SAND2009-2533P

Impact of Interfaces on Thermal Transport

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Thermal Interface Resistance

Field effect transistors

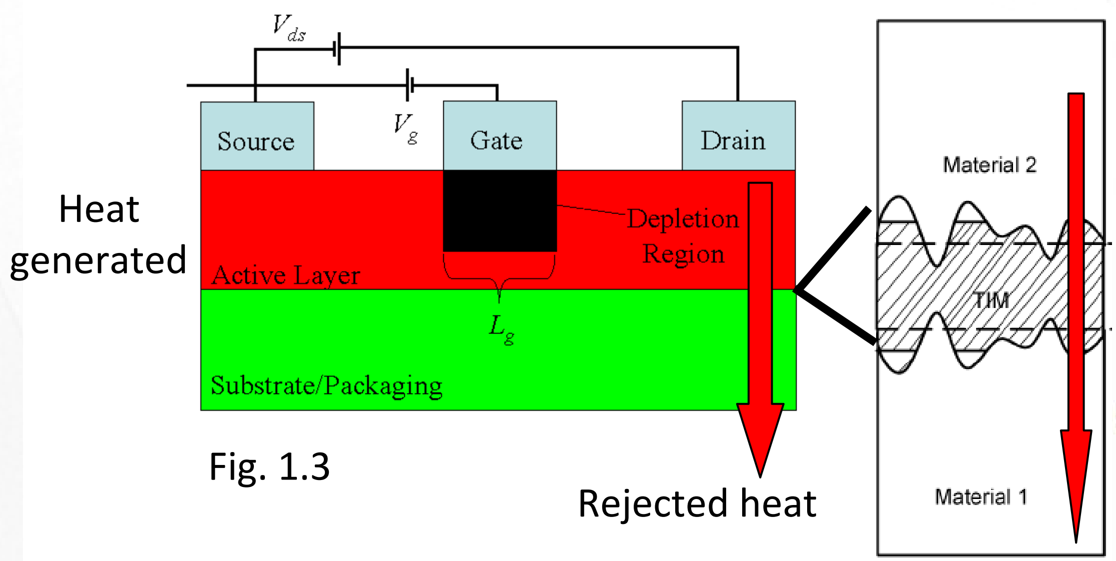
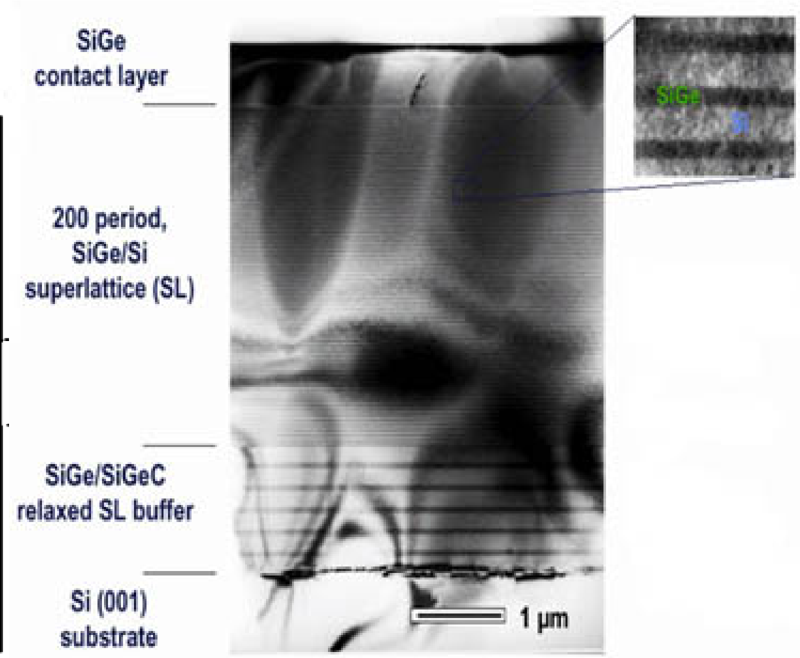


Fig. 1.3

Superlattices



Thermal management is highly dependent on the boundary of two materials

$$ZT = \frac{S^2 \sigma T}{k}$$

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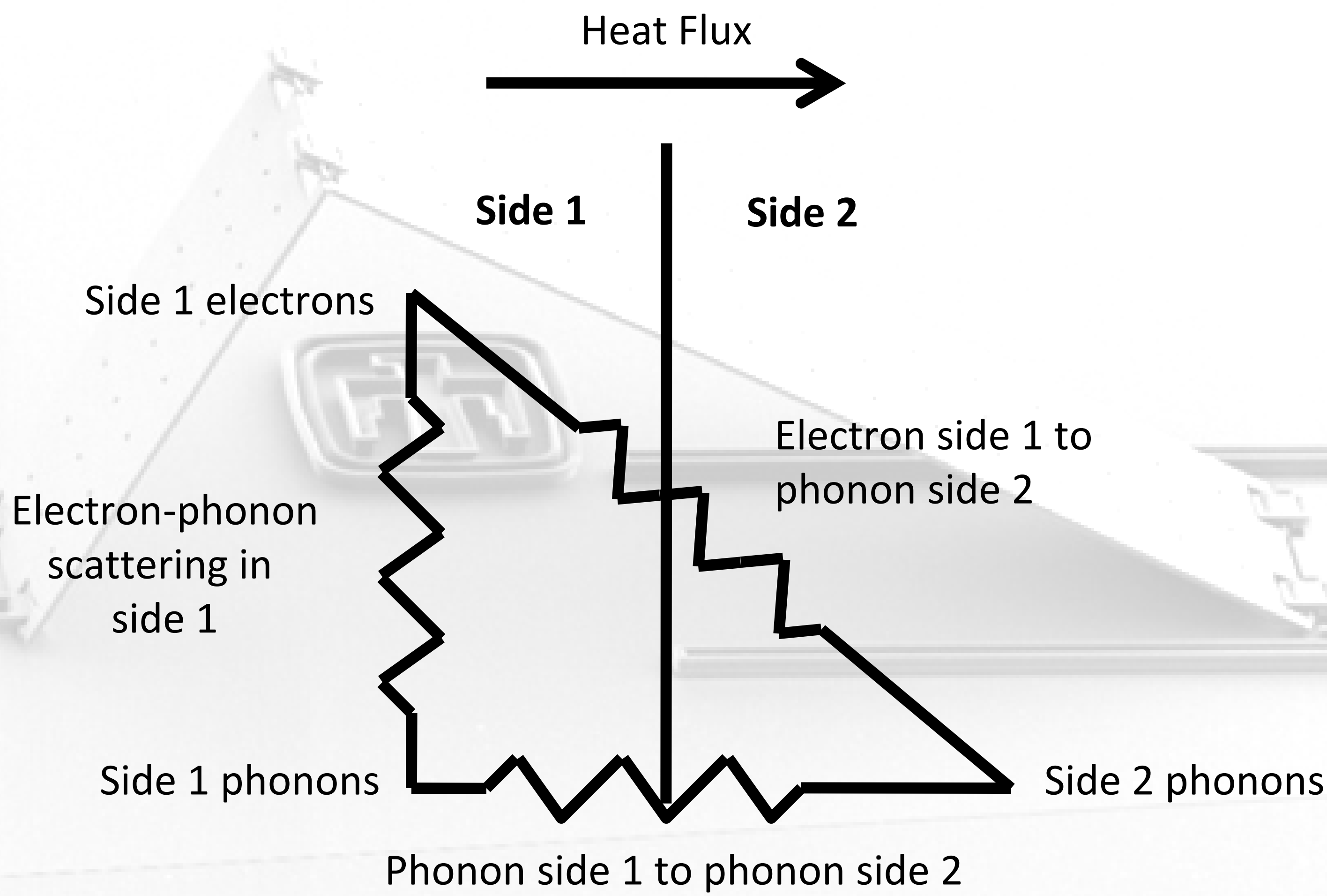
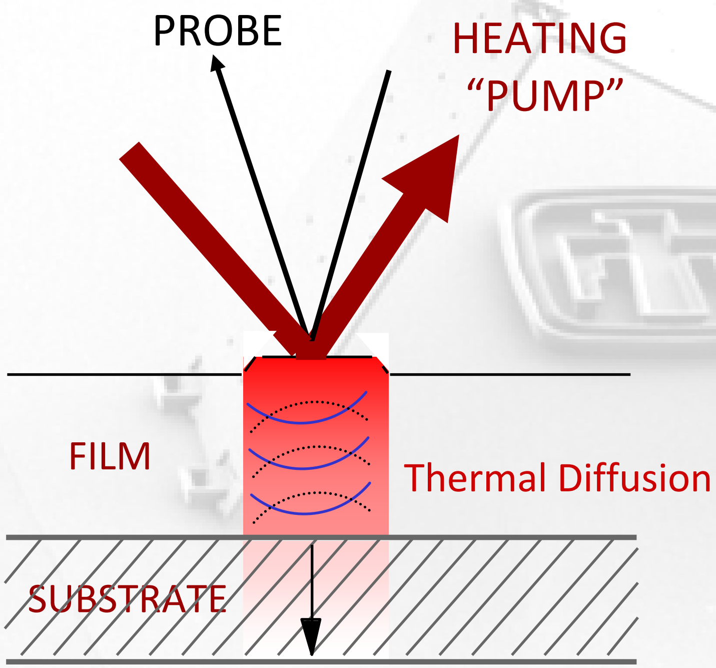
Limiting Forms of Resistance



