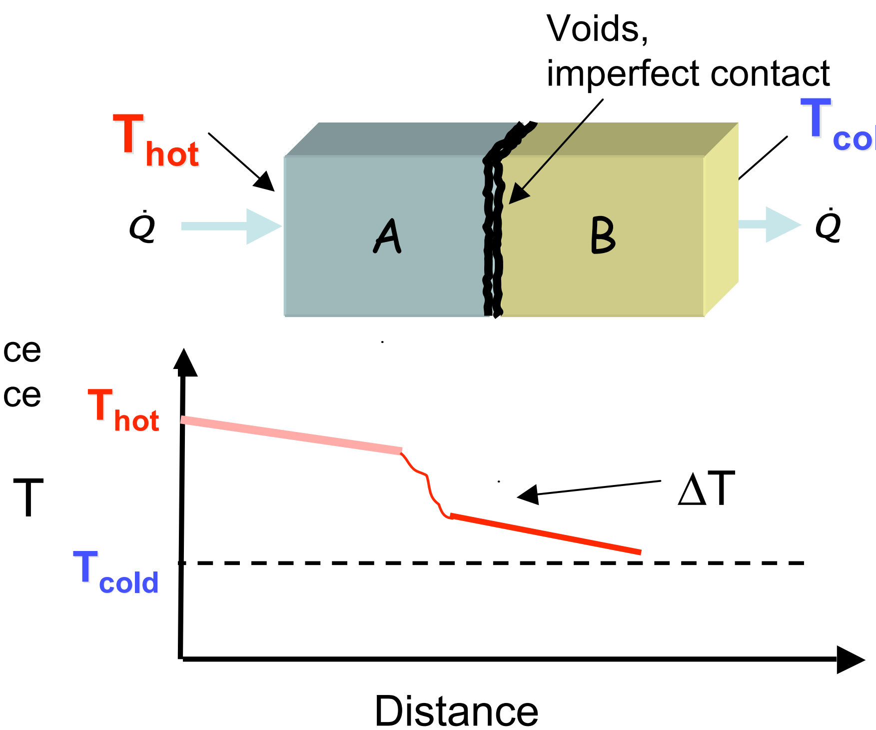
Thermal Constriction Resistance

- Important for bulk surfaces
- Macroscopic quantity

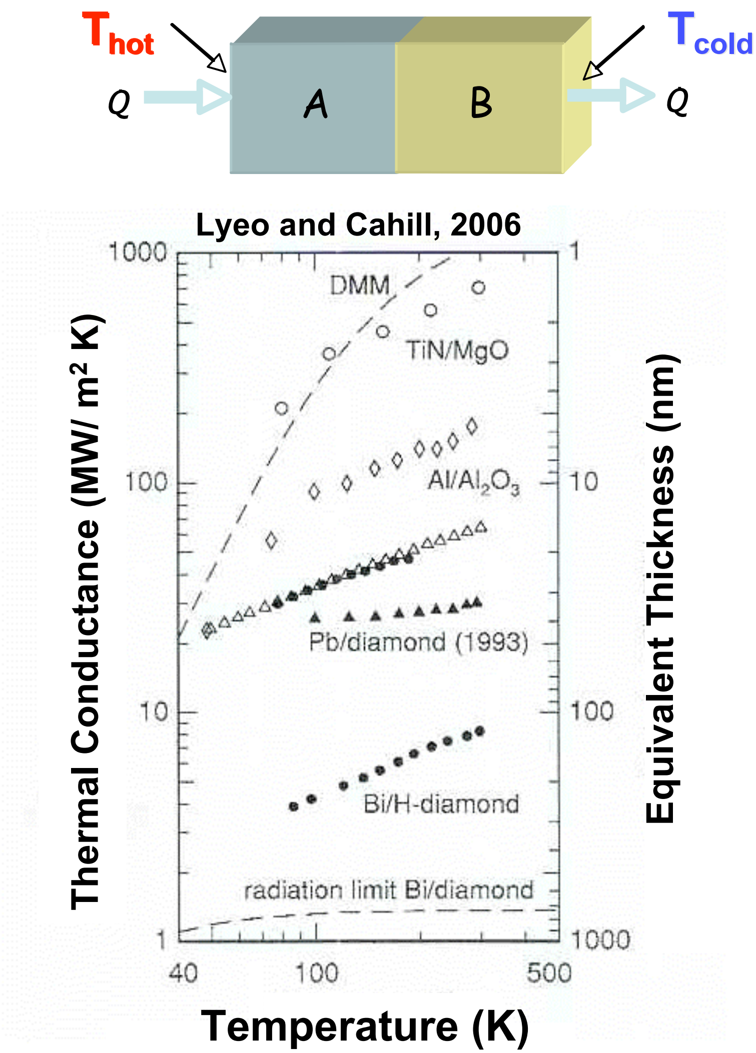
$$h_{BD} = \frac{\dot{Q}}{A\Delta T}$$

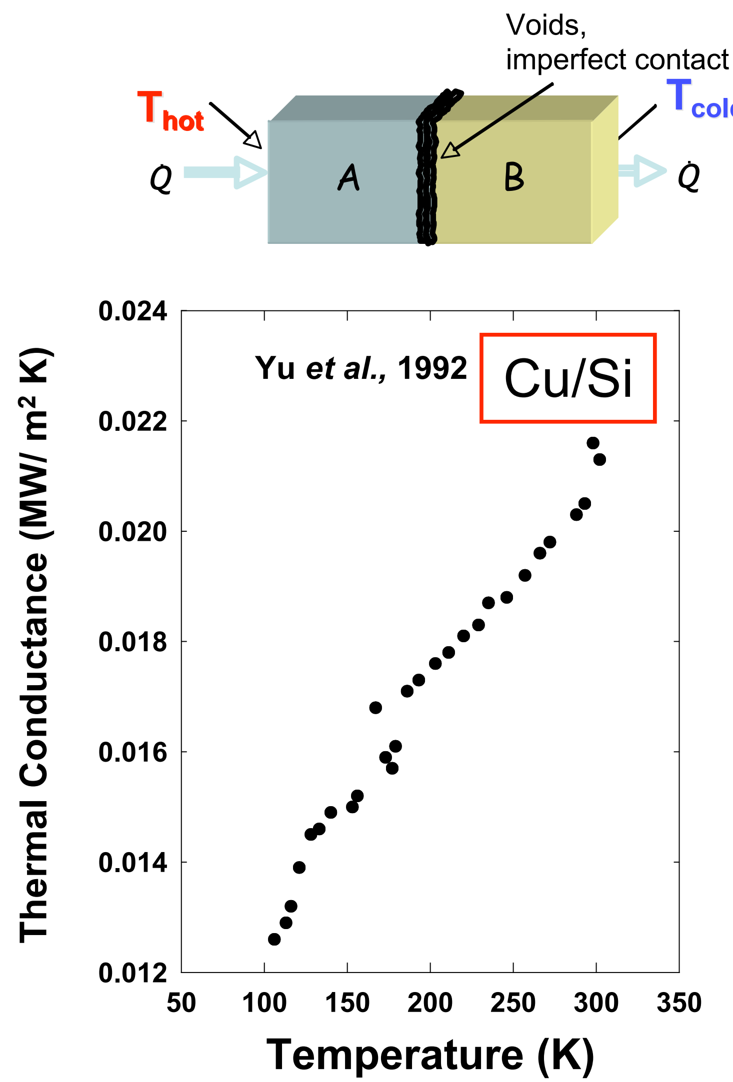


h_{BD}= thermal boundary conductance
$1/h_{BD}$ = thermal boundary resistance

