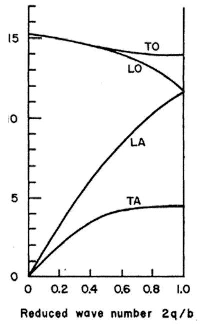
Transport Phenomena in Multi-Scale, Heterogeneous Materials & Systems

$$k = \frac{1}{6\pi^2}\sum_j \int v_j(q)\, c_{v,j}(q)\, \Lambda_j(q)\, q^2 dq \rightarrow \frac{1}{3} c_v v \Lambda$$

"Grey"

$$\Lambda_j(q) = v_j(q)\ \tau_j(q)$$

$\Lambda_{j,\text{ bulk}}$



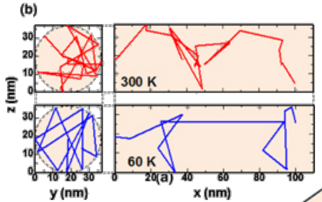
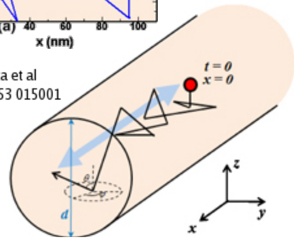
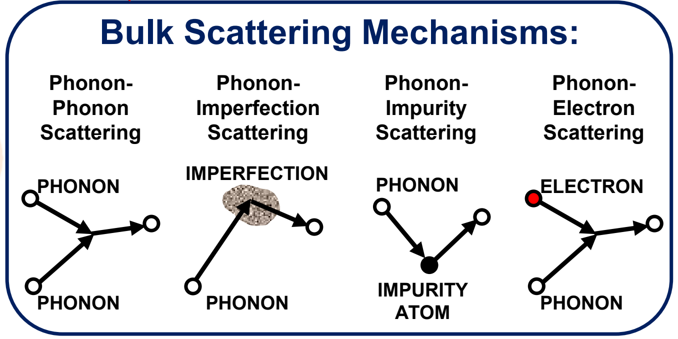
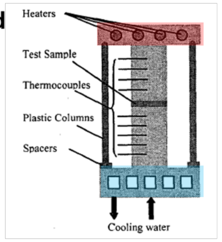


Fig. 4 from Kentaro Kukita et al 2014 Jpn. J. Appl. Phys. 53 015001

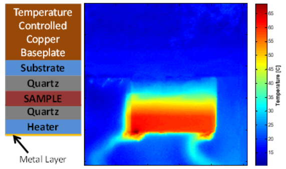


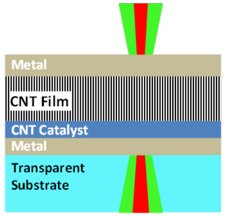


Reference Bar Method (ASTM D5470)

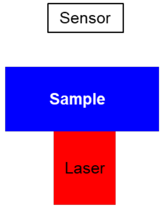


Infrared Microscopy



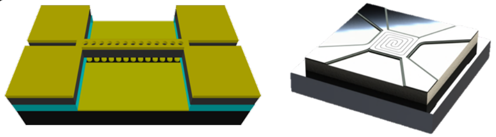


Thermoreflectance

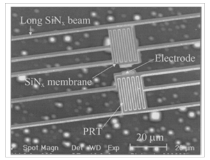


Flash Diffusivity

Electrothermal Metrology



3ω Technique and others



Li Shi *et al.*, JHT 2003

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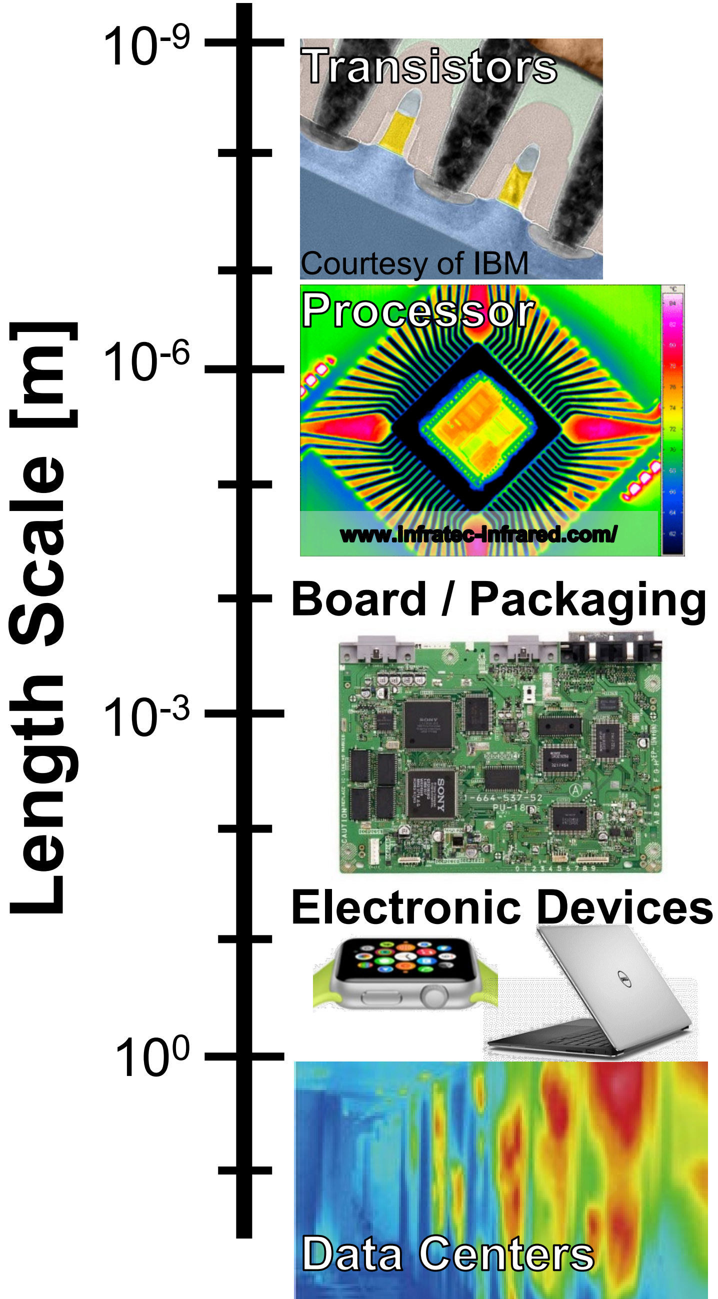
Tutorial Overview

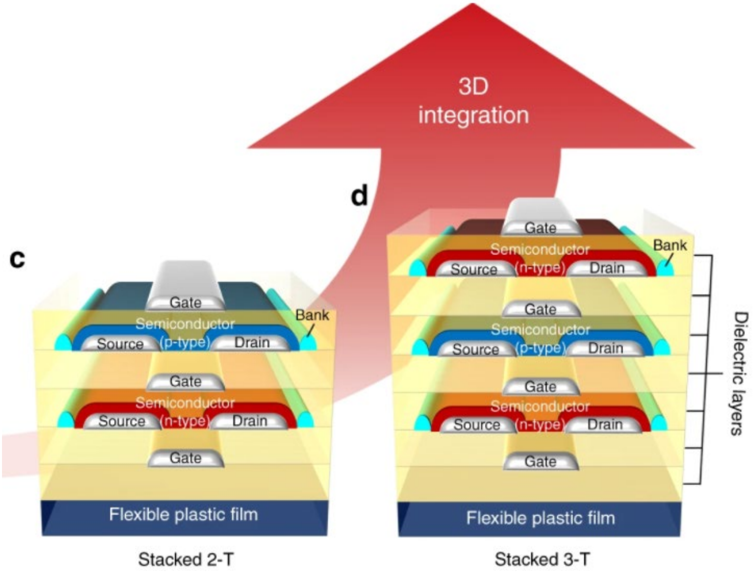
Part 0: Motivation / Introduction

Part 1: Introduction to Thermal Transport
- Overview of Thermal Energy Carriers
- Predicting Thermal Conductivity & Interfacial Thermal Transport

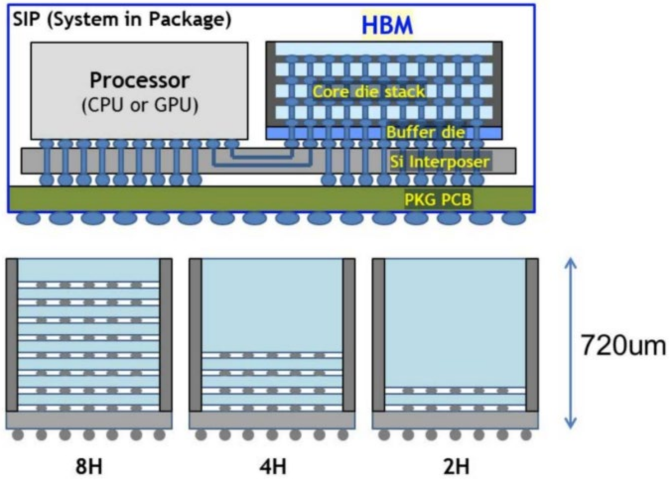
Part 2: Measuring Thermal Transport
- Introduction to Metrology Techniques

Multi-Scale & Heterogeneous System

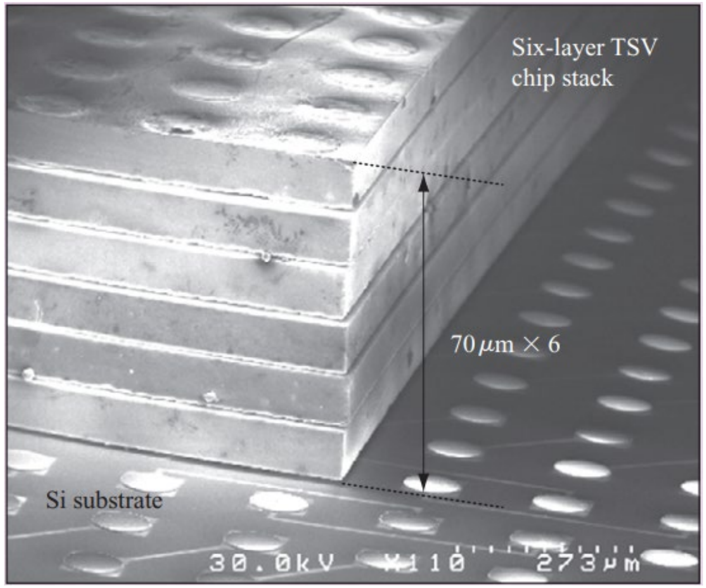




Kwon et. al. Nature (2019)

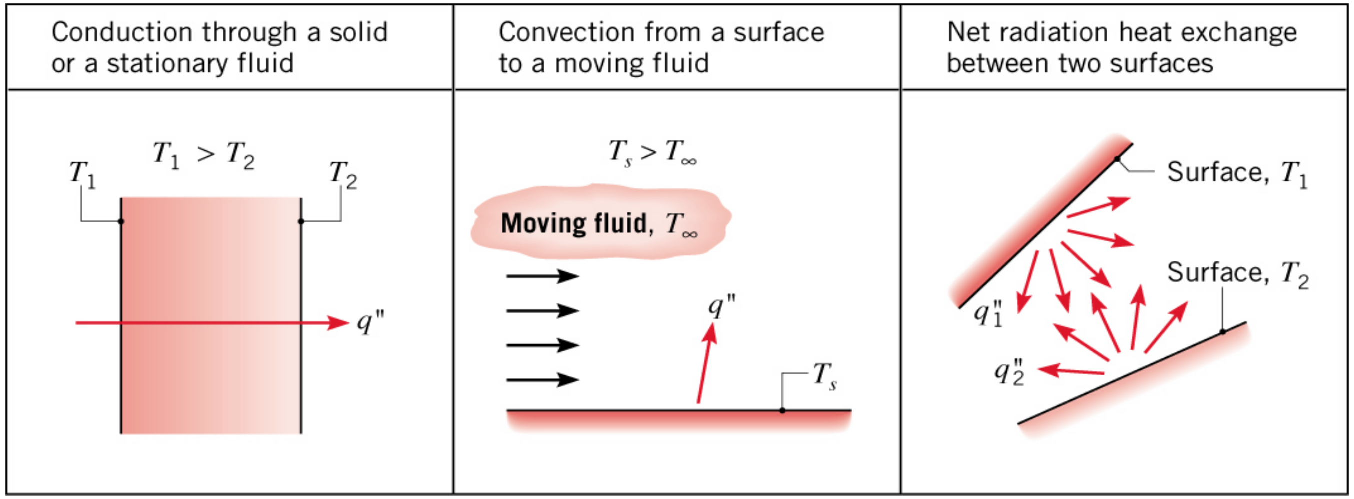


IEEE Heterogenous Integration Roadmap (2021)



Sakuma, K., et al., IBM J. of Res. & Dev. (2008)

Conduction / Convection / Radiation



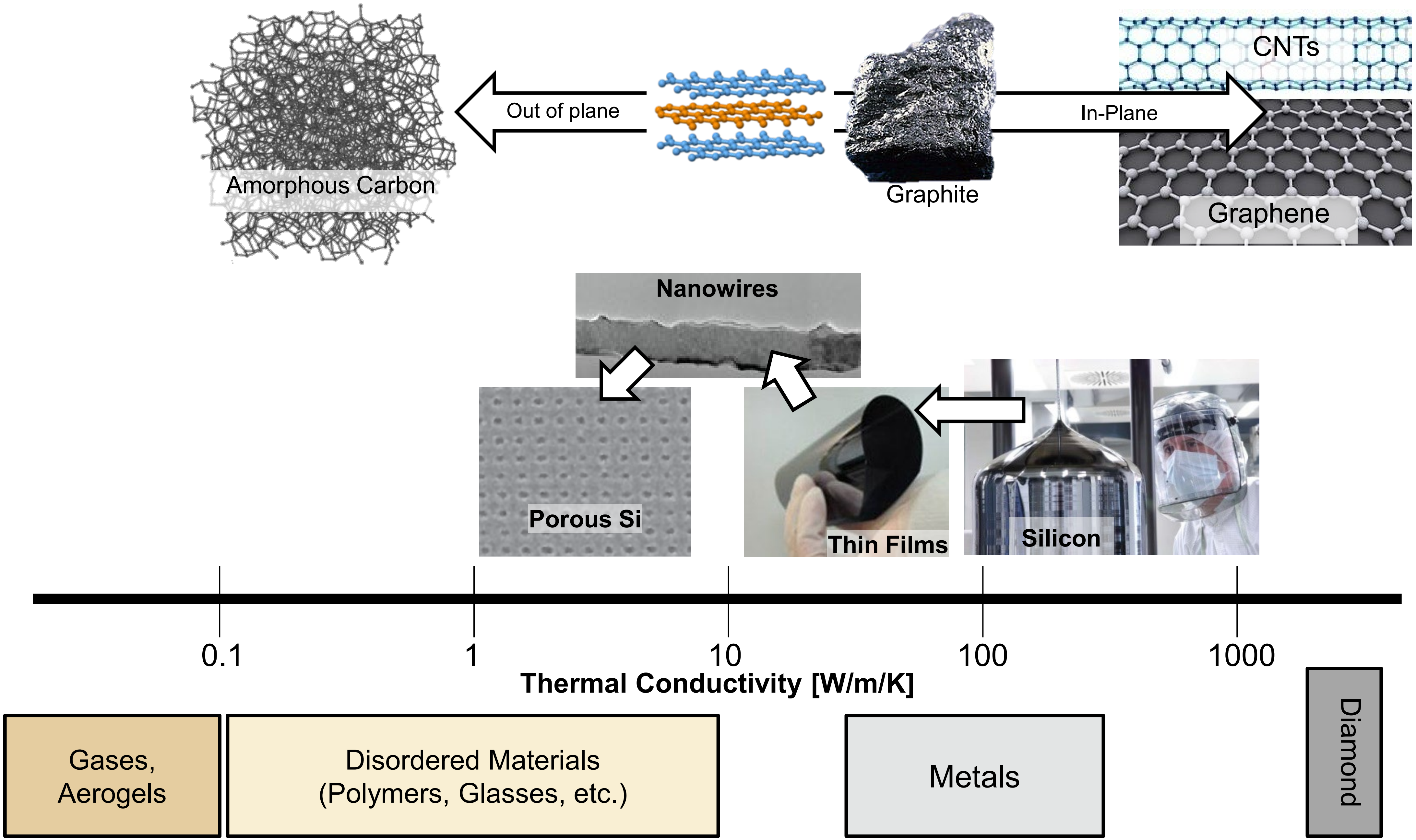
Heat Transfer = Transfer of **energy** resulting from a **temperature difference**

Each mode has specific mechanisms and rate equations

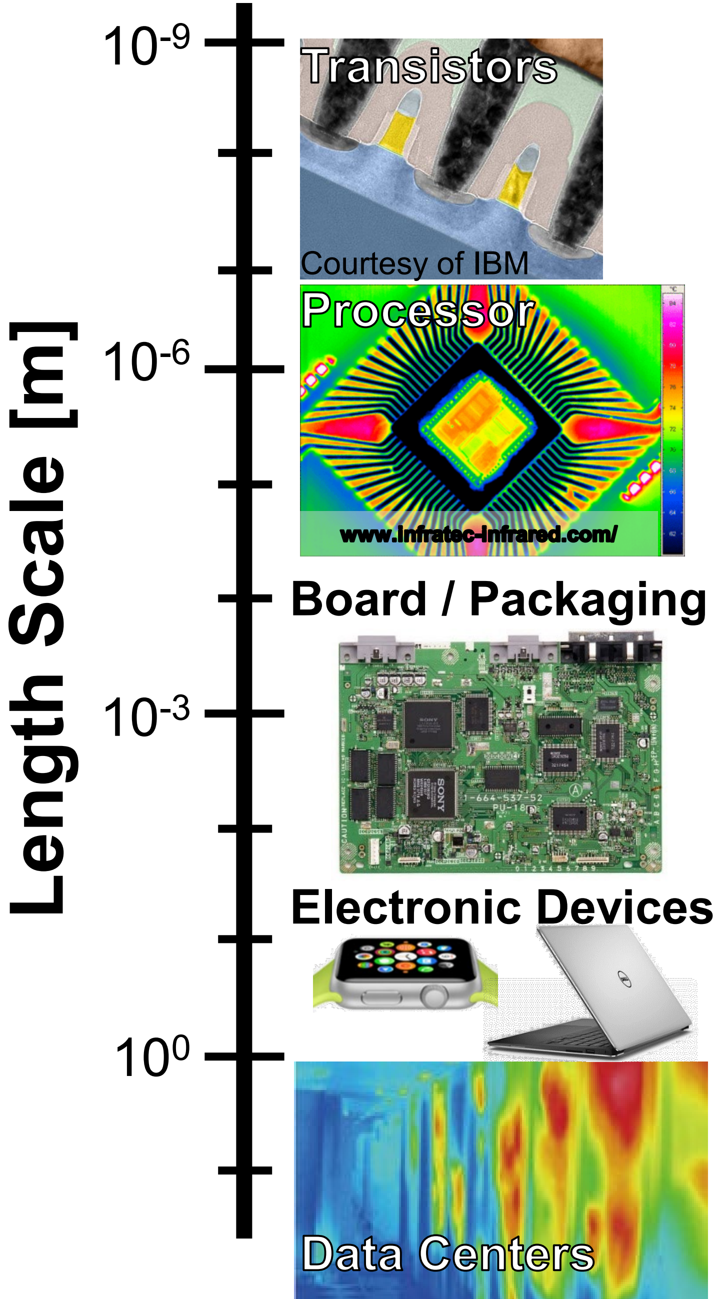
CONDUCTION MECHANISM

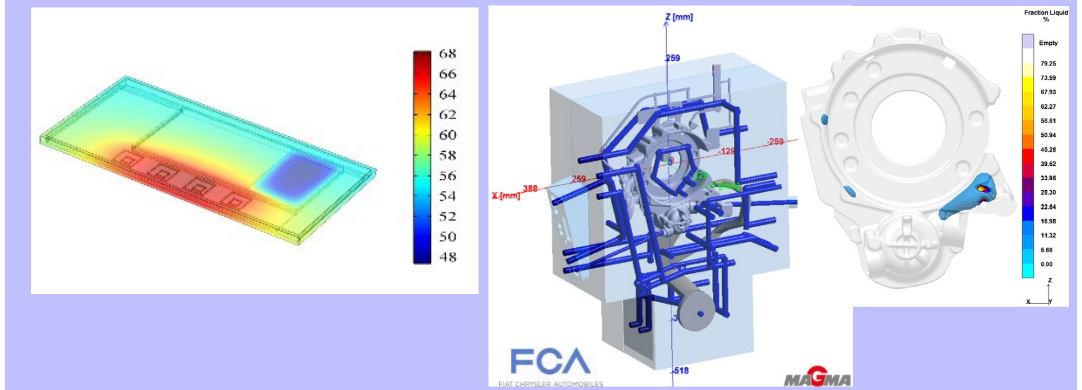
- Atomic, molecular, or electronic activity in the medium
- Conduction requires the presence of temperature variations in a material

Nanostructuring to Control ConductiveThermal Transport



Modeling Thermal Transport



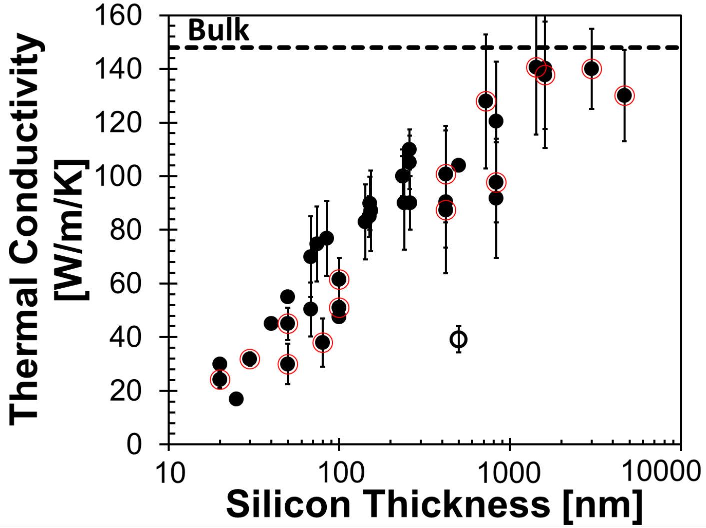


Continuum

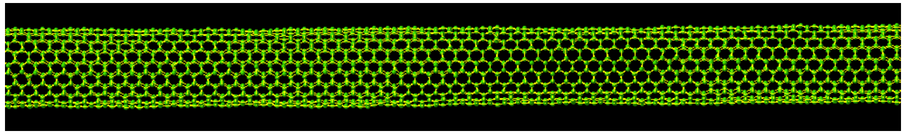
(Heat Diffusion Equation: Analytical & Numerical Methods)

When Does Continuum Analysis Fail?

Small Length Scales

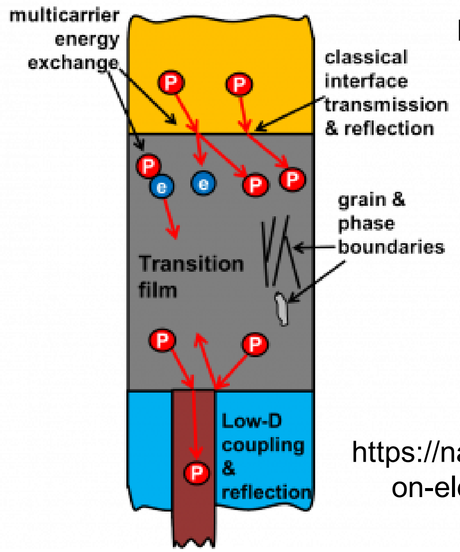


Marconnet, Asheghi, and Goodson, “From the Casimir Limit to Phononic Crystals: Twenty Years of Phonon Transport Studies using Silicon-on-Insulator Technology” *Journal of Heat Transfer* (2013).



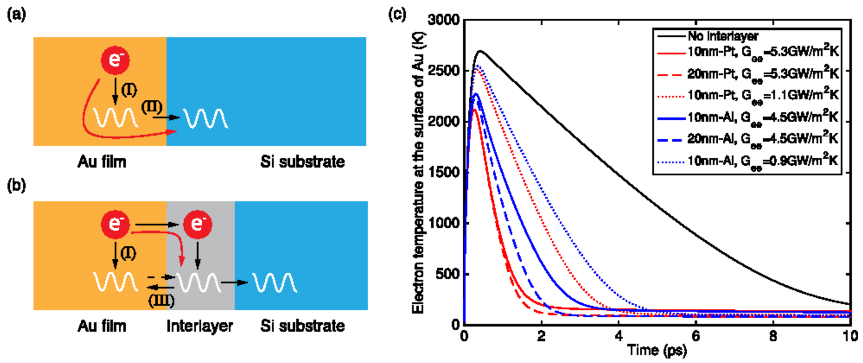
CNT animation from http://www.photon.t.u-tokyo.ac.jp/~maruyama/kikan2002/kikan2002.html

Short Time Scales



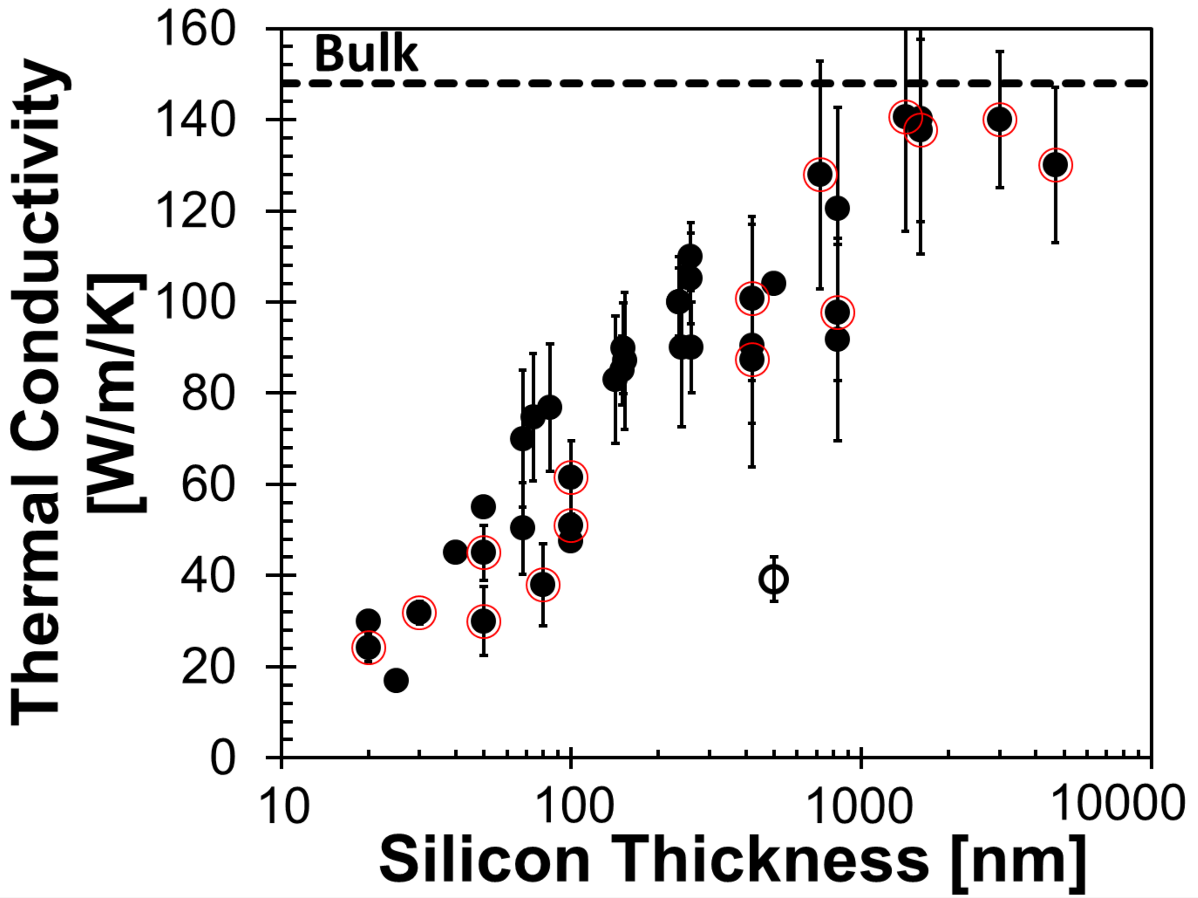
Example: Laser pulses absorbed at metal – non-metal interfaces

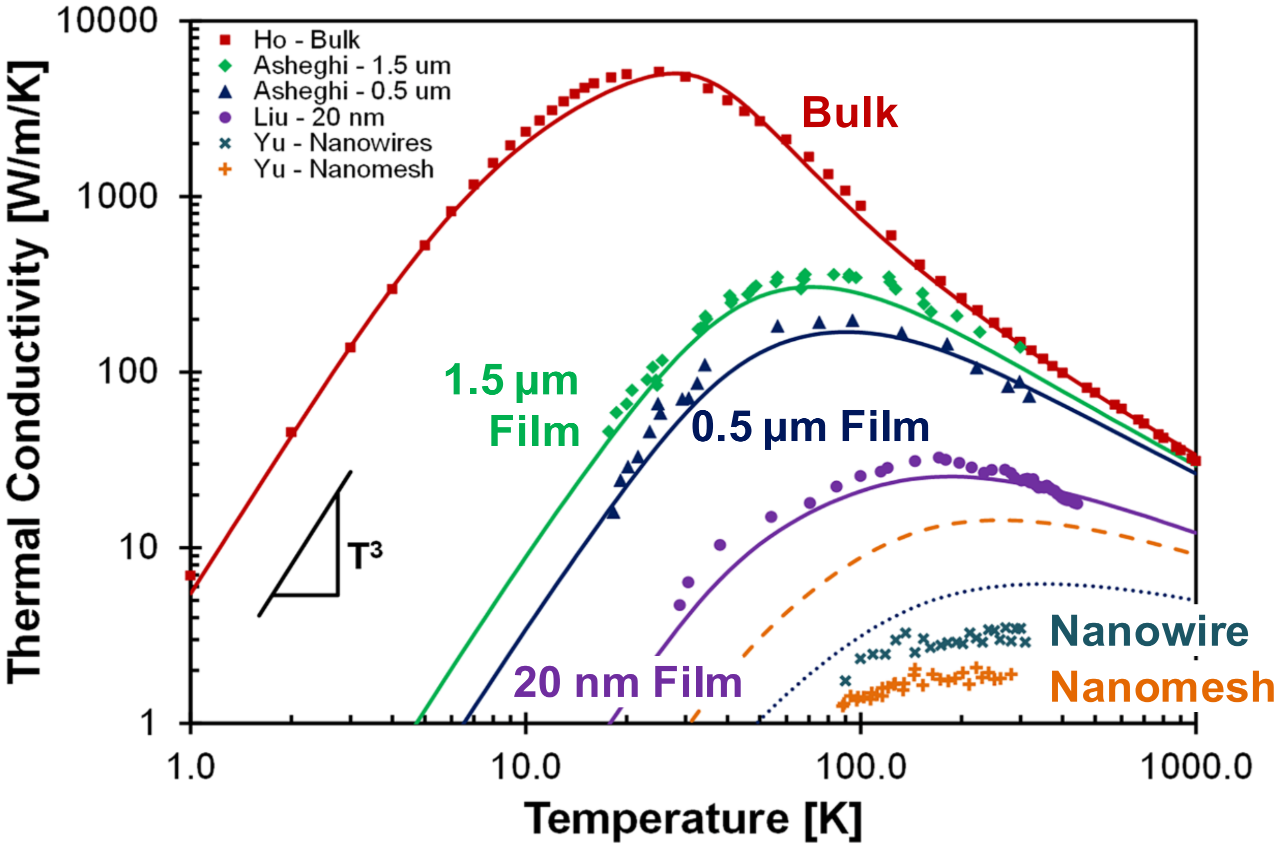
https://nanoheat.stanford.edu/projects/phonon-electron-nonequilibrium-interfaces



Wang, Lu, Roy, and Ruan, “Effect of interlayer on interfacial thermal transport and hot electron cooling in metal-dielectric systems : An electron-phonon coupling perspective”, *Journal of Applied Physics* **119**, 065103 (2016).

Experimental Evidence of the Size Effect in Silicon





Marconnet, Asheghi, and Goodson, "From the Casimir Limit to Phononic Crystals: Twenty Years of Phonon Transport Studies using Silicon-on-Insulator Technology" *Journal of Heat Transfer* (2013).

MECHANISM

- Atomic, molecular, or electronic activity in the medium
- Conduction requires the presence of temperature variations in a material

ENERGY CARRIERS FOR CONDUCTIVE HEAT TRANSFER:

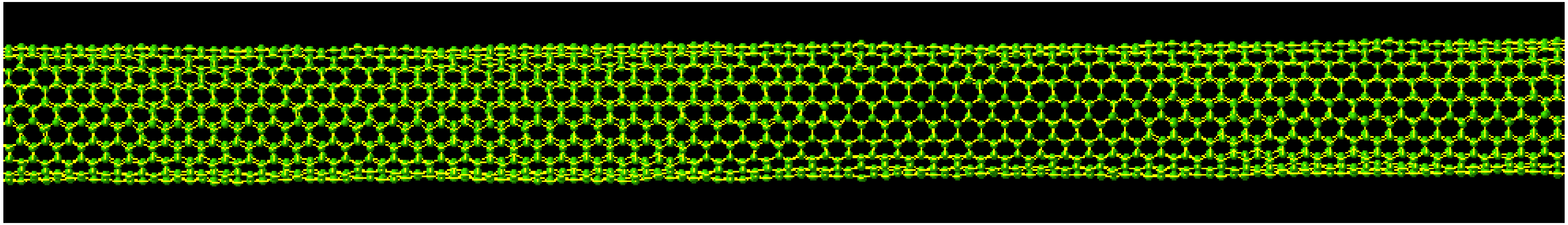
Medium	Example	Energy Transport Mechanisms	Energy Carrying Particles	Mean Free Path[2] [m]	Wavelength[2] [m]
Gases[1]	Hydrogen	Molecule motion	Molecule	$\sim 10^{-7}$	$\sim 10^{-11}$
Liquids[1]	Water	Atomic vibrations	Undefined		
Solids					
Metal	Aluminum	Electron motion	Electrons	$\sim 5 \times 10^{-8}$	$\sim 10^{-10}$
Semiconductor	Silicon	Atomic vibrations	Phonons	$\sim 5 \times 10^{-8}$	$\sim 5 \times 10^{-10}$
		Electron motion	Electrons and holes	$10^{-8} – 10^{-6}$	$10^{-9} – 10^{-7}$
Dielectric	Quartz	Atomic vibrations	phonons	$\sim 5 \times 10^{-8}$	$\sim 5 \times 10^{-10}$

[1]STATIONARY [2]ROOM TEMPERATURE AND PRESSURE

Table from Goodson, 2011

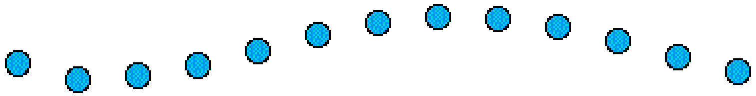
Underlying Energy Carriers: Phonons

Thermal Phonons in CNT:

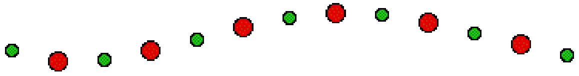


Longitudinal Acoustic

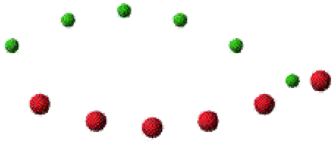
Transverse Acoustic

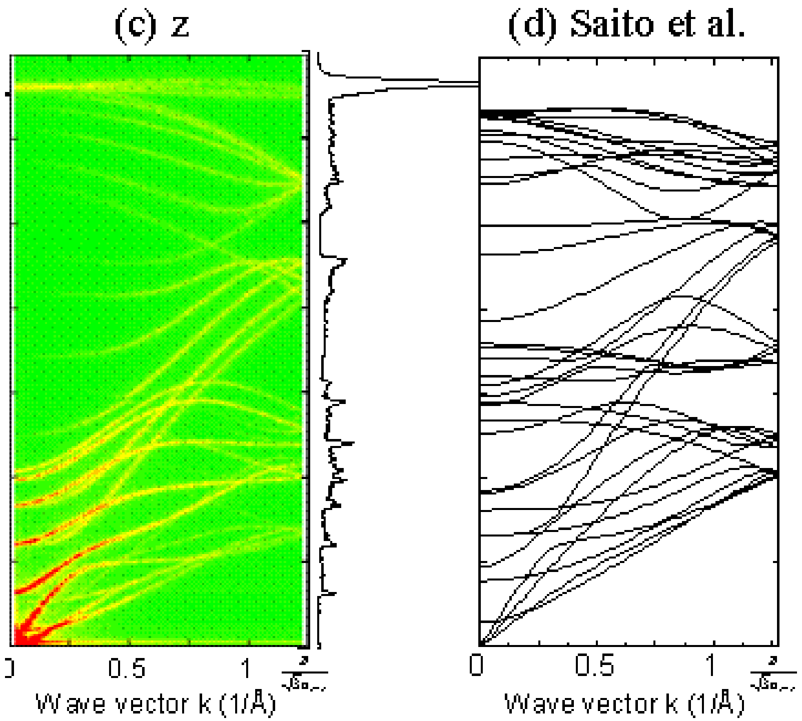


Transverse Acoustic (Diatomic Chain)



Transverse Optical





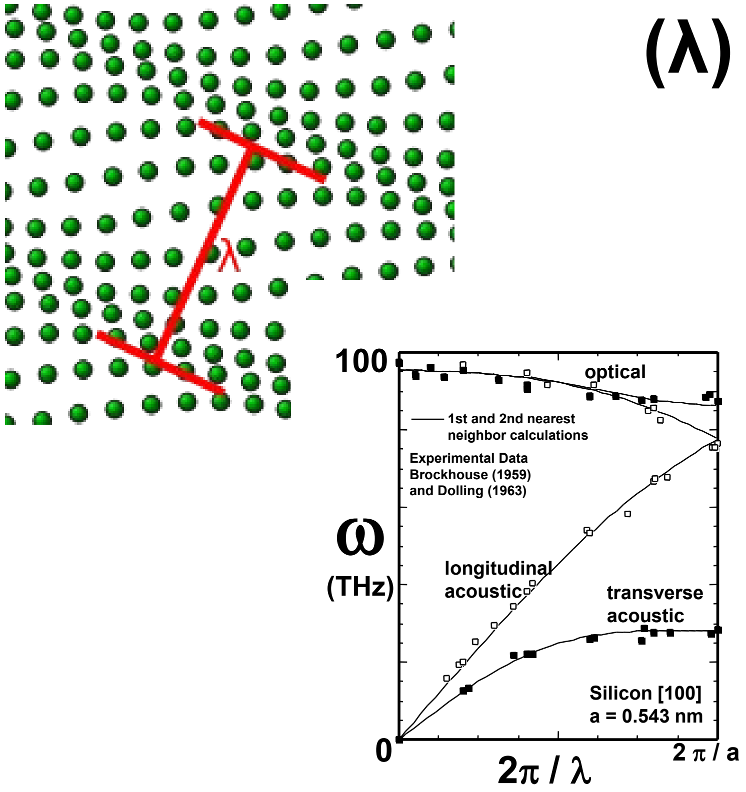
Dispersion Relationship

CNT animation and dispersion relation from http://www.photon.t.u-tokyo.ac.jp/~maruyama/kikan2002/kikan2002.html