Time Scales in Transient Thermal Reflectance (TTR) - Metal Film/Substrate



Free Electrons Absorb Laser Radiation

↓

Ballistic electron transport

↓

Electrons Transfer Energy to the Lattice | Thermal Diffusion by Hot Electrons — Electron-Phonon Coupling (~2 ps)

↓

Thermal Equilibrium

↓

Thermal Diffusion within Thin Film — Thermal Diffusion (~100 ps)

↓

Thermal Conductance across the Film/Substrate Interface — Thermal Boundary Conductance (~2 ns)

↓

Thermal Diffusion within Substrate — Substrate Thermal Diffusion (~100 ps – 100 ns)

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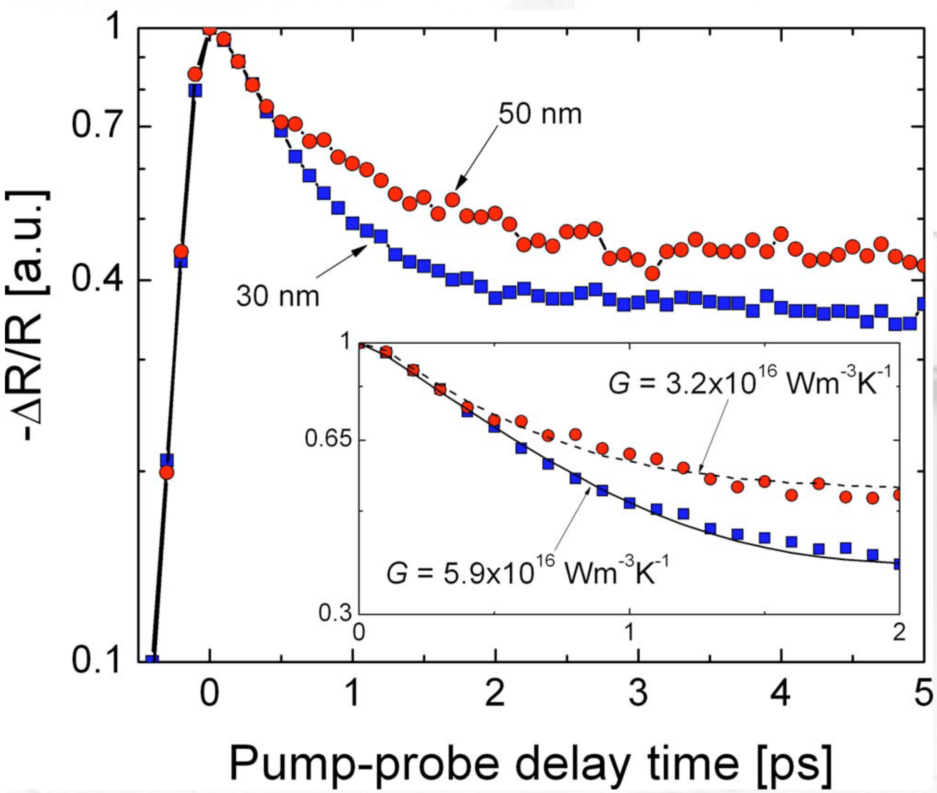
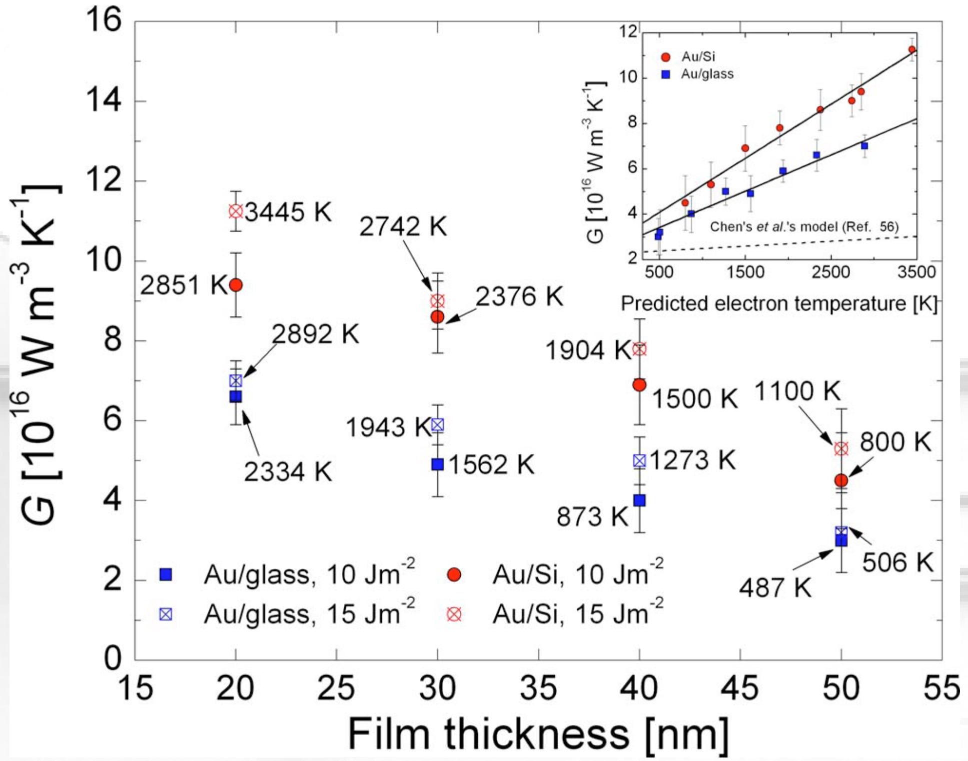
Electron-Phonon Coupling at Metal-Semiconductor Interfaces





Hopkins , Kassebaum, and Norris, 2009, *Journal of Applied Physics*, **105**, 023710.

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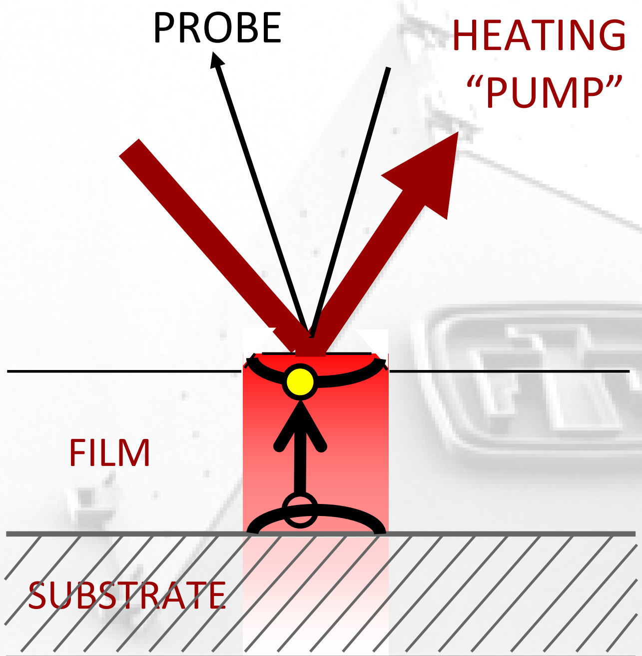
Time Scales in TTR - Semiconductors



TIME SCALES FOR THERMALIZATION AND RELAXATION OF HOT CARRIERS

Coherent Regime ($\lesssim$200 fs)

- momentum scattering
- carrier-carrier scattering
- hole-optical phonon scattering

Nonthermal Regime ($\lesssim$2 ps)

- electron-hole scattering
- electron-optical phonon scattering

Hot Excitation Regime ($\sim$1$\sim$100 ps)

- carrier-acoustic phonon scattering
- decay of optical phonons

Isothermal Regime ($\gtrsim$100 ps)