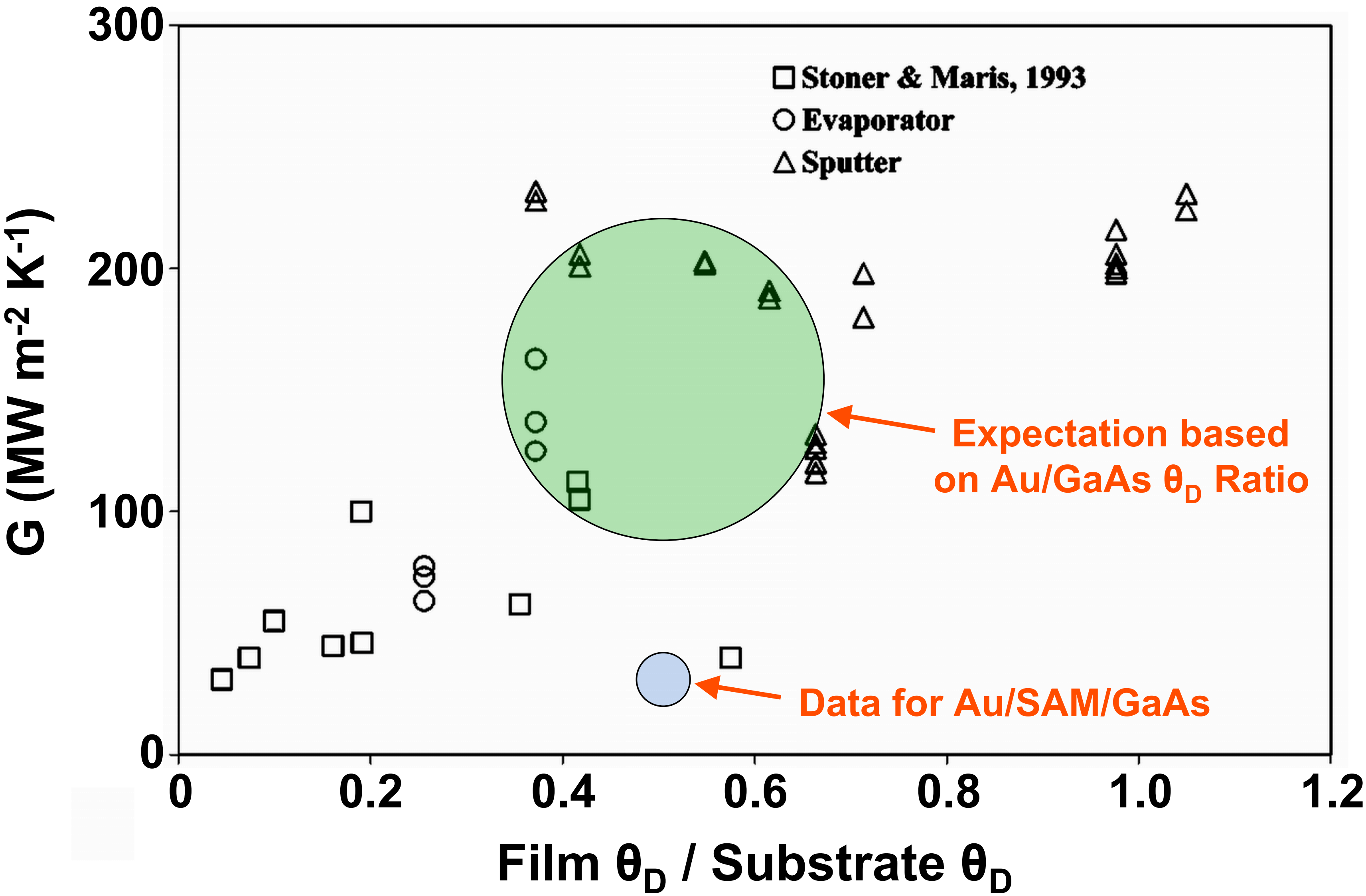


Both Constriction Resistance and Thermal Boundary Resistance Are Important



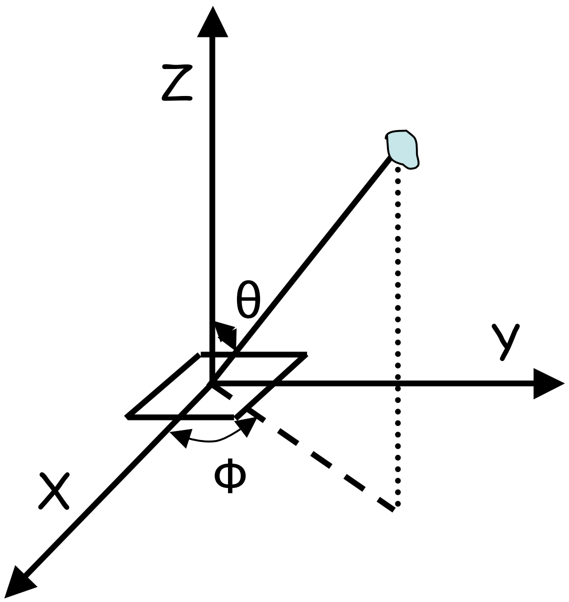


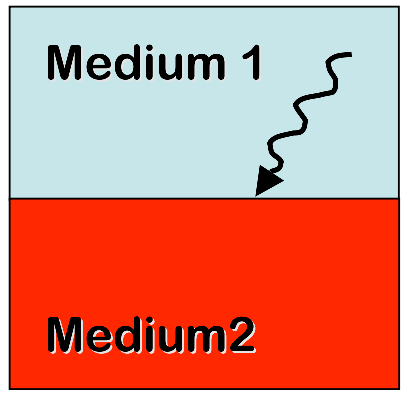
Conductance vs. Debye Temperature Ratio



Stevens et al., Journal of Heat Transfer, **127**, 315 (2005)