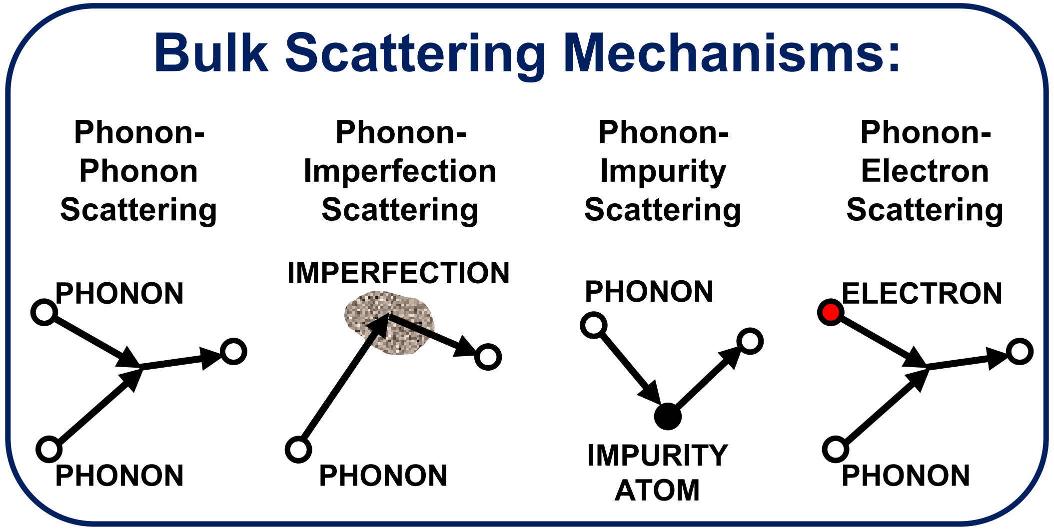
Atomic animations from http://www.chembio.uoguelph.ca/educmat/chm729/Phonons/

Length Scales for Phonon Transport

Phonon Wavelength (λ)

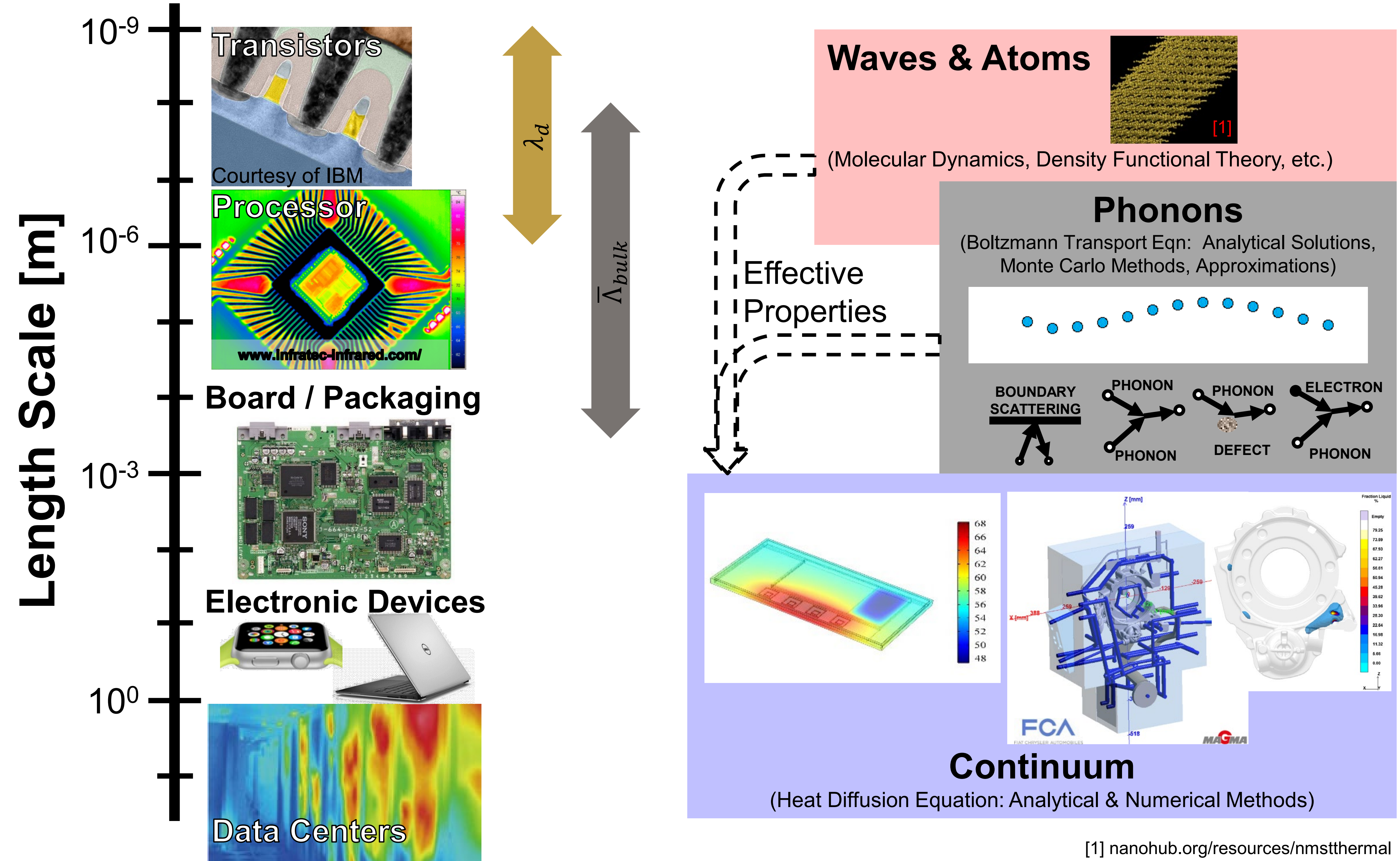


Phonon Mean Free Path (Λ)



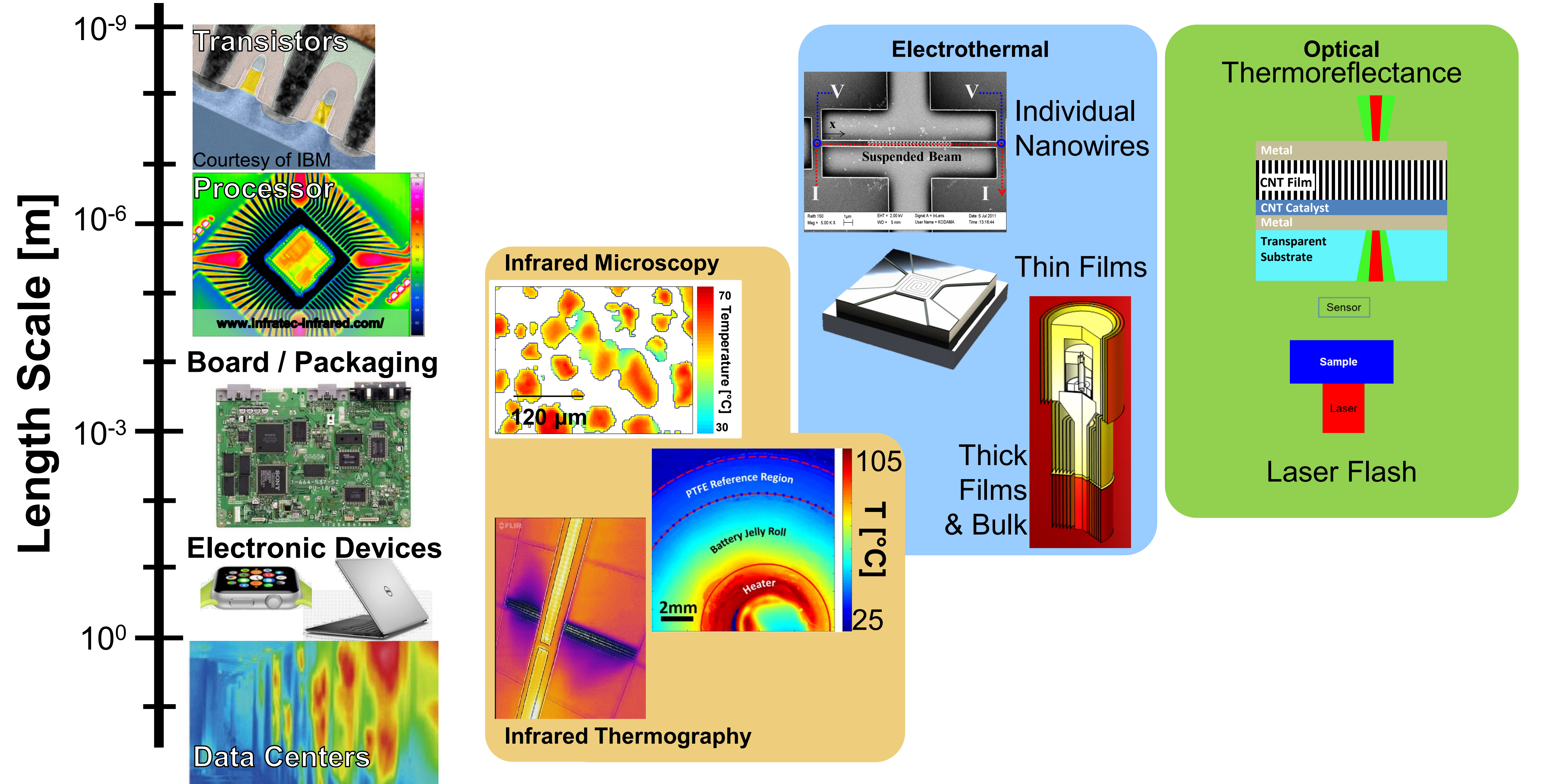
@ 300 K	Silicon	$\lambda_d \sim 1$ nm	$\Lambda \sim 300$ nm
	CNT	$\lambda_d \sim 3$ nm	$\Lambda \leq 1500$ nm

Part 1: Modeling Thermal Transport



[1] nanohub.org/resources/nmstthermal

Part 2: Measuring Thermal Transport



Part 1: Introduction to Thermal Transport

Modeling Phonon Thermal Transport

d ~ Λ

Λ ~ 300 nm in
Bulk Si at 300 K

d ~ λ_d

λ_d ~ 1 nm in
Bulk Si at 300 K

Continuum
(Fourier's Law, etc.)

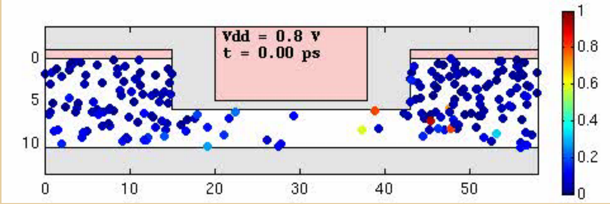
Phonons

Waves & Atoms

Boltzmann Transport Eqn:

$$\frac{\partial n_q}{\partial t} + \vec{v}_q \cdot \nabla n_q = \frac{n_q - \overline{n}_q}{\tau_q}$$

Monte Carlo Models:

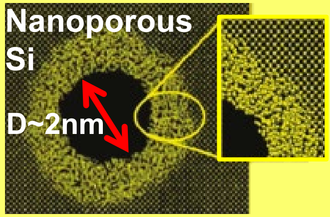


E. Pop et al, J. Appl. Phys. 96, 4998 (2004)

Thermal Conductivity Integral:

$$k = \frac{1}{6\pi^2} \sum_j \int C_j(q) v_j(q)^2 \tau_j(q) q^2 dq$$

Molecular Dynamics:



He, *et. al.*, ACS Nano (2011)

Lin *et al.*, http://nanohub.org/resources/nmstthermal

Phonon-Based Models for Thermal Conductivity

Simple Kinetic Theory

+ Consider energy carriers like particles
+ Determine energy flux across a plane

$$k = \frac{1}{3} C v \Lambda$$

Heat Capacity — Group Velocity — Mean Free Path

Boltzmann Transport Equation

"Multi-dimensional" Particle Balance

+ Near equilibrium
+ Steady state
+ Neglect spatial gradients in f_{DE}
+ Relaxation time approximation (RTA)
+ Isotropic
+ Constant τ and v

$$k = \frac{1}{3} \int_0^{\infty} E \frac{\partial f_{EQ}}{\partial T} v^2 \tau \, D_s 4\pi k_w^2 \, dk_w$$

You can omit the assumption of isotropy and find an expression for the anisotropic thermal conductivity tensor.

$$k = \frac{1}{3} C v \Lambda$$

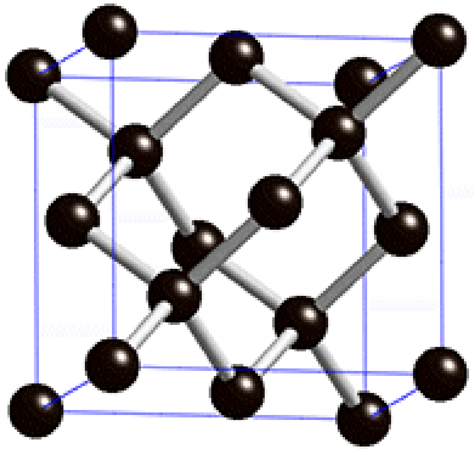
Landauer Transport Formalism

+ Assuming simple diffusive scattering (constant τ and v)

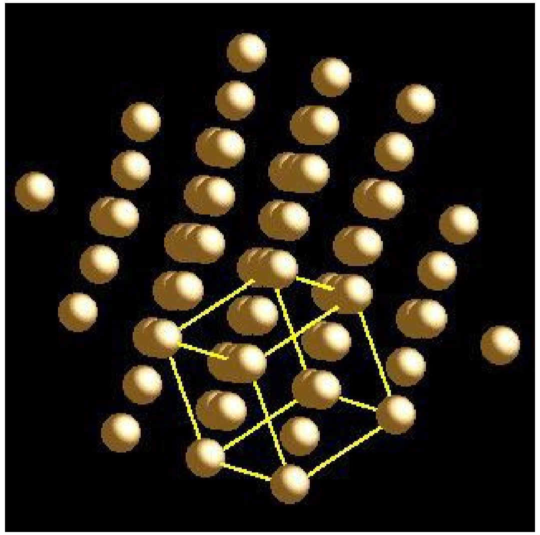
$$k = \frac{1}{2} \langle v_g \rangle \Lambda \underbrace{\int_0^{\infty} \hbar \omega D_{dD}(\omega) \frac{\partial f_{BE}}{\partial T} d\omega}_{c_v \text{ of a phonon branch}}$$

Coefficient is different because we didn't look at geometry (e.g., MFP in direction of interest)

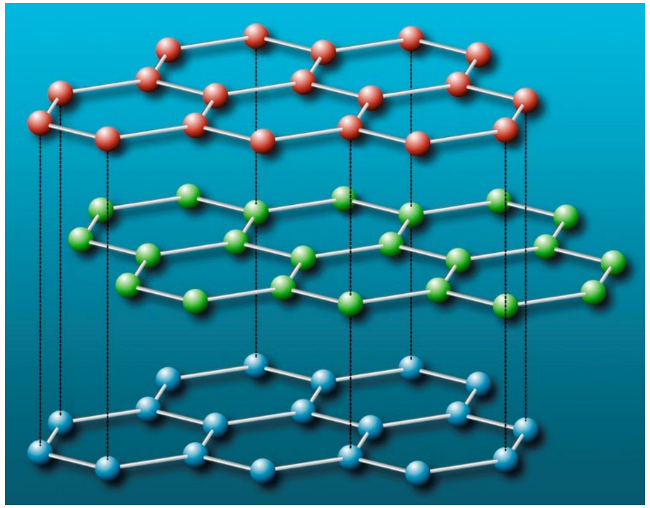
Lattice – Crystal Structure



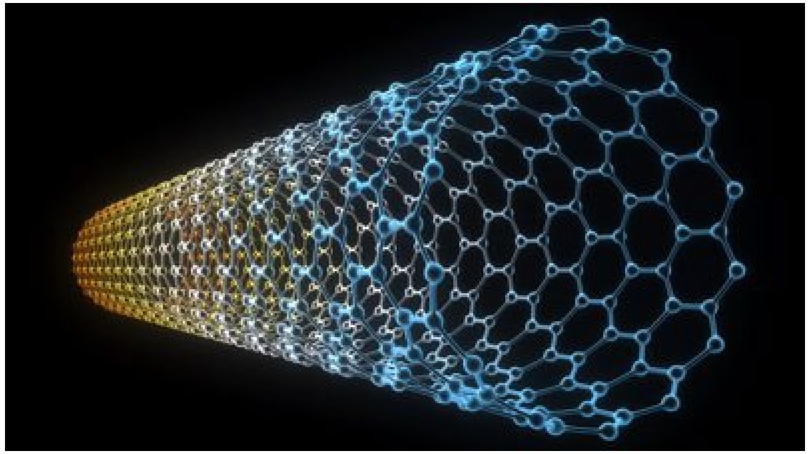
Diamond



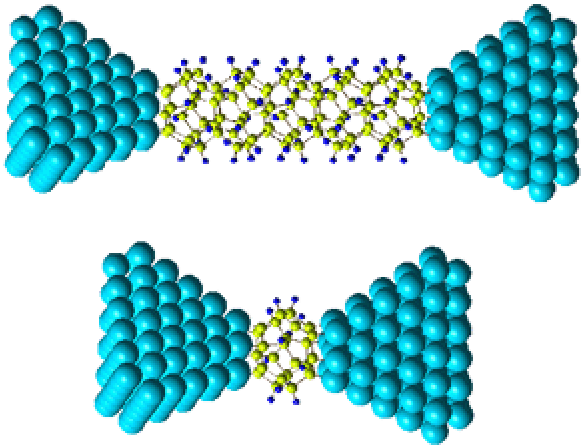
Gold



Graphite



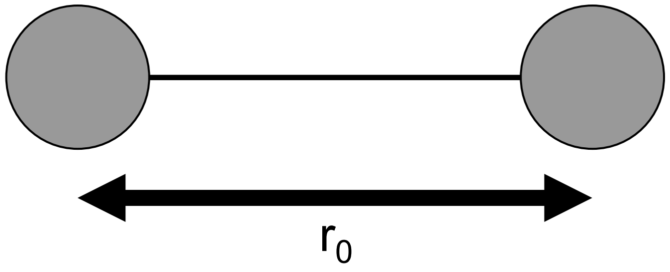
CNTs



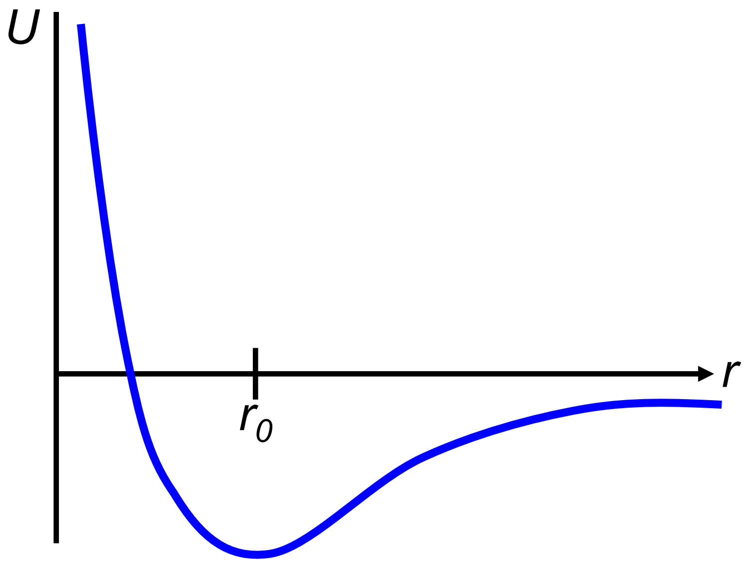
Molecular Junctions

Atomic Bonding

- Consider two neighboring atoms that share a chemical bond

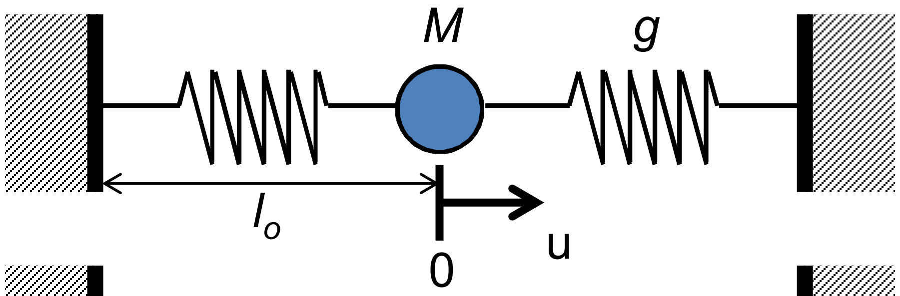


- The bond is not rigid, but rather like a spring with an energy relationship such as …

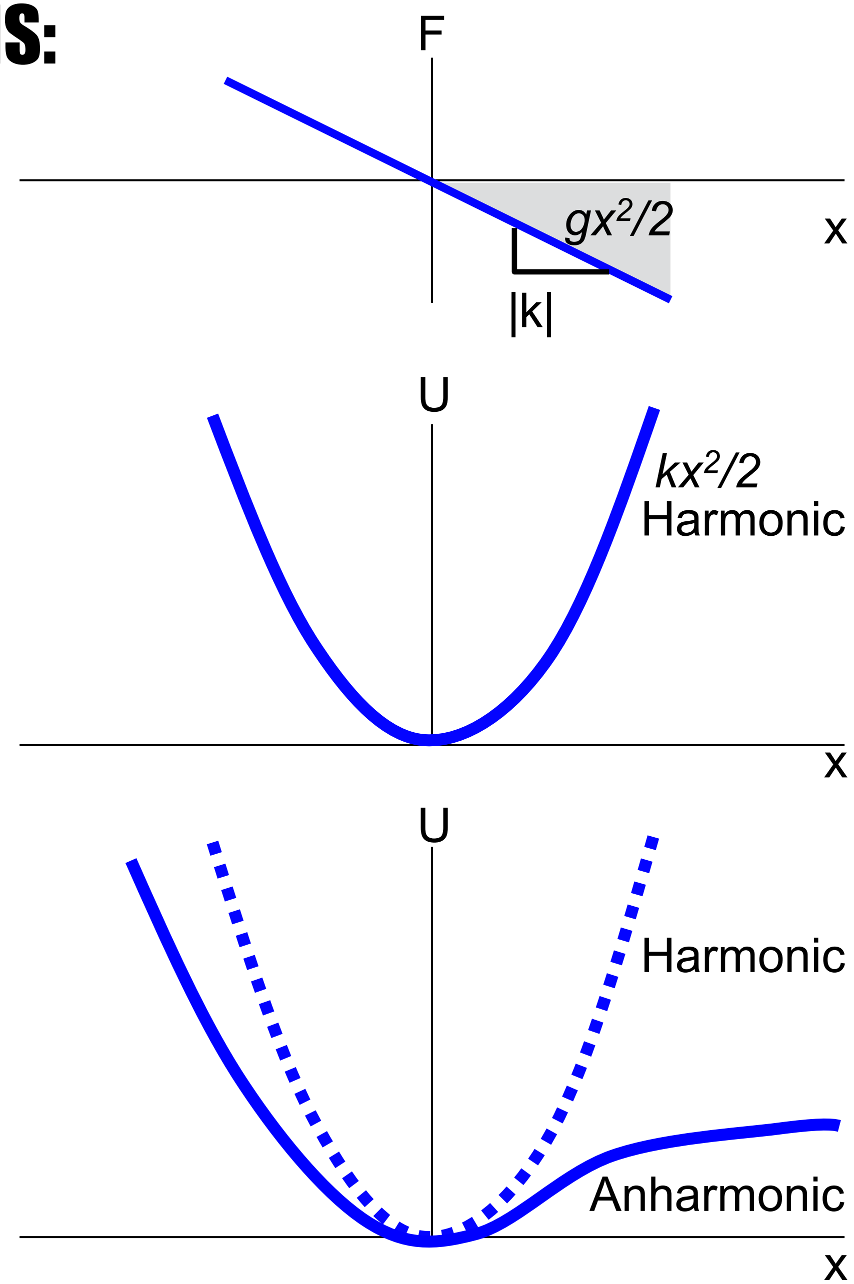


Harmonic Approximation

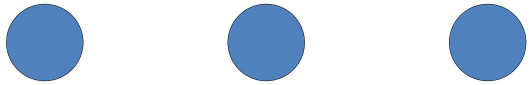
RECALL, FROM PHYSICS, SPRING-MASS SYSTEMS:



U: Elastic Potential Energy



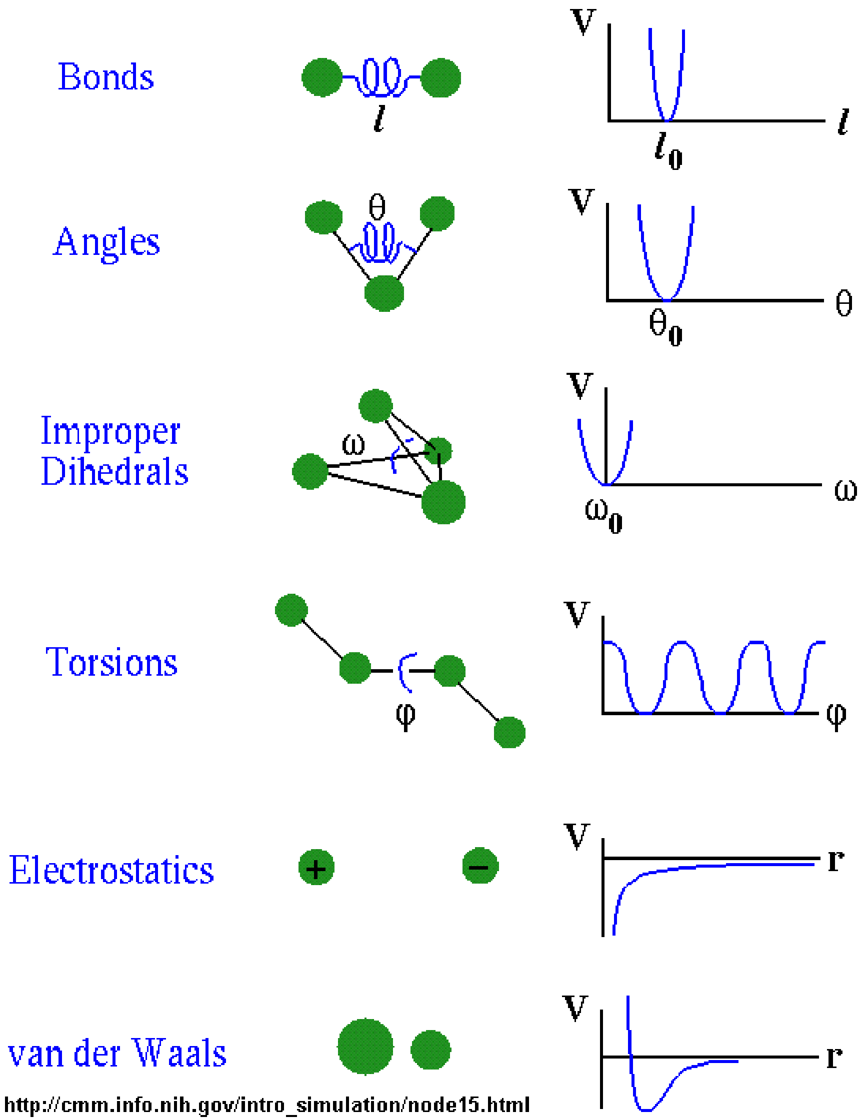
ATOMS



Forces:
+ van der Waals attraction
+ electrostatic interactions
+ etc.

Atomic Bonds

Empirical Potential Energy Function



http://cmm.info.nih.gov/intro_simulation/node15.html

Leonard Jones Potential:

$$U(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Born Model of Ionic Lattice:

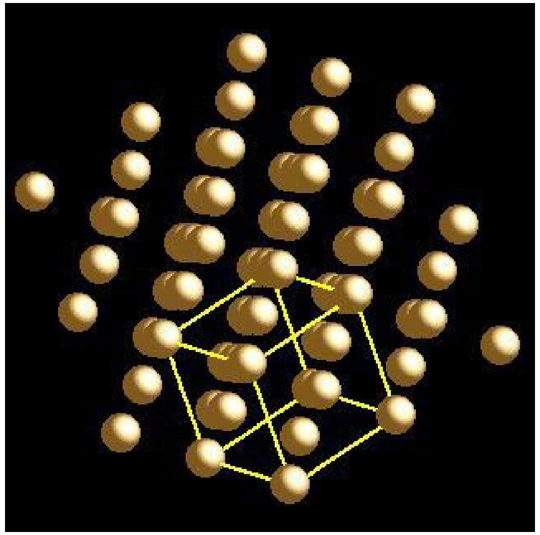
$$U_{ij}(r_{ij}) = \sum \frac{z_i z_j}{4\pi\epsilon_0}\frac{1}{r_{ij}} + \sum A_l \exp\frac{-r_{ij}}{p_l} + \sum C_l r_{ij}^{-n_l} + \cdots$$

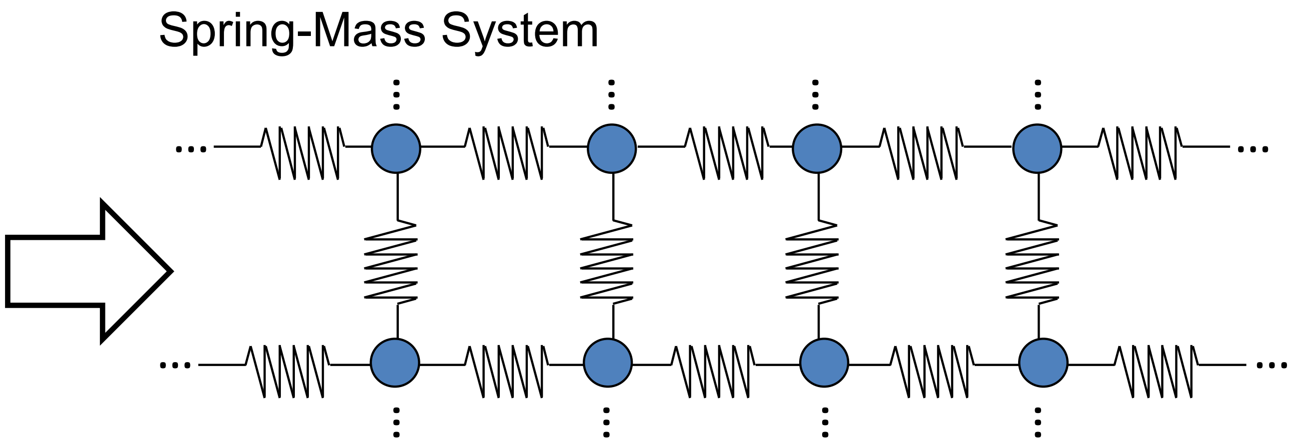
Coulomb's Law

Short Range Repulsion
(Pauli's Exclusion Principle)

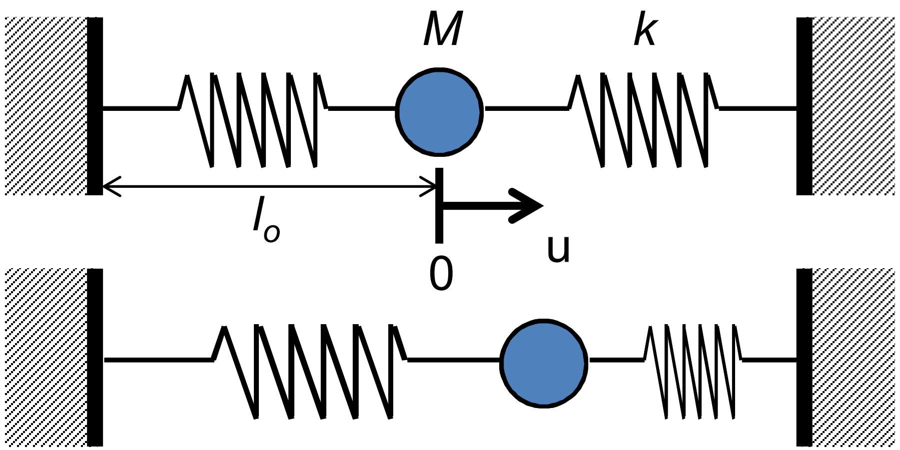
Dispersion
Interaction

Simple "Toy" Model





Simple Case: 1 Mass + 2 Springs



Newton's Law: $\sum F = Ma = M\ddot{u}$

Linear Springs: (Hooke's Law) $F = k(l - l_0) = -uk$

Has one solution:

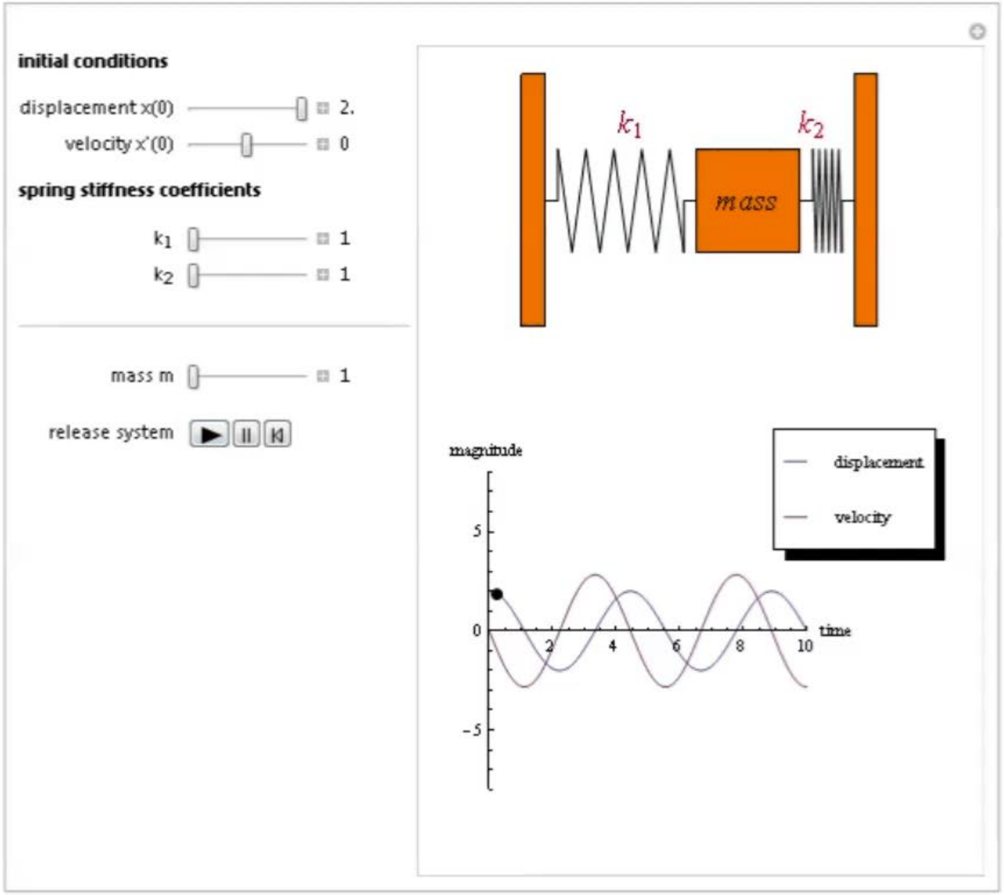
Combining: $-2uk = M\ddot{u} \Rightarrow -2ku_0 = -M\omega^2 u_0 \Rightarrow \omega = \sqrt{\frac{2k}{M}}$

Periodic Solutions: $u = u_o \exp(-i\omega t)$

This system has 1 mode of vibration.
Whatever you do, it always ends up in a sinusoidal motion about the equilibrium position at a frequency $f = \omega / 2\pi$.

Simple Case: 1 Mass + 2 Springs

Mass Oscillating between Two Springs

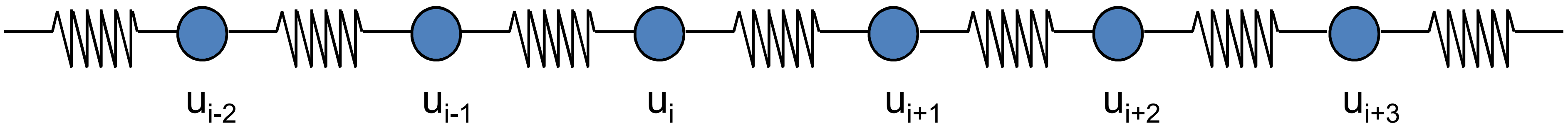


A block is connected to two fixed walls by two springs. The equation of motion is

$$m\frac{d^2x}{dt^2} + (k_1 + k_2)x = 0,$$

where m is the mass of the block, x is the displacement of the mass, t is time, and k_1 and k_2 are spring stiffness coefficients independent of x and t.