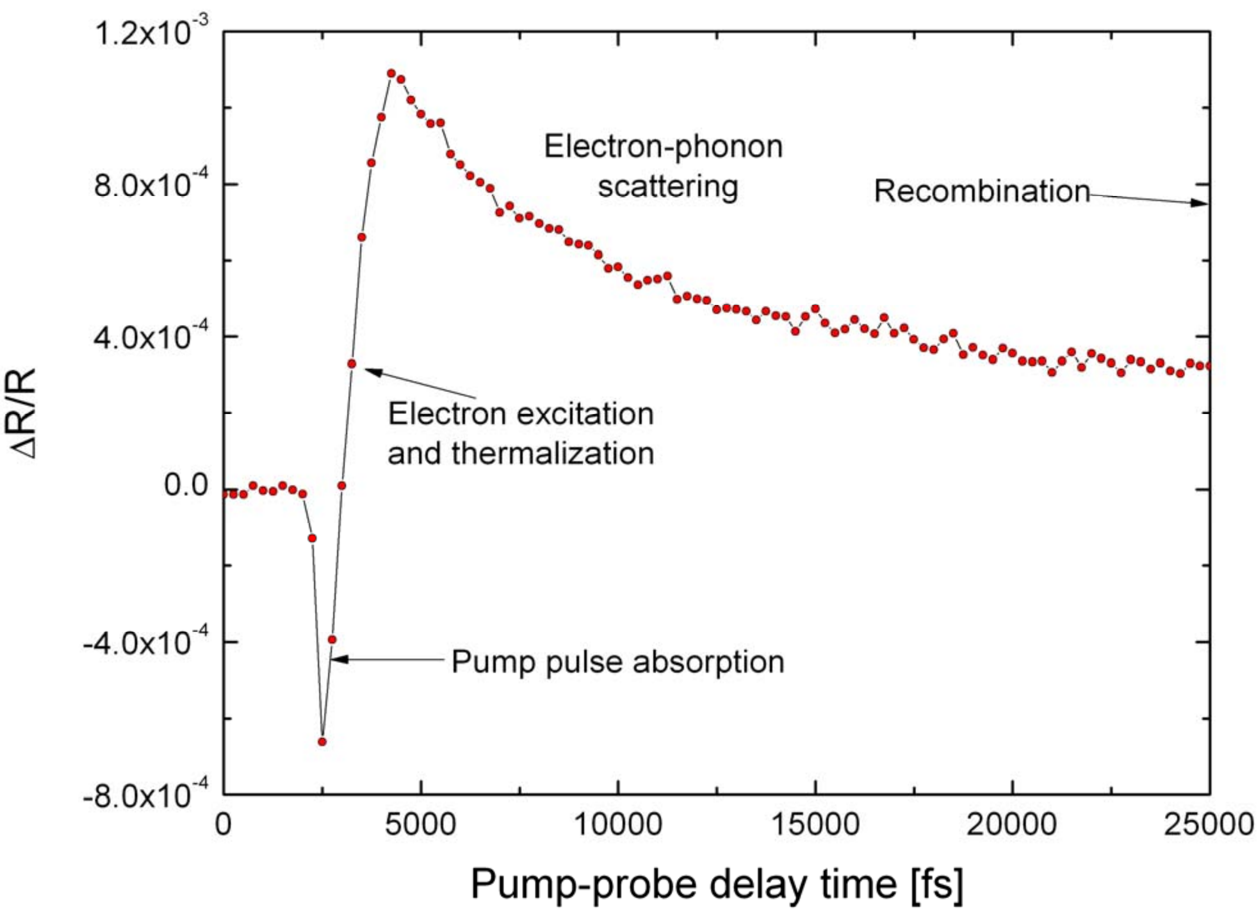
- carrier recombination

↓ *Time*

Klopf and Norris, 2005, *International Journal of Thermophysics*, **26**, p. 127.

EP Relaxation in Semiconductors

Fe doped InP, 400 nm pump, 750 nm probe



Typical thermoreflectance scan on semiconductor when pump and probe energies are greater than the band gap energy

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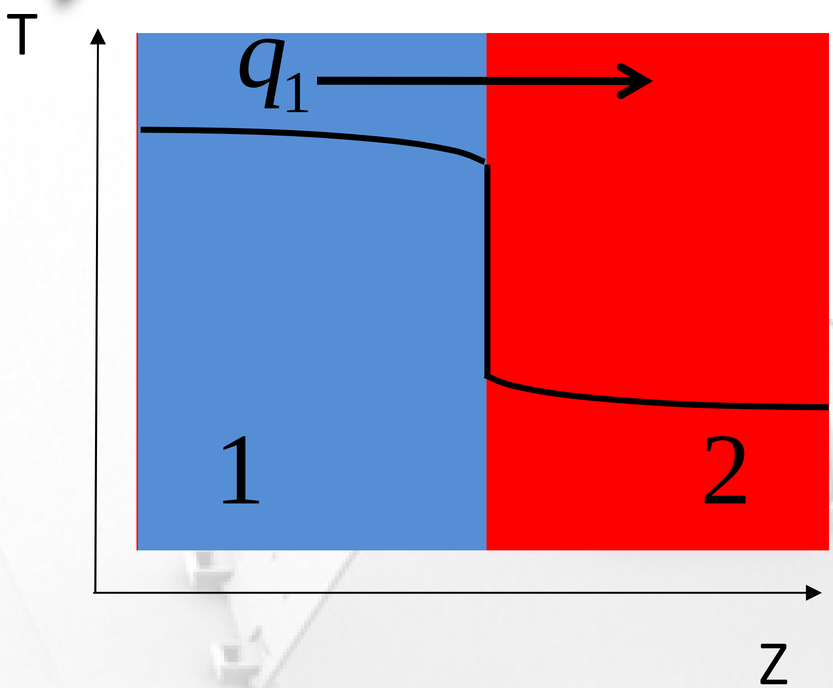
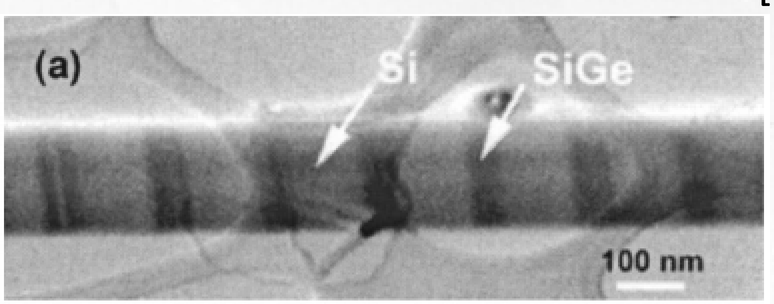
Thermal Boundary Conductance



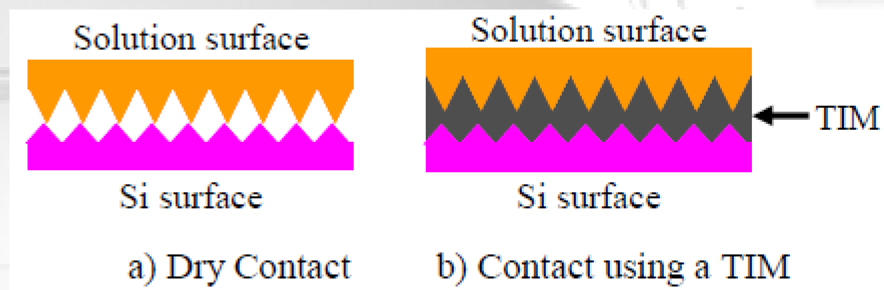
- G_K dominant thermal transport mechanism in nanostructures with thicknesses less than carrier mean free path
- Current nanoapplications rely on controlling phonon scattering in G_K

$$q_1 = G_K \Delta T$$

G_K= Thermal boundary conductance [$Wm^{-2}K^{-1}$]



Li, Wu, Fan, Yang, and Majumdar, 2003, *APL* **85**, 3186.



Samson *et al.*, 2005, *Intel Technology Journal*, **9**, 75.