Gross Phonon Heat Flux at Interfaces





Thermal Boundary Conductance

$$h_{BD} = \frac{q_{1\to 2}(T_1) - q_{2\to 1}(T_2)}{(T_1 - T_2)}$$

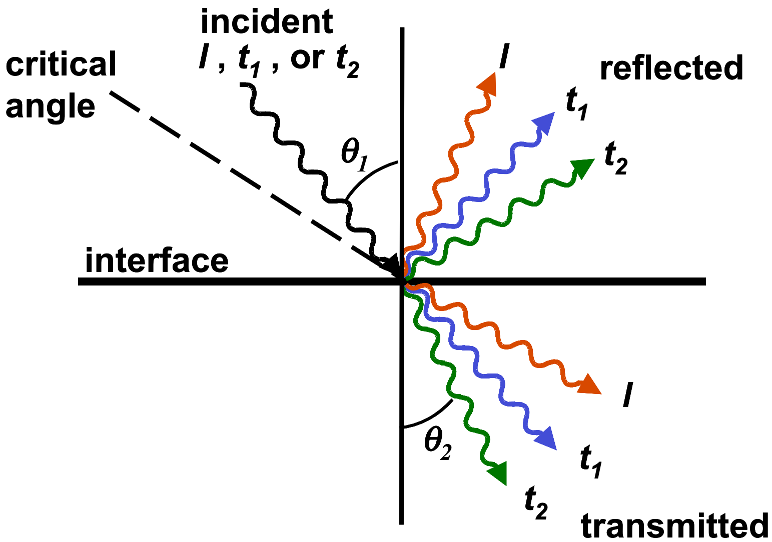
$$q_{1\to 2} = \sum_j \int_0^{2\pi} \int_0^{\frac{\pi}{2}} \int_0^{\omega_{max}} \underbrace{\alpha_{1\to 2}(\theta, j, \omega)}_{\text{Transmission Probability}} \underbrace{N_{1,j}(\omega, T)\hbar\omega}_{\text{Energy Distribution}} \underbrace{\frac{1}{4\pi} \upsilon_{g,1,j}(\omega) \cos\theta \sin\theta d\theta d\phi d\omega}_{\text{Geometric Considerations}}$$

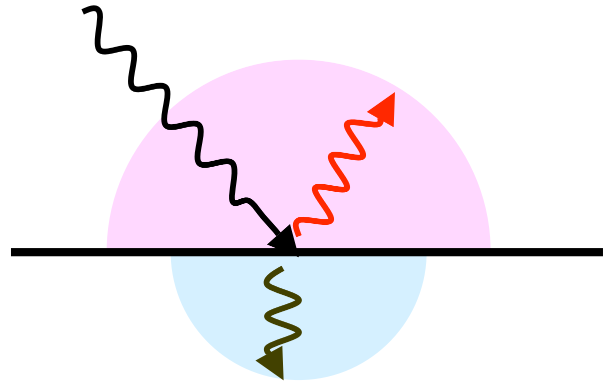
Transmission Probability

Energy Distribution

Geometric Considerations

Transmission Probabilities





Acoustic Mismatch Model (AMM)

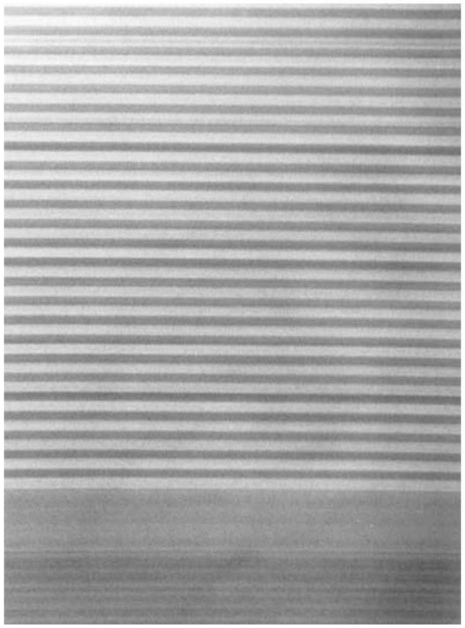
$$\alpha_{1\to2} = \frac{4Z_1Z_2}{(Z_1+Z_2)^2}$$

$$Z_i = \rho_i c_i$$

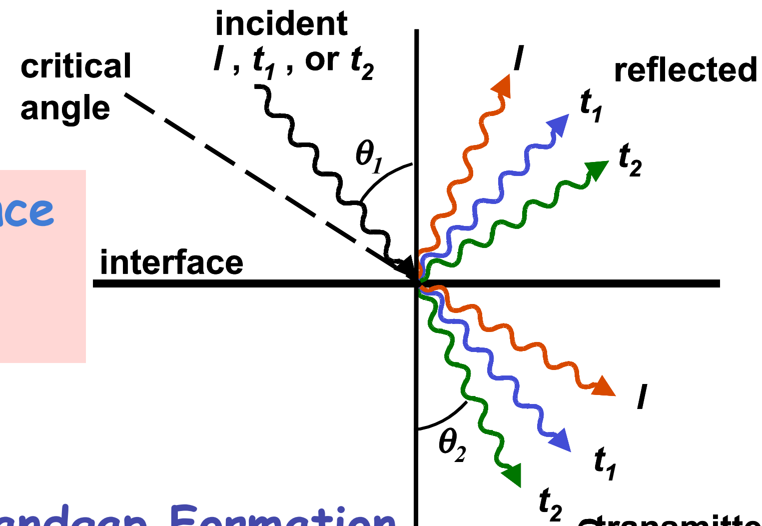
Diffuse Mismatch Model (DMM)

$$\alpha_{1\to2}(\omega) = \frac{[\sum_j N_{2,j}(\omega)c_{2,j}(\omega)]}{[\sum_{i,j} N_{i,j}(\omega)c_{i,j}(\omega)]}$$