Toy Model - Mathematically



Newton's Law + Hooke's Law: $(u_{i-1} - u_i)k + (u_{i+1} - u_i)k = M\ddot{u}_i$

Periodic Oscillations: $u_i = u_0 \exp(iKx)\exp(-i\omega t)$

Algebra: $\left(\exp(-iKa)u_i - u_i\right)k + \left(\exp(+iKa)u_i - u_i\right)k = -\omega^2 M u_i$

$$\left(\exp(-iKa) - 1\right)k + \left(\exp(+iKa) - 1\right)k = -\omega^2 M$$

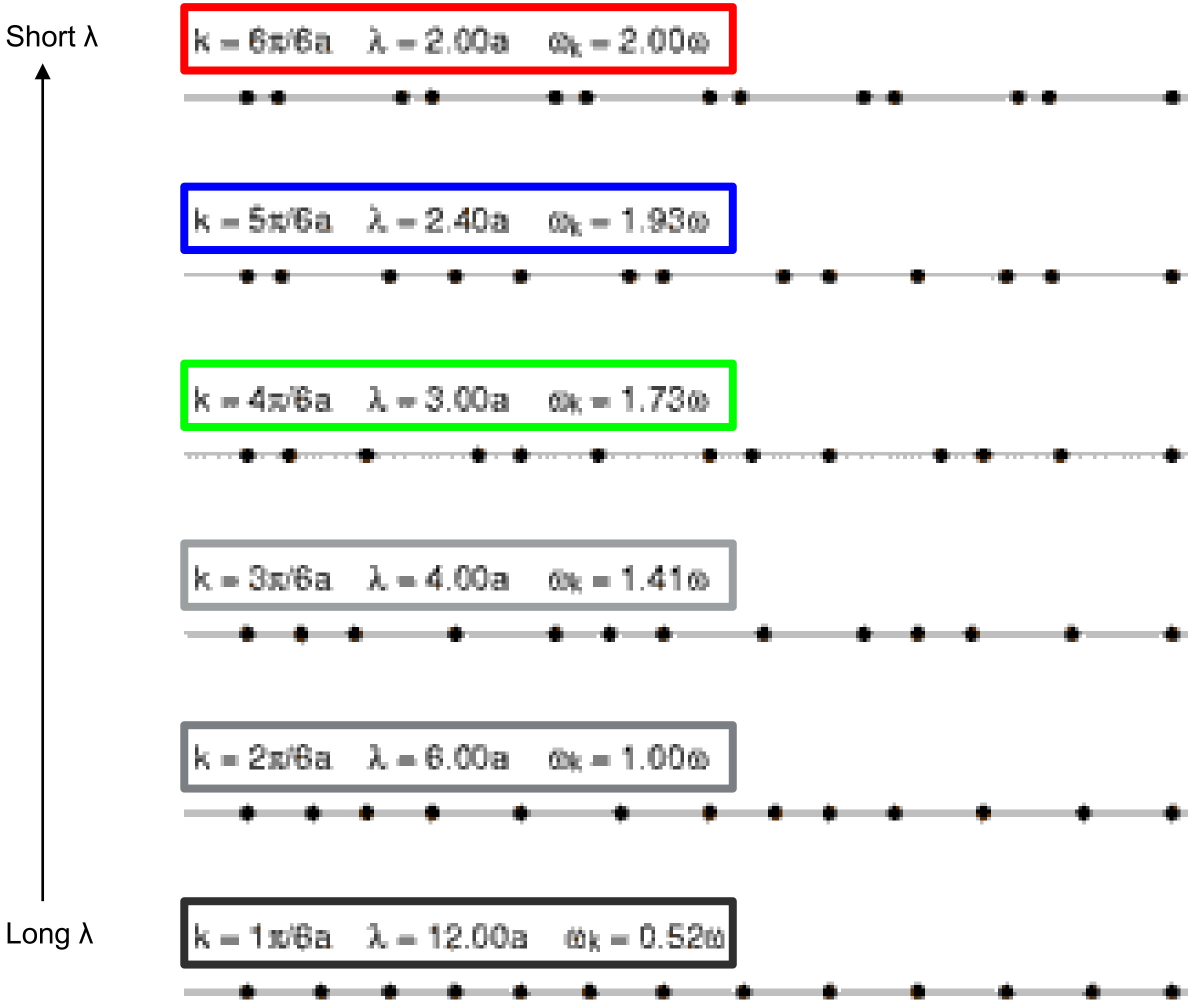
$$\omega^2 = 2\frac{K}{M}\left(1 - \cos(Ka)\right)$$

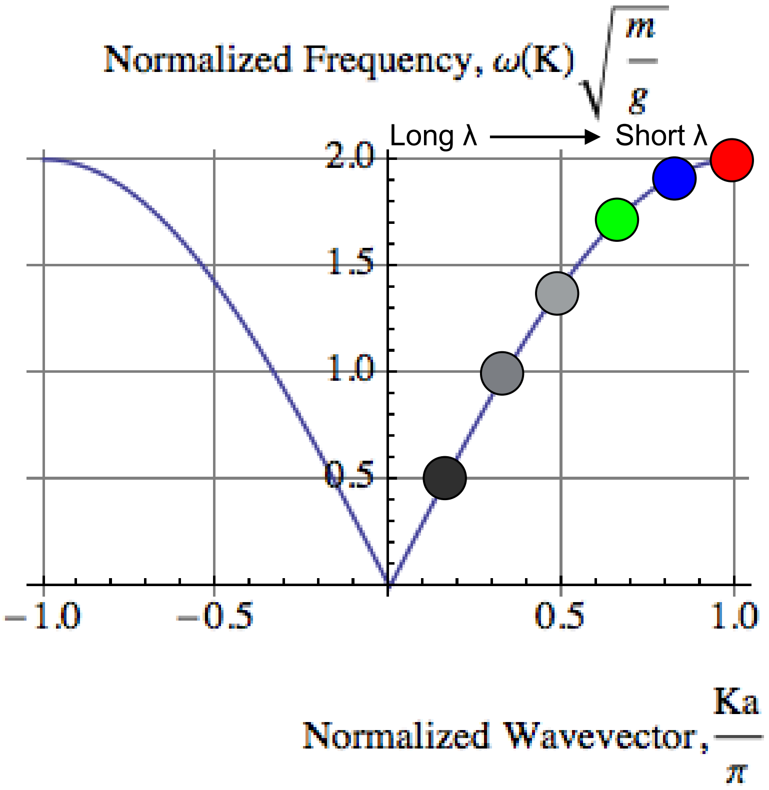
Frequencies: $\omega = \sqrt{2\frac{k}{M}\left(1 - \cos(Ka)\right)} = \sqrt{4\frac{k}{M}}\left|\sin\left(\frac{Ka}{2}\right)\right|$

<u>"Frequency"</u>
T = period (s)
ω = 2π/T = angular frequency (s^{-1})

<u>Spatial "Frequency"</u>
K = 2π/λ = wavevector (m^{-1})
λ = wavelength (m)

Dispersion Relationship: Toy Model

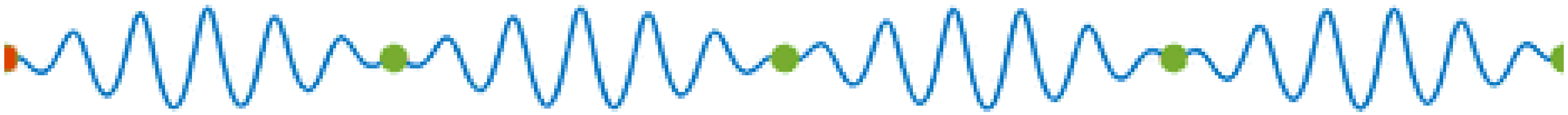




Badseed, https://commons.wikimedia.org/wiki/File:1D_normal_modes_(280_kB).gif

Side Note: Wave Packet Velocity

Wave packets contain superposition of many different waves



Red square moves with the phase velocity

Green circles propagate with the group velocity.

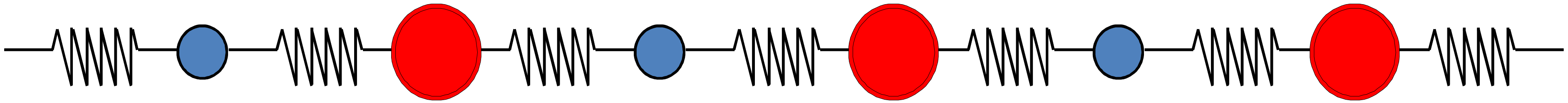
Phase velocity: Rate at which phase goes through space and time

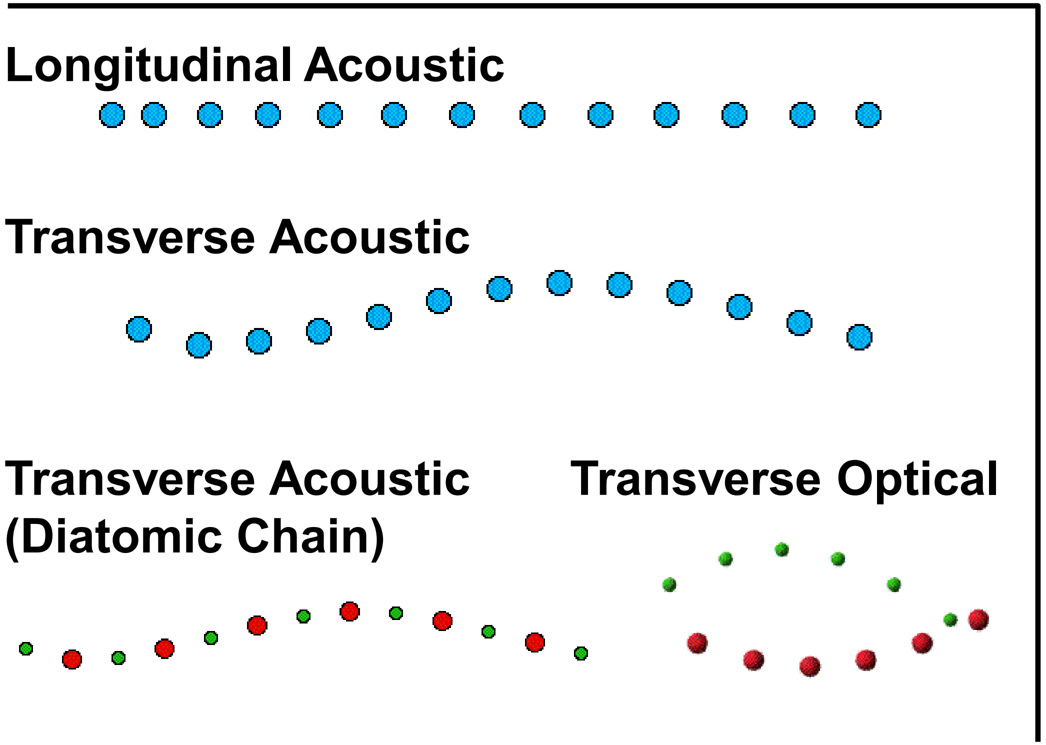
$$v_p = \frac{\omega}{k} = \frac{2\pi\nu}{\frac{2\pi}{\lambda}} = \lambda\nu$$

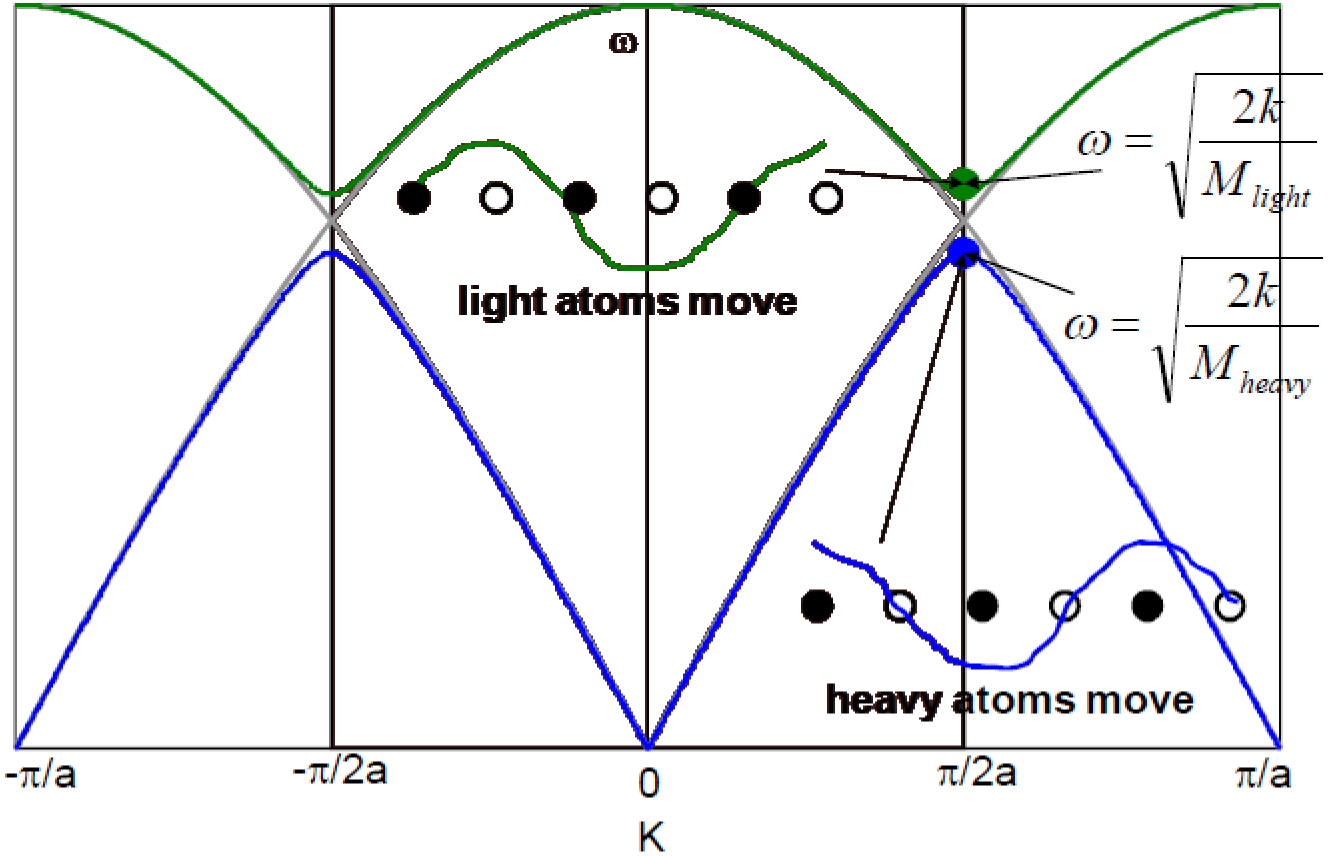
Group velocity: Rate at which the packet moves through space and time. **Determines rate of energy transport**

$$v_g = \frac{\partial\omega}{\partial k}$$

What if you have 2 different atoms?

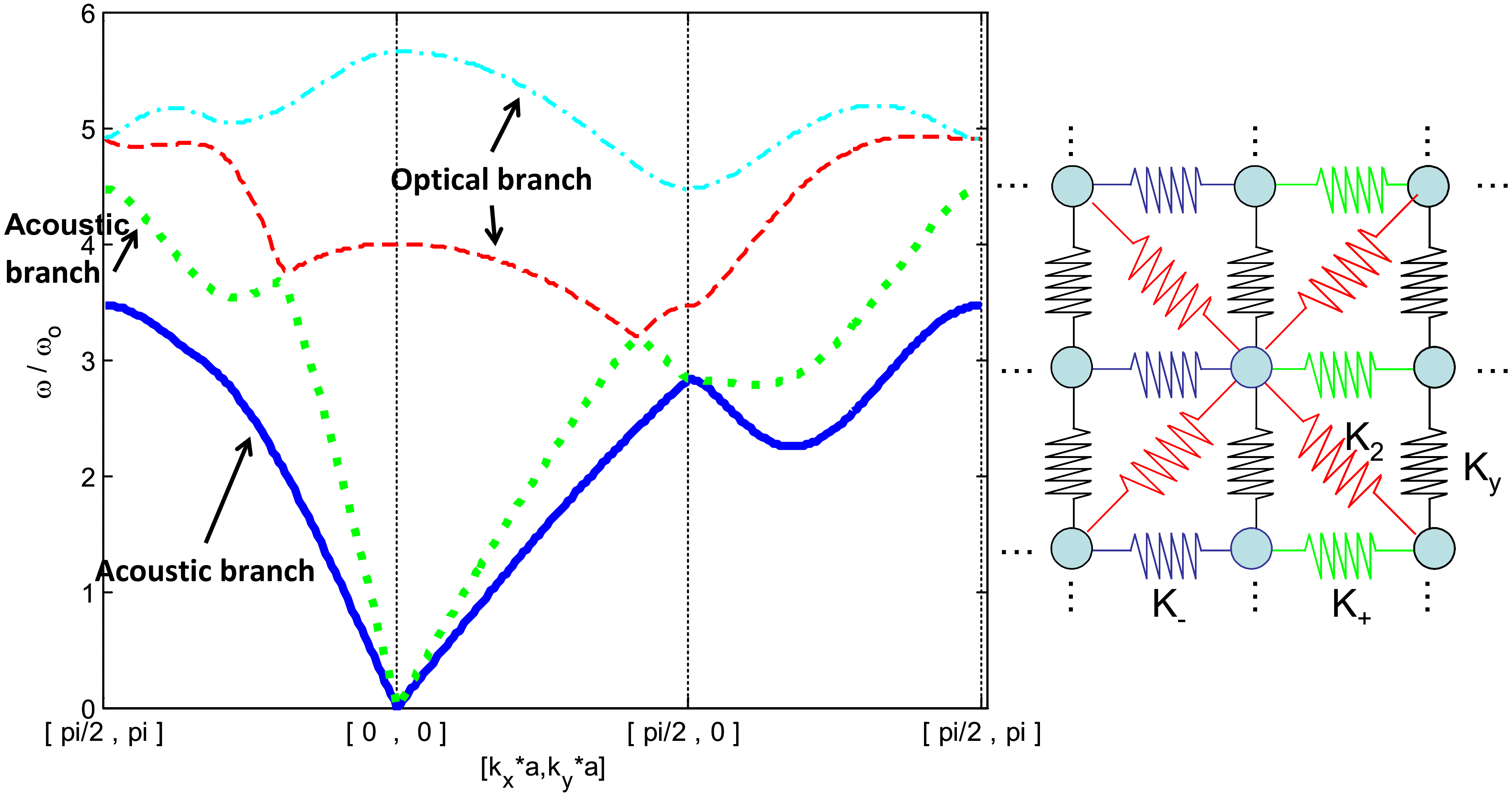






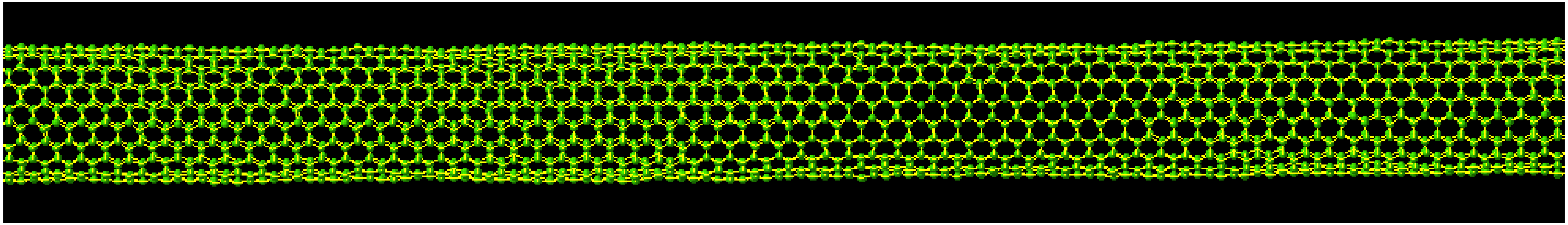
Two solutions → Acoustic Modes and Optical Modes

More Complex Mass + Spring Phonon Models



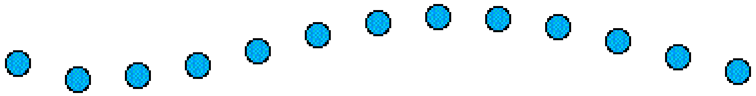
Atomistic Simulations to Compute Dispersion Relationships

Thermal Phonons in CNT:

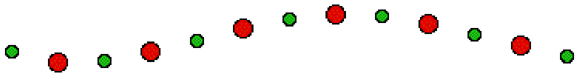


Longitudinal Acoustic

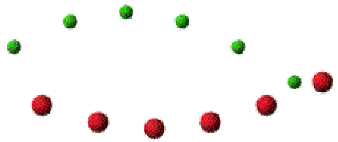
Transverse Acoustic

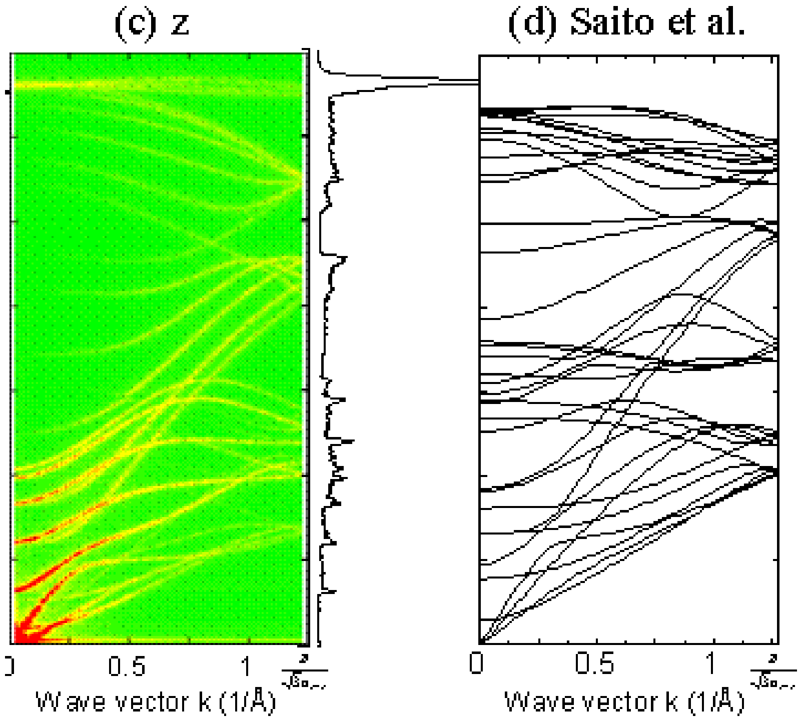


Transverse Acoustic (Diatomic Chain)



Transverse Optical





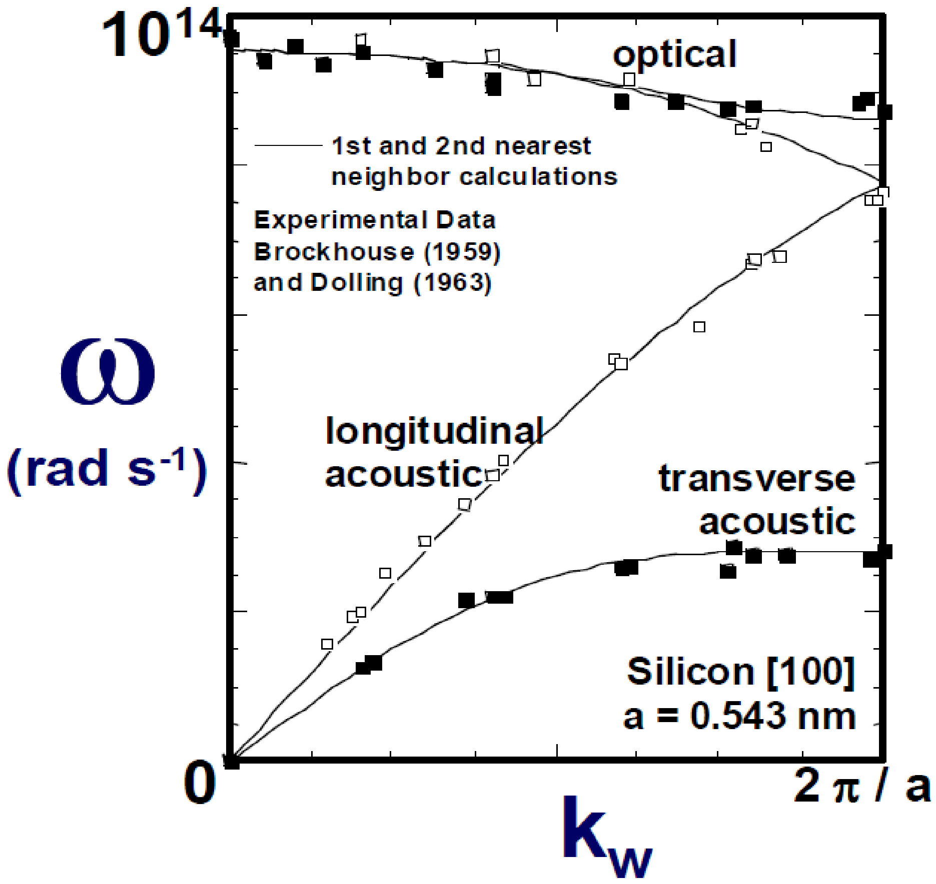
Dispersion Relationship

CNT animation and dispersion relation from http://www.photon.t.u-tokyo.ac.jp/~maruyama/kikan2002/kikan2002.html

Atomic animations from http://www.chembio.uoguelph.ca/educmat/chm729/Phonons/

Atomistic Simulations → Predicting Conductivity

Phonons Dispersion in Si



The crystal structure of many solids yields more than one atom for each lattice site.

In bulk materials, phonons can possess one of three polarizations: 1 longitudinal and 2 transverse modes

The phonon dispersion relations show a nonlinear variation of the angular frequency with the wavevector.

Longitudinal polarization have larger **group velocities** than those with transverse polarizations.

Thermal Conductivity Integral

$$k = \frac{1}{6\pi^2}\sum_j \int v_j(q)\, c_{v,j}(q)\, \Lambda_j(q)\, q^2 dq \rightarrow \frac{1}{3} c_v v \Lambda$$

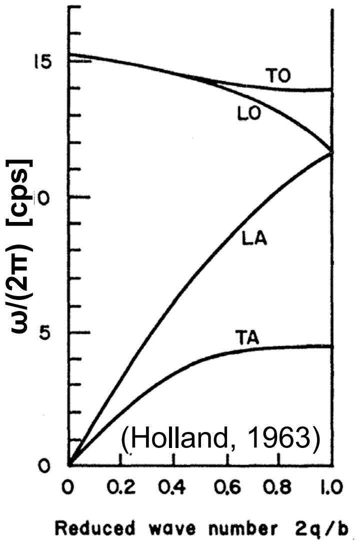
"Grey"

Group Velocity — **Heat Capacity** — **Mean Free Path**

$$\Lambda_j(q) = v_j(q)\;\tau_j(q)$$

$\Lambda_{j,\,bulk}$

Phonon Band Structure (Silicon)



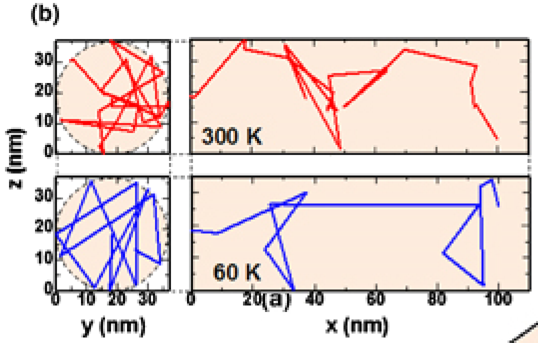
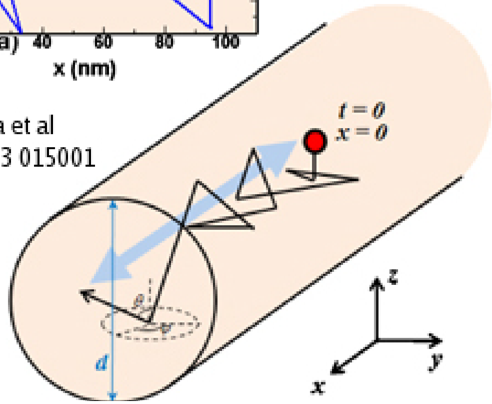
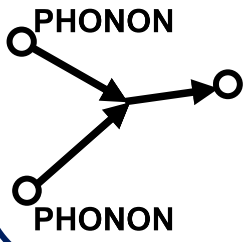


Fig. 4 from Kentaro Kukita et al
2014 Jpn. J. Appl. Phys. 53 015001

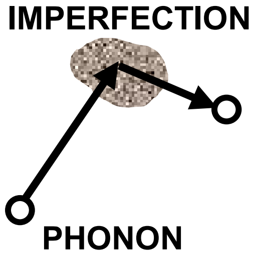


Bulk Scattering Mechanisms:

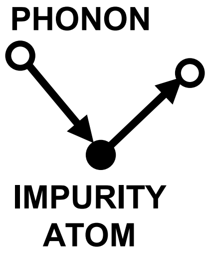
Phonon-Phonon Scattering



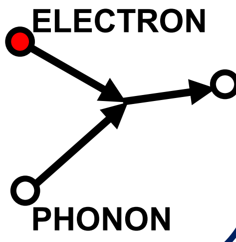
Phonon-Imperfection Scattering



Phonon-Impurity Scattering



Phonon-Electron Scattering



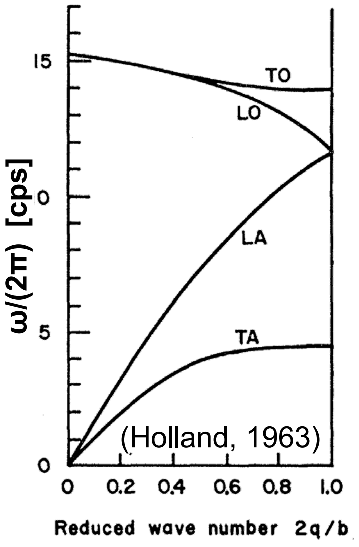
Thermal Conductivity Integral

$$k = \frac{1}{6\pi^2}\sum_j \int v_j(q)\, c_{v,j}(q)\, \Lambda_j(q)\, q^2 dq$$

Group Velocity | **Heat Capacity** | **Mean Free Path**

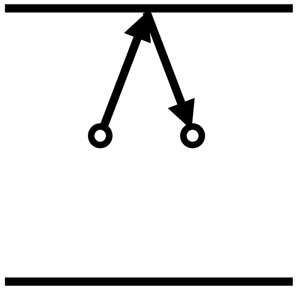
$$\Lambda_j(q) = v_j(q)\ \tau_j(q)$$

Phonon Band Structure (Silicon)

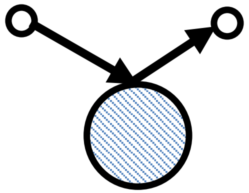


$\Lambda_{j,\ nano}$

Phonon-Boundary Scattering



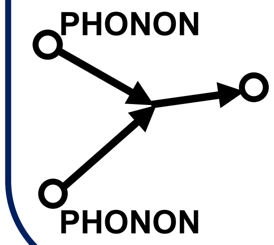
Phonon-Pore Scattering



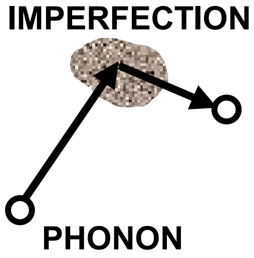
$\Lambda_{j,\ bulk}$

Bulk Scattering Mechanisms:

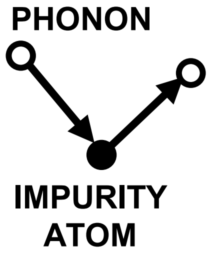
Phonon-Phonon Scattering



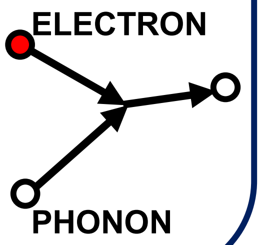
Phonon-Imperfection Scattering



Phonon-Impurity Scattering



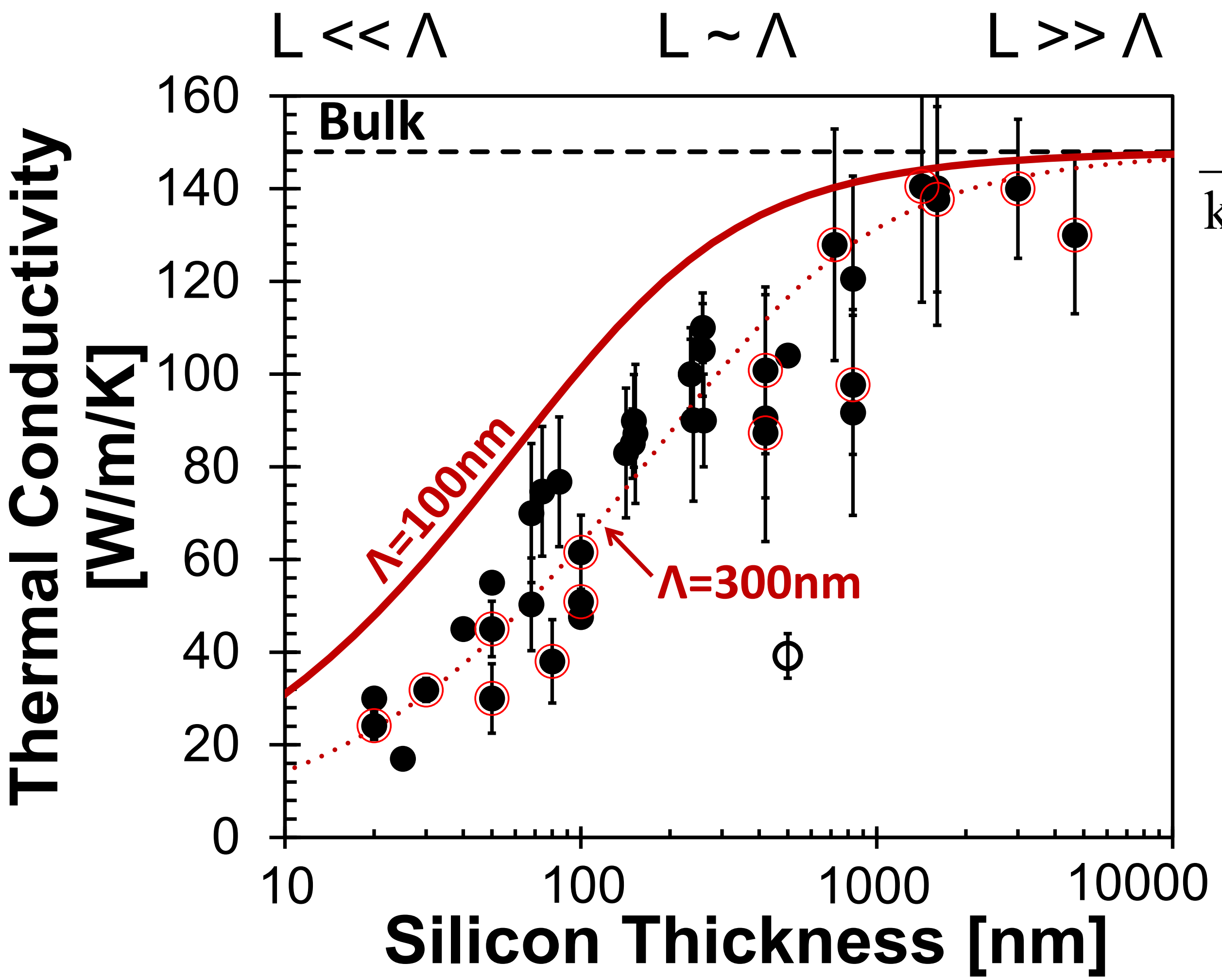
Phonon-Electron Scattering



Marconnet, Kodama, Asheghi, and Goodson, “Phonon Conduction in Periodically Porous Silicon Nanobridges“ *Nanoscale and Microscale Thermophysical Engineering* (2012).

Size Effect in Silicon

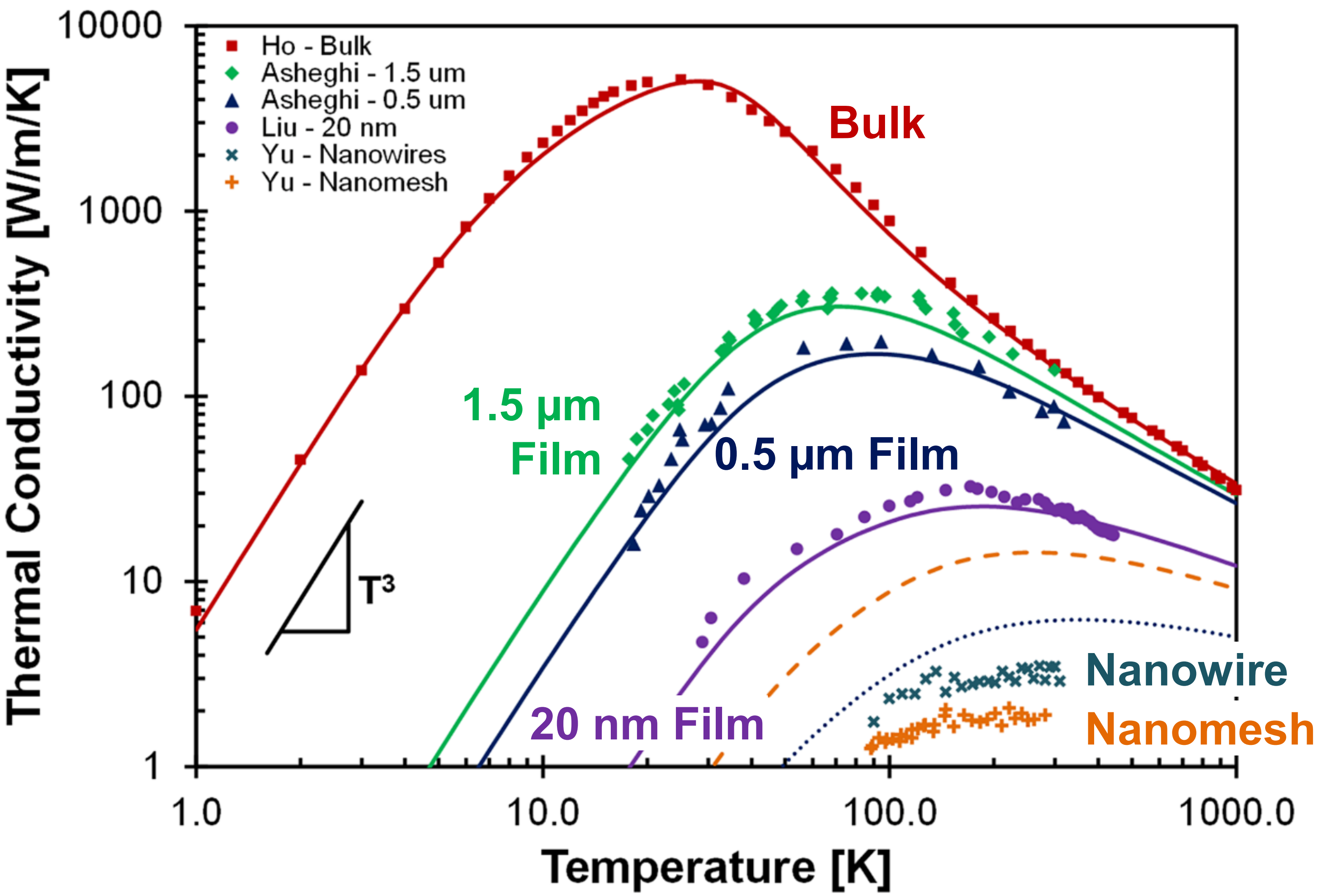
Approximation: Assume Spectral Independence



$$\frac{k}{k_{bulk}} = \frac{\overline{\Lambda}}{\Lambda_{bulk}} = F\left(\overline{\Lambda_{bulk}}, \{G\}\right)$$

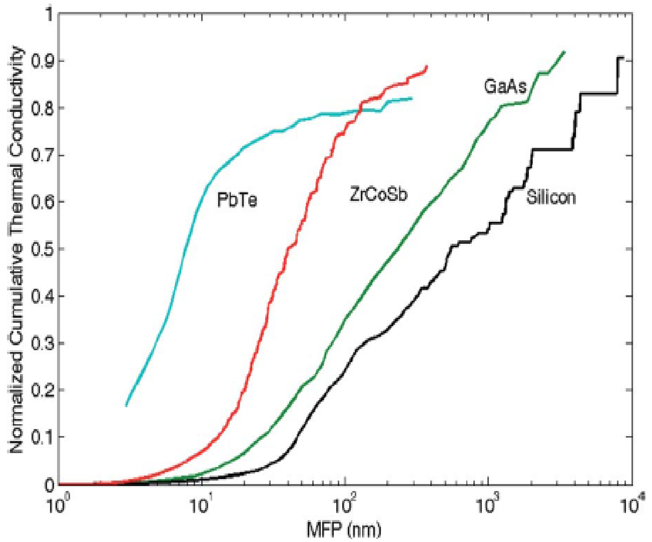
Marconnet, Asheghi, and Goodson, "From the Casimir Limit to Phononic Crystals: Twenty Years of Phonon Transport Studies using Silicon-on-Insulator Technology" *Journal of Heat Transfer* (2013).

Size Effect in Silicon



Marconnet, Asheghi, and Goodson, “From the Casimir Limit to Phononic Crystals: Twenty Years of Phonon Transport Studies using Silicon-on-Insulator Technology” *Journal of Heat Transfer* (2013).