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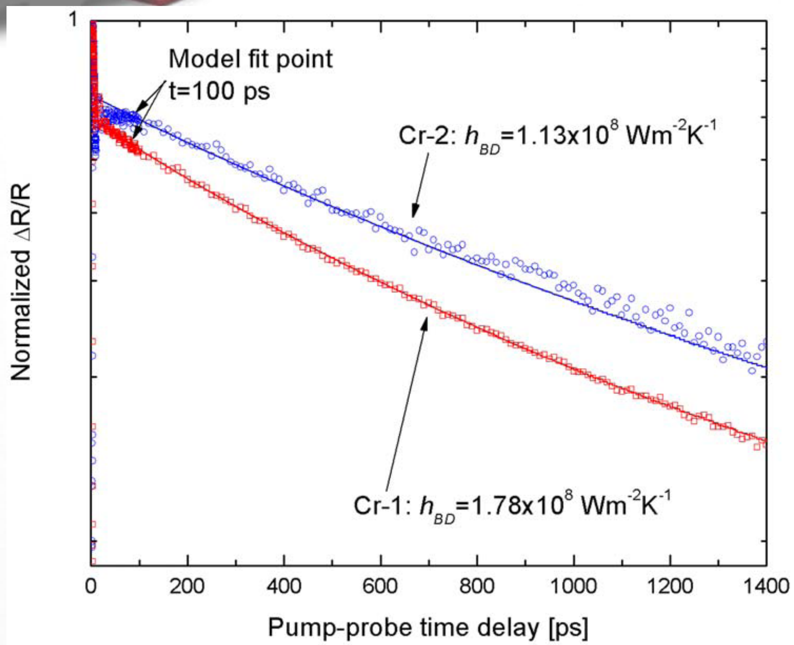
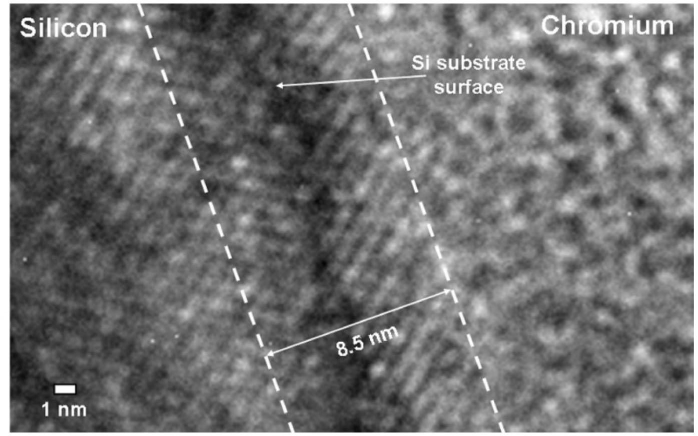
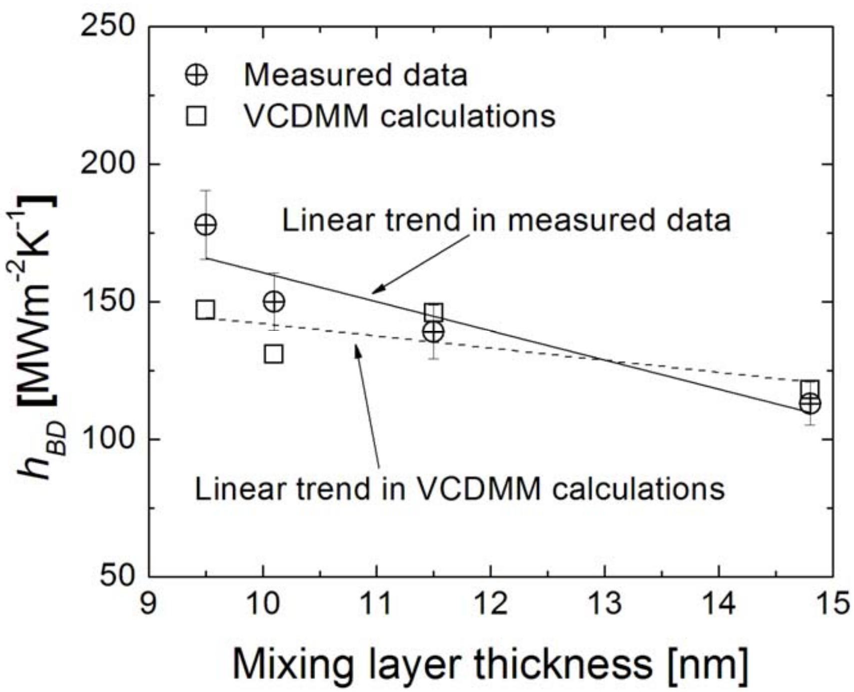
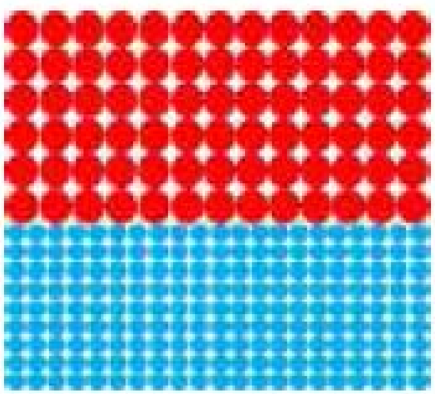
Phonon Scattering at Rough Interfaces



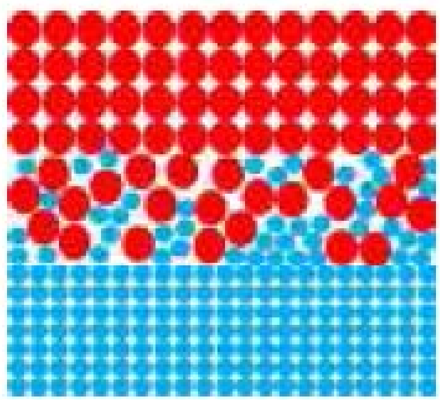




Typical assumption



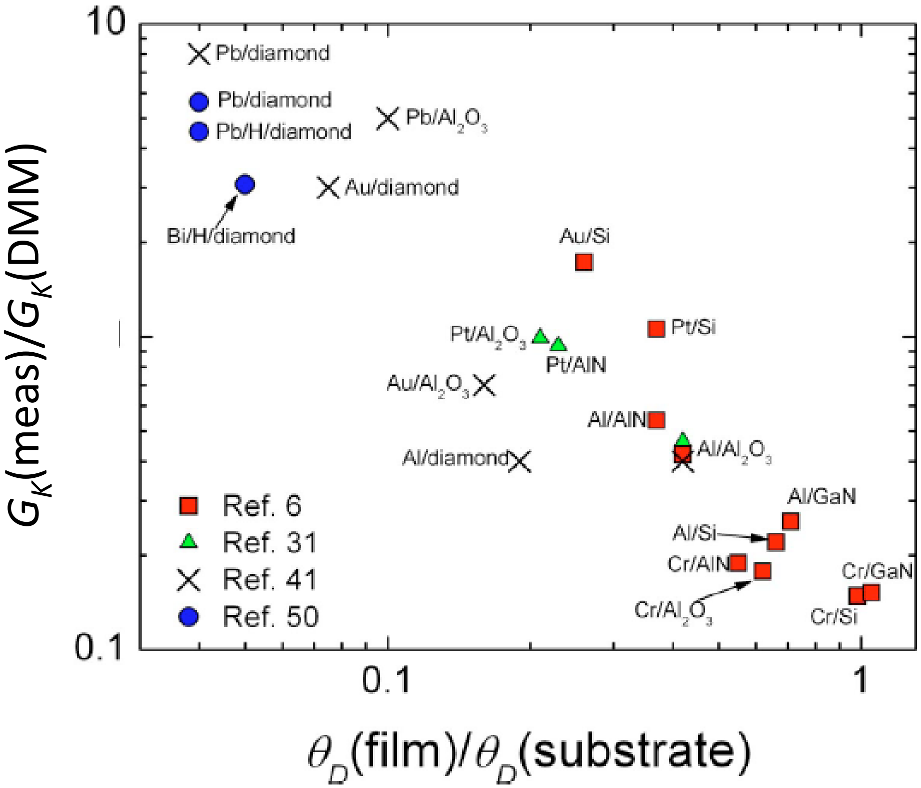
Realistic interface

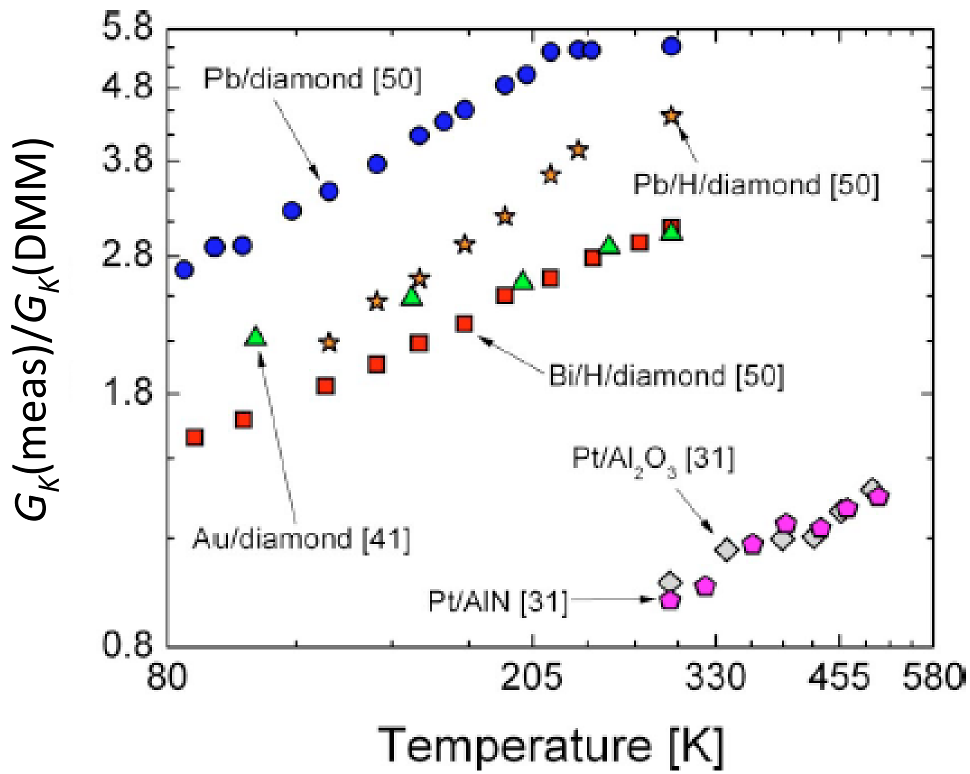


Hopkins, Norris, Stevens, Beechem, and Graham, 2008, *Journal of Heat Transfer*, **130**, 062402.

Laboratories

Consequences





Norris and Hopkins, 2009, *JHT*, **131**, 043207.

Ref. 6 – Stevens et al., 2005, *JHT*, **127**, 315.; **Ref. 31** – Hopkins *et al*., 2008, *JHT*, **130**, 022401.
Ref. 41 – Stoner and Maris, 1993, *PRB*, **48**, 16373.; **Ref. 50** – Lyeo and Cahill, 2006, *PRB*, **73**, 144301.