TEM



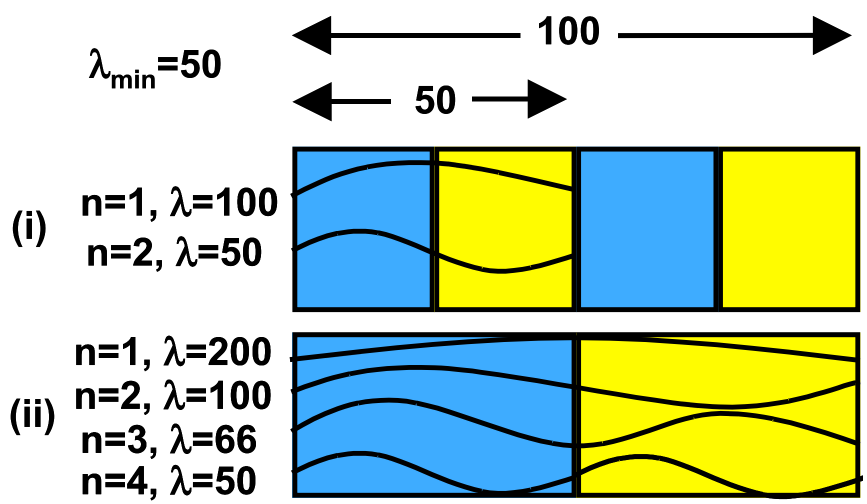
Phonon Reflection/Transmission



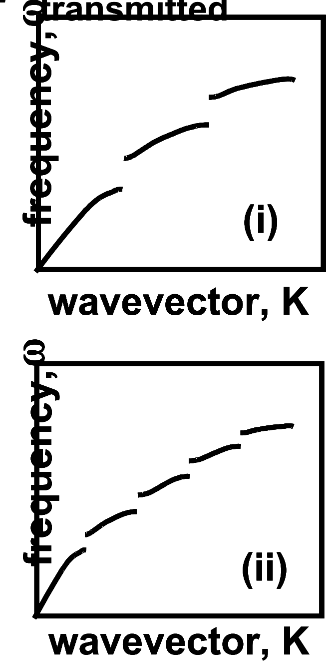
Acoustic Impedance Mismatch (AIM)
= $(\rho v)_1/(\rho v)_2$

Phonon Bandgap Formation

$$n\lambda = 2d \sin\theta$$



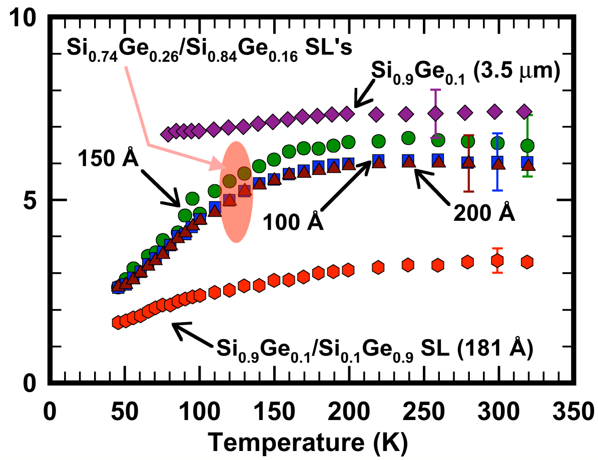
(A)



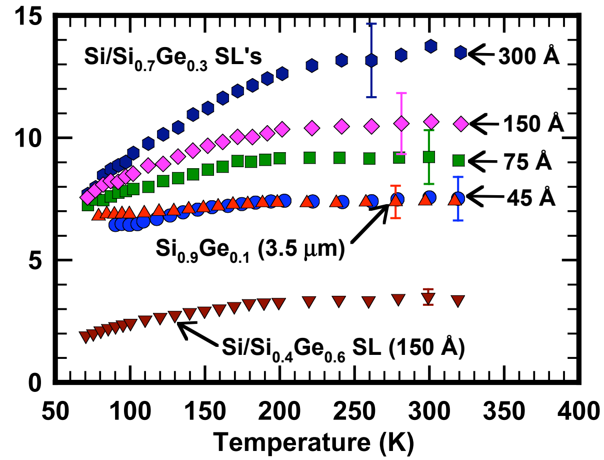
(B)

Si-Ge Superlattices

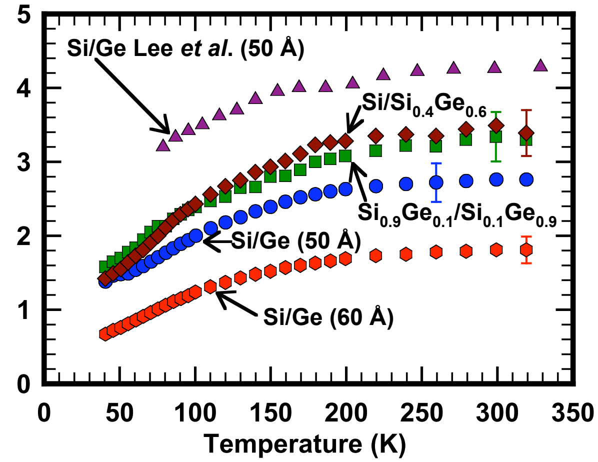
$Si_xGe_{1-x}/Si_yGe_{1-y}$: $|x-y| \leq 0.1$

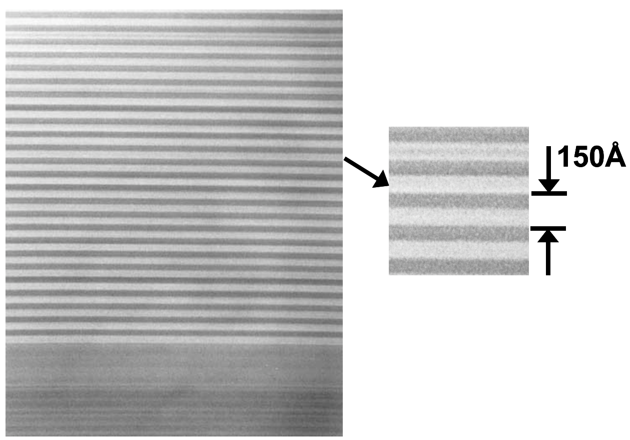


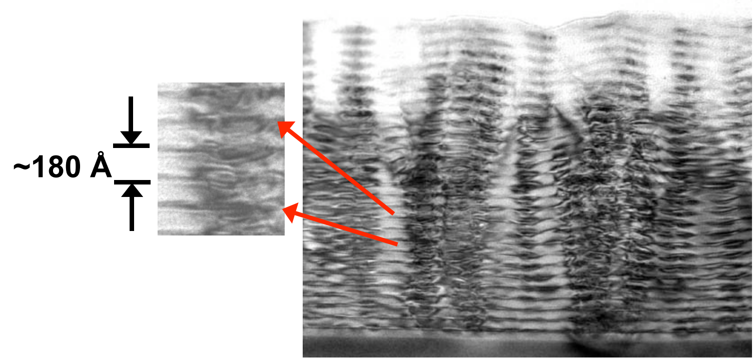
$Si_xGe_{1-x}/Si_yGe_{1-y}$: $|x-y| = 0.3$