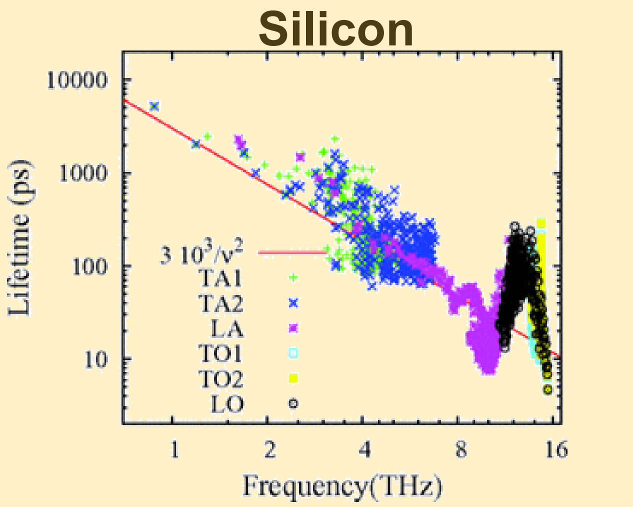
Spectral Dependence



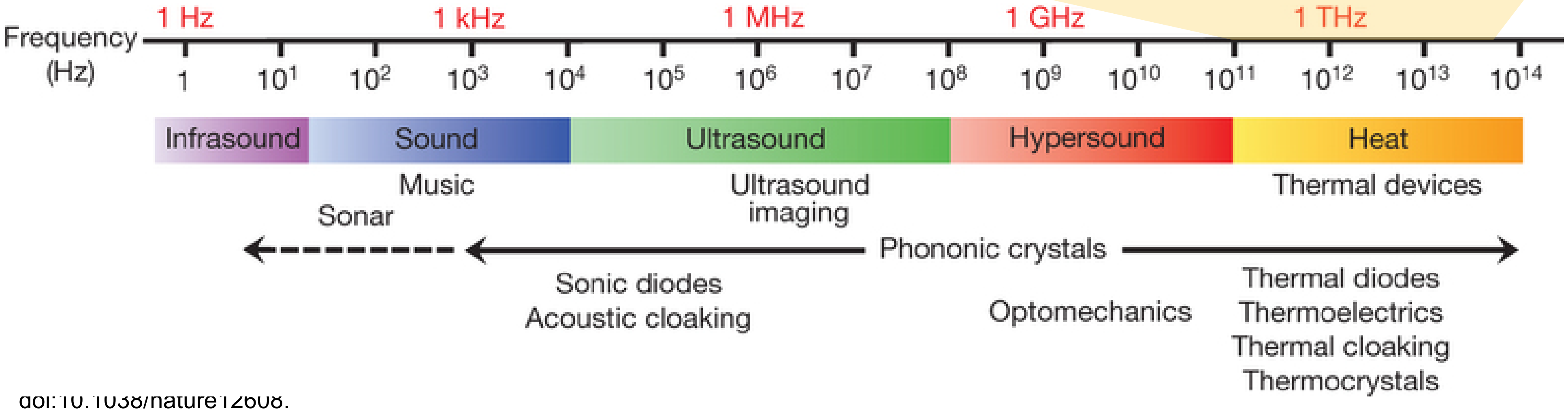
M. Zebarjadi et al., Energy & Environ. Sci. 5, 5147-5162 (2012). A. Henry et al., J. Comp. and Theor. Nanoscience, Vol. 5, pp. 141-152 (2008).

$$k = \frac{1}{6\pi^2}\sum_j \int v_j(q)\, c_{v,j}(q)\, \Lambda_j(q)\, q^2 dq$$

$$\Lambda_j(q) = v_j(q)\ \tau_j(q)$$

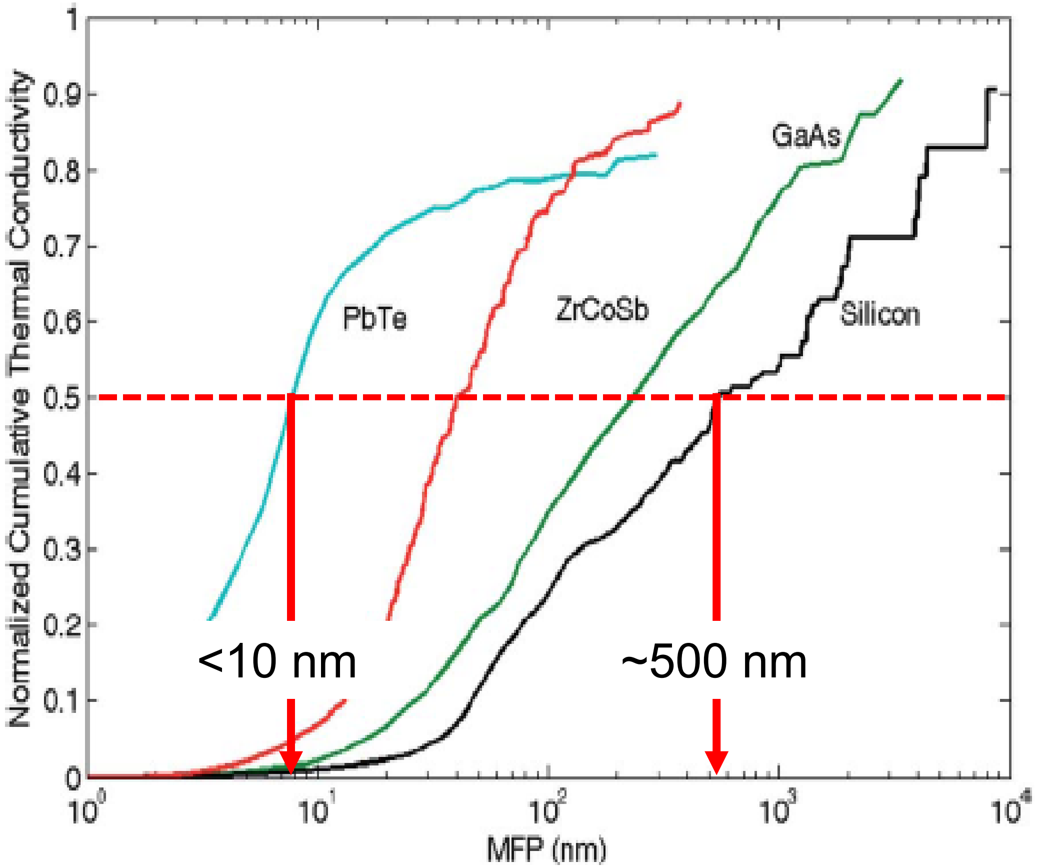


Esfarjani and Chen., "Heat transport in silicon from first-principles calculations," DOI: 10.1103/PhysRevB.84.085204



doi:10.1038/nature12608.

MFP Spectrum – Materials

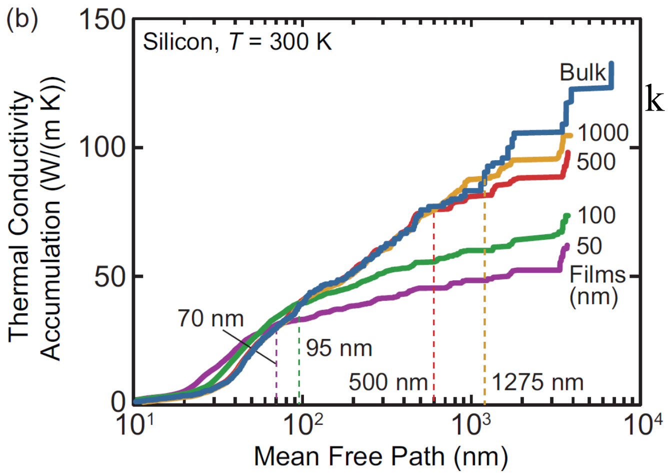


M. Zebarjadi et al., Energy & Environ. Sci. 5, 5147-5162 (2012).

A. Henry et al., J. Comp. and Theor. Nanoscience, Vol. 5, pp. 141-152 (2008).

To strongly impact the thermal conductivity, structures with appropriate length scales must be introduced into the system.

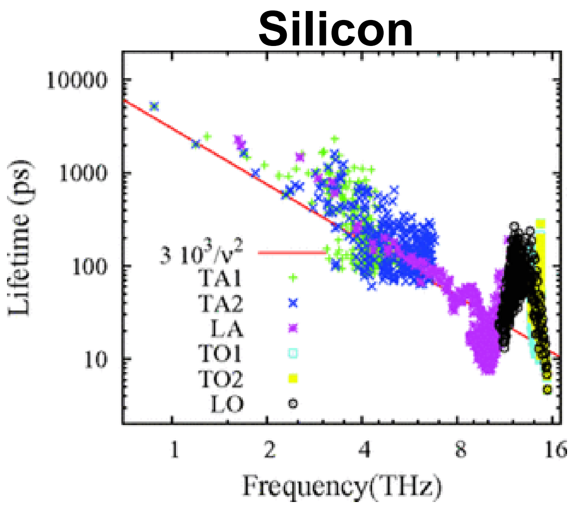
Silicon Thin Films



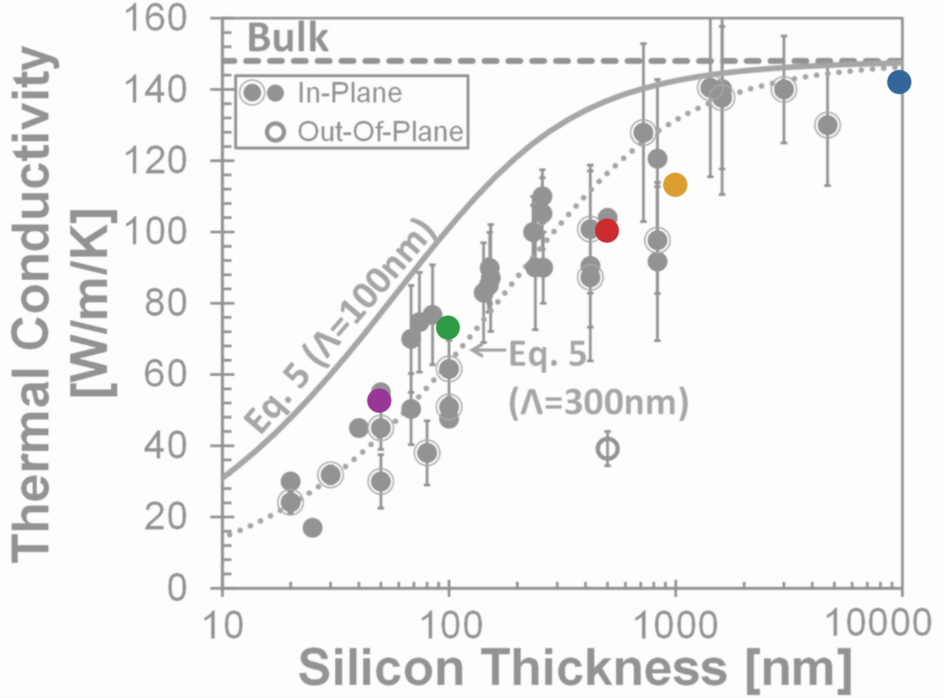
Jain *et al.*., "Phonon transport in periodic silicon nanoporous films with feature sizes greater t
DOI: 10.1103/PhysRevB.87.195301

$$k = \frac{1}{6\pi^2} \sum_j \int v_j(q) c_{v,j}(q) \Lambda_j(q) q^2 dq$$

$$\Lambda_j(q) = v_j(q) \quad \tau_j(q)$$

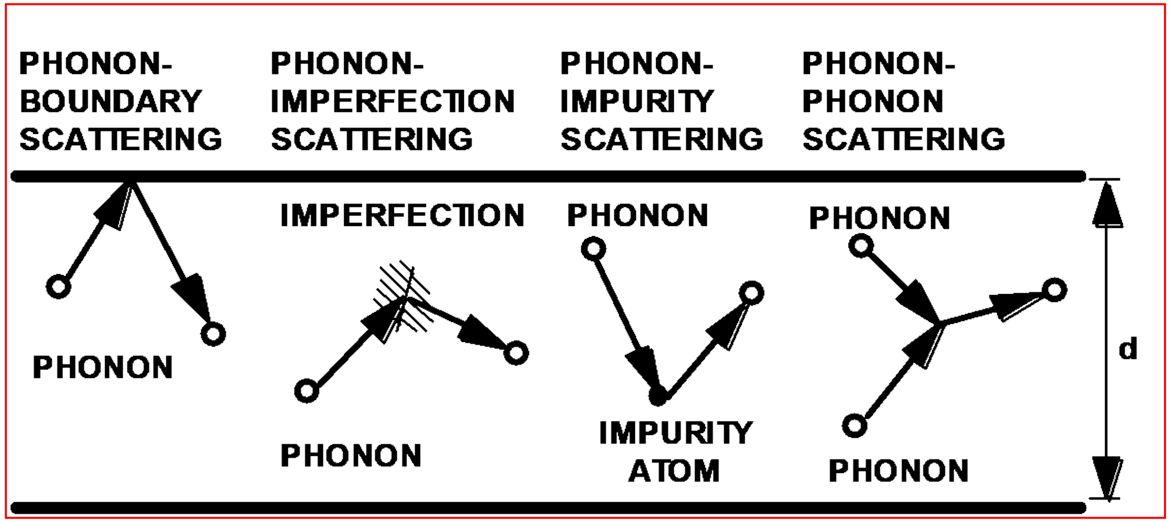


Esfarjani and Chen., "Heat transport in
con from first-principles calculations,"
OI: 10.1103/PhysRevB.84.085204



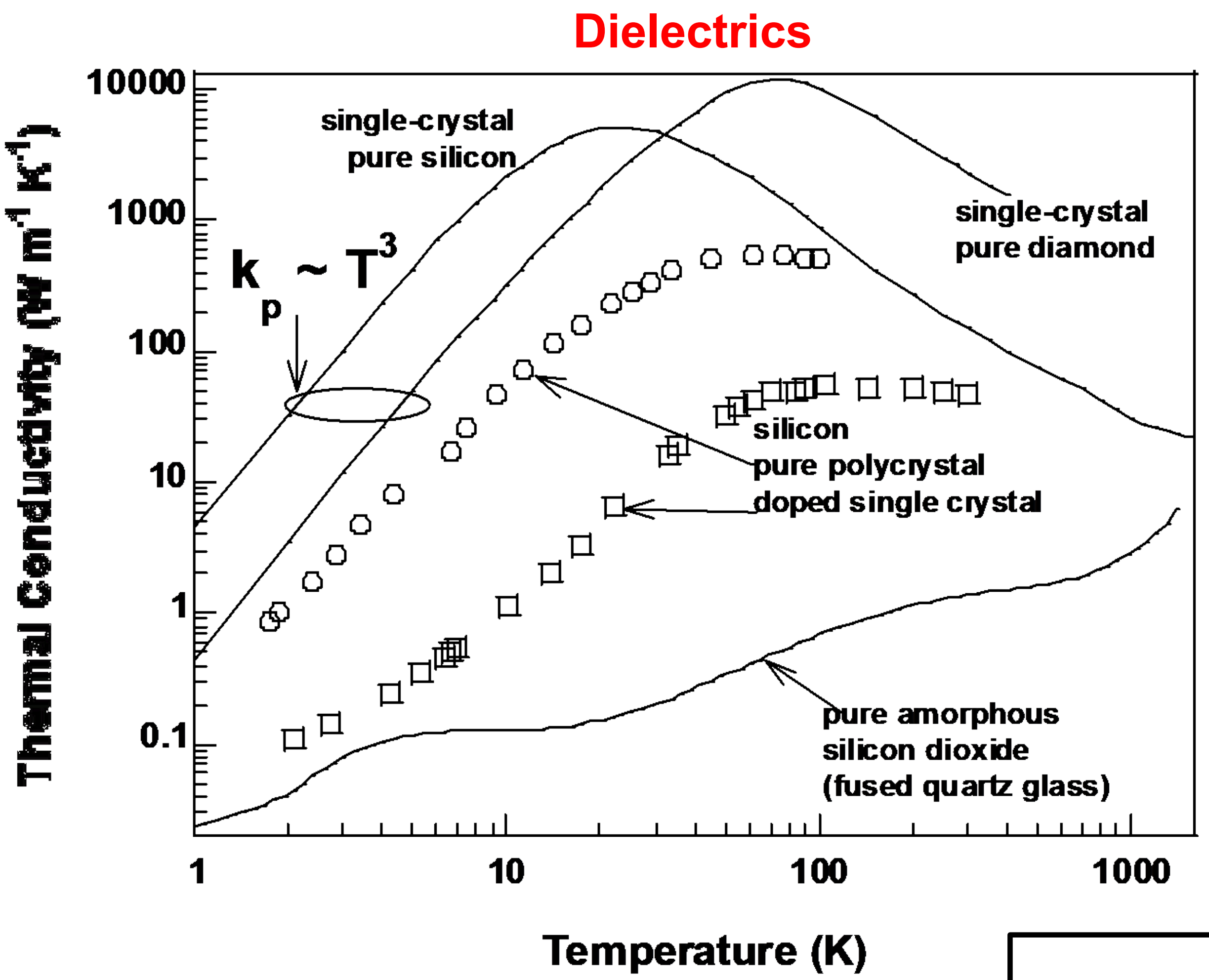
Effective Relaxation Time

- Defect Scattering (τ_i)
- U (Umklapp) Scattering (τ_U)
- Boundary Scattering $\left(\tau_b \sim \frac{L}{v_g}\right)$



- **Effective relaxation time**, τ_{eff}, by the Matthiessen's rule
  - $\frac{1}{\tau_{eff}} = \frac{1}{\tau_i} + \frac{1}{\tau_b} + \frac{1}{\tau_U}$
    - Assumes no interaction between scattering processes
- Effective mean free path: $\Lambda_{eff} = v_g \tau_{eff}$

Temperature Dependence of *k*: Dielectrics



$$k_p = \frac{1}{3} C_p v_p \Lambda_p$$

Specific Heat

Low-Temperature Limit ($T \ll \theta_D$):

$$C_s = \frac{12\,\pi^4}{5} n_a k_B \left(\frac{T}{\theta_D}\right)^3$$

High Temperature Limit ($T > \theta_D$):

$$C_s = 3\, n_a k_B \quad \text{(a constant)}$$

Debye Temperature:

$$\theta_D = \frac{\hbar\, v}{k_B} \sqrt[3]{6\pi\eta_a}$$

Scattering Time:

$$\frac{1}{\tau_p(\omega, T)} = \frac{1}{\tau_{p\text{-}p}(\omega, T)} + \frac{1}{\tau_{p\text{-}i}(\omega)} + \frac{1}{\tau_{p\text{-}b}}$$

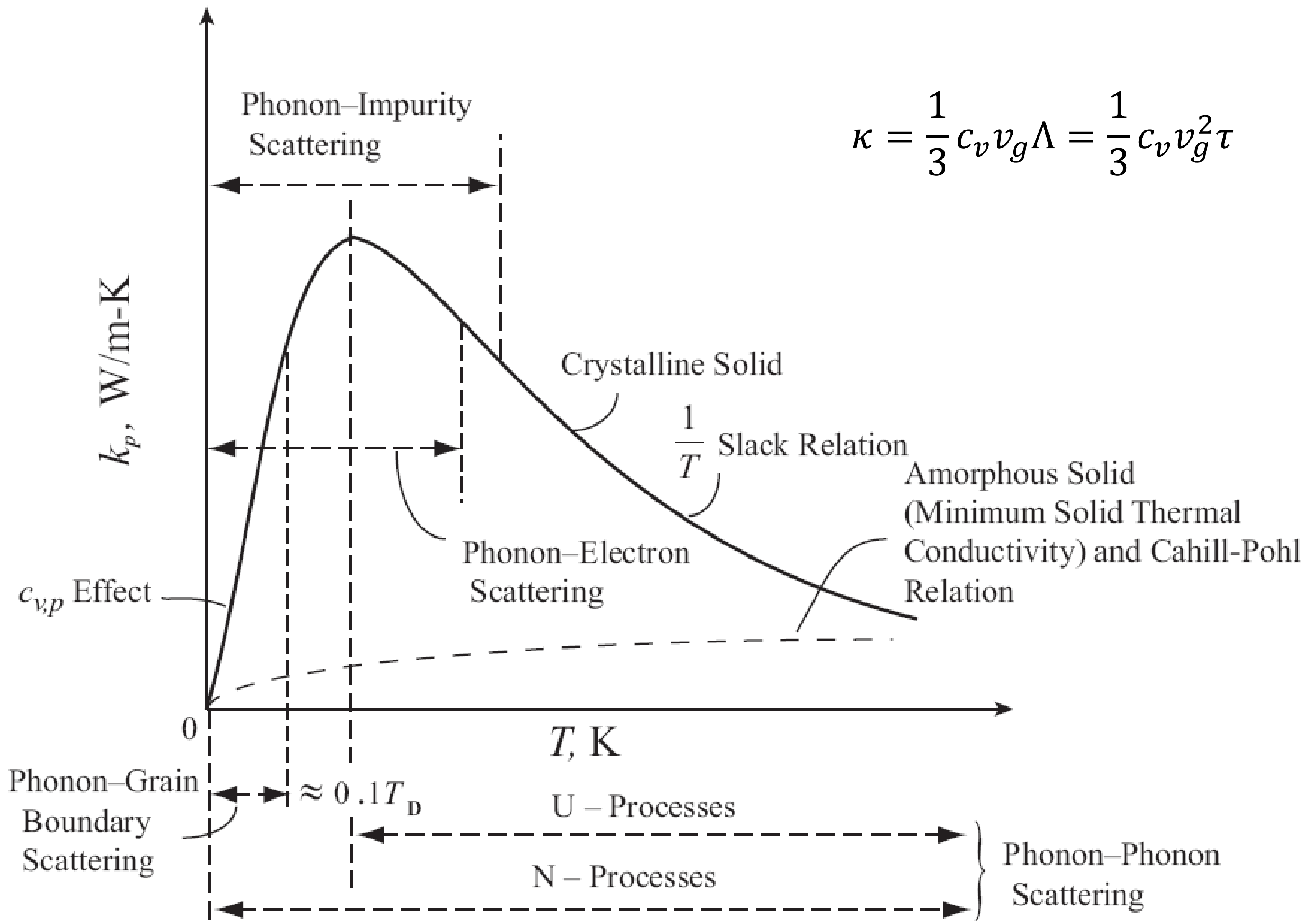
phonon-phonon, -impurity, -boundary

$$= c_{phonon}\, T^\gamma \exp(-B\ x_\omega) + c_{impurity}(T\ x_\omega)^4 + c_{boundary}\frac{v_p}{d}$$

Source: Goodson, Microscale Heat Conduction, 2008

Temperature Dependence of *k*: Dielectrics

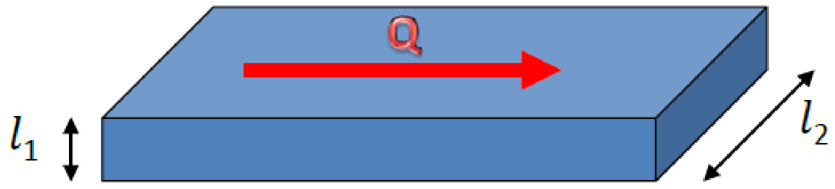
$$\kappa = \frac{1}{3} c_v v_g \Lambda = \frac{1}{3} c_v v_g^2 \tau$$



Source: Kaviany, Heat Transfer Physics, 2008

Simple Model for Boundary Scattering

$$\tau_b^{-1} = \frac{v_g}{FL}$$

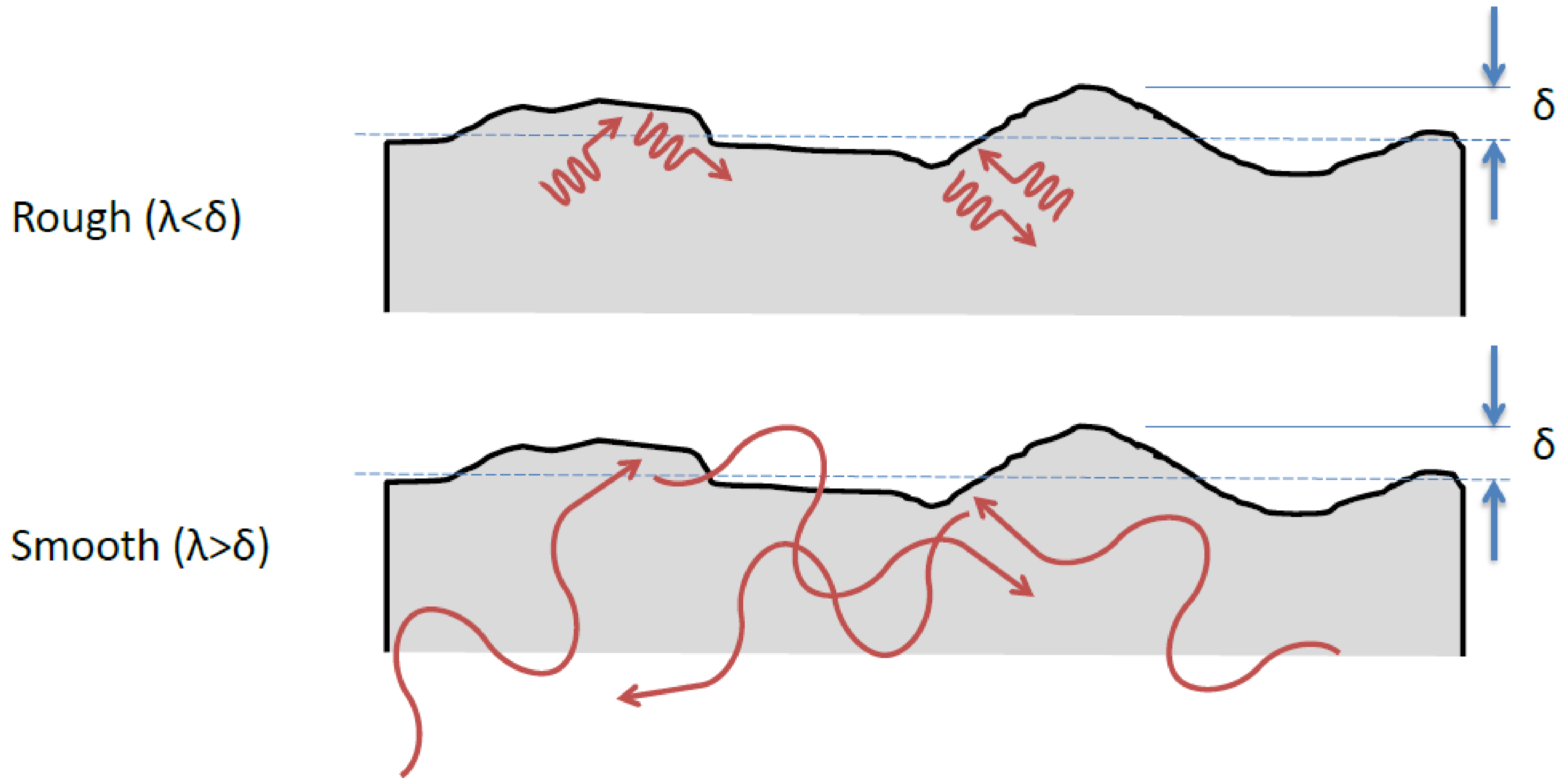


where $L = 2\sqrt{\frac{l_1 l_2}{\pi}}$

F is a geometric "fitting" parameter

Scattering depends on the smoothness of the boundary

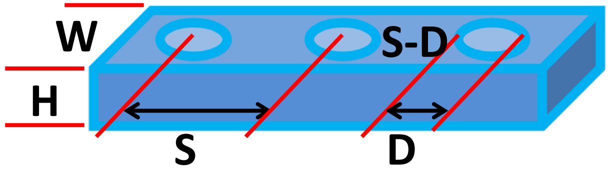
Boundary Specularity



Approaches for the Size Effect

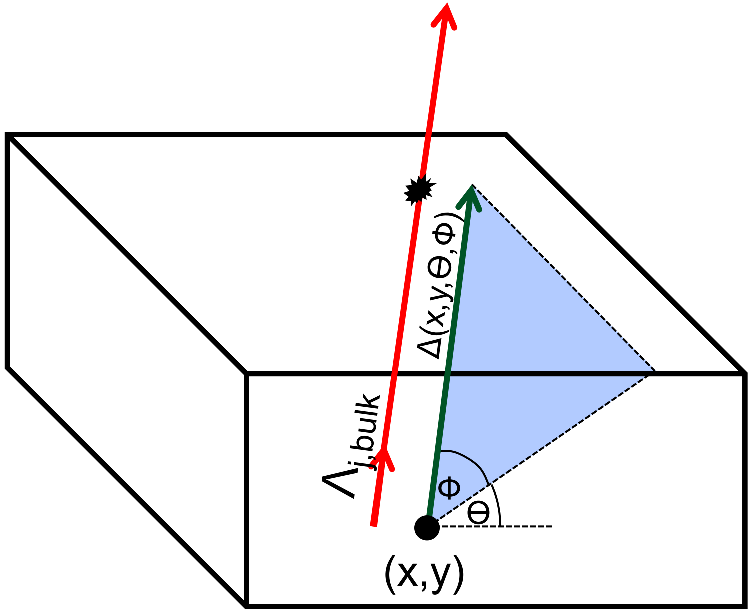
Method 1: Boundary Scattering Times + Matthiessen's Rule:

$$\tau_{j,NW} = \frac{d_h}{v_j(q)} \qquad \tau_{j,pores} = \frac{S-D}{v_j(q)}$$



$$\tau_j^{-1} = \tau_{j,pores}^{-1} + \tau_{j,NW}^{-1} + \tau_{j,bulk}^{-1}$$

Method 2: Conductivity Reduction Function:



$$\Lambda_{j,nano}\left(\Lambda_{j,bulk}(q),\{G\}\right) = F\left(\Lambda_{j,bulk}(q),\{G\}\right)\Lambda_{j,bulk}(q)$$

$$k = \frac{1}{6\pi^2}\sum_j \int v_j(q)\, c_{v,j}(q)\, F\left(\Lambda_{j,bulk}(q),\{G\}\right)\Lambda_{j,bulk}(q)\, q^2 dq$$

Integral Approach (Sondheimer, 1952):

$$F(\Lambda) = 1 - \frac{3}{4\pi A_c}\int_{A_c}\int_0^{2\pi}\int_0^{\pi} \sin\phi\cos^2\phi \exp\left(-\Delta/\Lambda\right) d\phi\, d\theta\, dS$$

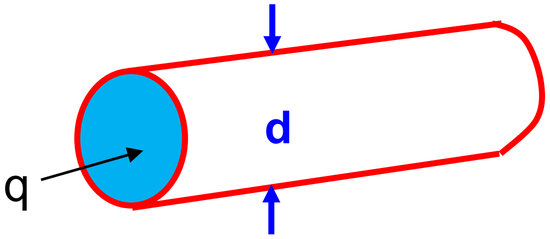
Originally derived for electrons use BTE.
Also applies to phonon transport.

Full model can include effect of "specularity" (related to roughness)

Conductivity Reduction Function

Gray Approximation: $\Lambda_{bulk} = constant \rightarrow k_{nano}/k_{bulk} \approx \Lambda_{nano}/\Lambda_{bulk}$

Solid wires:



$$\frac{k_{eff}}{k_{bulk}} = \left[1 + \frac{\Lambda}{d}\right]^{-1}$$

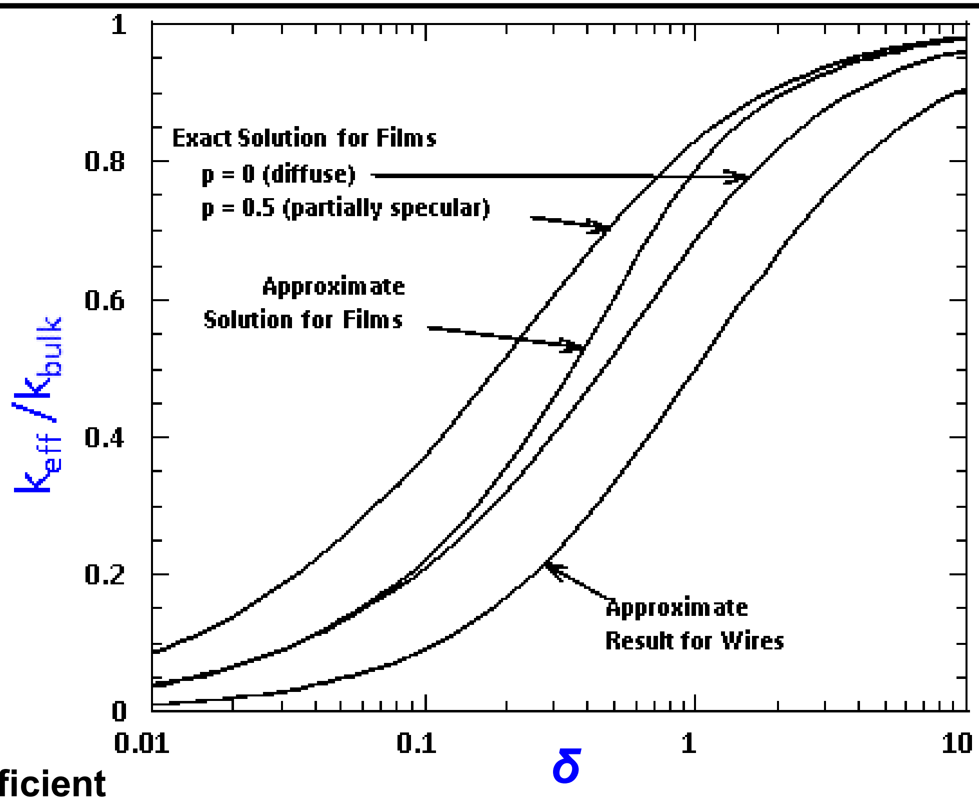
Nordheim, 1934, in "Die Theorie der Thermoelektrischen Effekte," Act. Scie et Ind., No. 131, Hermann, Paris.

Solid films:

Exact: $$\frac{k_{eff}}{k_{bulk}} = 1 - \frac{3(1-p)}{2\delta}\int_1^{\infty}\left(\frac{1}{\xi^3} - \frac{1}{\xi^5}\right)\frac{1-\exp(-\delta\xi)}{1-p\exp(-\delta\xi)}d\xi$$

where with $\delta = d/L$ and p ($0 < p < 1$) is the specular reflection coefficient

Sondheimer, 1952, "Mean Free Path of Electrons in Metals," from Advances in Physics, Vol. 1, pp. 1-42.