When $T>\theta_D$, Inelastic scattering causes linear trend in G_K

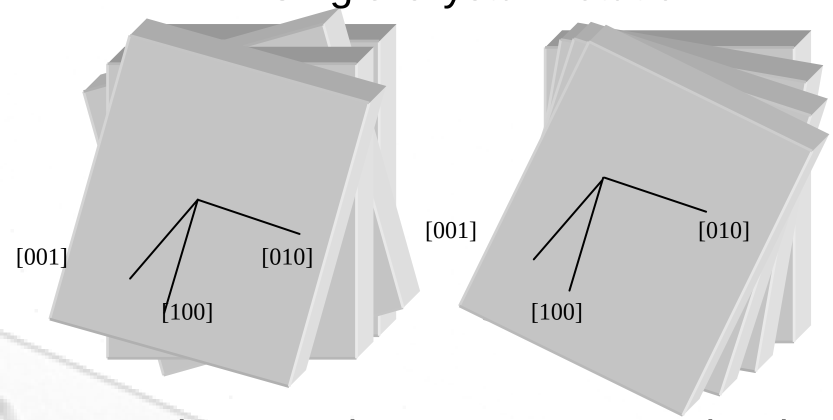
DMM predicts constant trend in G_K

Scattering at Grain Boundaries

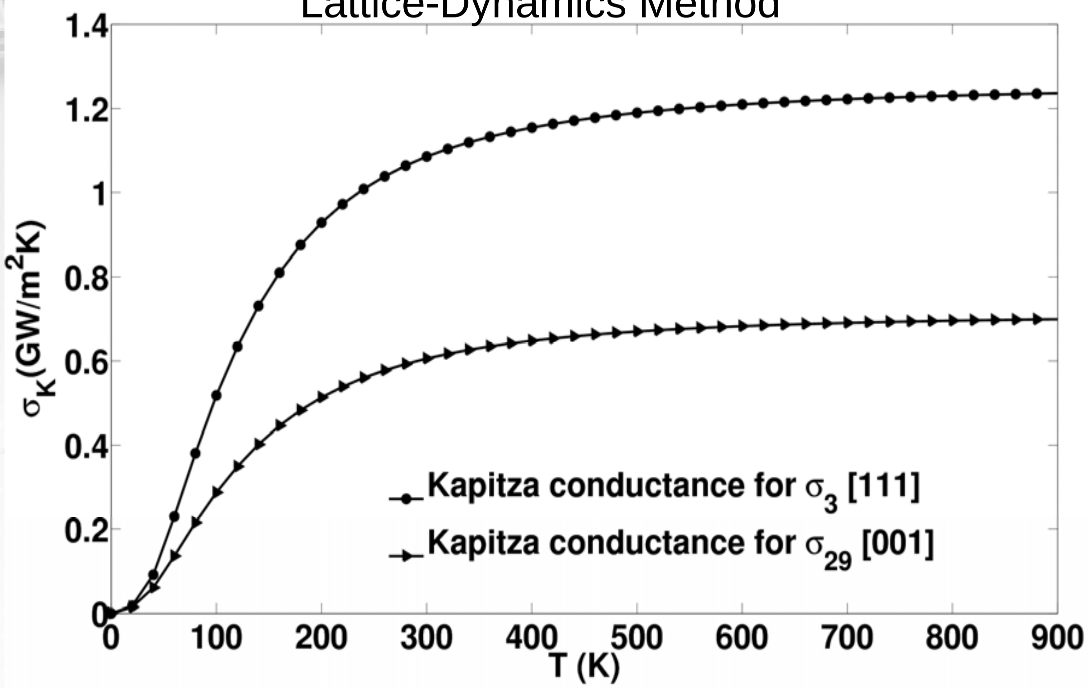
- Phonon scattering at interfaces calculated
- Molecular-dynamics simulations determine transmission coefficients at interfaces
- Thermal conductance then calculated via lattice-dynamics or Monte Carlo simulations

Figures courtesy of E. Piekos, S. Aubry, and S. Shinde

Examples of Twist Boundaries Created by Single Crystal Rotation

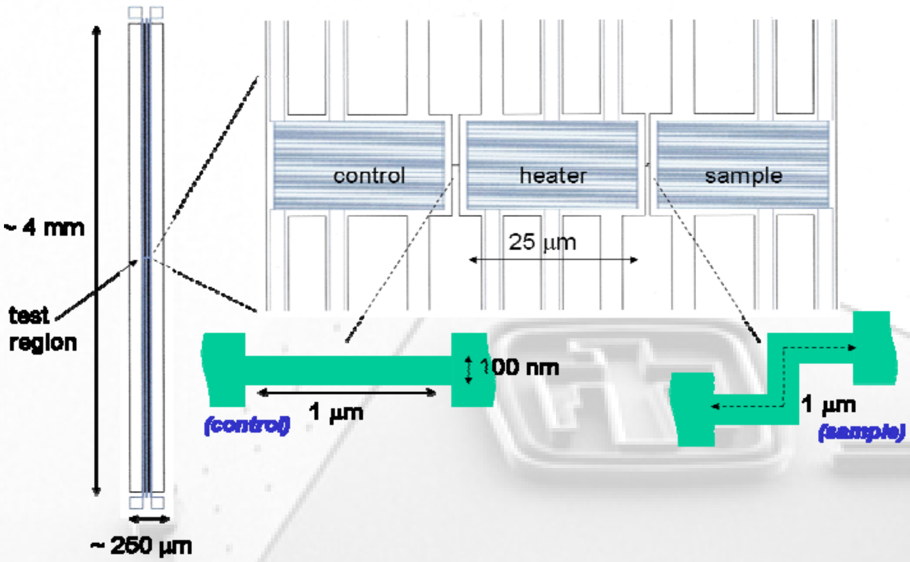


Kapitza Conductance Computed Using Lattice-Dynamics Method

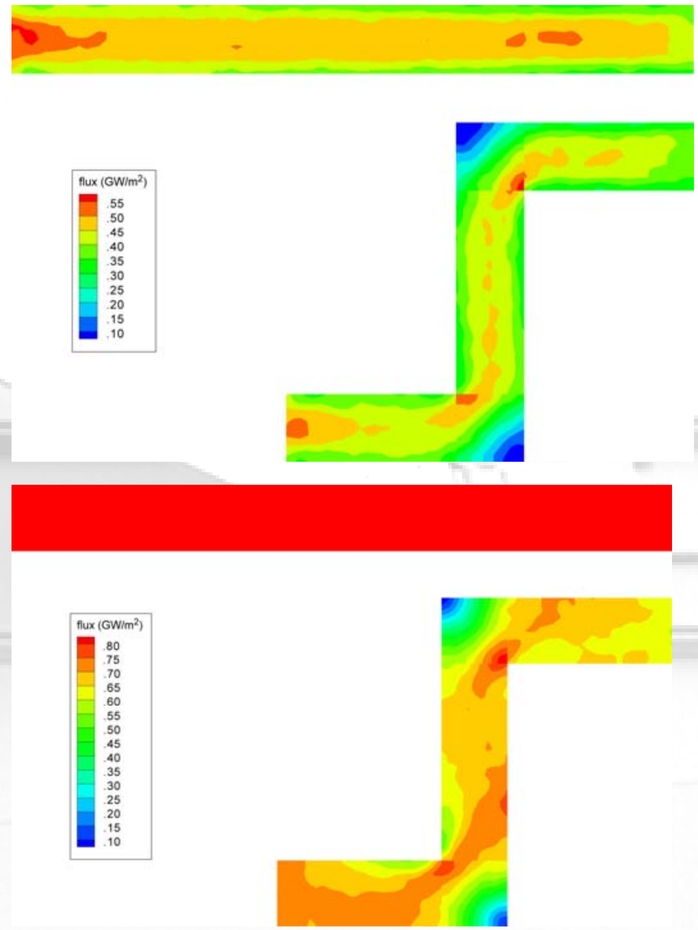


Phonon Scattering at Boundaries

Differential Thermal Test Structure for Measuring Phonon Scattering along Boundaries



Monte Carlo Flux Prediction for Test Ligaments



- Understand the Effect of Boundary Scattering on Thermal Transport
- Plans to Measure Accomodation Coefficient Using Differential Structure and Confirm via Simulation Results