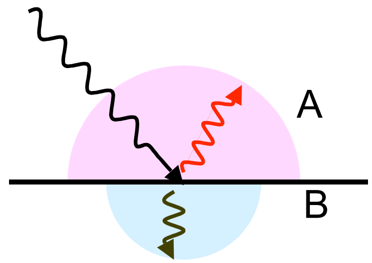
$Si_xGe_{1-x}/Si_yGe_{1-y}$: $|x-y| \geq 0.6$



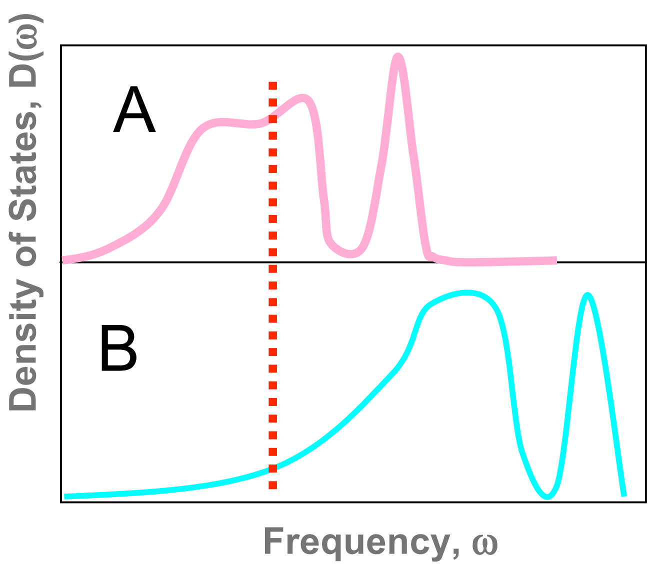




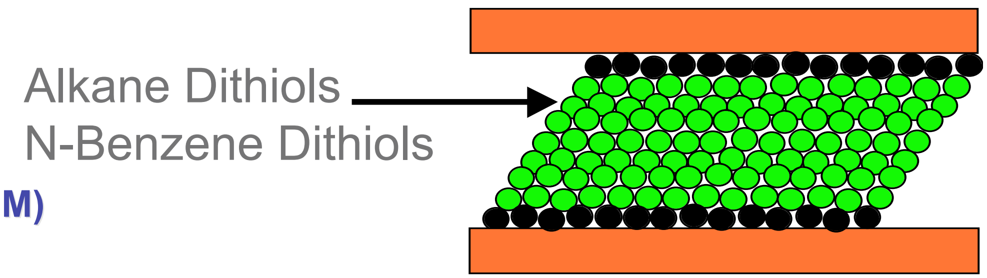
Molecular Heterostructures

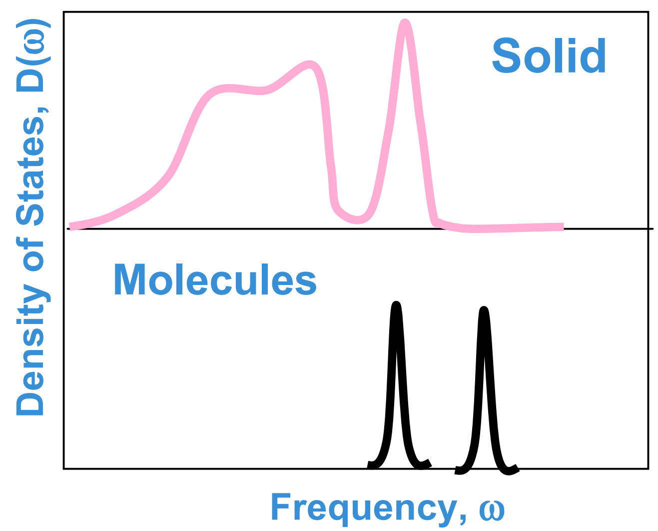


Diffuse Mismatch Model (DMM)
Swartz and Pohl (1989)