Approx.:

$$\frac{k_{eff}}{k_{bulk}} = 1 - \frac{2}{3\pi\delta} \quad \text{for } \delta < 1$$

$$\frac{k_{eff}}{k_{bulk}} = 1 - \frac{2(1-S^3)}{3\pi\delta} + \frac{2\delta}{\pi}\ln\left[\frac{1+\delta+S}{1+\delta-S}\right] - \frac{2}{\pi}\arccos(\delta) \quad \text{for } \delta > 1$$

Flik and Tien, 1990, J. Heat Transfer, Vol. 112, pp. 872-881. **with $\delta = d/L$ and $S = (1 - \delta^2)^{0.5}$**

Thermal Conductivity of Metals

- **Electrons are now our energy carriers**

- **Simple estimate of metal thermal conductivity:**

- $k_e = \frac{1}{3} c_e \, v_F \, \Lambda_e = \frac{1}{3}(\gamma T) v_F \Lambda_e$ where $\gamma = \frac{\pi^2 n_e k_B^2}{m_0 v_F^2}\left(\frac{m^*}{m_0}\right)$

- **What can electrons scatter on?**
  + Phonons
  + Impurities & Imperfections
  + Boundaries (what size matters? $\Lambda_e(300\ \mathrm{K}) \sim 50\mathrm{nm}$)

$$\frac{1}{\Lambda_e} = \frac{1}{\Lambda_{e-p}} + \frac{1}{\Lambda_{e-i}}$$

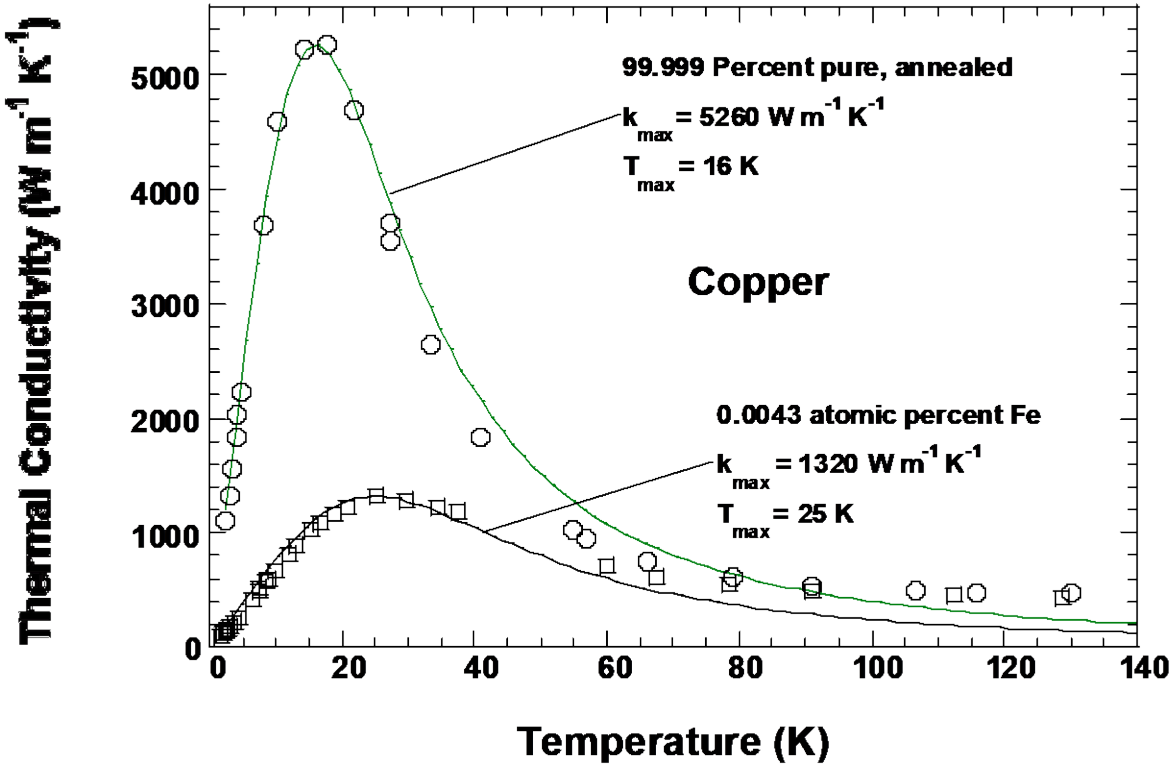
Wiedemann Franz Lorenz Law (WFL)

- Relates electrical and thermal conductivity
- Electrical Conductivity: $\sigma_e = \frac{n_e q^2 \Lambda_e}{v_F m^*}$
- Thermal Conductivity: $\mathrm{k_e} = \frac{1}{3}\frac{\pi^2 n_e k_B^2}{m_0 v_F^2}\left(\frac{m^*}{m_0}\right) T v_F \Lambda_e$

$$\frac{k_e}{\sigma_e} = \frac{\frac{1}{3}\left(\frac{\pi^2 n_e k_B^2}{m_0 v_F^2}\left(\frac{m^*}{m_0}\right) T\right) v_F \Lambda_e}{\frac{n_e q^2 \Lambda_e}{v_F m^*}} = \frac{\pi^2 k_B^2}{3q^2} T = L_0 T = \left(2.45 \times 10^{-8} W\,\Omega\,K^{-2}\right) T$$

(assuming m approximately m_0)*

Low Temperature Conductivity

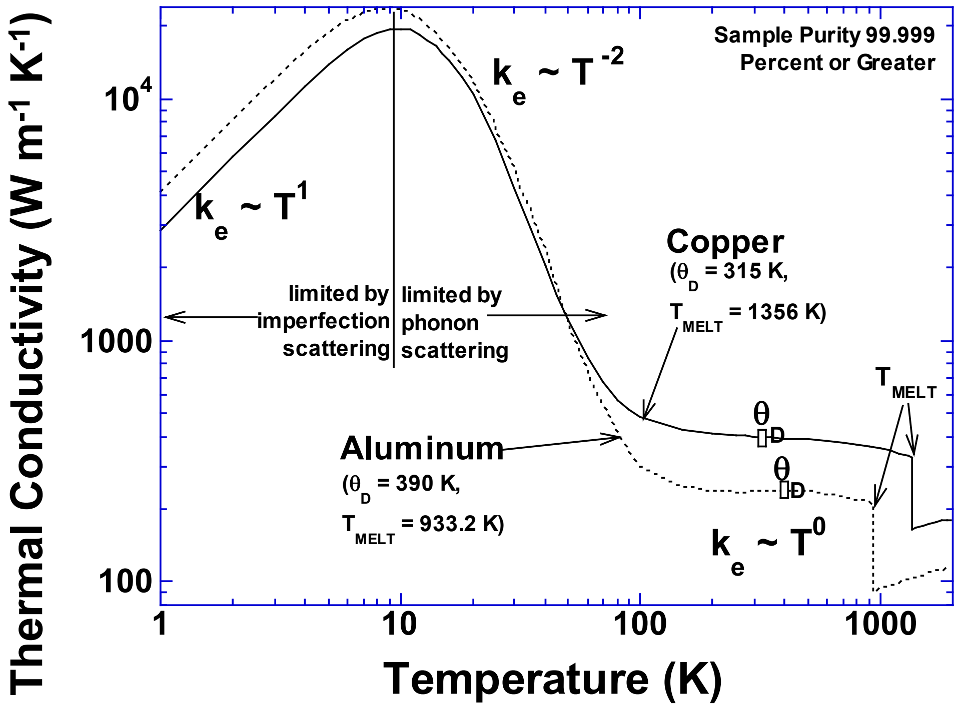


$$k_e = \frac{1}{3} c_e \, v_F \, \Lambda_e = \frac{1}{3} c_e v_F \left[\frac{1}{\Lambda_{e-i}} + \frac{1}{\Lambda_{e-p}}\right]^{-1} = \frac{1}{\alpha T^2 + \frac{\beta}{T}}$$

$$T_{max} = \left(\frac{\beta}{2\alpha}\right)^{1/3}$$

Source: Goodson, Microscale Heat Conduction, 2008

Temperature Dependence



$$k = 0.989\ k_\theta\ \exp\left[\frac{0.0117}{(T/\theta)^{2.5}}\right] \quad , \quad 0.3\ \theta < T < 0.86\ \theta$$

$$k = k_\theta\left(1.05 - 0.05\ \frac{T}{\theta}\right) \quad , \quad 0.86\ \theta < T < 3\ \theta$$

Source: Goodson, Microscale Heat Conduction, 2008

Parameters for High-T Model

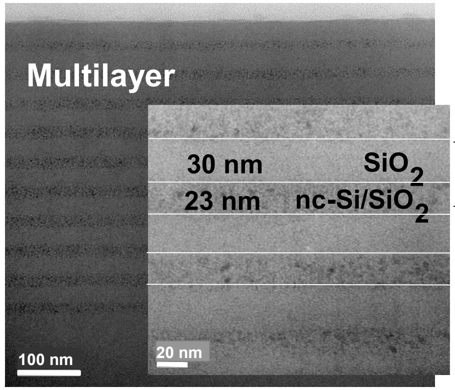
Metal	Z	A_r	θ, K	T_{melt}, K	k_θ, W m^{-1} K^{-1}	$k_{\theta\ i}$, W m^{-1} K^{-1}
Ag	47	107.870	215	1234	420	380
Al	13	26.982	390	933.2	230	210
Au	79	196.97	170	1336.2	348	320
Cd	48	112.40	220	594.2	113	84
Cu	29	63.54	315	1356	414	330
Ir	77	192.2	285	2716	160	130
Mg	12	24.31	290	923	170	140
Pb	82	207.19	88	600.58	47	35
Pd	46	106.4	275	1825	72	60
Rh	45	102.91	370	2233	160	130
Ti	22	47.90	350	1953	25	15
Tl	81	204.4	100	576.2	60	44
W	74	183.85	310	3653	170	160
Zn	30	65.37	250	692.7	140	105
Zr	40	91.22	280	2125	26	19
Co	27	58.93	385	1765	130	100
Cr	24	51.99	485	2118	84	65
K	19	39.10	100	336.8	120	100
Li	3	6.939	400	453.7	80	65
Mo	42	95.94	380	2883	150	120
Na	11	22.99	150	371.0	150	120
Pt	78	195.1	225	2042	60	65
Rb	37	85.47	85	312.04	75	60
Re	75	186.2	300	3453	55	45

Source: Goodson, Microscale Heat Conduction, 2008

Nanoelectronic Interfaces

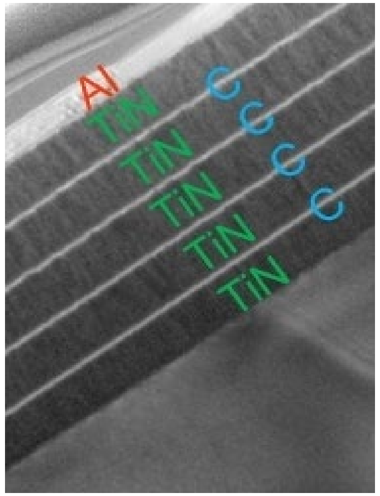
CMOS Optical Interconnects

Physical Review B
(Rowlette et al. 2009)

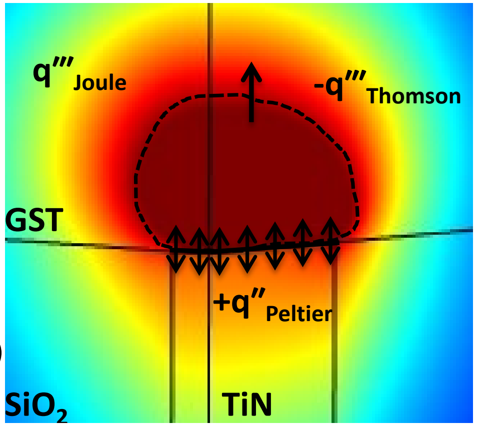


Composite Substrates

Electron Device Letters
(Cho et al., 2011)



Electron Device Letters
(Bozorg-Grayeli et al. 2011)

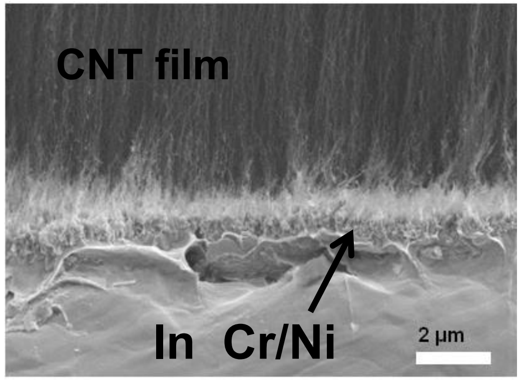


Electron Device Letters
(Reifenberg et al. 2008, 2010)

Nanotechnology
(Lee et al., under review)

Low-Energy PCRAM

Applied Physics Letters
(Reifenberg et al. 2007)

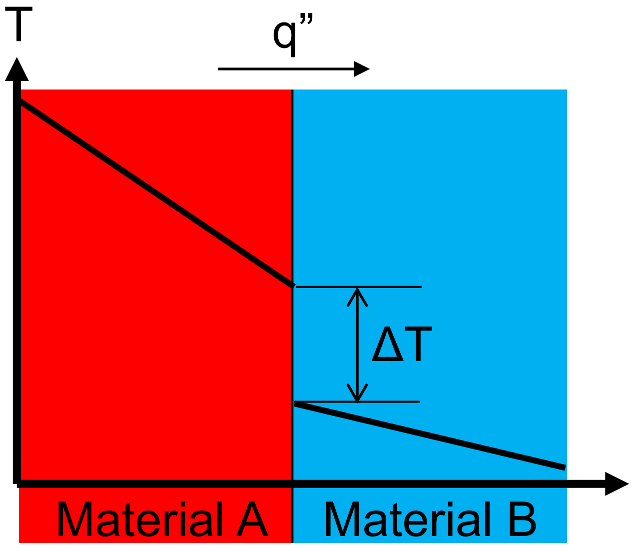


Nanotube Interfaces

Nano Letters
(Panzer et al. 2010)

ACS Nano
(Marconnet et al. 2011)

Boundaries & Interfaces



Thermal Resistance

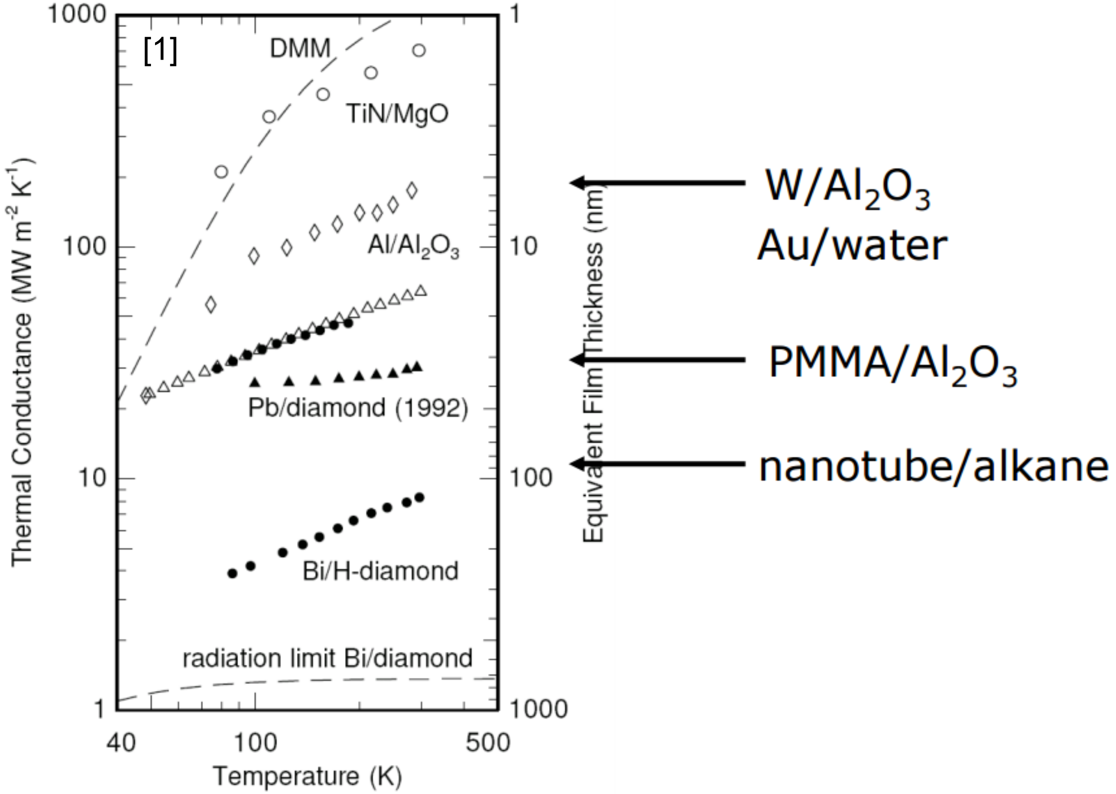
$$R = \frac{\Delta T}{q} \quad \text{in [K/W]}$$

$$R'' = \frac{\Delta T}{q''} \quad \text{in [m}^2\text{ K/W]}$$

Thermal Conductance

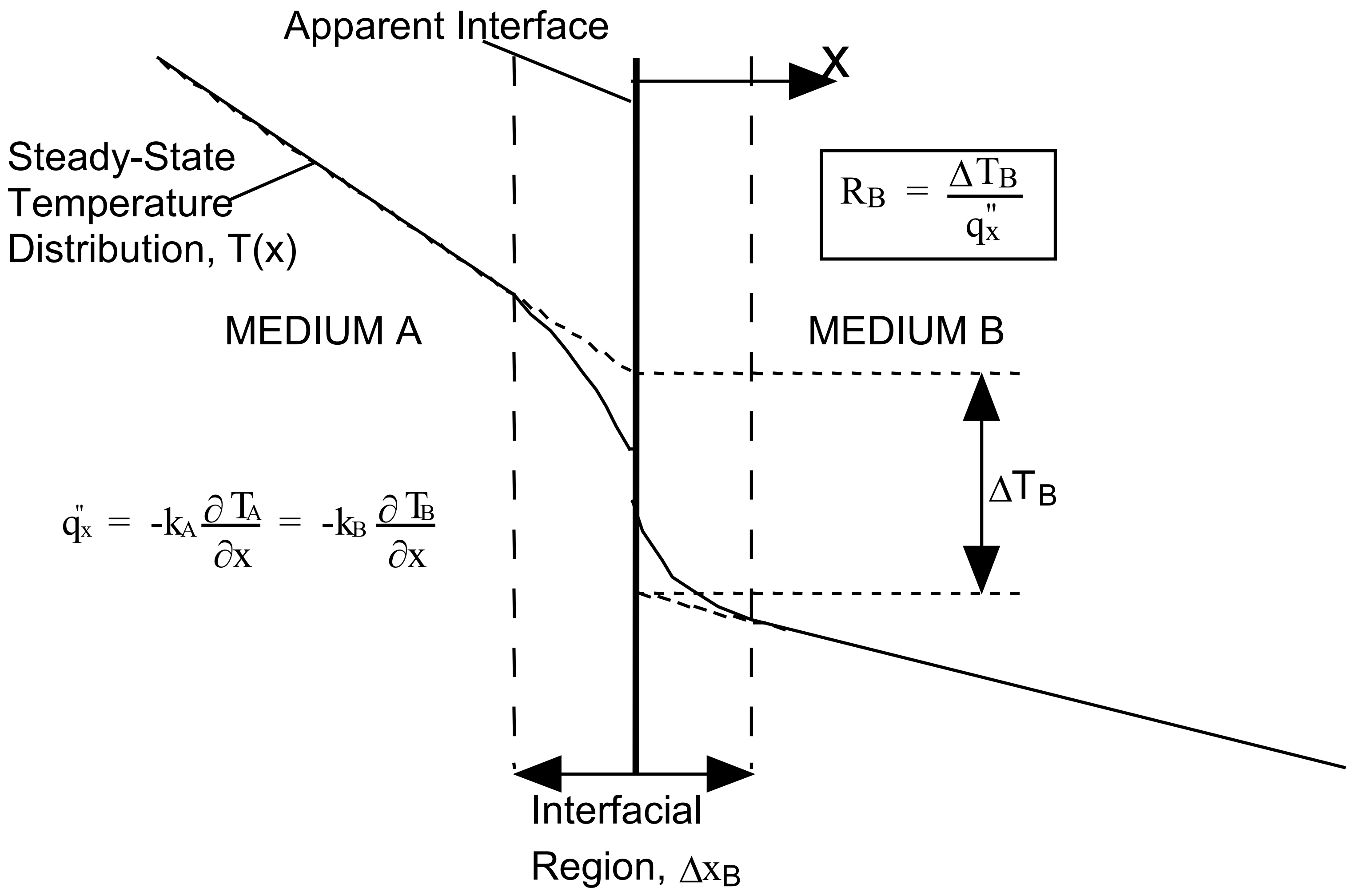
$$= \frac{q}{\Delta T} \quad \text{in [W/K]}$$

$$G = \frac{q''}{\Delta T} \quad \text{in [W/(m}^2\text{ K)]}$$



[1] http://users.mrl.illinois.edu/cahill/tongji_tdtr_fundamentals.pdf

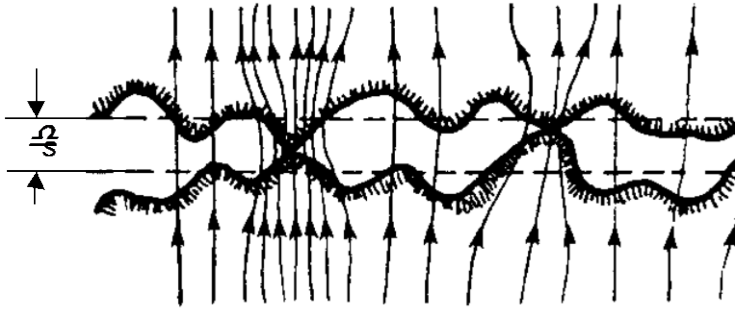
Thermal Boundary Resistance



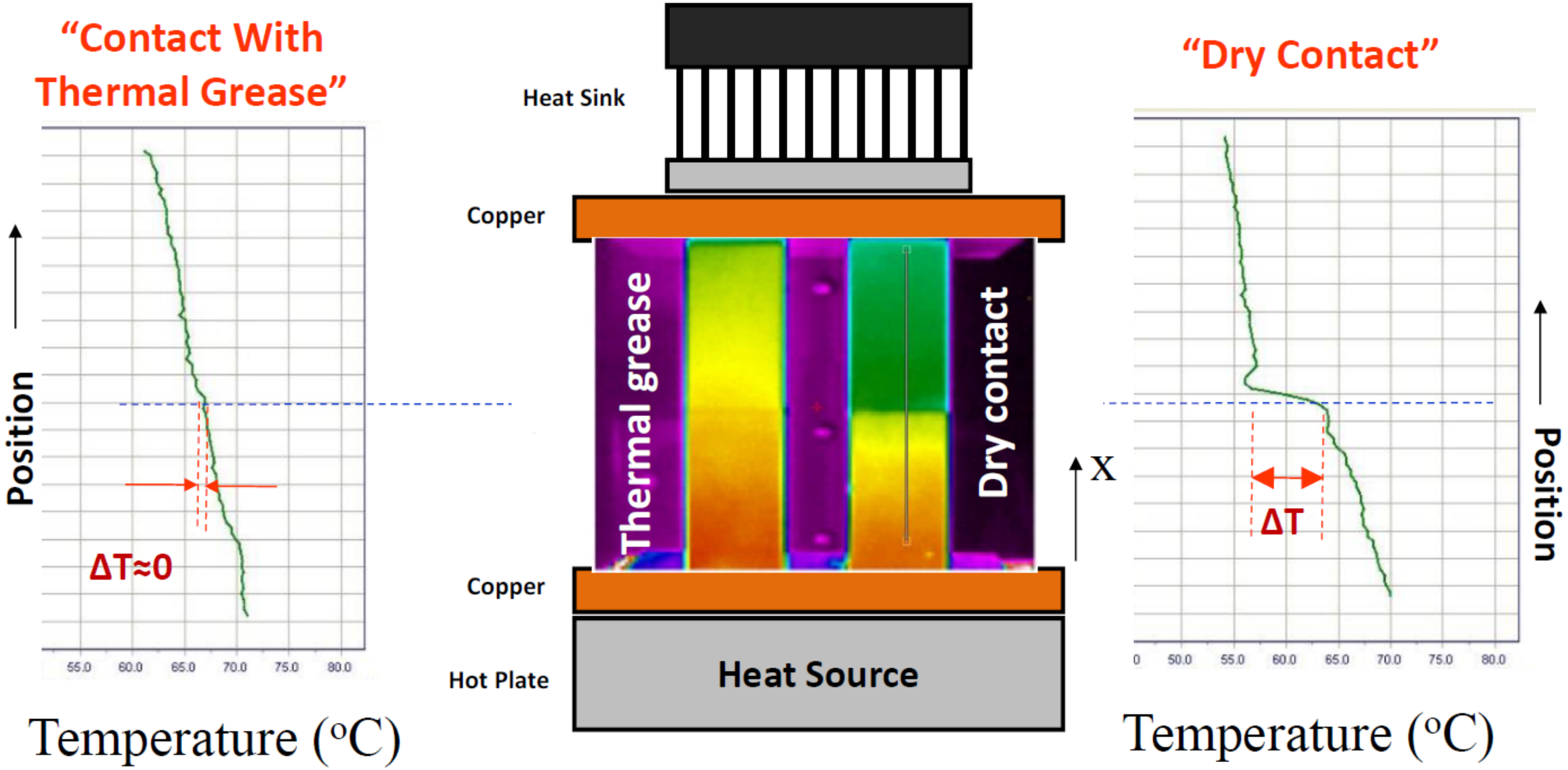
Ref: Goodson ME 352B (2011)

Thermal Boundary Resistance

1. Incomplete Contact:
Constricts heat flow through the contact regions

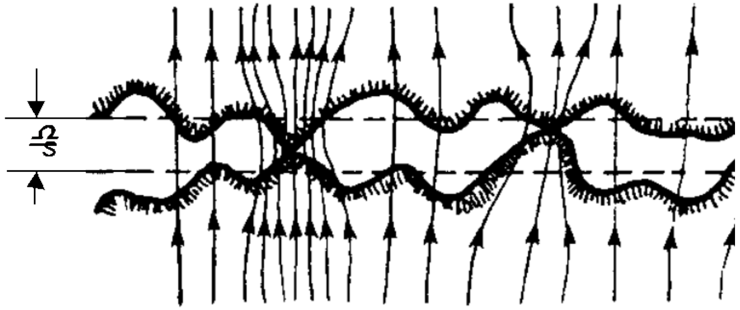


Dealing with Incomplete Contact



Courtesy of Michael Barako and Mehdi Asheghi (Stanford)

1. Incomplete Contact:
Constricts heat flow through the contact regions



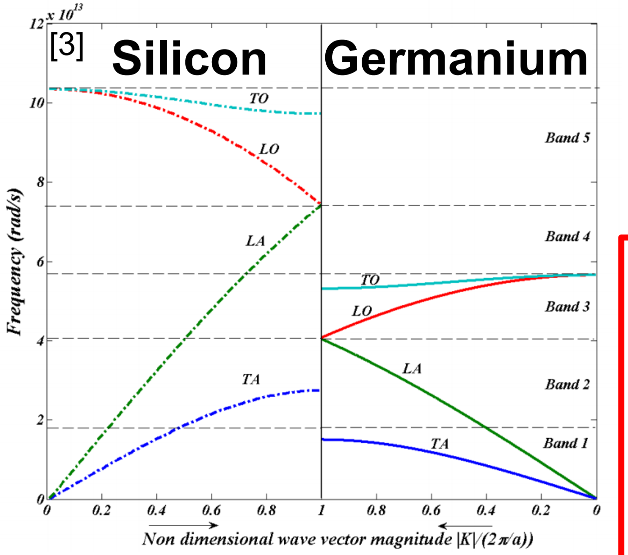
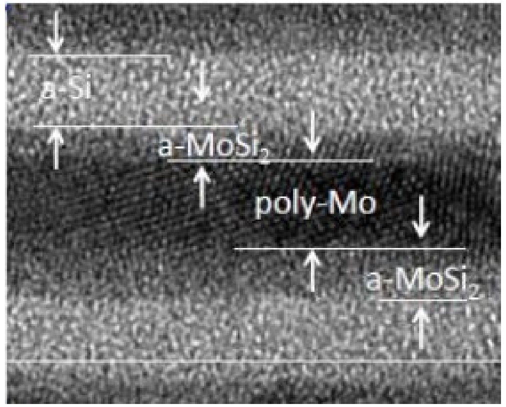
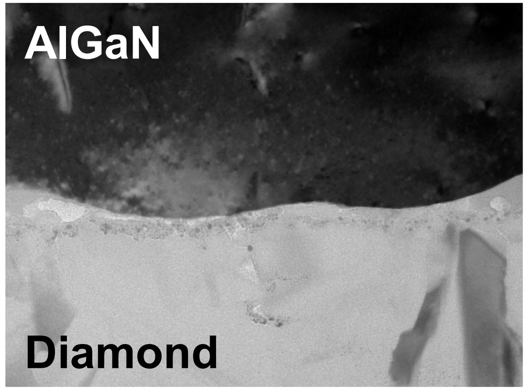


Fig. 4(a): Phonon dispersion in Si and Ge along [100] direction

2. Near Interfacial Disorder:
Microstructural defects and phase or stoichiometric disorder scatter electron and phonon heat carriers



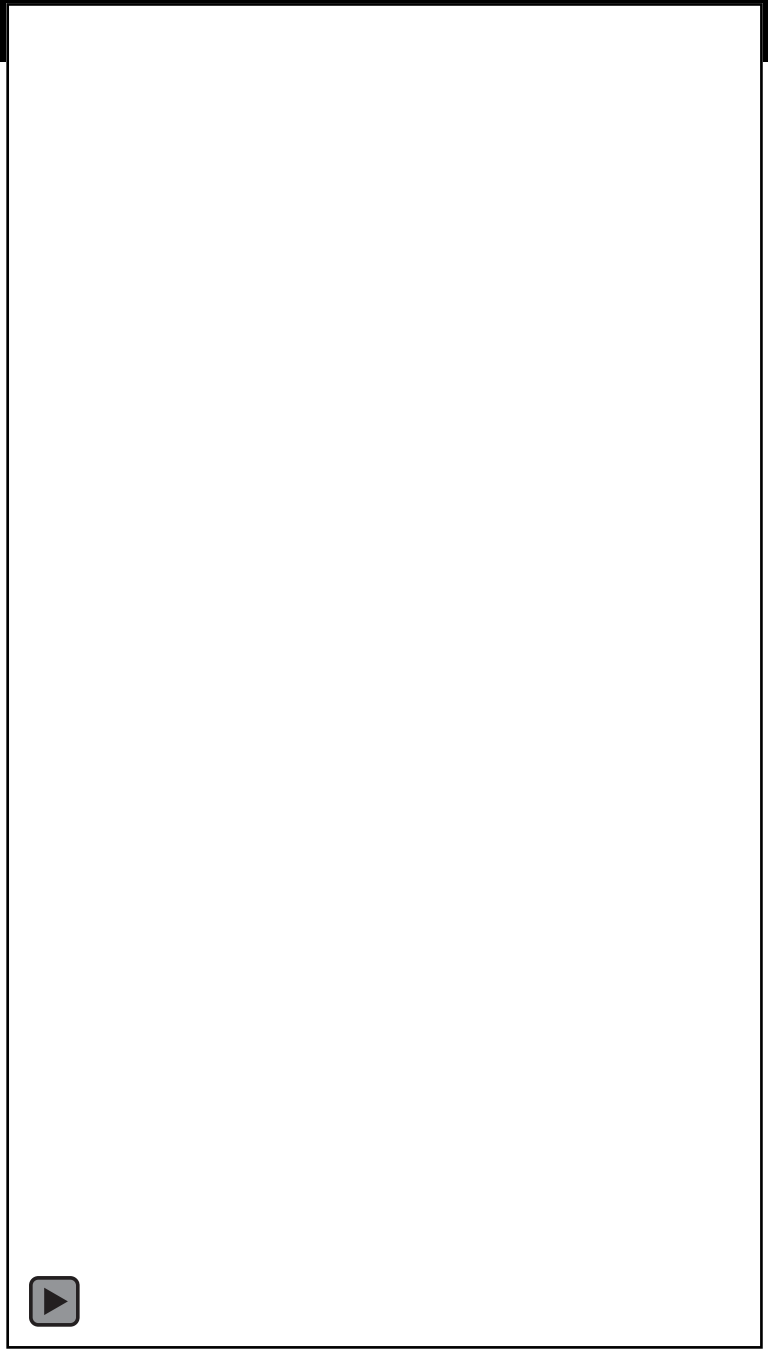
Lee et al., JAP, 2011

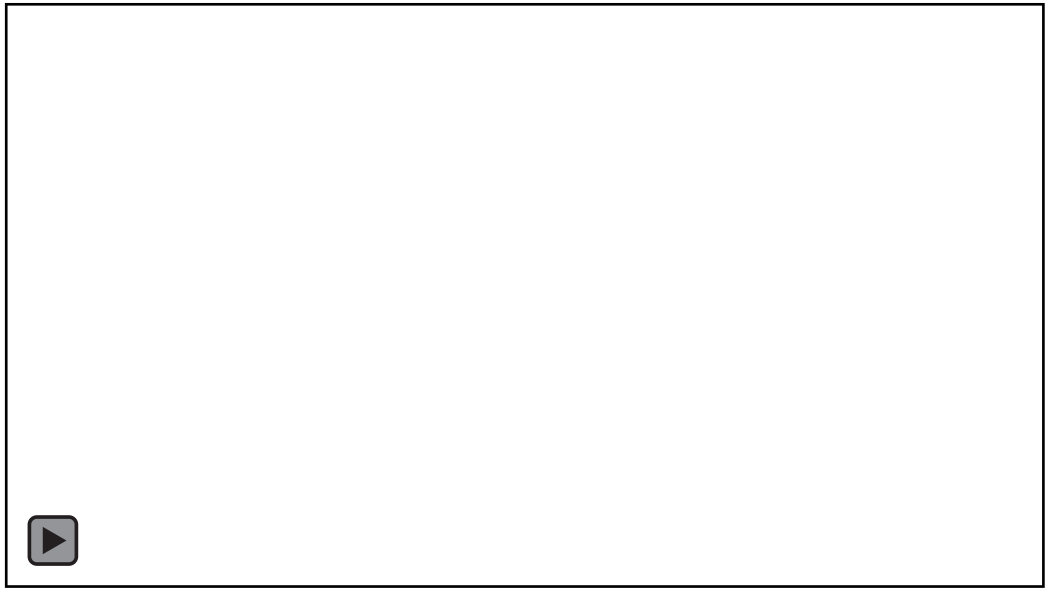


Cho et al., EDL, 2011

3. Boundary Scattering & Transmission
Difference in the spectra and possibly type of energy carriers on each side of the interface yields partial transmission of the energy carriers

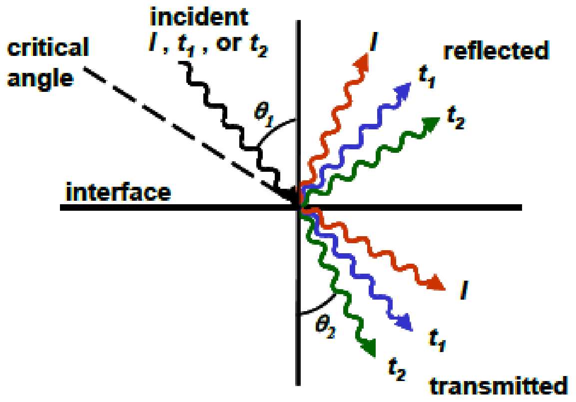
[3] Singh et al. arXiv:1005.2578





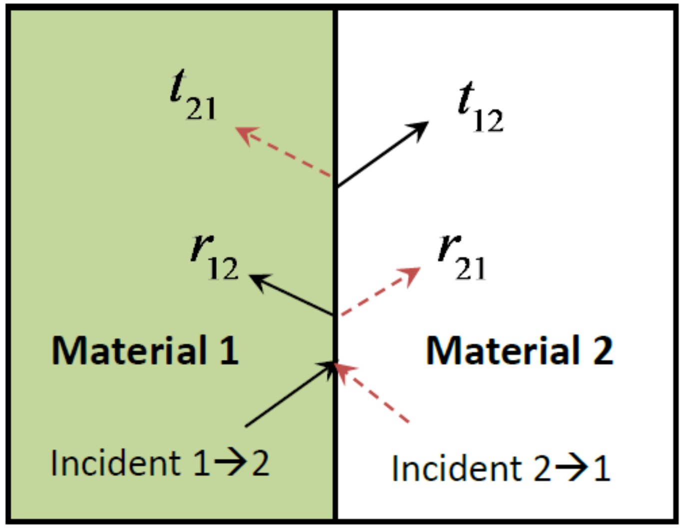
Acoustic Mismatch Model:

- Phonons treated by continuum acoustics with a planar interface (Wavelength >> Interatomic Spacing)
- Phonons specularly reflect, reflect and mode convert, refract, or refract and mode convert.
- Acoustic mismatch model in 3D uses the equivalent of Fresnel equations (A. Little, Canadian Journal of Physics, **37** 334, 1959). Often, approximate averages are
  used for transmission (Swartz & Pohl, Rev. Mod. Phys. **61** 605, 1989)
- Energy transmission probability: $\alpha_{1\rightarrow 2} = \frac{Z_2 Z_1}{(Z_1+Z_2)^2}$



Diffusive Mismatch Model:

- In diffuse scattering a phonon loses the memory of its origin and its type (branch)
- Applies well to interfaces that are rough compared to the carrier wavelength
- Therefore, a carrier moving away from the interface does not ‘know’ whether it was transmitted or reflected



Diffuse vs. Acoustic Mismatch

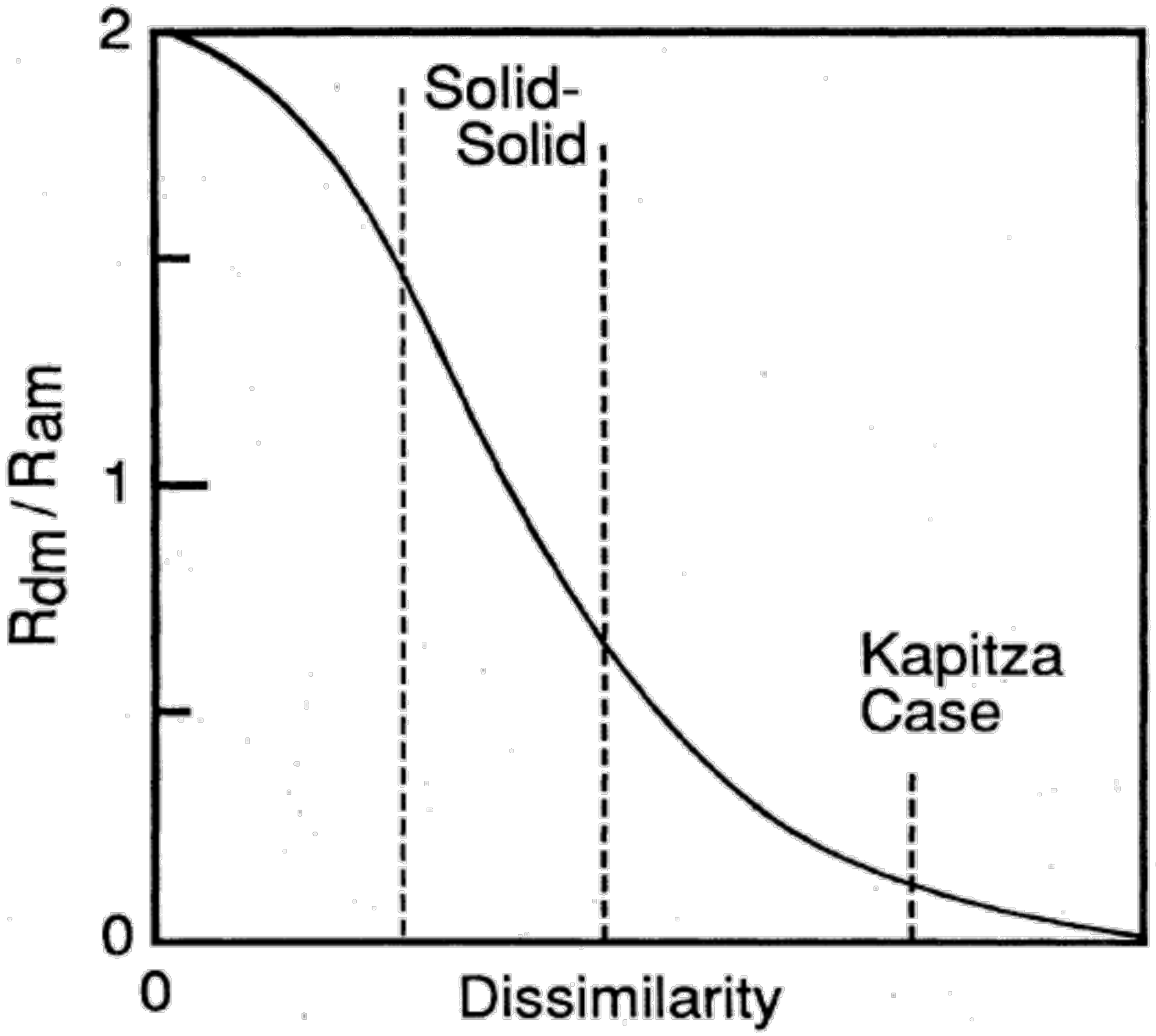


FIG. 14. Plot of the ratio of the diffuse mismatch model thermal boundary resistance to the acoustic mismatch model thermal boundary resistance vs the "amount of mismatch." The horizontal scale is qualitative and has arbitrary units; see text. The leftmost dotted line exemplifies a solid-solid boundary with relatively little dissimilarity, such as aluminum on quartz, the middle dotted line exemplifies a solid-solid boundary with large dissimilarity, such as platinum on quartz, and the rightmost dotted line marks the beginning of the region of extremely large dissimilarity, as found in the Kapitza (liquid helium-to-solid) case. The plot serves to summarize qualitatively the results of several calculations, including those in Table II. From Swartz (1987).