Figures courtesy of E. Piekos and J. Sullivan

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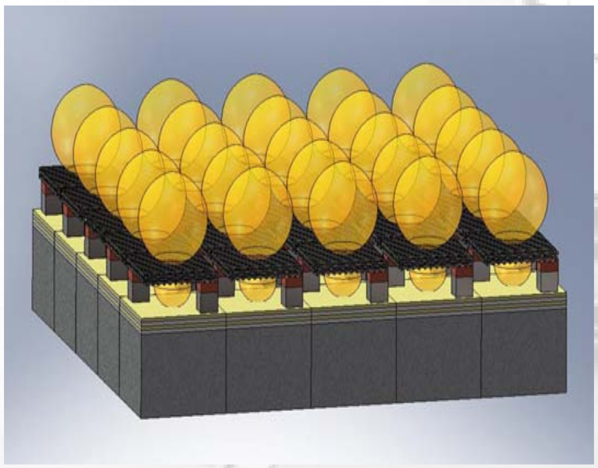
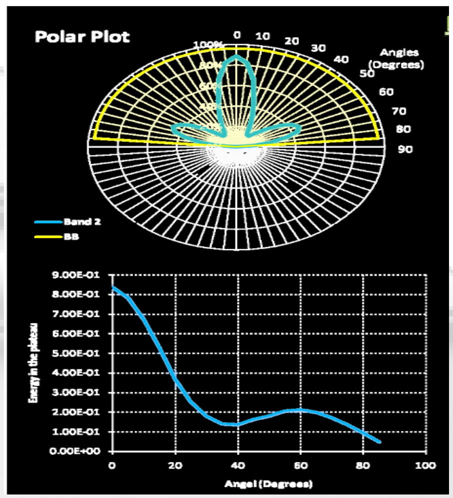
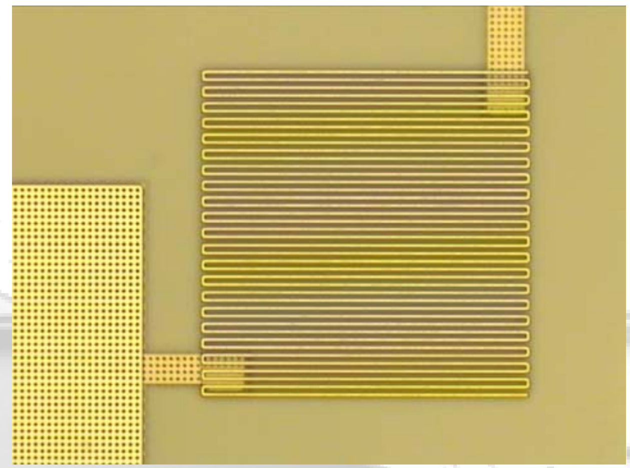
Engineered Thermal Emission

Advanced Modeling, Design, and Fabrication utilizing Sandia's MESA Facility

Theory → Modeling & Design → Fabrication & Test







$$I(\Omega_q,\omega) = c\rho(\omega)\mathscr{T}(\vec{q},\omega),$$

$$\mathscr{T}(\vec{q},\omega) = \frac{1}{2}\sum_{nm}\sum_{n'm'}\tau_{nm}\tau_{n'm'}\left[c_{TE}(\vec{k}_{nm})c_{TE}(\vec{K}_{n'm'})\frac{(\mathbf{q}\times\hat{k}_{nm})\cdot(\mathbf{q}\times\hat{K}_{n'm'})}{q_z^2} + c_{TM}(\vec{k}_{nm})c_{TM}(\vec{K}_{n'm'})\frac{k^z_{nm}K^z_{n'm'}(\hat{k}_{nm}\cdot\hat{K}_{n'm'})}{k^2\varepsilon}\right],$$

- Theoretical Modeling for Design of Structured Emitters
- Integration of Structured Emitters with drive electronics

Submitted to Optics Express: Direct Thermal Emission from a Planar Structured Emitter:Kirchoff's Law and Generalized Emissivity, P. S. Davids.

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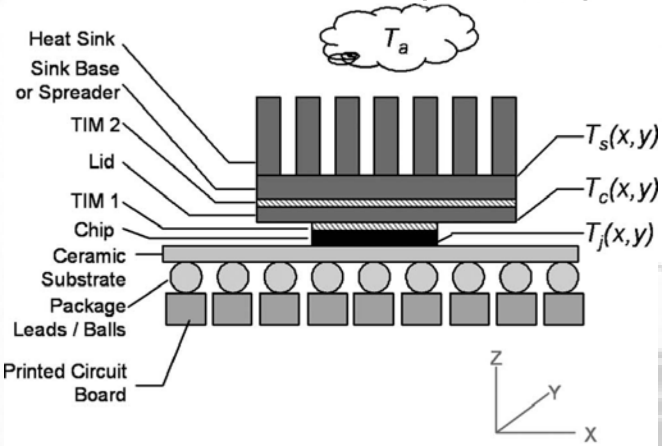
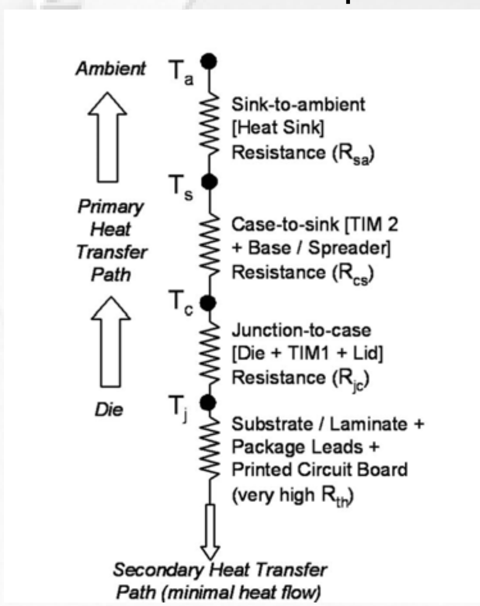
Exergy Analysis of Microelectronics Chip Package

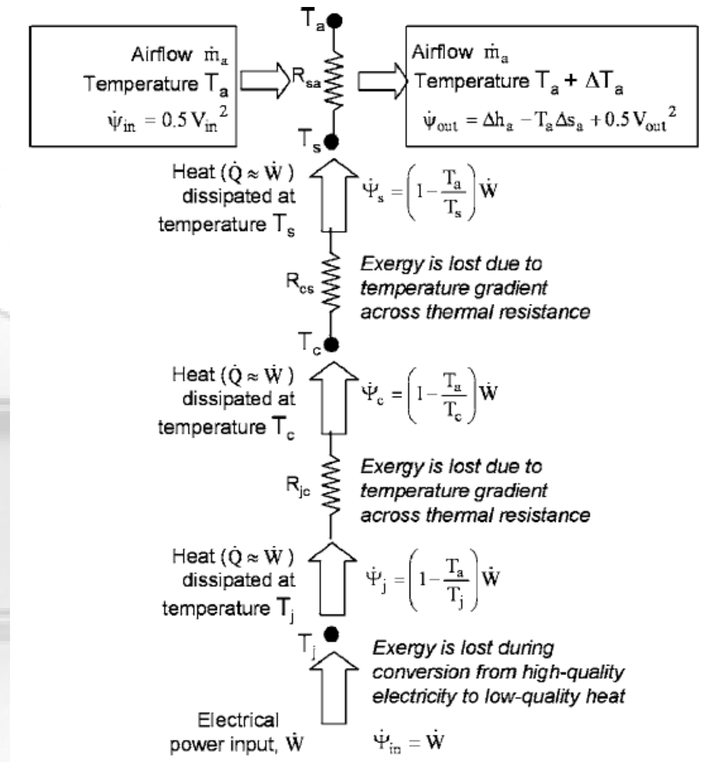
Microelectronics Chip Package



Thermal Resistance Network of Microelectronics Chip Package



Junction-to-Ambient Energy and Exergy Flow for Microelectronics Chip Package



Exergy – maximum theoretical work obtainable as a system comes into equilibrium with a reference environment

Reference and Figures: Shah, Carey, Bash, and Patel, 2006, *Journal of Electronic Packaging*, **128**, 360-369

Unanswered Questions on Thermal Transport

- How does roughness and mixing affect electron and phonon heat transfer at interfaces?
- Can we isolate effects of electron and phonon heat transfer at interfaces?
- What are the electron and phonon thermophysical properties of nanomaterials?
- How can we quantify and contronl the effects of interfaces on thermal transport?
- How do interfaces impact the availability of energy from microelectronics for harvesting and/or conversion?

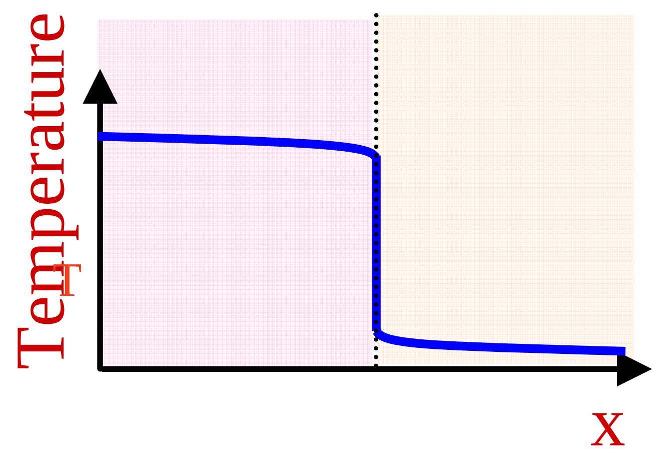
Thermal boundary resistance

•Thermal boundary resistance creates a temperature drop, ΔT, across an interface between two different materials when a heat flux is applied.

•First observed by Kapitza for a solid and liquid helium interface in 1941.

$$q = h_{BD}\Delta T$$

$$h_{BD} = {}^{1}\!/\!_{R_{BD}}$$



A typical resistance of

10^{-9}-10^{-7} m^2K/W

is equivalent to

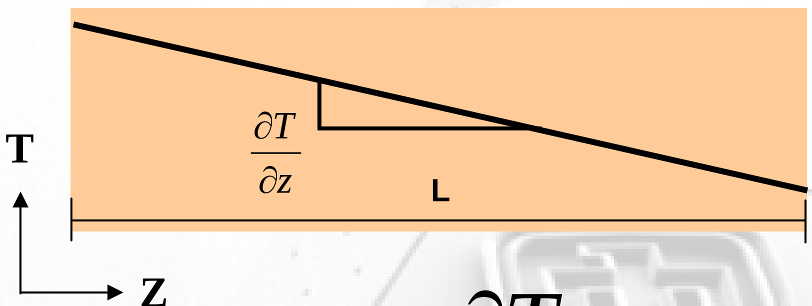
~ 0.15-15 μm Si

~ 1-100 nm SiO_2

Mismatch in materials causes a resistance to heat flow across an interface.