Molecular Heterostructures



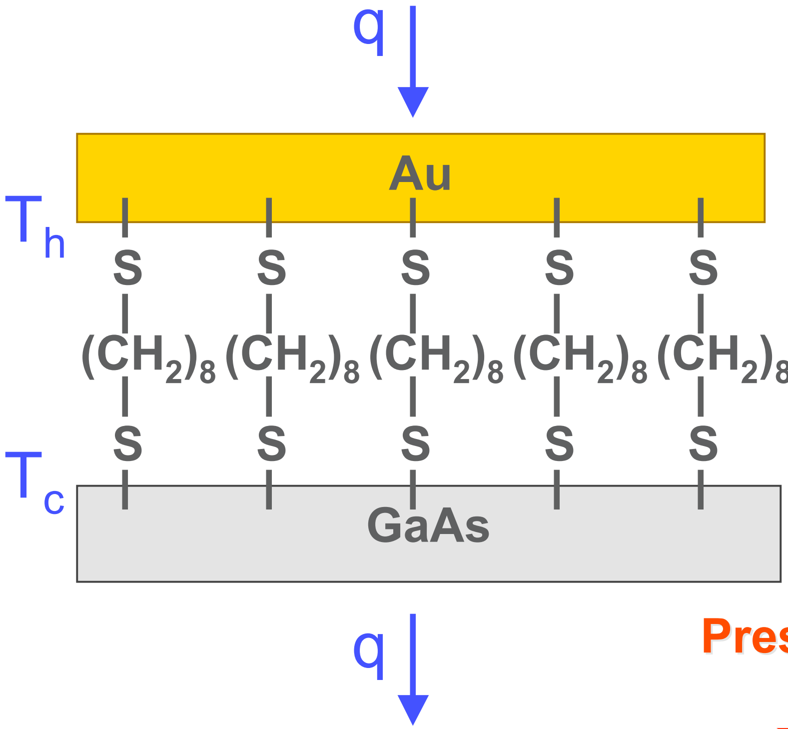


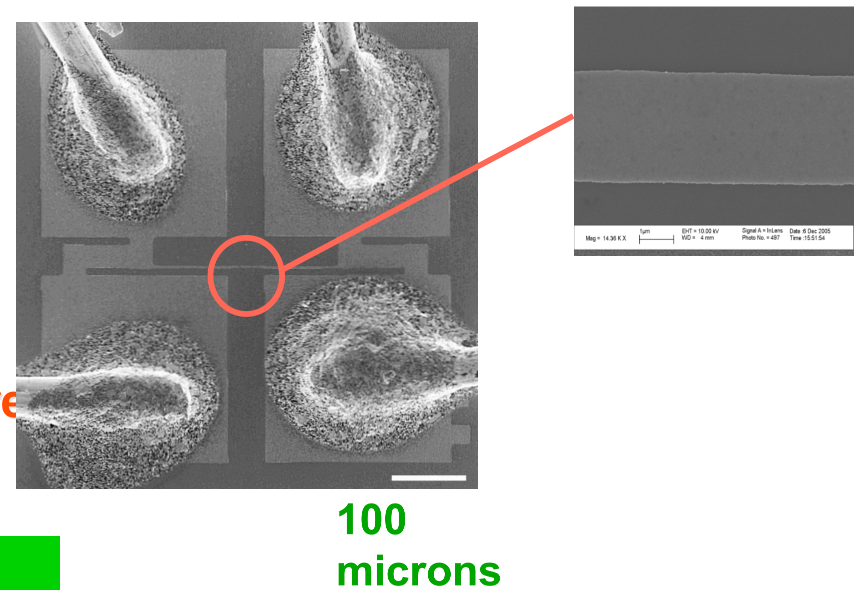
Collaboration:
Rachel Segalman (ChemE, UCB) - Synthesis
Pawel Keblinski (Matl Sci-RPI) - Theory
Jack Lloyd (ME, MSU) - Theory