Low temperature limits:

Acoustic Velocities

Function of transmission probability

AMM:

$$R_{\mathrm{Bd}} = \left[\frac{\pi^2}{15}\frac{k_B^4}{\hbar^3}\left[\sum_j c_{1,j}^{-2}\Gamma_{1,j}\right]\right]^{-1} T^{-3}$$

$$= \left[2.04\times 10^{10}\left[\sum_j c_{1,j}^{-2}\Gamma_{1,j}\right]\right]^{-1}\times T^{-3}\left[\frac{\mathrm{sec}^2}{\mathrm{cm}^2}\mathrm{K}^3\frac{\mathrm{K}}{\mathrm{W/cm}^2}\right]$$

DMM:

$$R_{dm} = \left[\frac{\pi^2}{15}\frac{k_B^4}{\hbar^3}\frac{1}{2}\frac{\left[\sum_j c_{i,j}^{-2}\right]\left[\sum_j c_{3-i,j}^{-2}\right]}{\sum_{i,j} c_{i,j}^{-2}}\right]^{-1} T^{-3}$$

$$= \left[1.02\times 10^{10}\frac{\left[\sum_j c_{i,j}^{-2}\right]\left[\sum_j c_{3-i,j}^{-2}\right]}{\sum_{i,j} c_{i,j}^{-2}}\right]^{-1}\times T^{-3}\left[\frac{\mathrm{cm}^2}{\mathrm{sec}^2}\mathrm{K}^3\frac{\mathrm{K}}{\mathrm{W/cm}^2}\right]$$

(Swartz & Pohl, Rev. Mod. Phys. **61** 605, 1989)

Multi-Carrier Interface effects

Multicarrier transport and non-equilibrium

Scattering on phase & grain boundaries and stoichiometric impurities

Coupling & reflection at low-dimensional interfaces

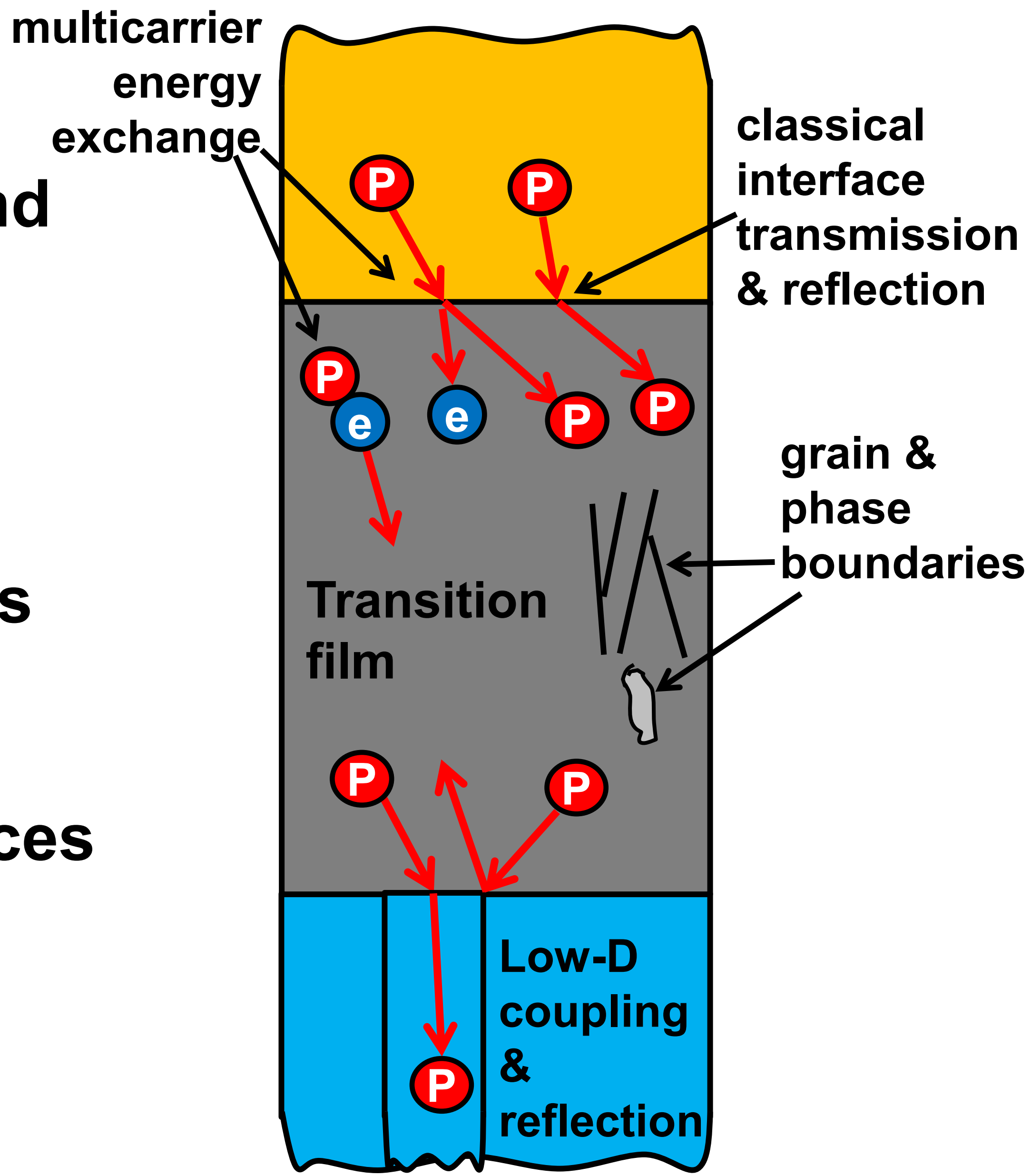
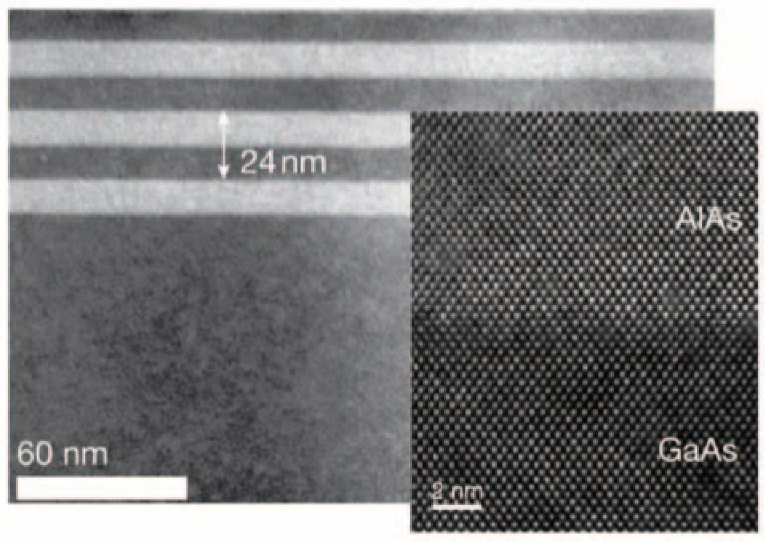
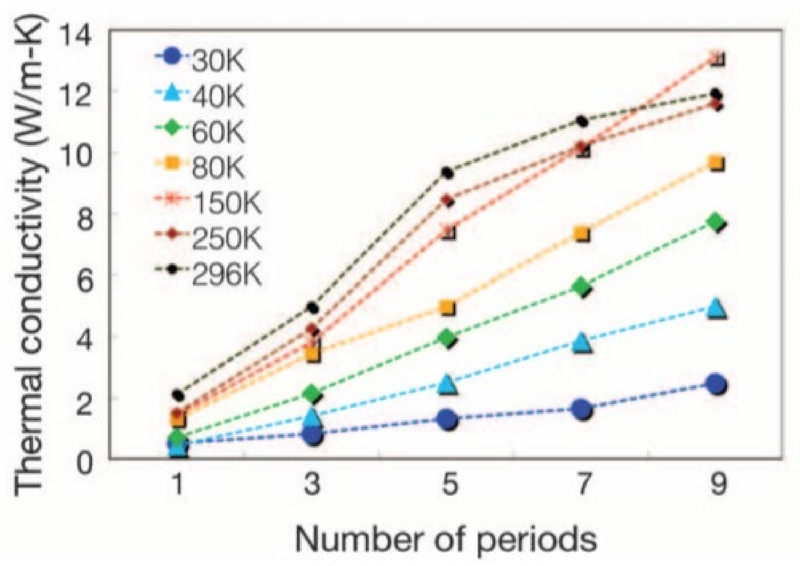


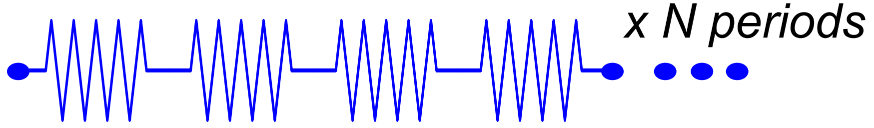
Figure from Goodson, 2011

Coherent Transport at Interfaces?





Diffusive Picture



R_{int} $\frac{L_{AlAs}}{k_{AlAs}}$ R_{int} $\frac{L_{GaAs}}{k_{GaAs}}$

Superlattice Period

→ k_{eff} independent of number of layers

Coherent Picture

"However, if the phase of the phonon is preserved at the interfaces of the SL and if anharmonic scattering is minimal, superposition of the Bloch waves creates stop bands and effectively modifies the phonon band structure (*10*). In this regime, phonon mean free paths (MFPs) are equal to the sample length, leading to a thermal conductivity that is linearly proportional to the total thickness of the SL."

Luckyanova *et al. Science* 2012. Doi: 10.1126/science.1225549

Part 2: Measuring Thermal Transport

Designing Thermal Measurements

Fourier's Law: $\overrightarrow{q''} = -k\,\nabla T$ Heat Diffusion Eqn: $\frac{1}{\alpha}\frac{\partial T}{\partial t}=\nabla^2 T$

1. How to measure **temperature**?

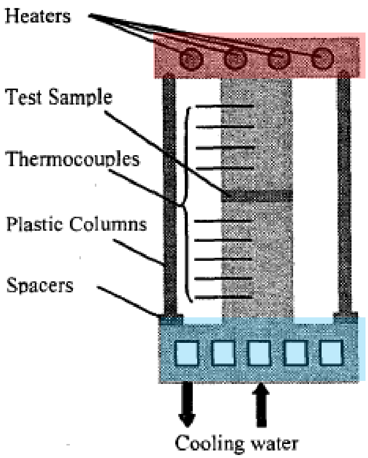
	Indirect [Heat Diffuses into Sensor]	**Direct** [Heat Diffusion Not Required]
Contact (generally electrical)	Thermocouples, electrical resistance thermometers, scanning probe techniques	Temperature sensitive device behavior (*e.g.* temperature dependent resistance of a nanowire)
Non Contact (generally optical)	Interactions with thin coatings (Fluorescence, Liquid Crystals, Thermoreflectance, etc.)	Temperature sensitive device or material behavior (IR emission, Raman spectroscopy, thermoreflectance)

2. How to measure **heat flux**?

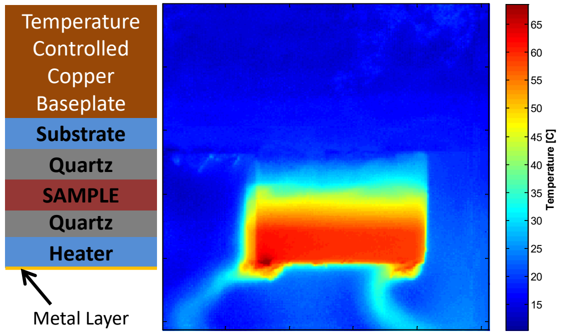
Joule heating, use reference materials, quantify optical absorption, …

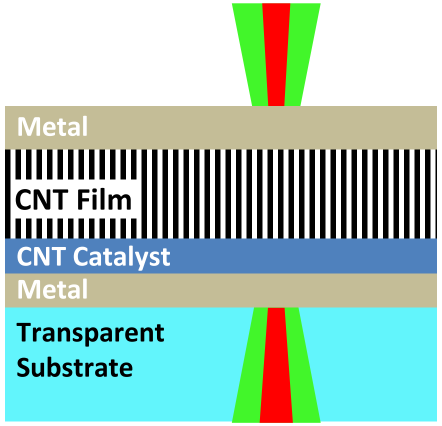
Common Thermal Metrology Tools

Reference Bar Method (ASTM D5470)

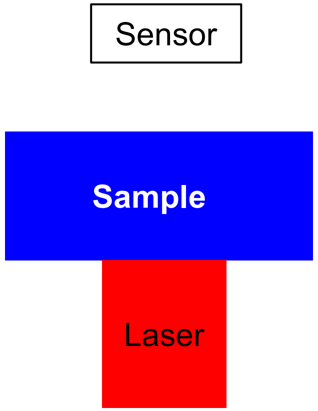


Infrared Microscopy



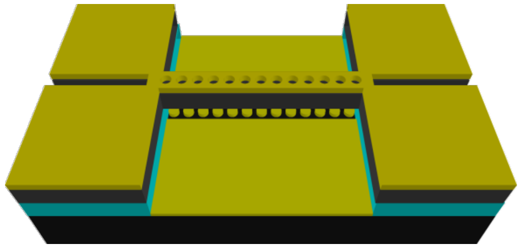


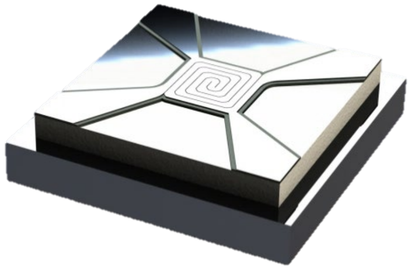
Thermoreflectance



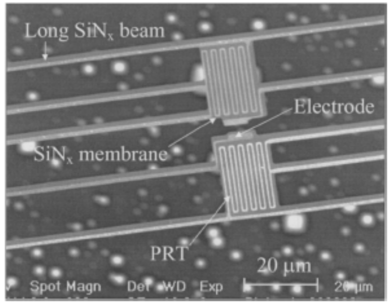
Flash Diffusivity

Electrothermal Metrology



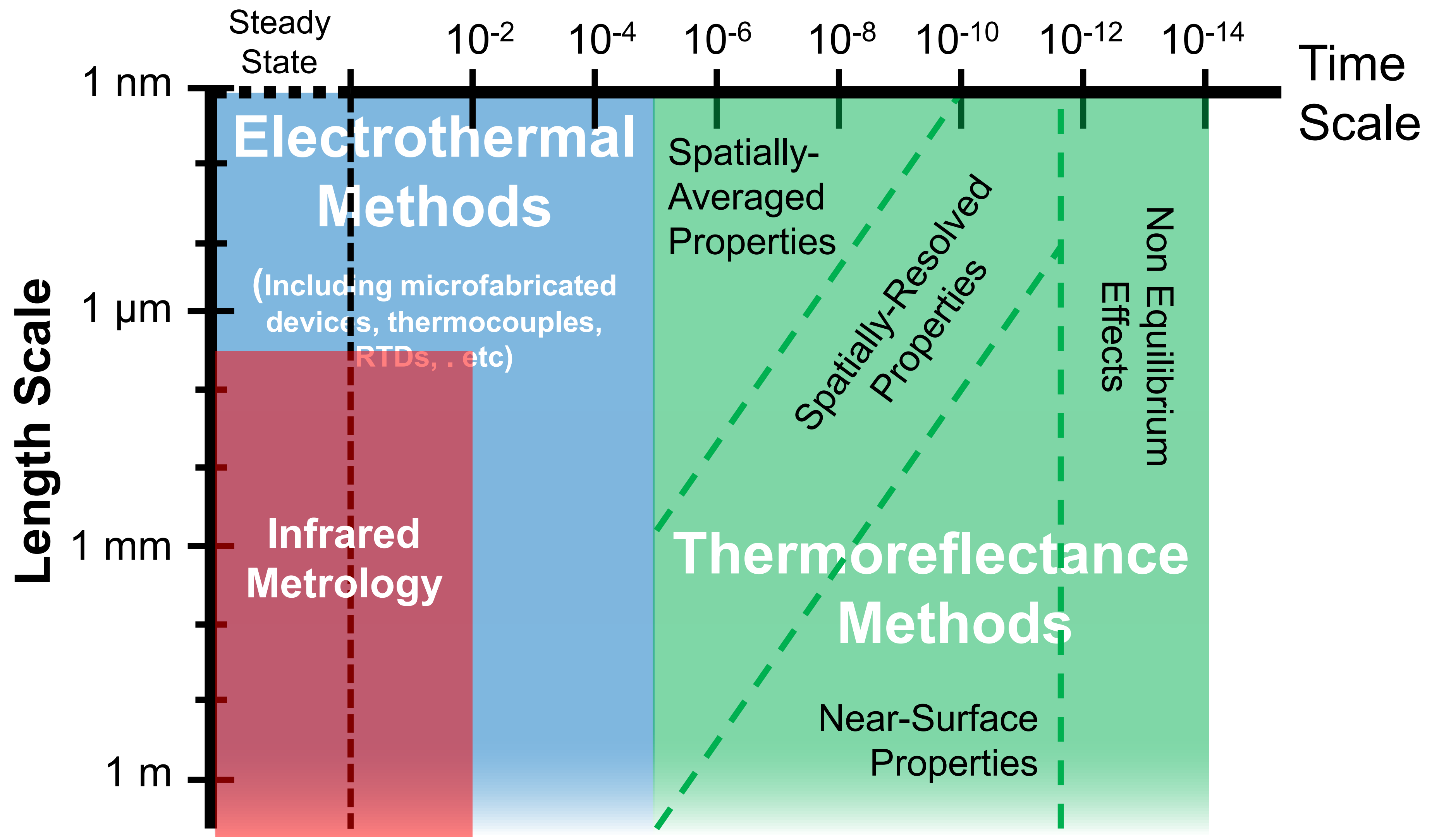


3ω Technique and others



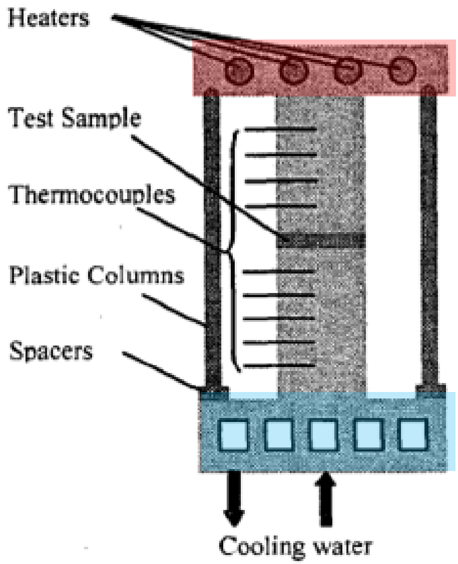
Li Shi *et al.*, JHT 2003

Measurement Time & Length Scales



STEADY STATE METHODS → Directly Measure k

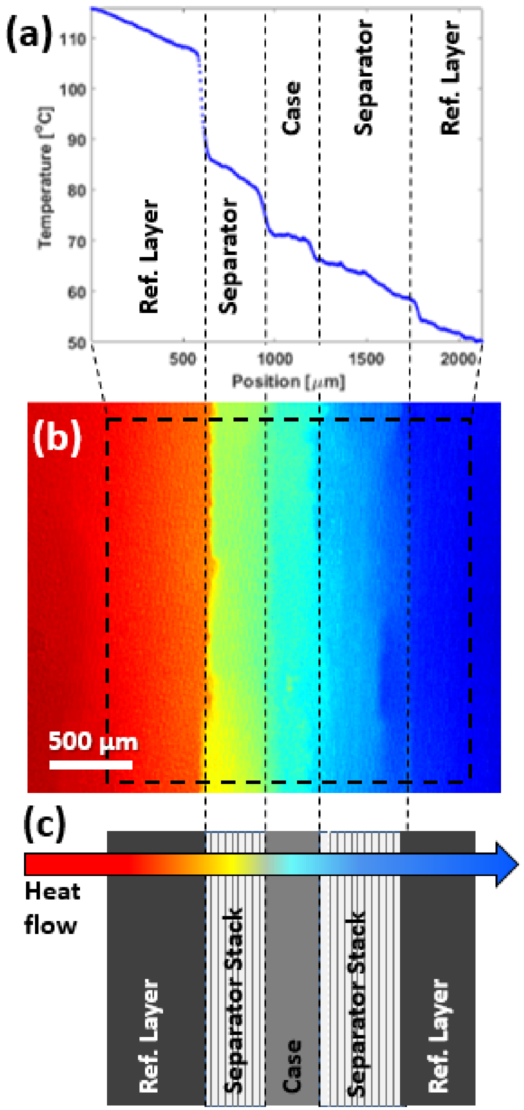
Reference Bar Method (ASTM D5470)

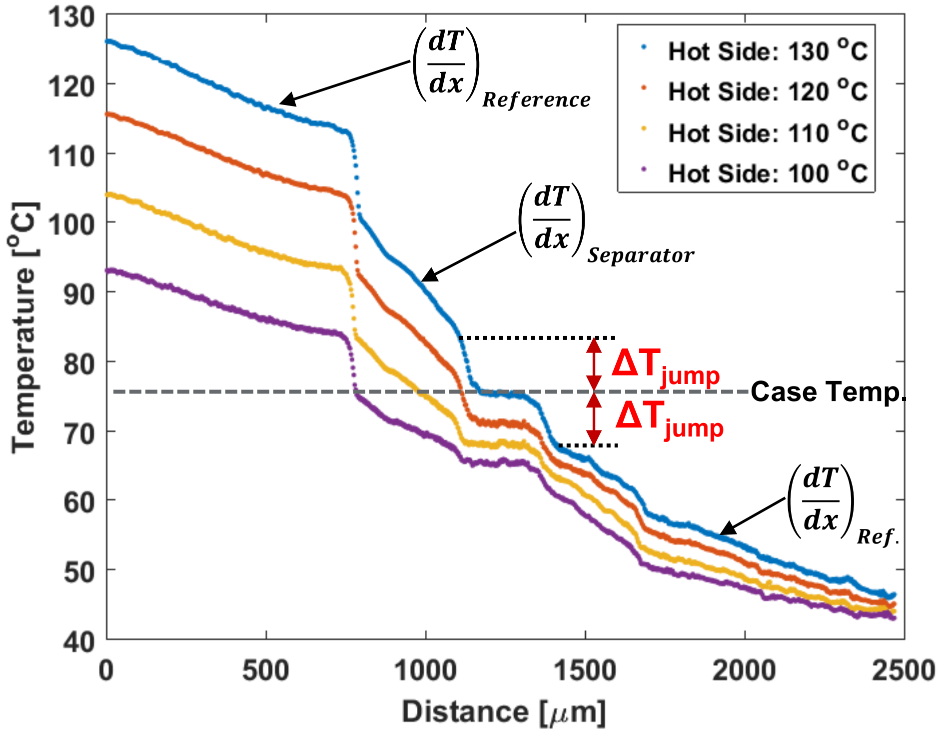


X. Hu *et al.*, *ITHERM* 2004.
DOI: 10.1109/ITHERM.2004.1319155
Barako *et al.*, *TCPMT* 2014.
DOI: 10.1109/ITHERM.2004.1319155

Heat Source:
- Resistive or Radiant Heaters
- Temperature Controlled Heat Exchangers

Temperature Measurement:
- Thermocouples
- RTDs
- Infrared imaging (resolve contacts)



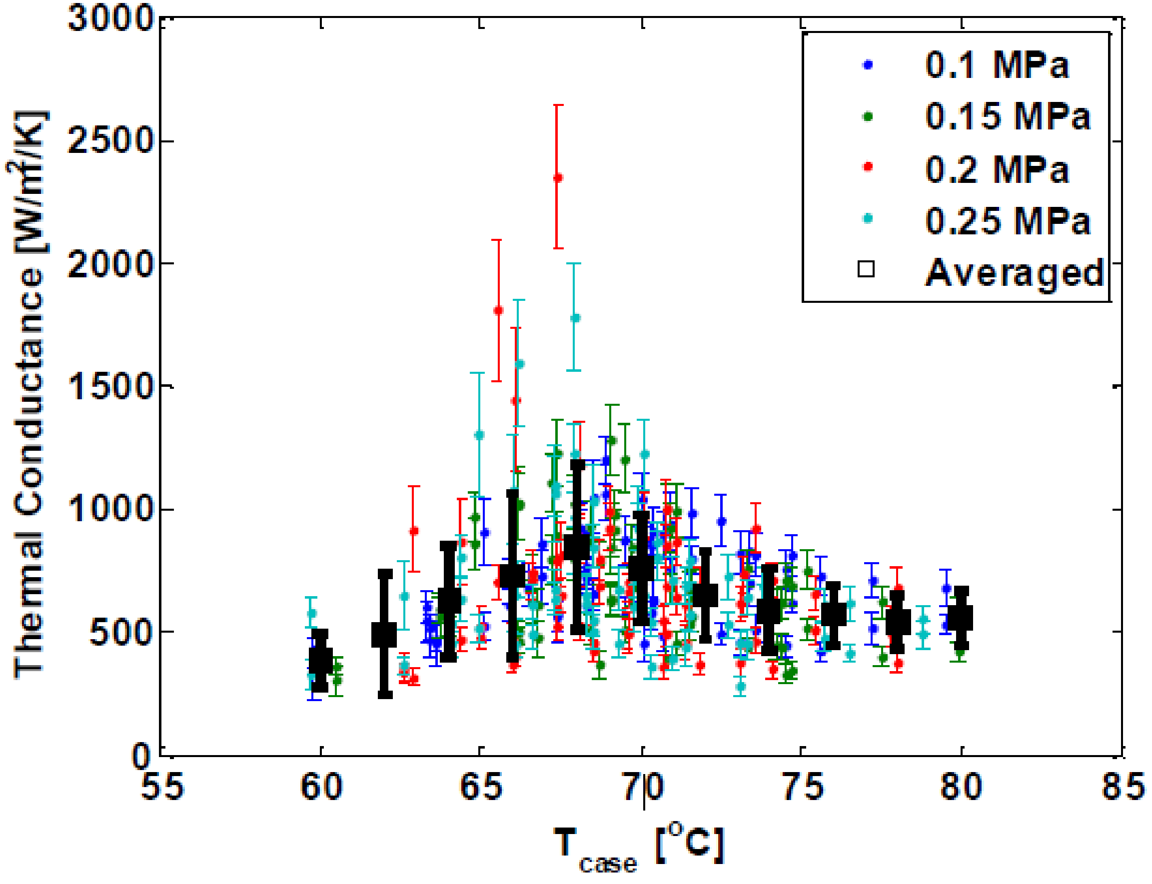


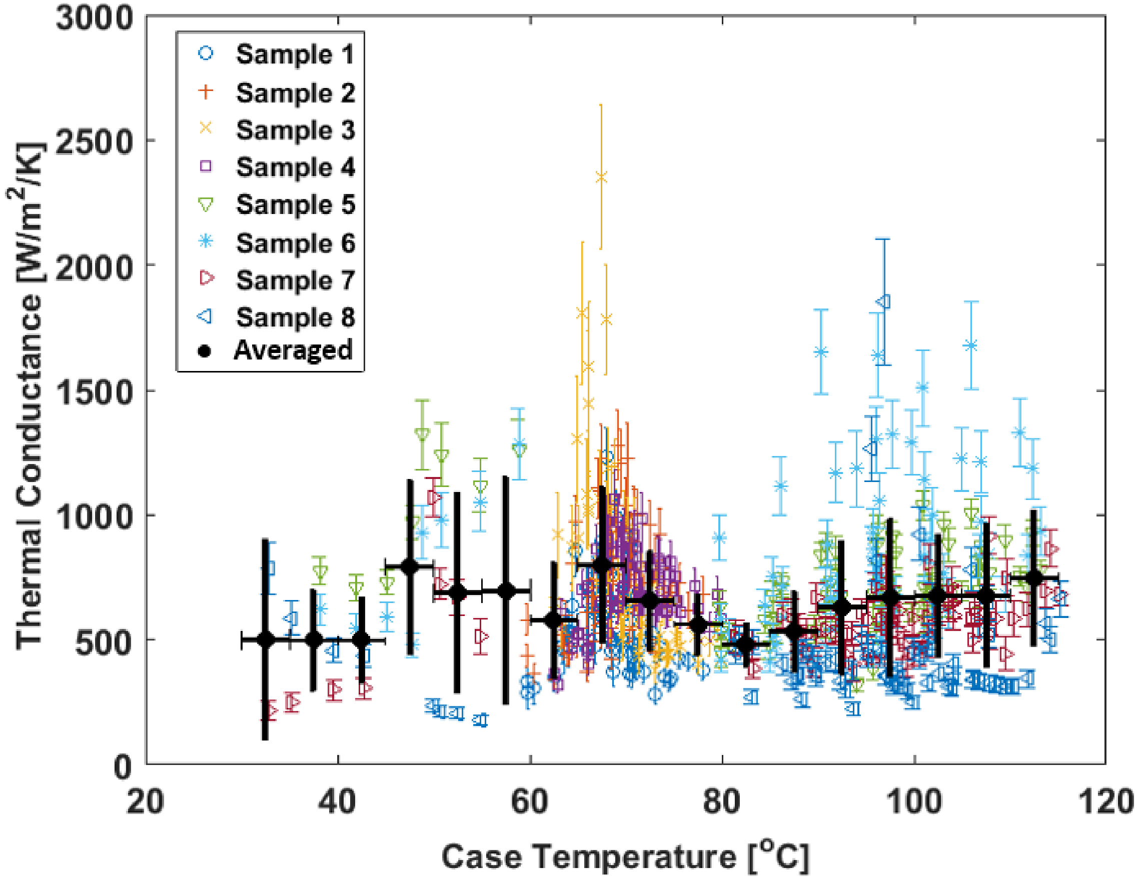
Temperature gradients across the sample stack, at four case temperatures

$$\text{Thermal Conductance}, G = \frac{q''}{\Delta T_{jump}}$$

Gaitonde, Nimmagadda, **Marconnet**: "Measurement of Thermal Conductance in Li-ion Batteries" *Journal of Power Sources* (2017).

Separator-Case Interfacial Thermal Conductance



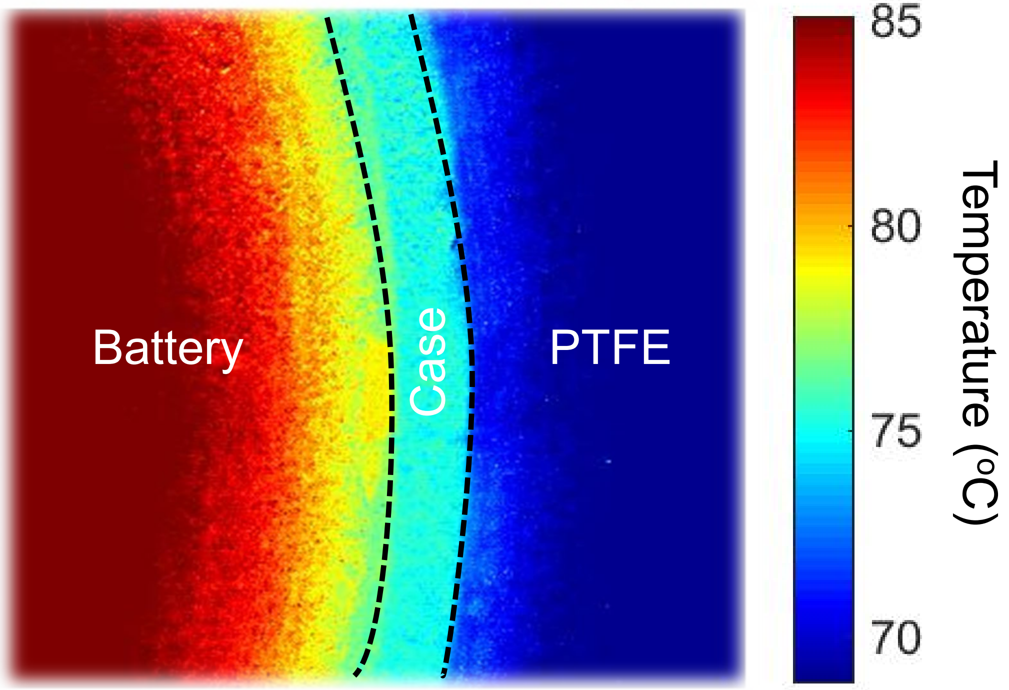


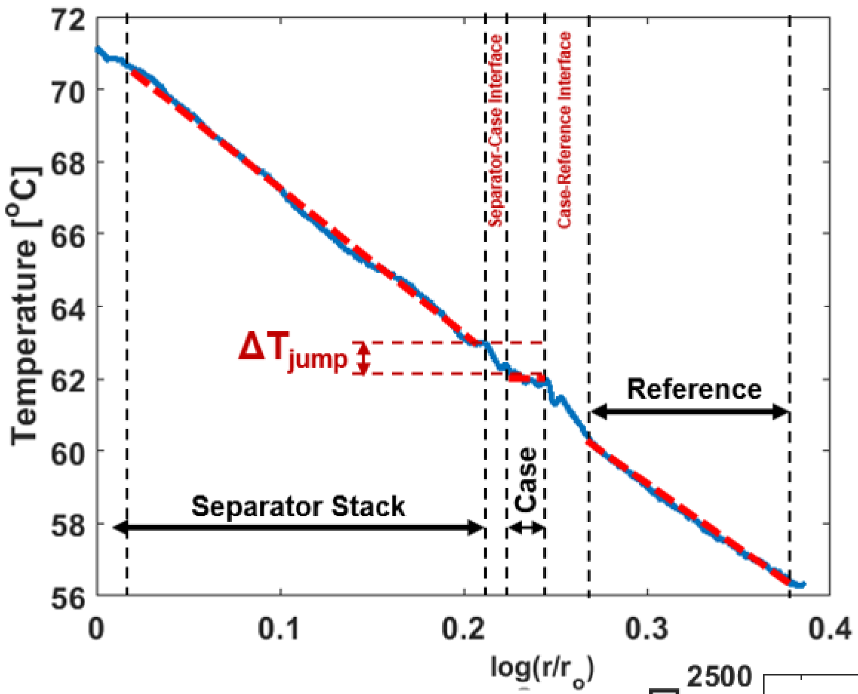
- **Interfaces Measured: 8**
- **Pressure Range: 0.1-0.25 MPa**
- **Case Temperatures: 30-120 °C**

Mean Thermal Conductance: 670 W/(m^2K)
Standard Deviation: 275 W/(m^2K)

Gaitonde, Nimmagadda, **Marconnet**: "Measurement of Thermal Conductance in Li-ion Batteries" *Journal of Power Sources* (2017).

Radial Battery Cell Measurement



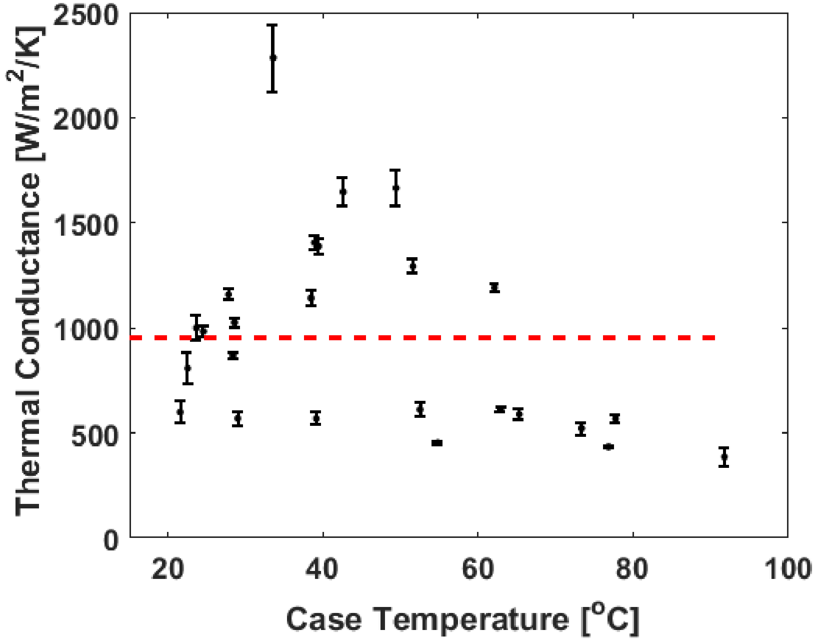


Cartesian Cell:

670 ± 275 W/(m²K)

Radial Cell:

920 ± 475 W/(m²K)



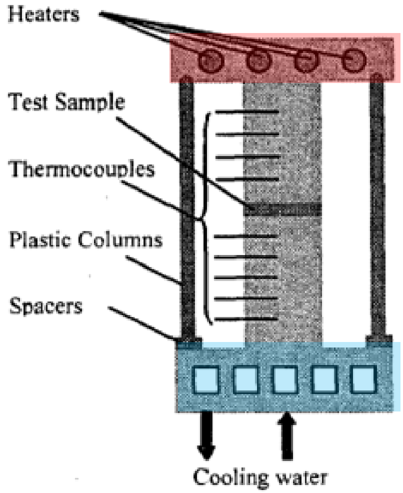
$$q_{in} = \frac{T_o - T_i}{R_{conduction}}$$

$$R_{conduction} = \left[\frac{\log\left(\frac{r_o}{r_i}\right)}{2\pi k}\right]_{sample}$$

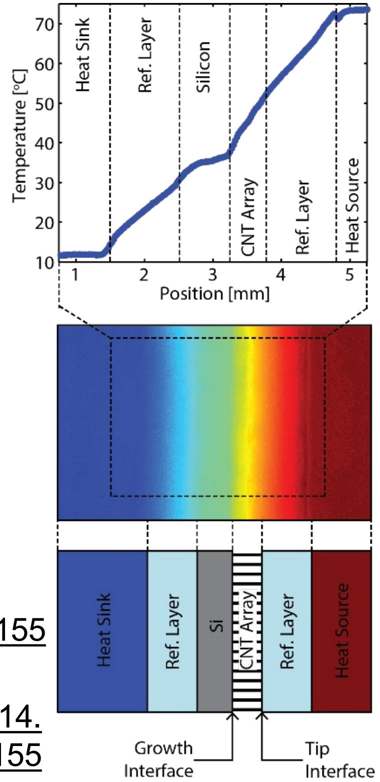
A. Gaitonde, A. Nimmagadda, and **A. Marconnet**, *2017 ITherm,* Orlando, FL.
DOI: 10.1109/ITHERM.2017.7992602

Steady State Methods → Directly Measure *k*

Reference Bar Method



X. Hu *et al.*, *ITHERM* 2004.
DOI: 10.1109/ITHERM.2004.1319155

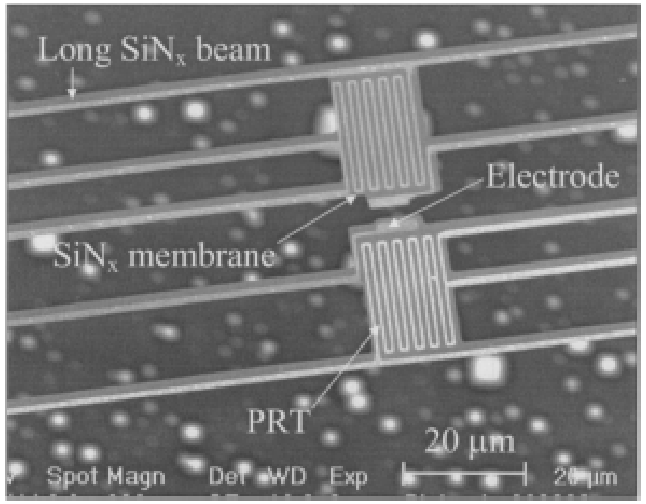


Barako *et al.*, *TCPMT* 2014.
DOI: 10.1109/ITHERM.2004.1319155

Heat Source:
- Resistive or Radiant Heaters
- Temperature Controlled Heat Exchangers

Temperature Measurement:
- Thermocouples
- RTDs
- Infrared imaging (resolve contacts)

Two-Platform Microdevice

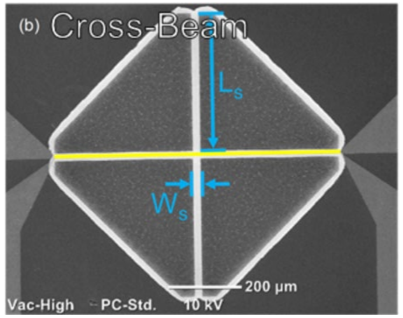


L. Shi *et al.*, *JHT*, 2003.
doi:10.1115/1.1597619

Heat Source:
- Resistive Heating

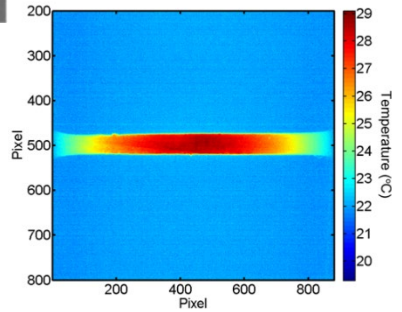
Temperature Measurement:
- Resistive Thermometry