Thermal conduction in bulk materials

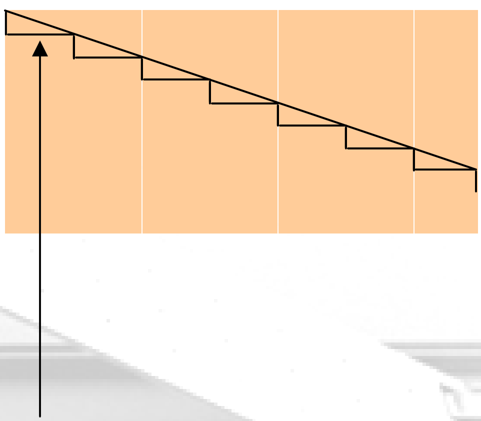
Thermal conduction



$$q_z = -k\frac{\partial T}{\partial z} = q$$

k = thermal conductivity [$Wm^{-1}K^{-1}$]
q = thermal flux [Wm^{-2}]

Microscopic picture



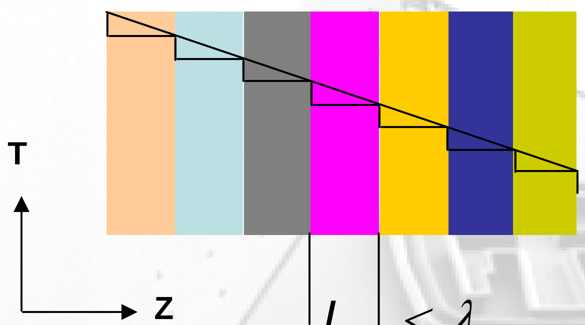
λ = mean free path [m]

phonon-phonon scattering length in homogeneous material

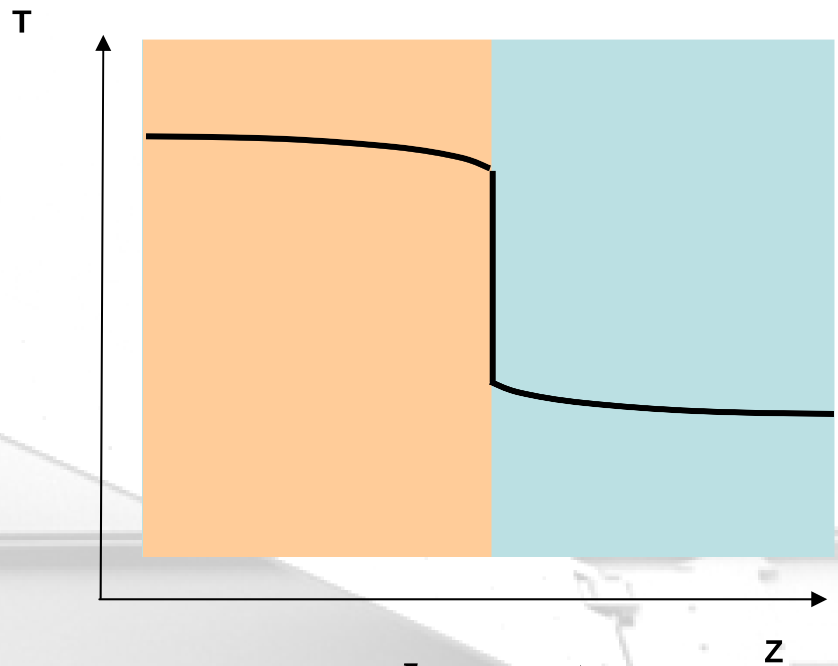
What happens if λ is on the order of L?

Thermal conduction in nanomaterials

Microscopic picture of nanocomposite



$L_n < \lambda_n$



$k_{effective}$ of nanocomposite does not depend on phonon scattering in the individual materials but on phonon scattering at the interfaces

$$q = h_{BD} \Delta T$$

h_{BD} = thermal boundary conductance [$Wm^{-2}K^{-1}$]

Change in material properties gives rise to h_{BD}

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Diffuse scattering

$$q_1 = \frac{1}{2}\sum_j \int_0^{\pi/2} \int_0^{\omega_{1,j}^{cutoff}} D_{1,j}(\omega) f(\omega, z, t) \hbar \omega v_{1,j} \alpha_{1,j}(\phi, j, \omega) \cos(\phi) \sin(\phi) d\omega d\phi = h_{BD} \Delta T$$

Diffuse Mismatch Model (DMM)

E. T. Swartz and R. O. Pohl, 1989, "Thermal boundary resistance," Reviews of Modern Physics, 61, 605-668.

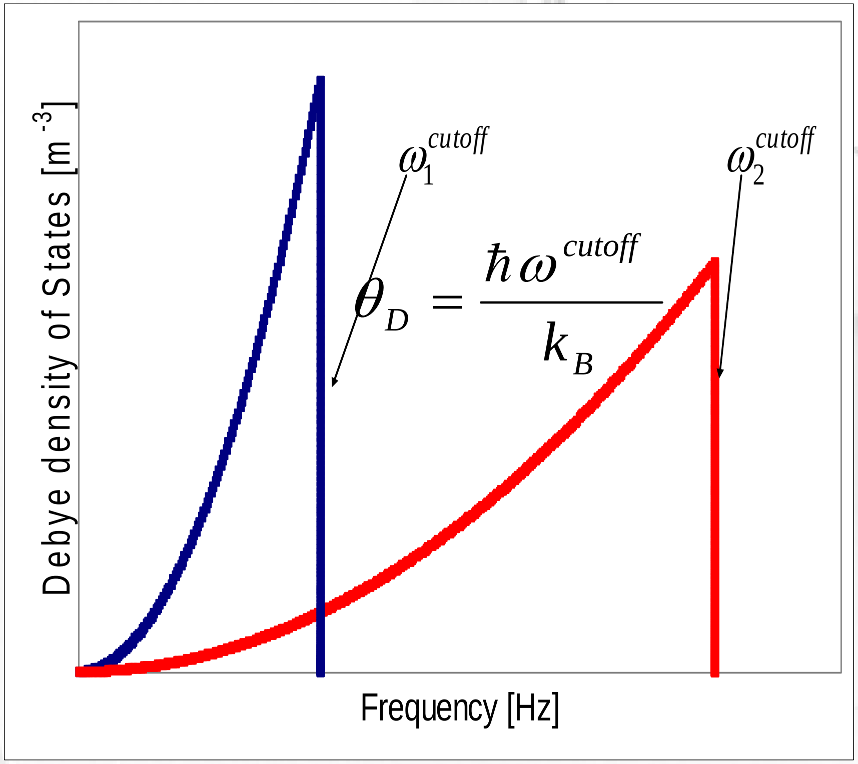
diffuse scattering – phonon "looses memory" when scattered

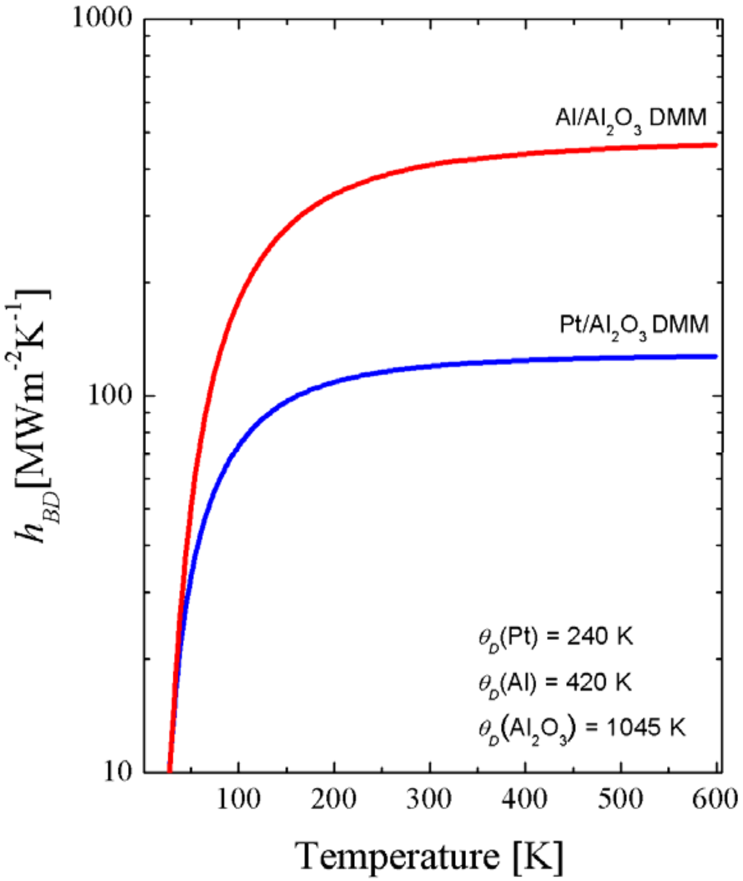
$$h_{BD,1} = \frac{1}{4}\sum_j \frac{\partial}{\partial T} \int_0^{\omega_{1,j}^{cutoff}} D_{1,j}(\omega) f(\omega, T) \hbar \omega v_{1,j} \alpha_1 d\omega$$