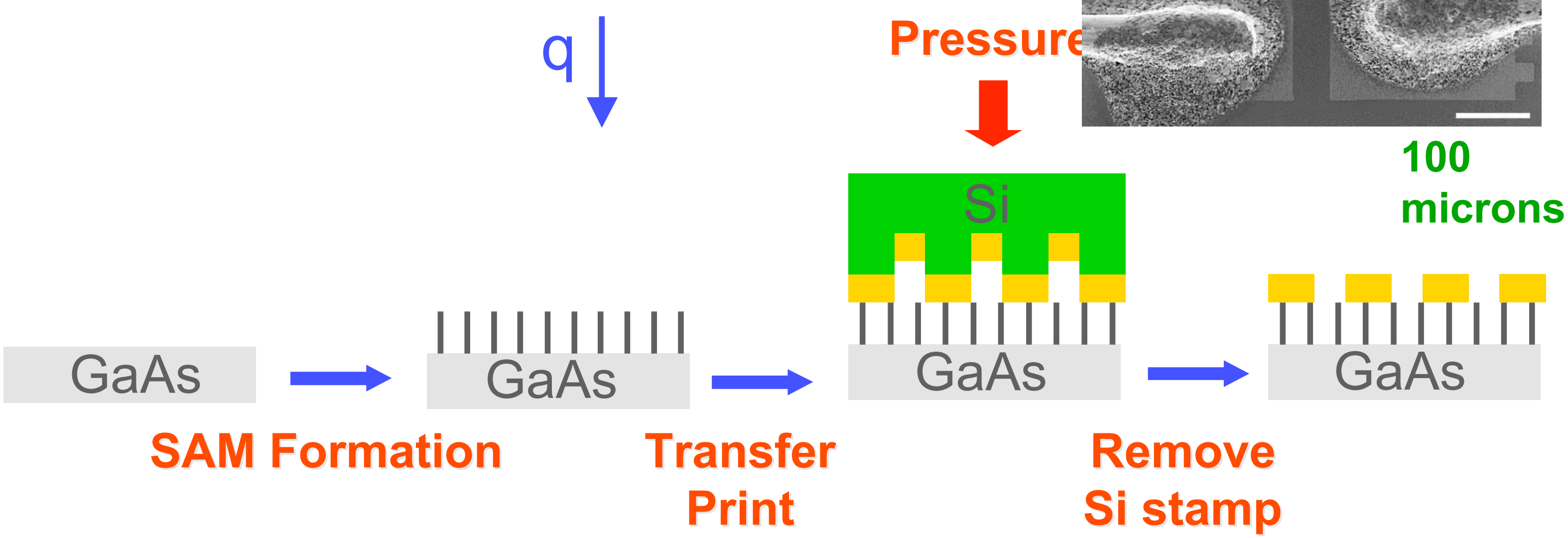
Molecular Interfaces

Robert Wang

$$G = \frac{q}{\Delta T}$$

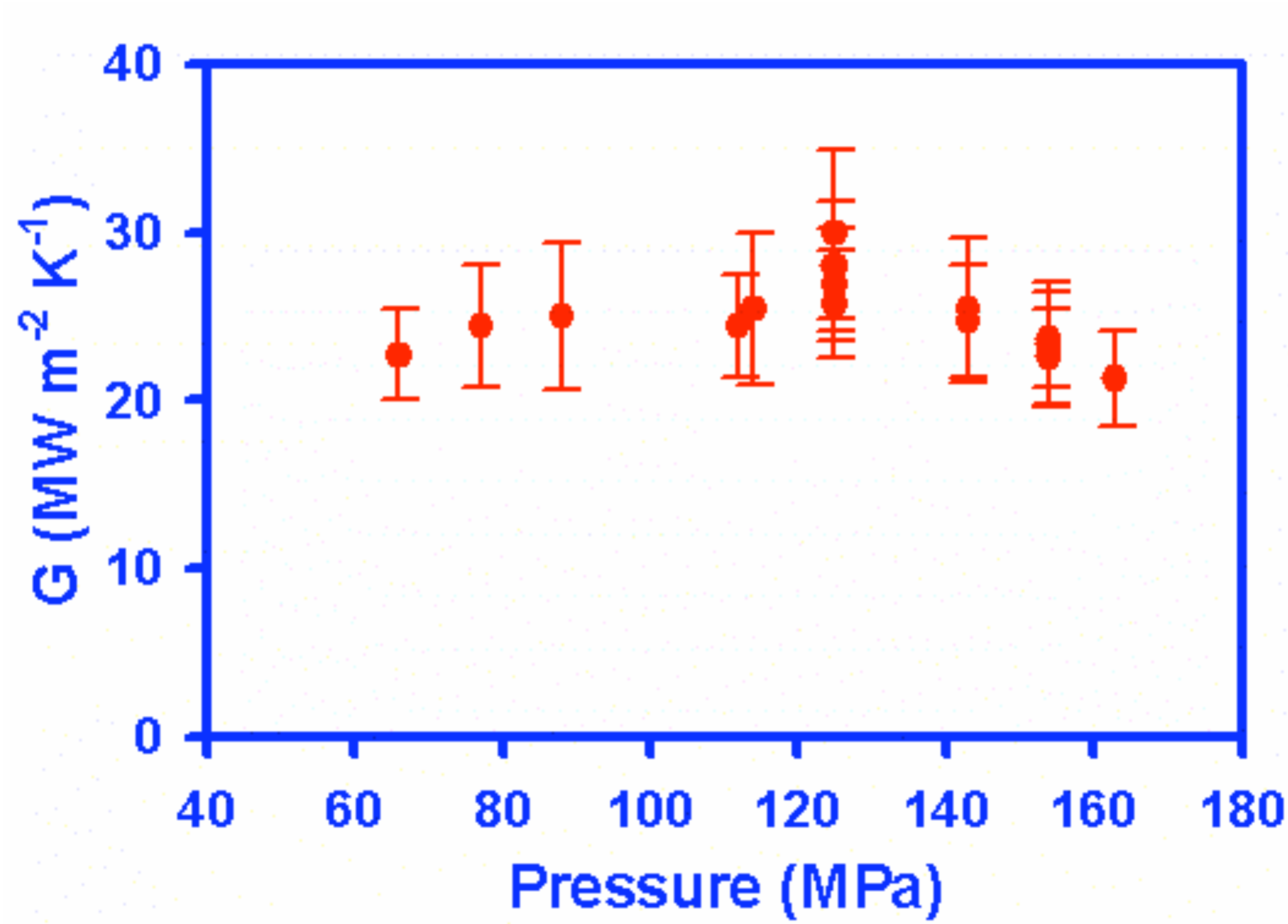






Loo et al., *J.Vac. Sci. Technol. B* **20**, 2853 (2002)

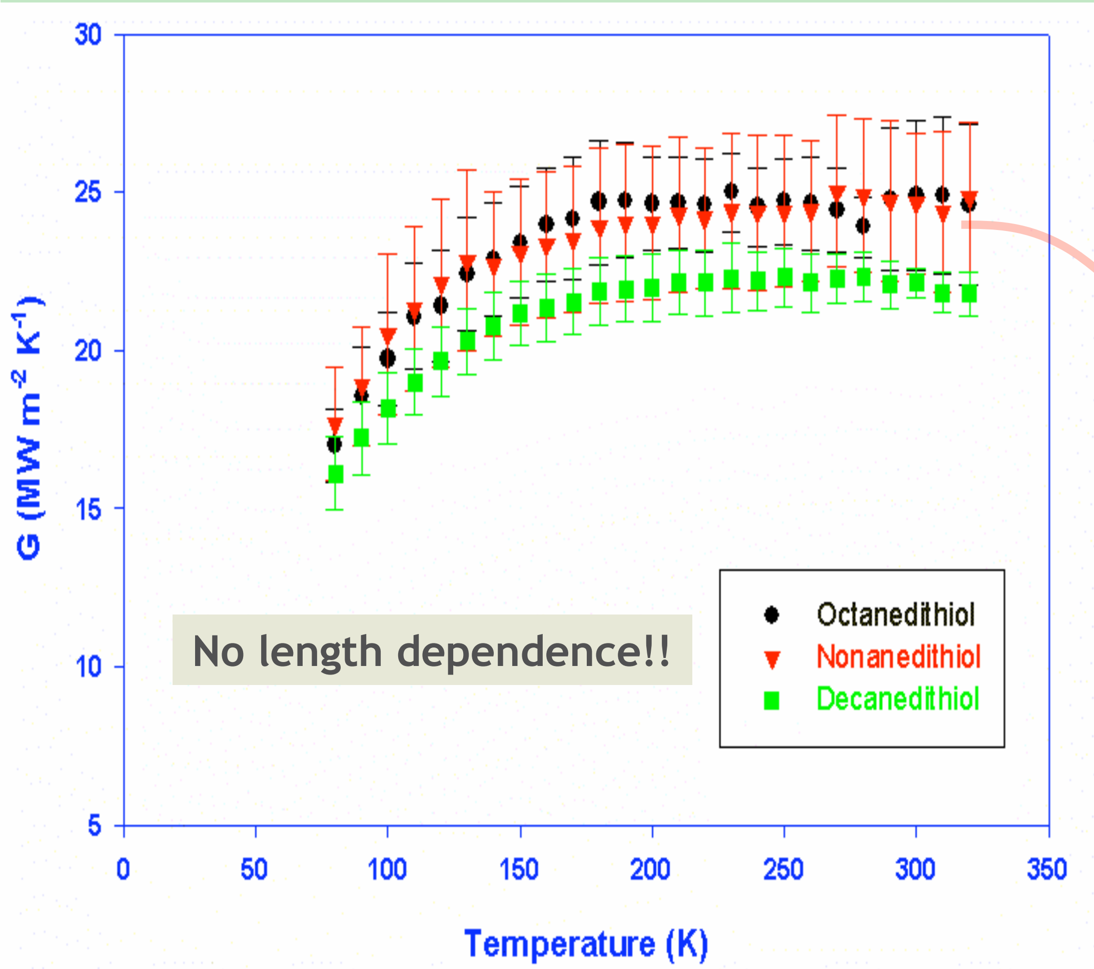
Effect of Fabrication Pressure

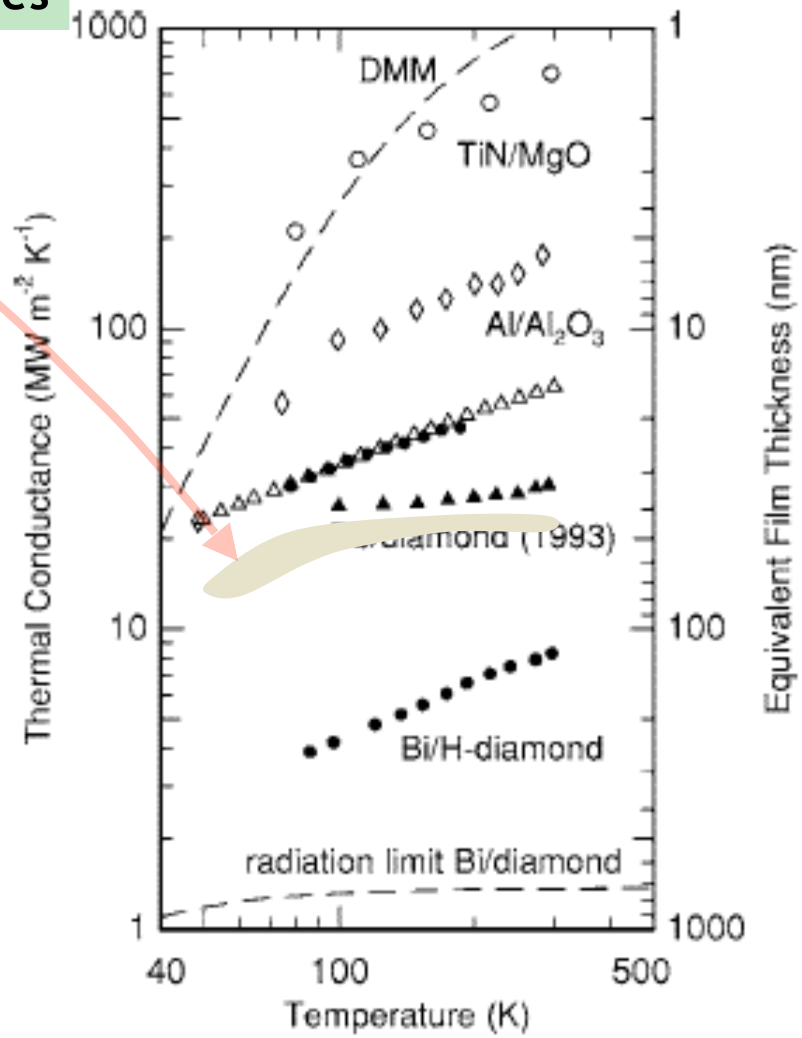


Wang, Segalman, Majumdar, *Appl. Phys. Lett.* (2006)