Custom Platforms



Zeng & Marconnet, *RSI*, 2018. doi:10.1063/1.4979163

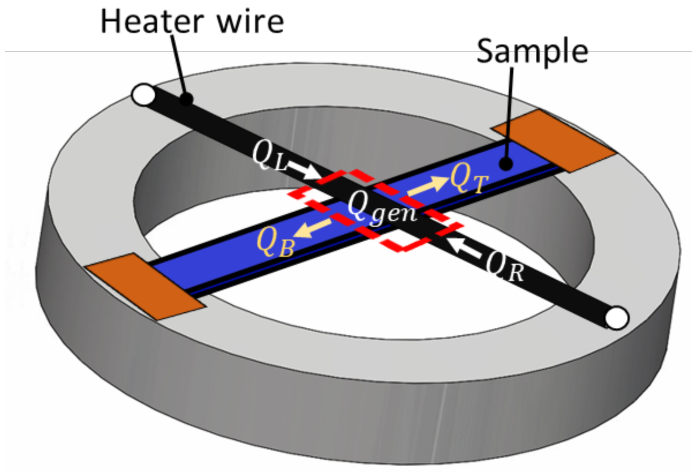
Liu *et al.*, *ACS AMI*, 2016.
doi:10.1021/acsami.6b04114

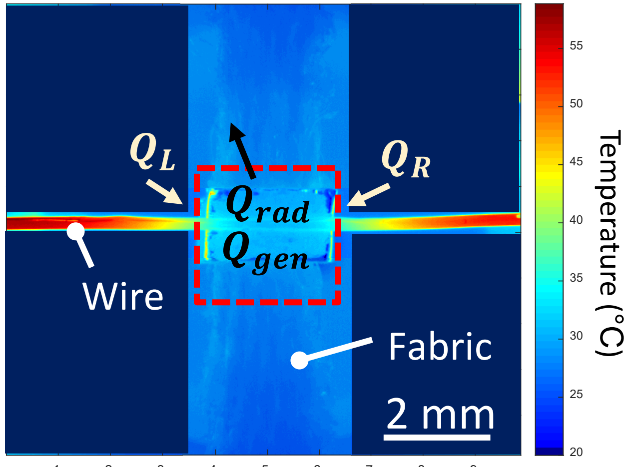


Heat Source:
- Resistive Heaters
- Lasers

Temperature Measurement:
- Point Measurements:
  - Resistive Thermometers
  - Raman Spectroscopy
- Surface Imaging:
  - Infrared Imaging
  - Raman Spectroscopy Imaging
  - Thermoreflectance Imaging

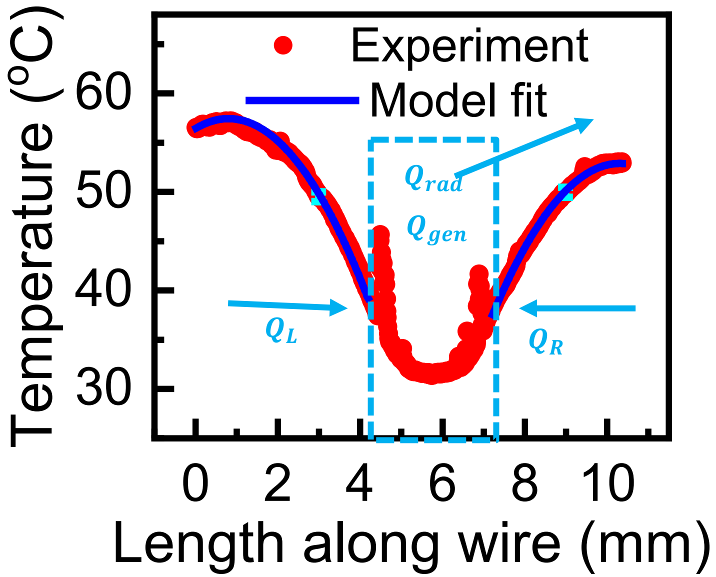
Heater Wire-Based Absolute Method

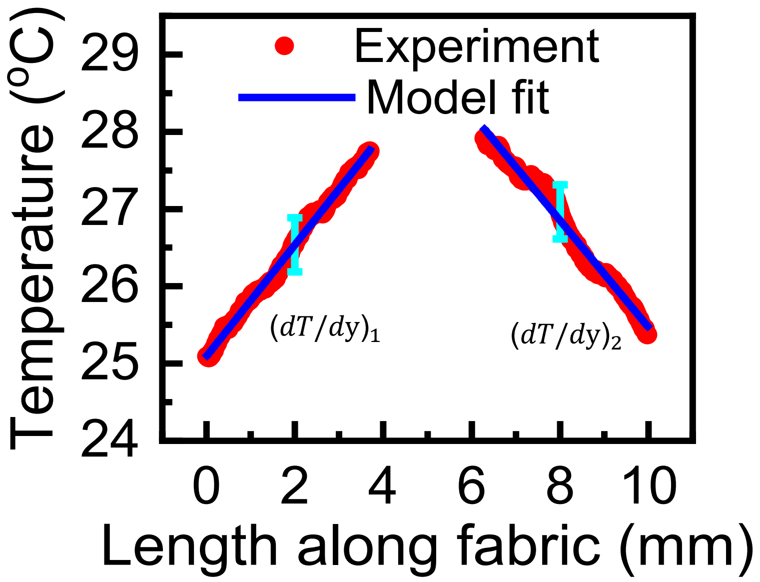




Sample Thermal Conductivity

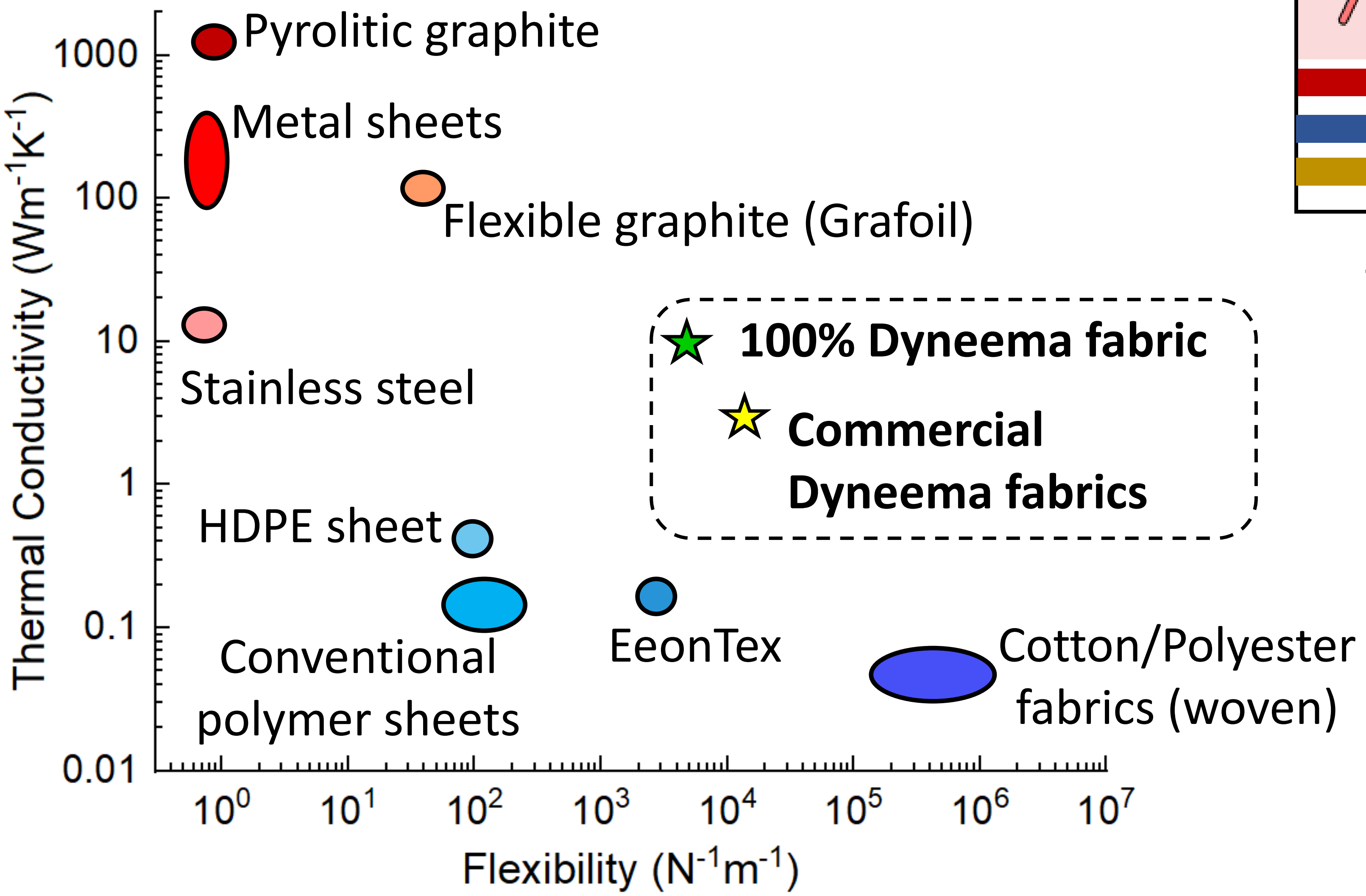
$$k_s = \frac{Q_L + Q_R + Q_{gen}}{A\left\{\left(\frac{dT}{dy}\right)_T + \left(\frac{dT}{dy}\right)_B\right\}}$$

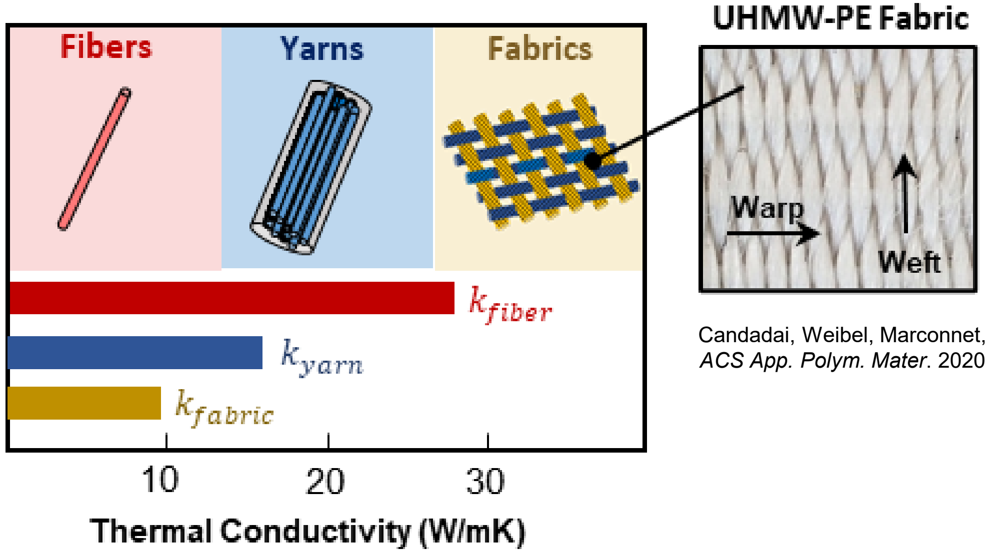




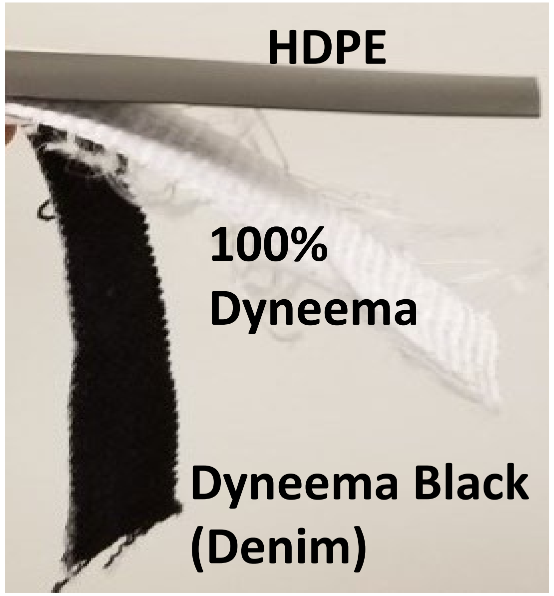
A.A. Candadai, J.A. Weibel, and A.M. Marconnet, "Thermal Conductivity of Ultra-High Molecular Weight Polyethylene: From Fibers to Fabrics," *ACS Applied Polymer Materials,* 2020.

Multi-Functional Properties





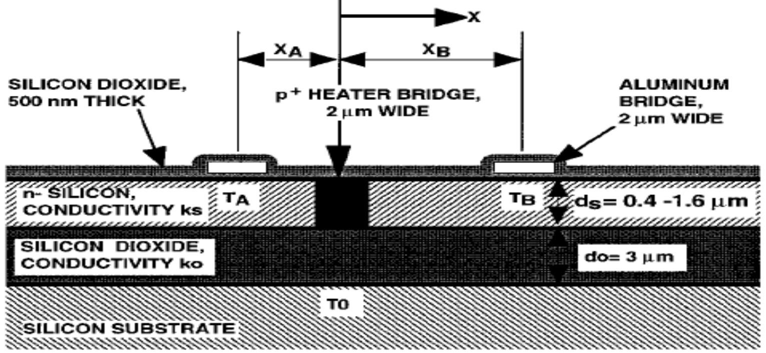
Candadai, Weibel, Marconnet, *ACS App. Polym. Mater.* 2020



Thin Film Measurements

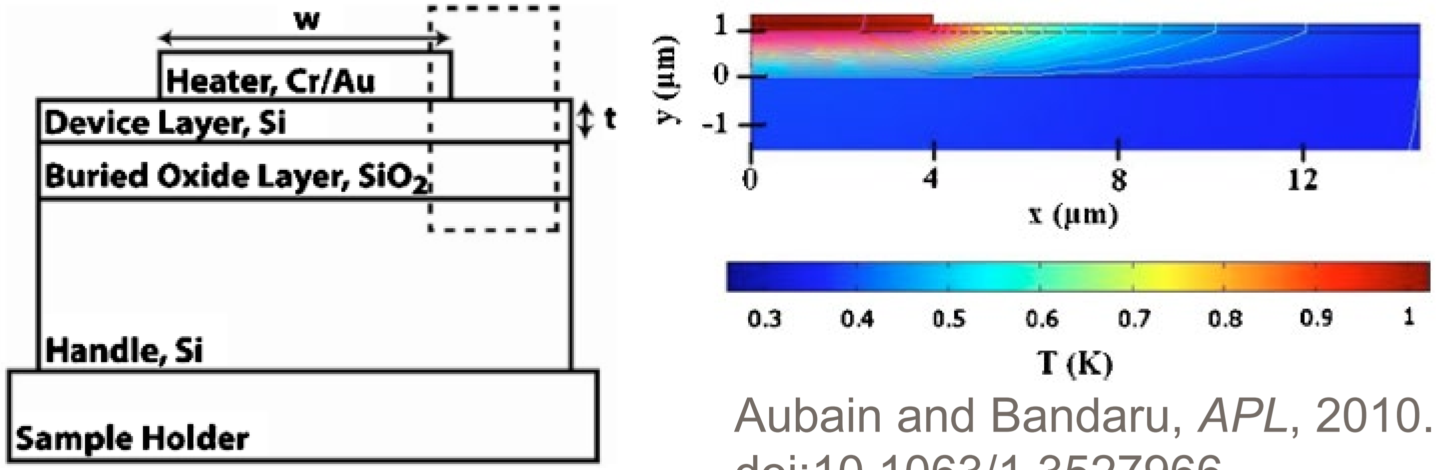
On-substrate (Si-SiO_2-Si)

Electrical Heating + Sensing



Asheghi *et al.*, *APL*, 1997.
doi:10.1063/1.119402

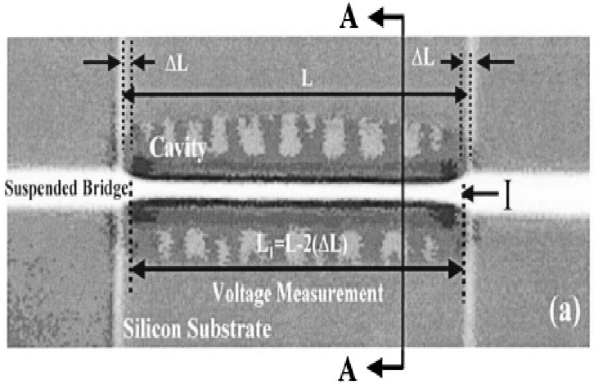
Electrical Heating + Optical Sensing



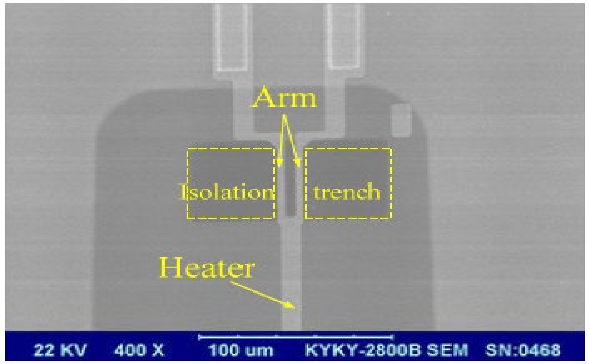
Aubain and Bandaru, *APL*, 2010.
doi:10.1063/1.3527966

Partially Suspended ($Si + SiO_2$)

Electrical Heating + Sensing

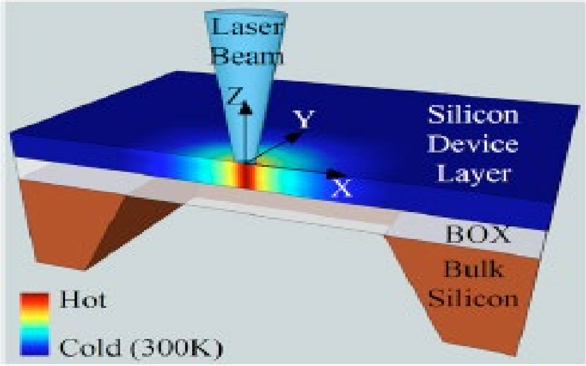


Liu and Asheghi, *APL*, 2004.
doi:10.1063/1.1741039



Hao *et al.*, 2006 8th International Conference on Solid-State and Integrated Circuit Technology Proceedings.
doi:10.1109/ICSICT.2006.306679

Optical Heating + Sensing



Liu *et al.*, *APL*, 2011.
doi:10.1063/1.3583603

TRANSIENT METHODS

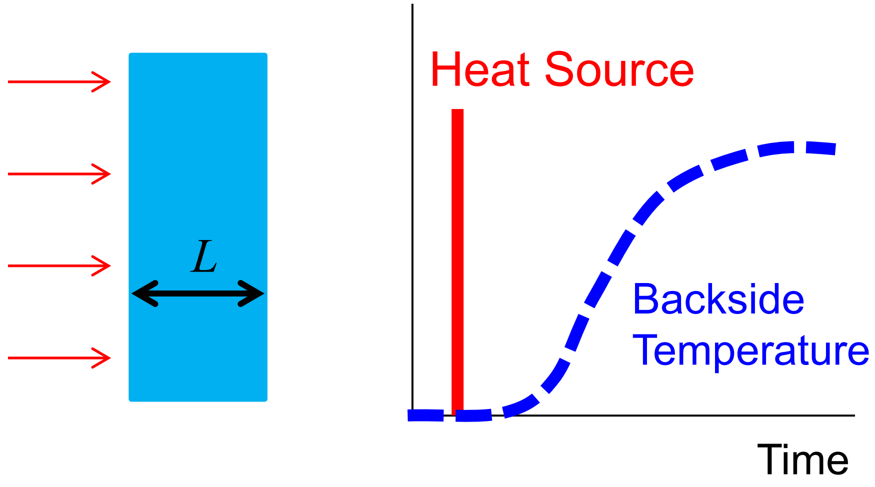
- Heat Diffusion Equation:
(one dimensional)

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\boxed{\alpha}} \frac{\partial T}{\partial t}$$

Thermal Diffusivity [m²/s] $\alpha = \frac{k}{\rho C_p}$

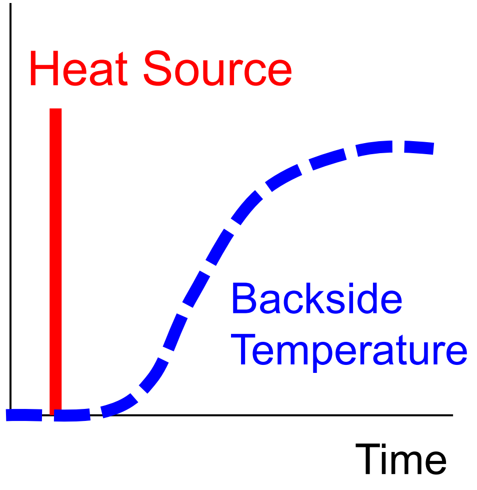
- Consider a pulse of heat at one surface of a slab, how long does it take for heat to diffuse to other surface?

$$\frac{T}{L^2} \sim \frac{1}{\alpha}\frac{T}{t} \Rightarrow t \sim \frac{L^2}{\alpha}$$



→ The flash method is sensitive to the thermal diffusivity

Pulsed Methods



Flash Diffusivity

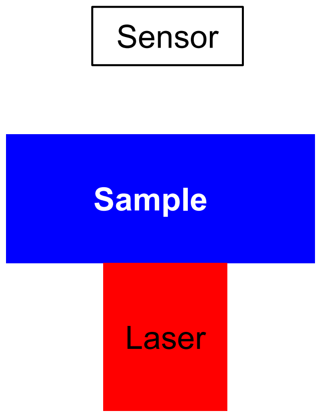
Heat Source:

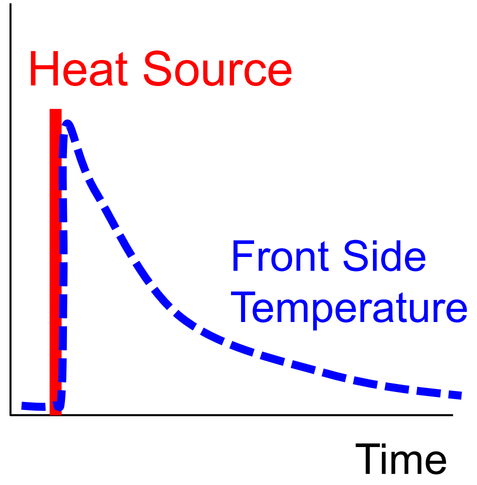
Pulsed optical heating at surface 1

Temperature Measurement:

Infrared sensing at surface 2

Sensitive to $\alpha = \frac{k}{\rho C_p}$





Time Domain and Transient Thermoreflectance (TDTR and TTR)

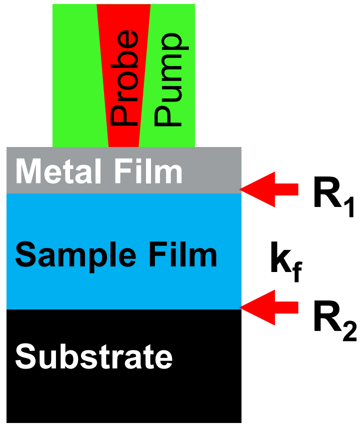
Heat Source:

Pulsed optical heating at surface 1

Temperature Measurement:

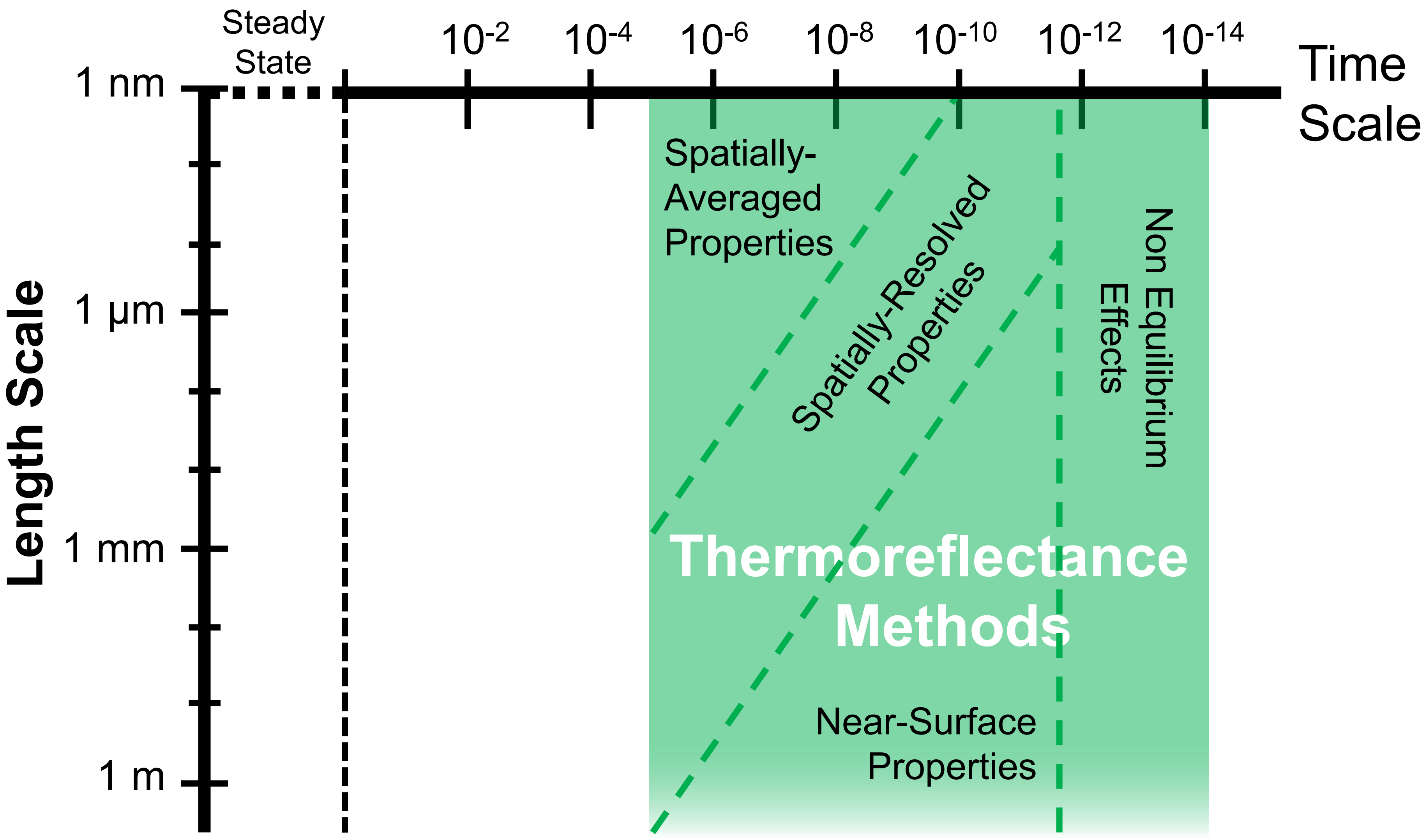
Optical sensing at surface 1

Sensitivity to properties (k, C_p, R'') depends on geometry and time scale. Often most sensitive to $\epsilon^2 = k\rho C_p$



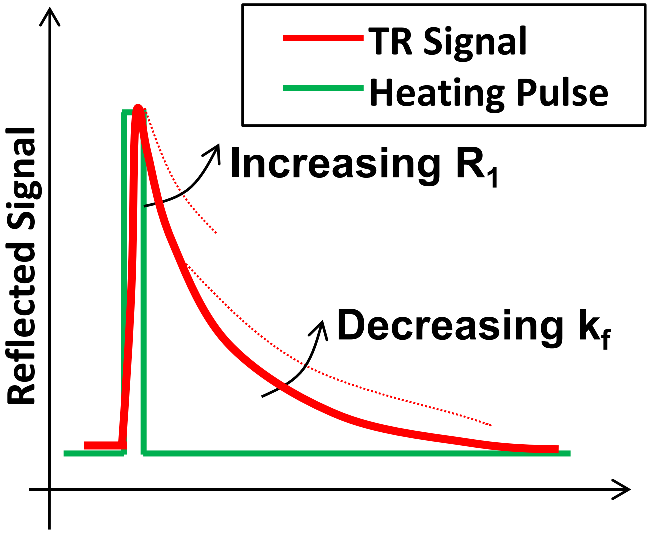
Transient Grating Measurements

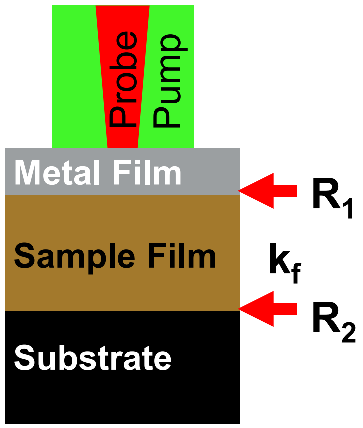
Measurement Time & Length Scales

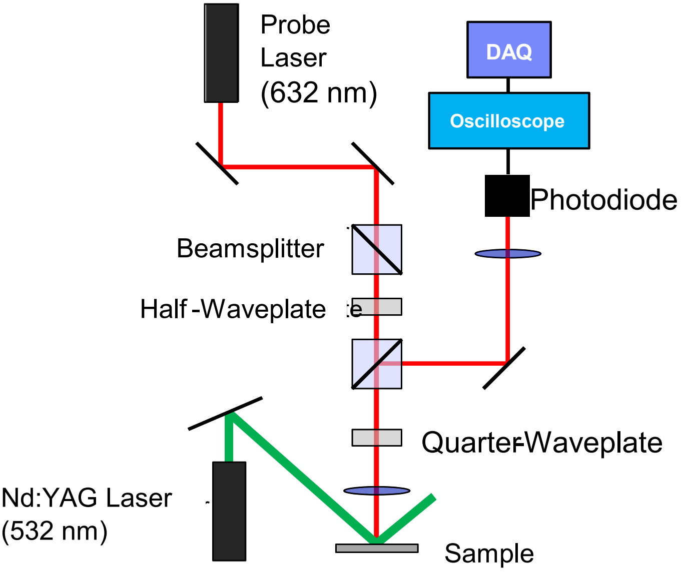


TTR vs. TDTR

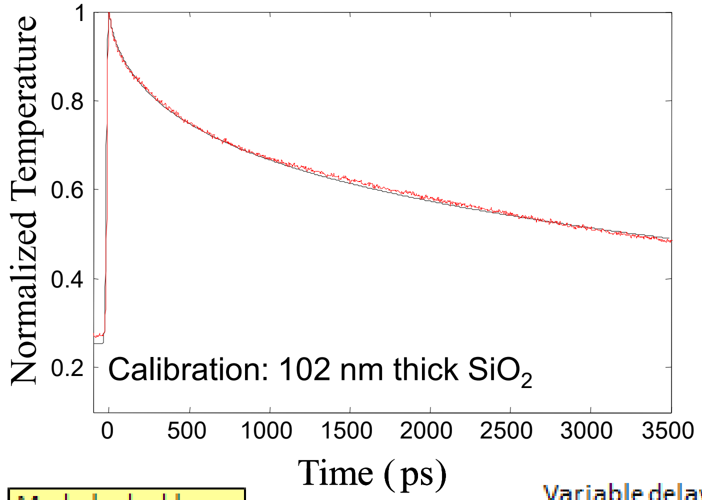
Nanosecond Transient Thermoreflectance (TTR)

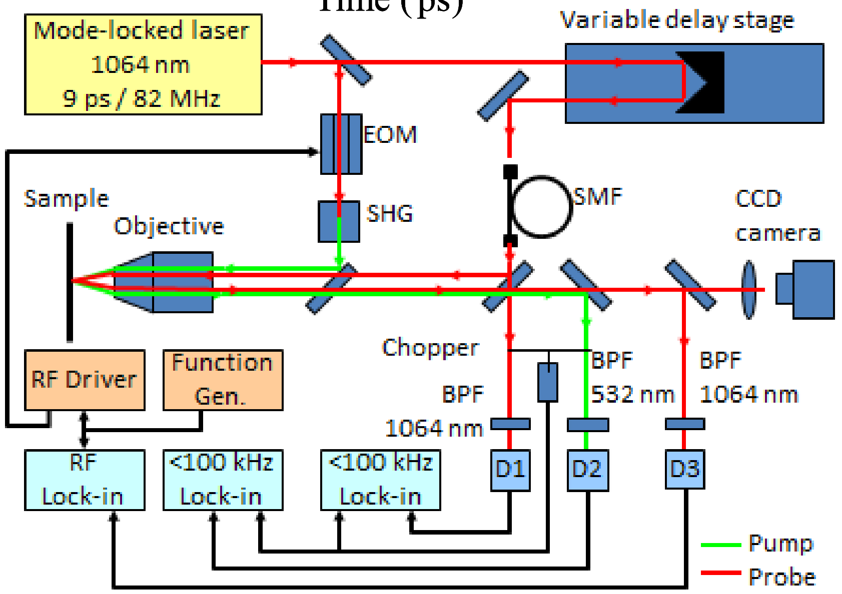


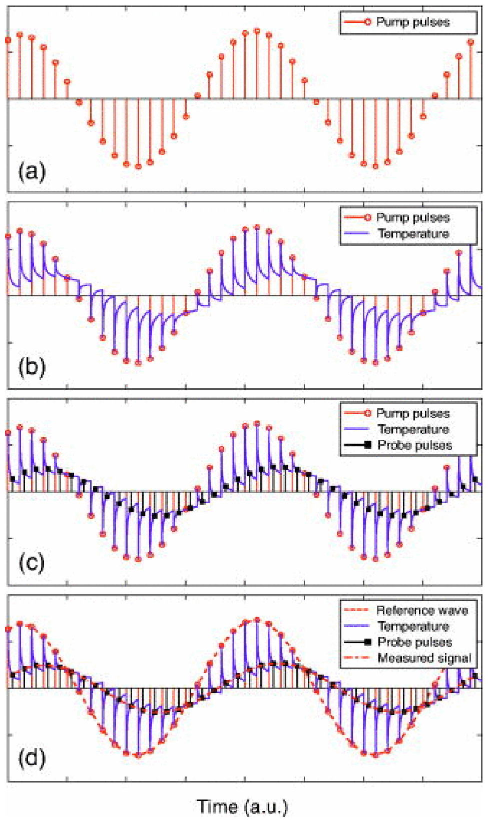




Picosecond Time-Domain ThermoReflectance (TDTR)

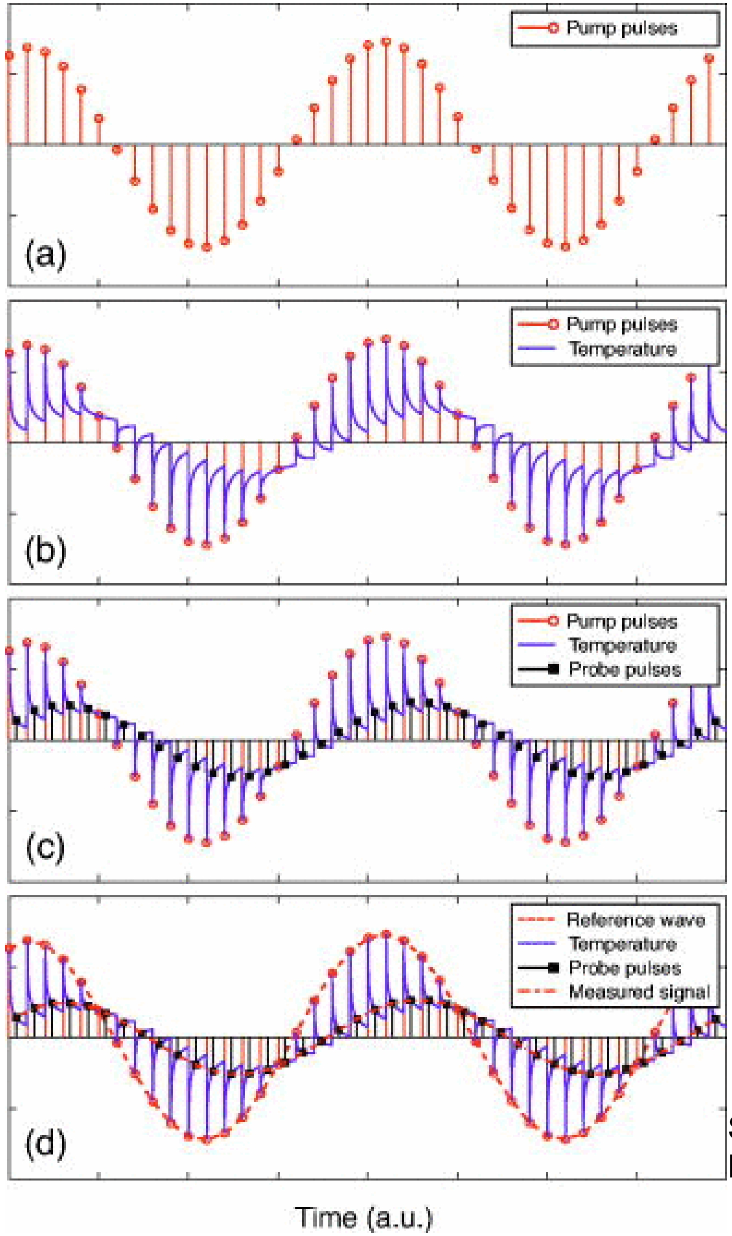






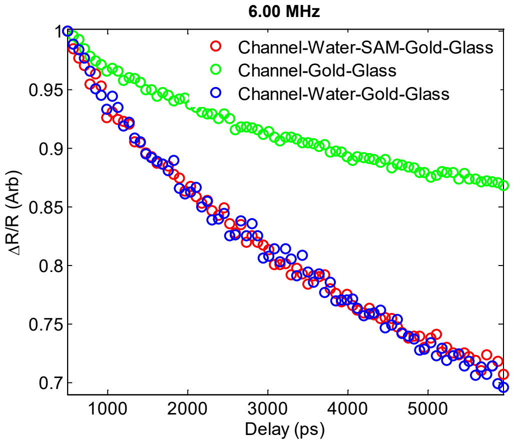
Schmidt *et al.*, *RSI*, 2008.
DOI:10.1063/1.3006335

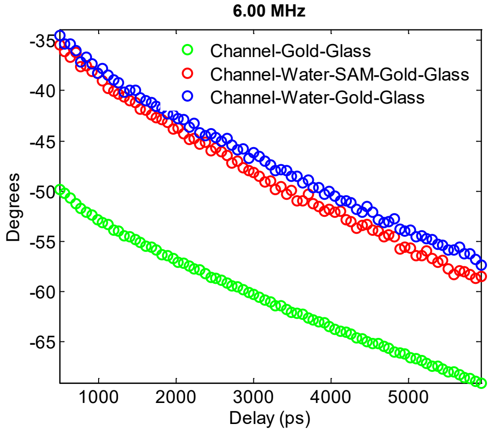
TDTR Signals



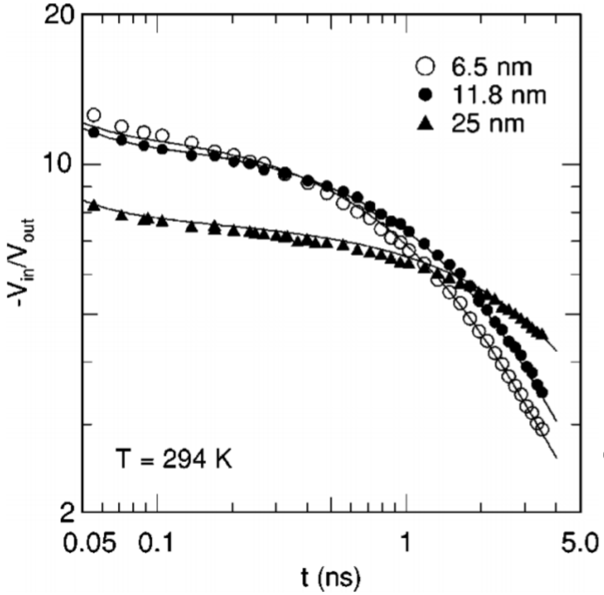
Schmidt *et al.*, *RSI*, 2008.
DOI:10.1063/1.3006335