Thermal Conductance of Molecular Interfaces

Next: Thermal conductance of aromatic molecules

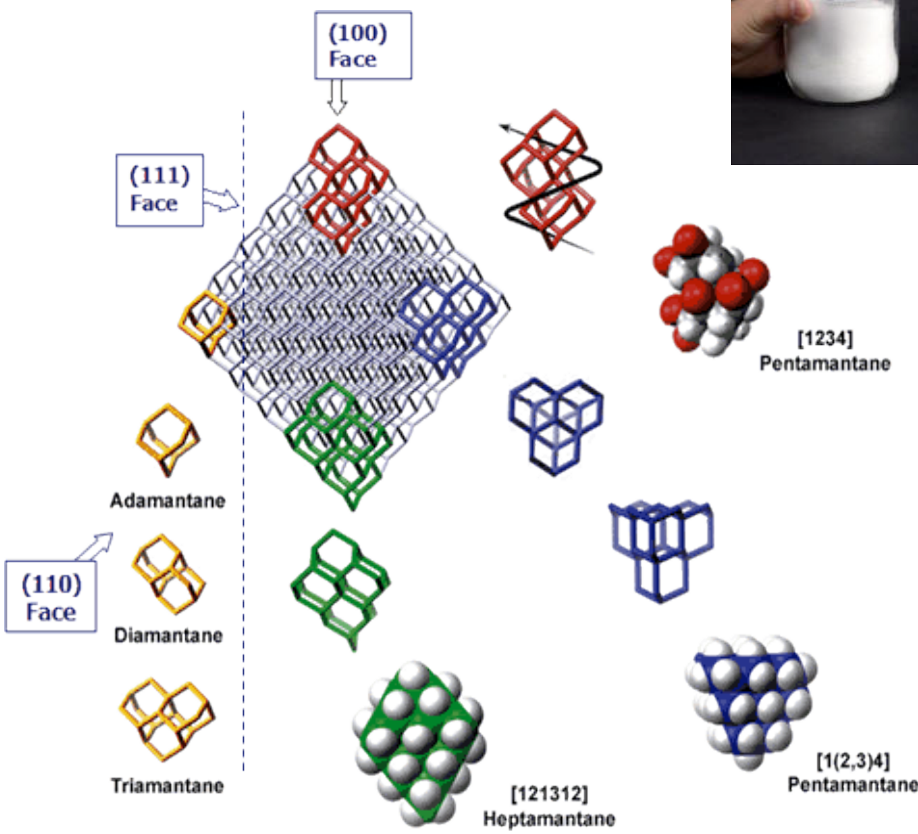




Lyeo, Cahill, Phys. Rev. B. **74**, 144301 (2006)

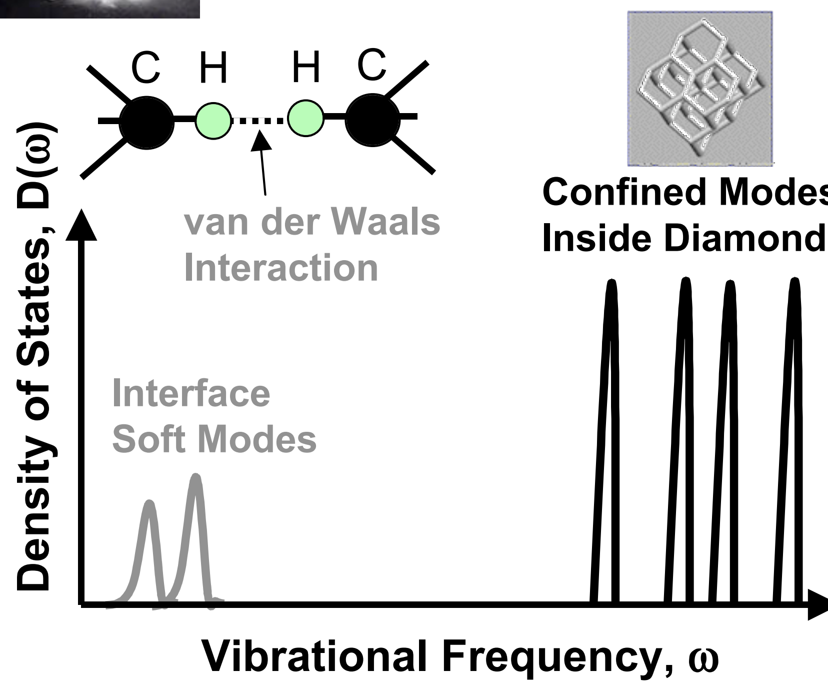
Molecular Heterostructures

Diamondoids
sp^3 bonded carbon nanostructures



Chevron

Possible Values
G ~ 1 MW/m^2-K
k ~ 1-10 mW/m-K



Collaboration:
Jeremy Dahl (C-T) - Synthesis
Pawel Keblinski (RPI) - Theory

Phonon Optics at Low Temperature (1970s--.)
(Narayanamurti, Dynes, et al; Wolfe et al.)

Quantum Phonon Conductance
(Schwab,Roukes, 2000)

Molecular Heterostructures	Nanowires & Arrays		Nanotubes
Phonon Filtering / Correlated scattering & diffusion		Uncorrelated scattering & diffusion	Waveguiding & ballistic transport

Ultralow — Polymers ⟷ Diamond — Ultrahigh

10^4 @300K

Phonon Length Scales (300K)
Wavelength = 1-10 nm
Mean Free Paths = 10-100 nm

Thermal Conductivity
$k = Cvl/3$

Information Technology

- Microelectronics
- Data Storage (> 1 TBits/in^2)
- Wireless (>100 GHz)

Energy Technology

- Insulation (k < 1 mW/m-K)
- High Cond (k > 5000 W/m-K)
- Thermoelectricity (ZT > 3)