Normalized Amplitude Phase





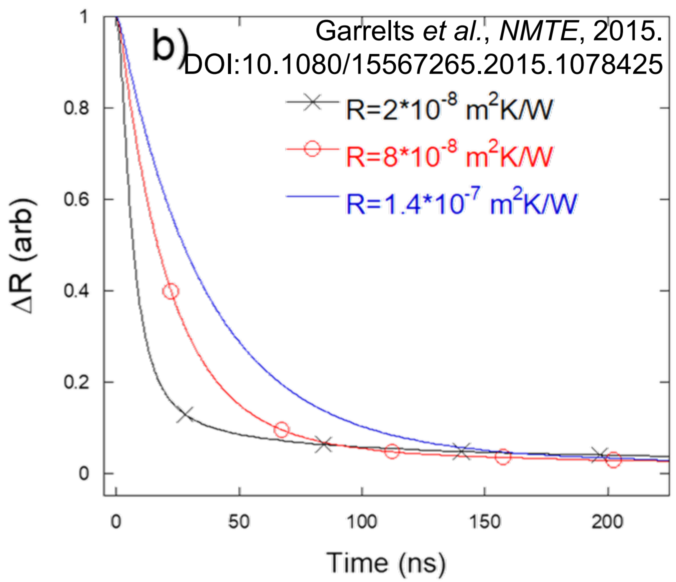
Ratic



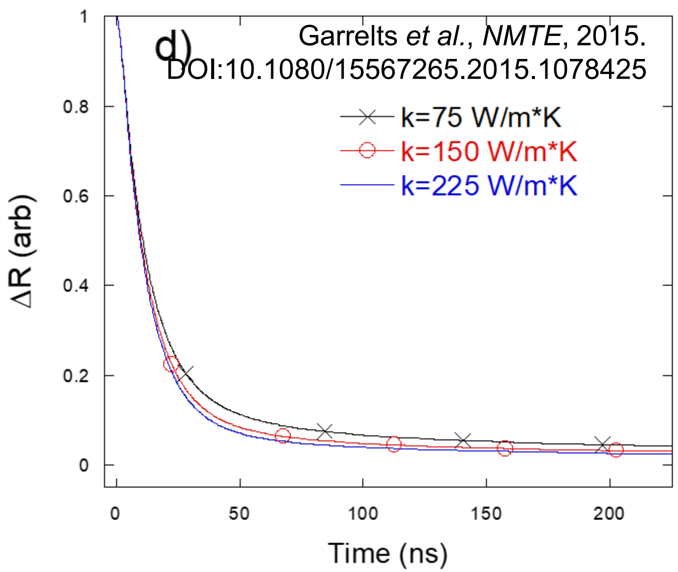
Costescu *et al.*, *PRB*, 2003.
DOI:10.1103/PhysRevB.67.054

Sensitivity & Uncertainty

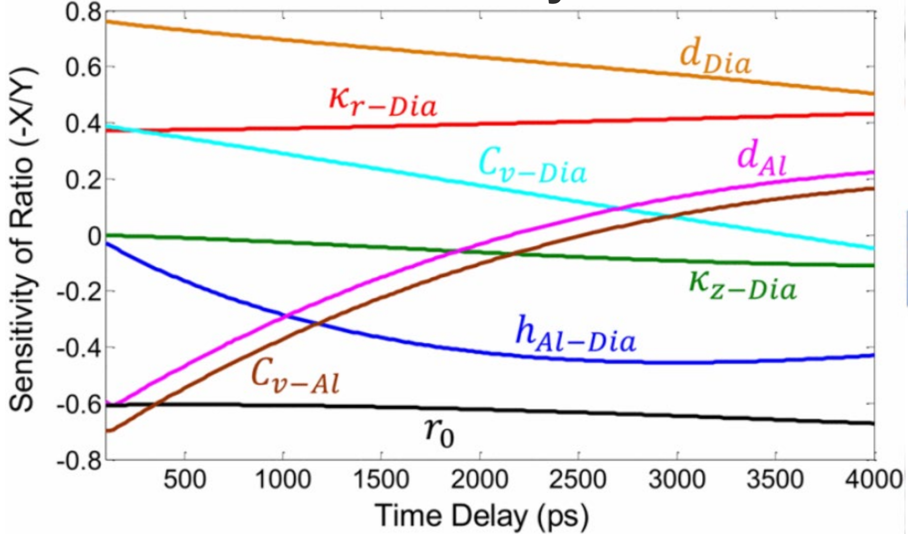
Changing *R”*

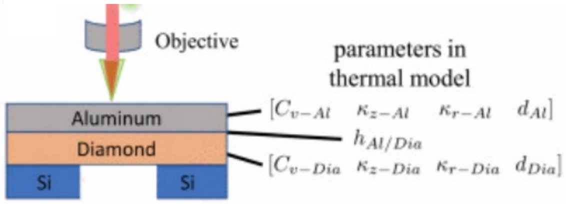


Changing k_{sample}



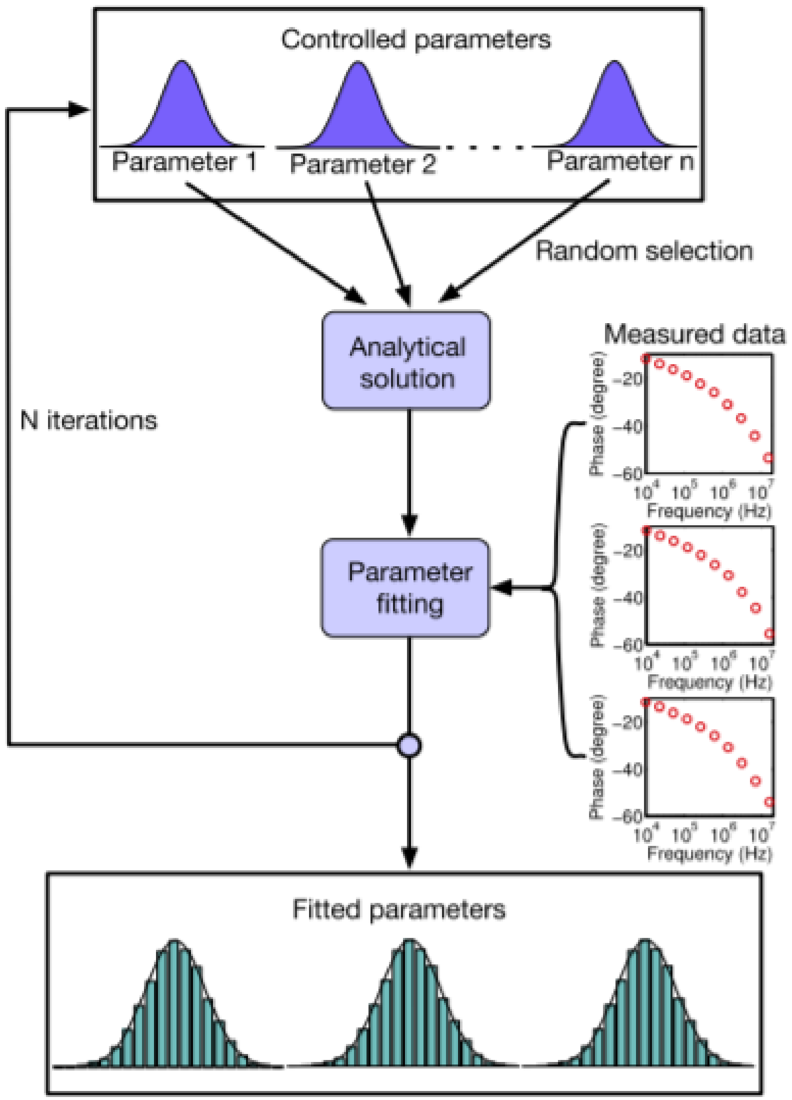
Sensitivity of Ratio to Different Parameters





Cheaito et al., *ITHERM 2017.*
DOI:10.1109/ITHERM.2017.7992555

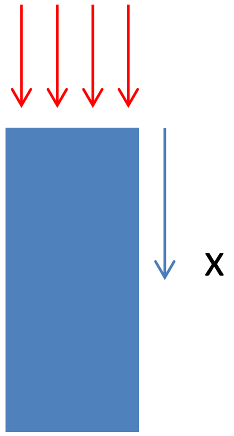
Monte Carlo Uncertainty Approach



Yang *et al.*, *RSI*, 2016.
DOI:10.1063/1.4939671

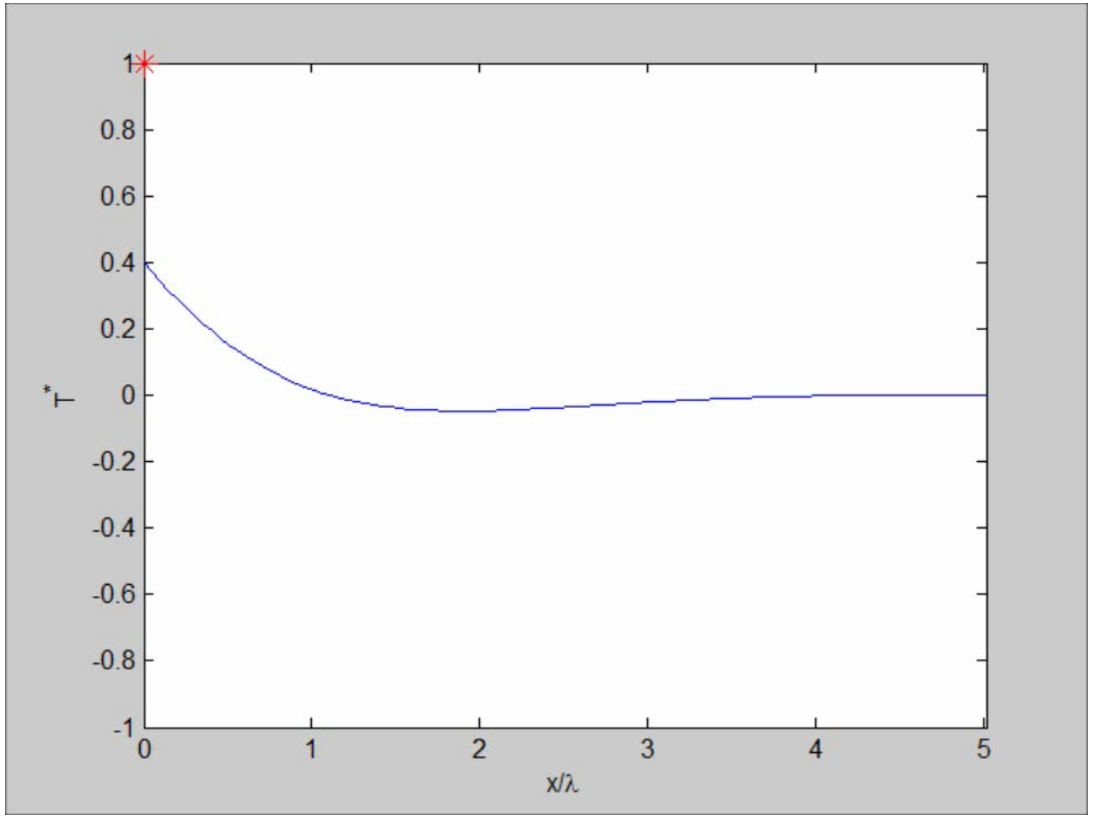
Example: Steady Periodic Convection B.C.

$$T_\infty(t) = T_0 + T_A \cos(\omega t)$$

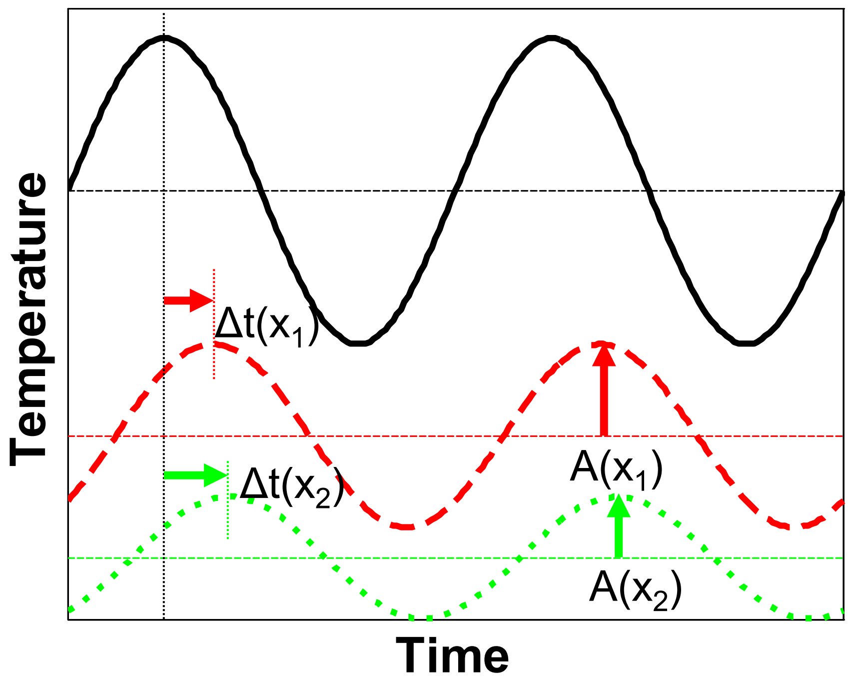


$$x^* = x \Big/ \sqrt{2\alpha/\omega}$$

$$\tau = \omega t$$



Diffusion depth $\propto \sqrt{2\alpha/\omega}$



Amplitude: $A(x)$

Phase Lag: $\phi = \frac{\Delta t(x)}{Period} = 2\pi f \Delta t(x)$

Transform to the Frequency-Domain

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t}$$

Assume a periodic solution $T = \tilde{T}(x)\exp(i\omega t)$

$$\frac{\partial^2}{\partial x^2}\left[\tilde{T}(x)\exp(i\omega t)\right] = \frac{1}{\alpha}\frac{\partial}{\partial t}\left[\tilde{T}(x)\exp(i\omega t)\right]$$

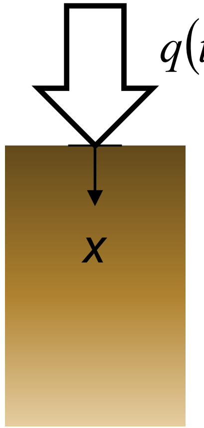
$$\cancel{\exp(i\omega t)}\frac{\partial^2 \tilde{T}}{\partial x^2} = \tilde{T}\frac{i\omega}{\alpha}\cancel{\exp(i\omega t)}$$

$$\boxed{\frac{d^2\tilde{T}}{dx^2} = \frac{i\omega}{\alpha}\tilde{T}}$$

ODE for $\tilde{T}(x)$ -- apply boundary conditions and solve for $\tilde{T}(x)$

Fourier Series & Transforms are your Friends!

Once you find the frequency domain solution: $\tilde{\theta}(x)$
You have the solution to any time dependent problem!

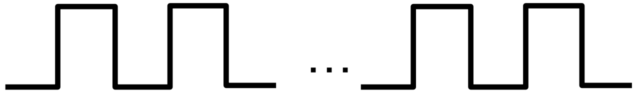


$q(t) = q_0 e^{i\omega t}$

$\theta_m(x,t) = \tilde{\theta}_m(x) e^{i\omega t}$

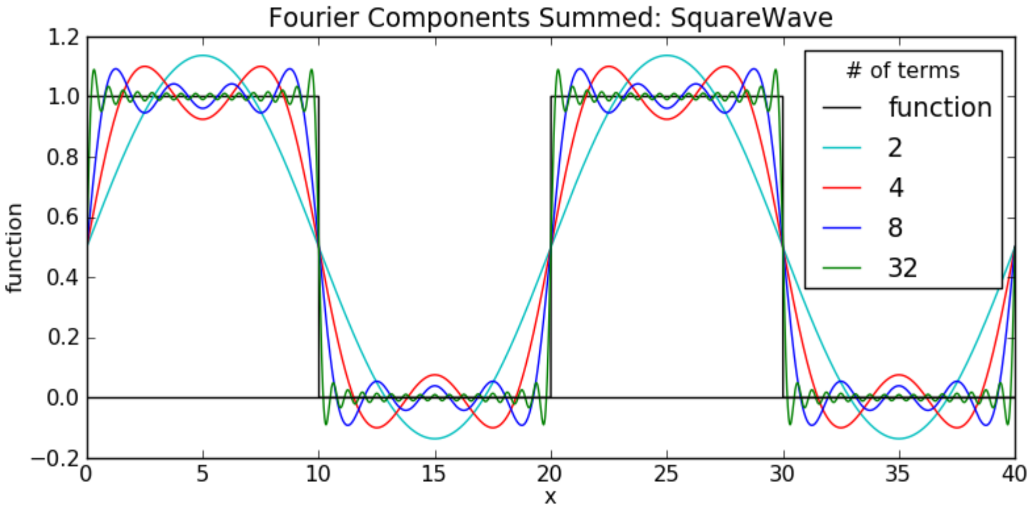
$T(x \to \infty, t) = T_0$

Periodic Function:



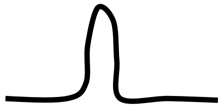
$$q(t) = \sum_m q_m e^{i\omega t}$$ Fourier Series

$$\theta(x,t) = \sum_m \frac{q_m}{q_0} \tilde{\theta}_m(x) e^{i\omega t}$$



http://2.bp.blogspot.com/_oklcsBieX4U/TRKogEZh16I/AAAAAAAAAIY/spYsURzN3d0/s1600/squarewave32terms.png

Single Event Heating:



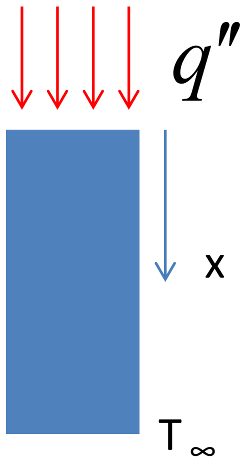
$$q(t) = \int_{-\infty}^{\infty} q(\omega) e^{i\omega t} \frac{d\omega}{2\pi}$$ Fourier Transform

$$\theta(x,t) = \int_{-\infty}^{\infty} \frac{q(\omega)}{q_0} \tilde{\theta}_m(x) e^{i\omega t} d\omega$$

Sinusoidal Heating

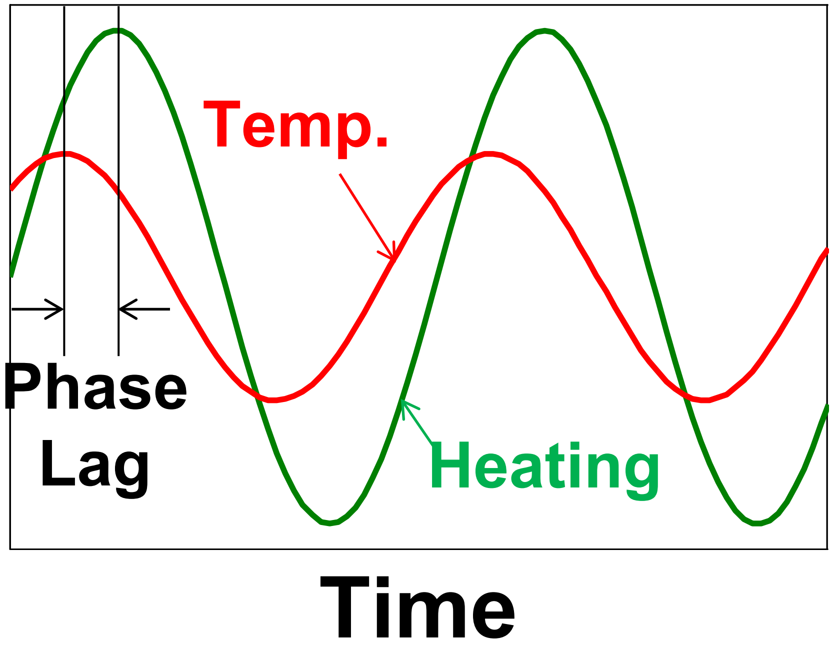
Surface Heat Flux at Frequency ω:

$$q'' \sim \cos(\omega t)$$



Temperature Response:

$$T(x,t) - T_\infty = A(x)\cos(\omega t + \phi)$$



Magnitude and Phase Lag Depend on Thermal Properties, Heating Frequency, and Depth into Sample

Frequency Domain Techniques

Sensitivity to properties (k, C_p, R'') depends on geometry and frequency

Three Omega (3ω) Method

Heat Source:
Sinusoidal electrical heating at surface 1

Temperature Measurement:
Electrical sensing at surface 1

Frequency Domain Thermoreflectance (FDTR)

Heat Source:
Sinusoidal optical heating at surface 1

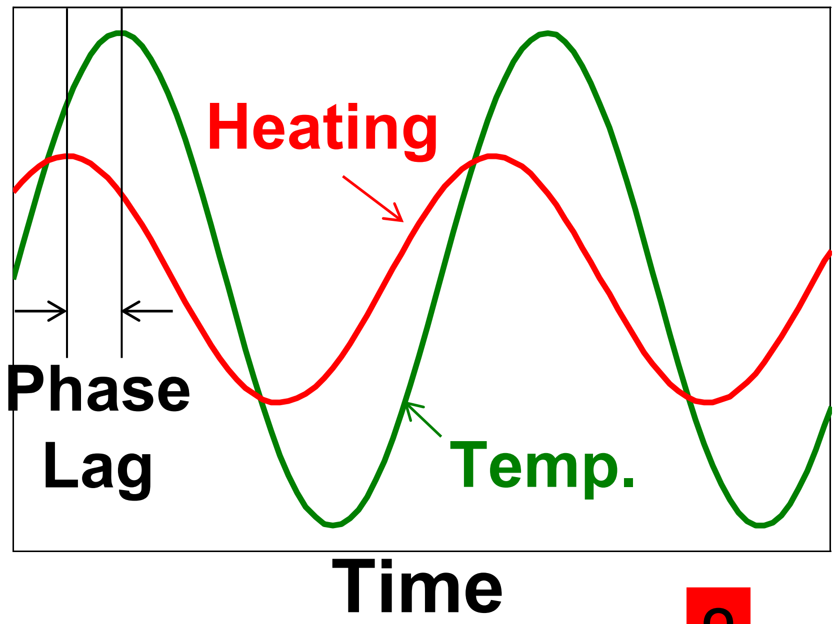
Temperature Measurement:
Optical sensing at surface 1

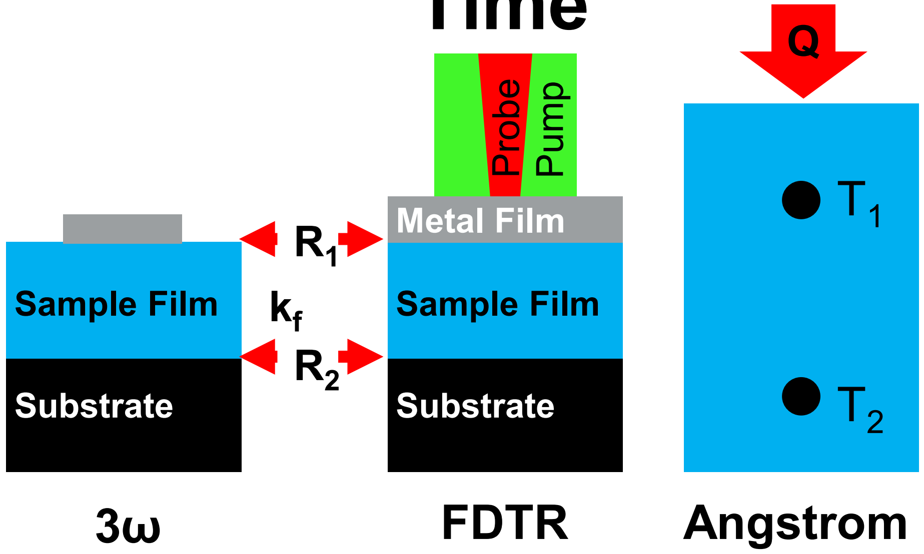
Sensitive to α

Angstrom Method

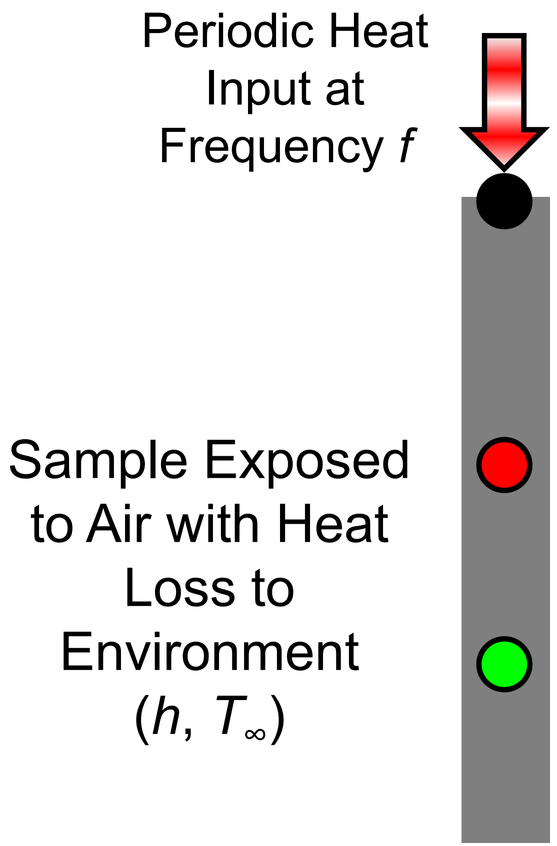
Heat Source:
Sinusoidal/Square wave heating at surface 1

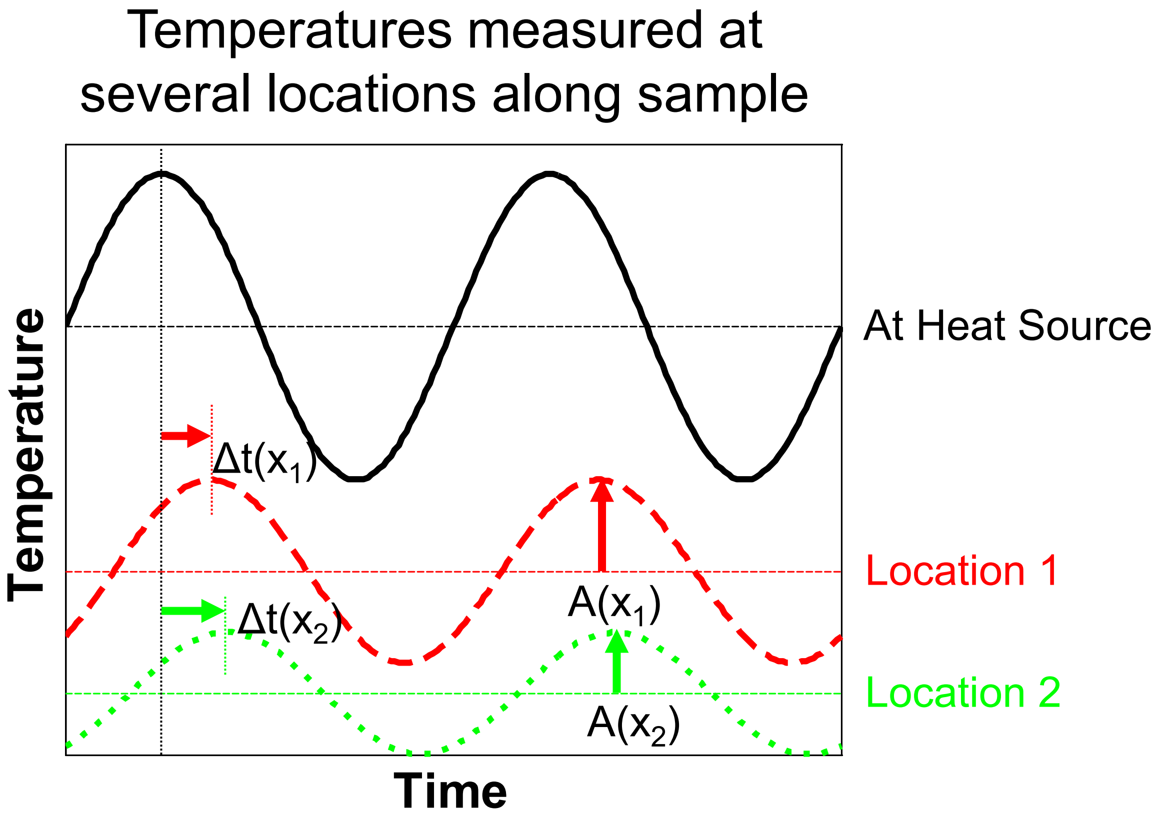
Temperature Measurement:
Sensing at ≥2 depths into sample (Thermocouples or IR)



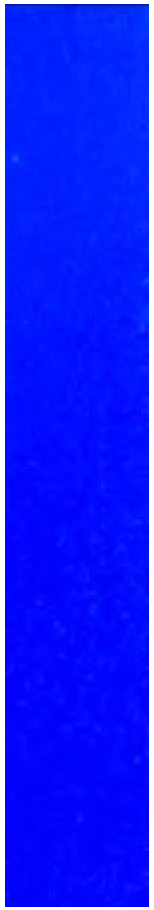


IR- Microscopy Enhanced Angstrom Method





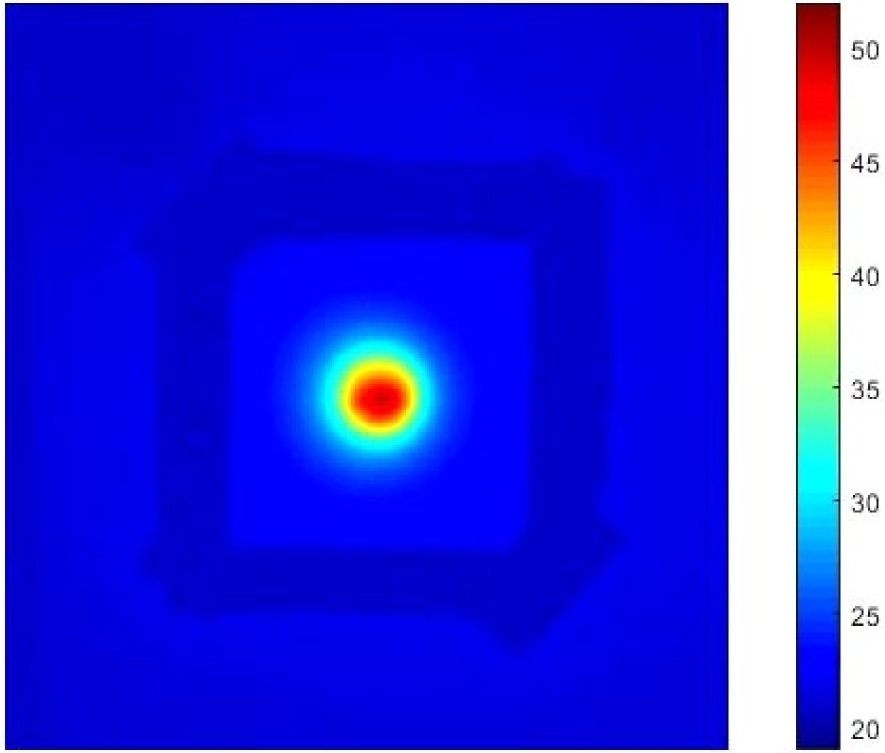
IR Data



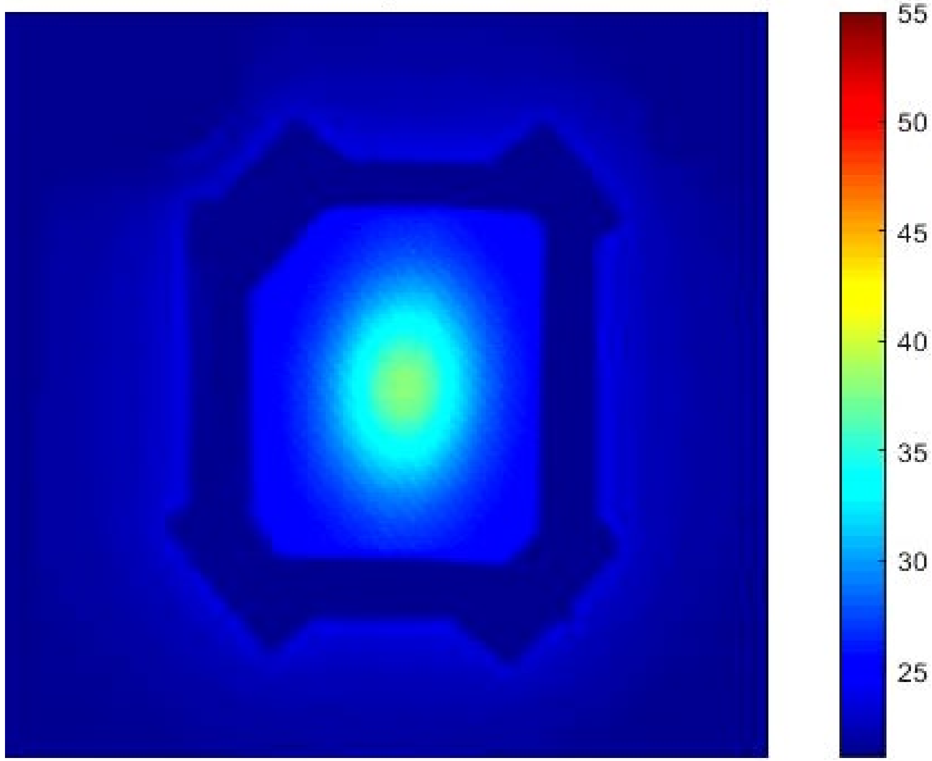
Hahn, Reid, and Marconnet, "Infrared microscopy enhanced Angstrom's method for thermal diffusivity of polymer monofilaments and films", *Journal of Heat Transfer*, Accepted and In Press.

In Plane Anisotropy

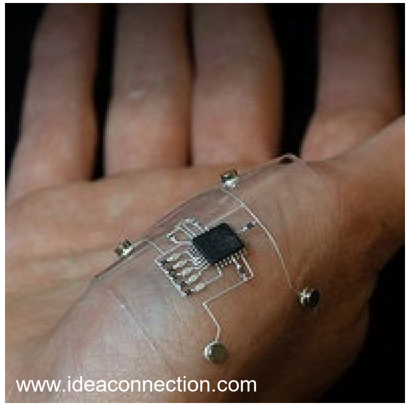
Isotropic, low *k*



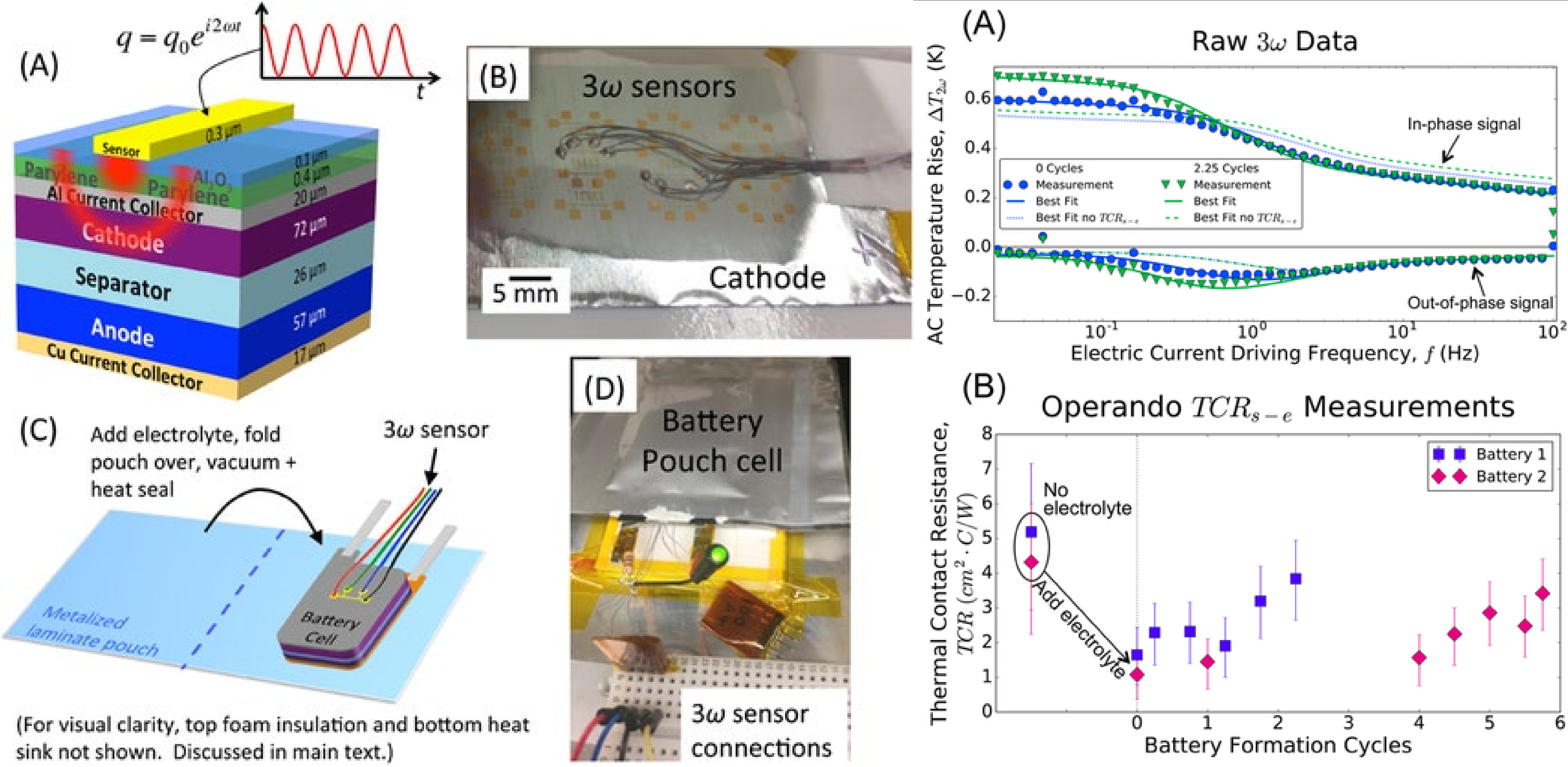
Anisotropic, high *k*



- Characterize and optimize material properties for composite heat spreaders
- Integrate flexible high conductivity heat spreaders into wearable electronics or situations needing conformal heat spreading



Operando 3ω sensors



Lubner et al., JAP, 2020. https://doi.org/10.1063/1.5134459

Selecting & Designing Measurements for a Particular Sample