- **Scattering completely diffuse** → T > 50 K and realistic interfaces
- **Elastically isotropic materials** → Averaged properties in different crystallographic directions
- **Single phonon elastic scattering** → **Is this assumption valid?**

Single phonon elastic scattering

$$h_{BD,1} = \frac{1}{4}\sum_j \frac{\partial}{\partial T} \int_0^{\omega_{1,j}^{cutoff}} D_{1,j}(\omega) f(\omega,T) \hbar\omega v_{1,j}\alpha_1 d\omega$$





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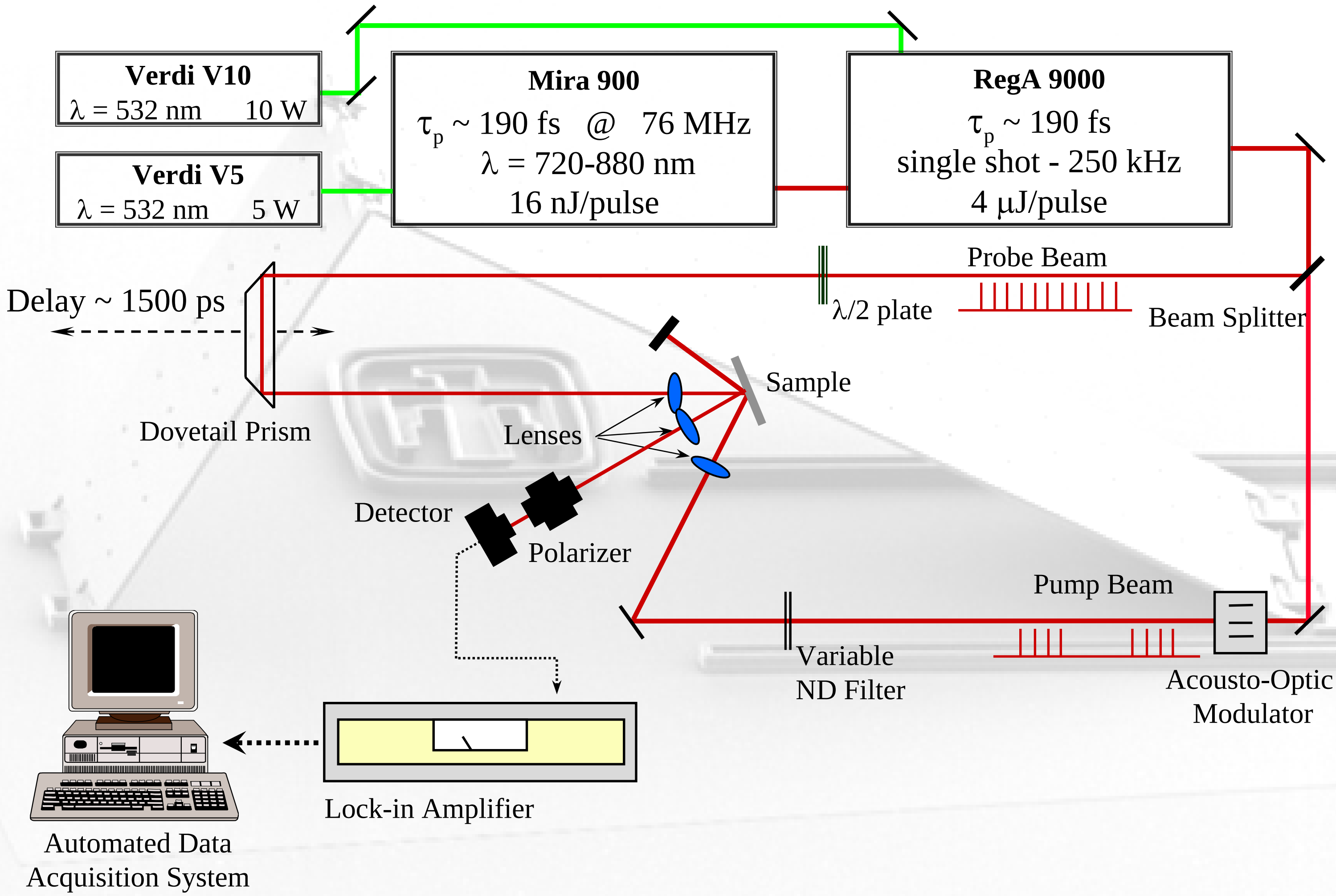
Ultrashort Pulsed Transient ThermoReflectance (UPTTR)



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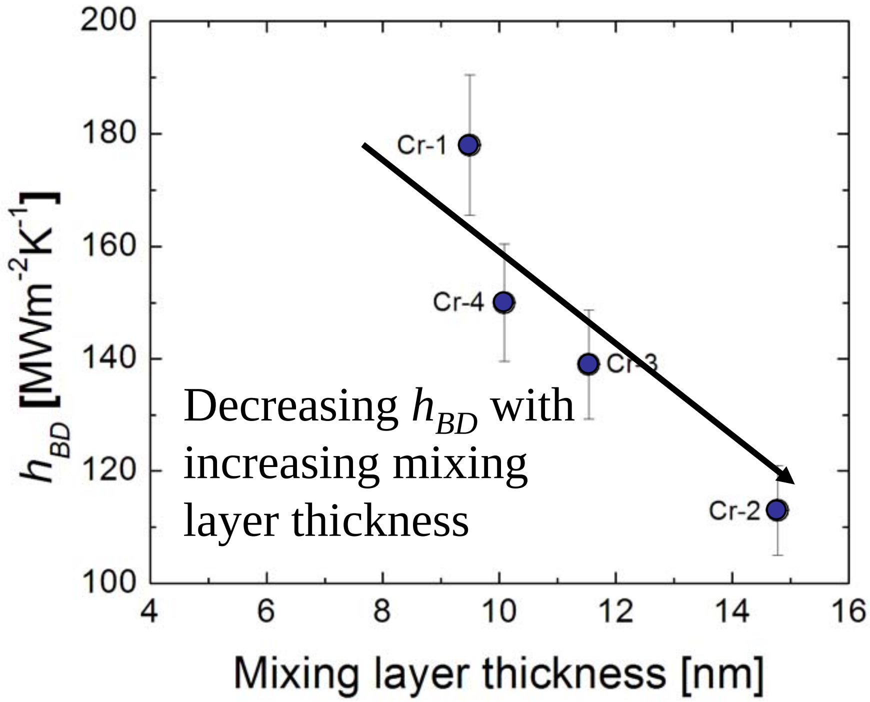
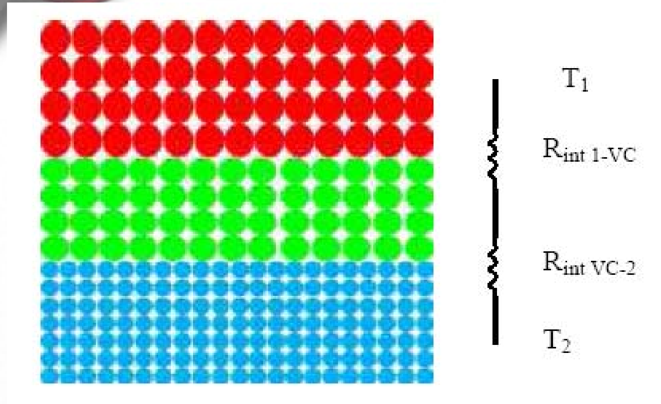
Effects of disorder on h_{BD}



DMM predicts a constant h_{BD} = 855 MWm^{-2}K^{-1}

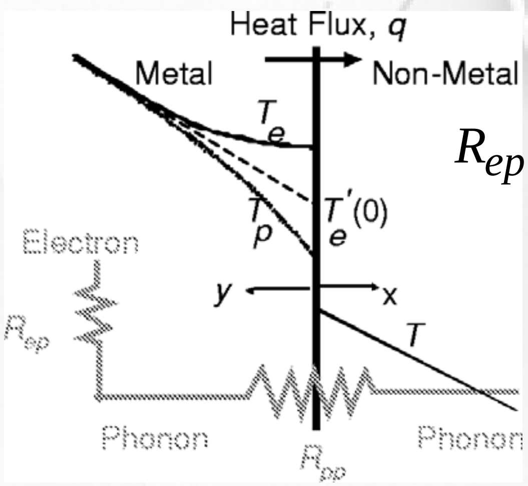
Hopkins, Norris, Stevens, Beechem, and Graham, to appear in the Journal of Heat Transfer, 2008

Effects of disorder on h_{BD}



$$R_{BD} = \frac{1}{h_{BD}} = \frac{D_{\text{int}}}{\lambda_{\text{int}}}\left[R_{pp,j}^{1\to VC} + R_{pp,j}^{VC\to 2}\right] = R_{pp}$$

$$\frac{D_{\text{int}}}{\lambda_{\text{int}}} \longrightarrow$$ multiple scattering events from interatomic mixing

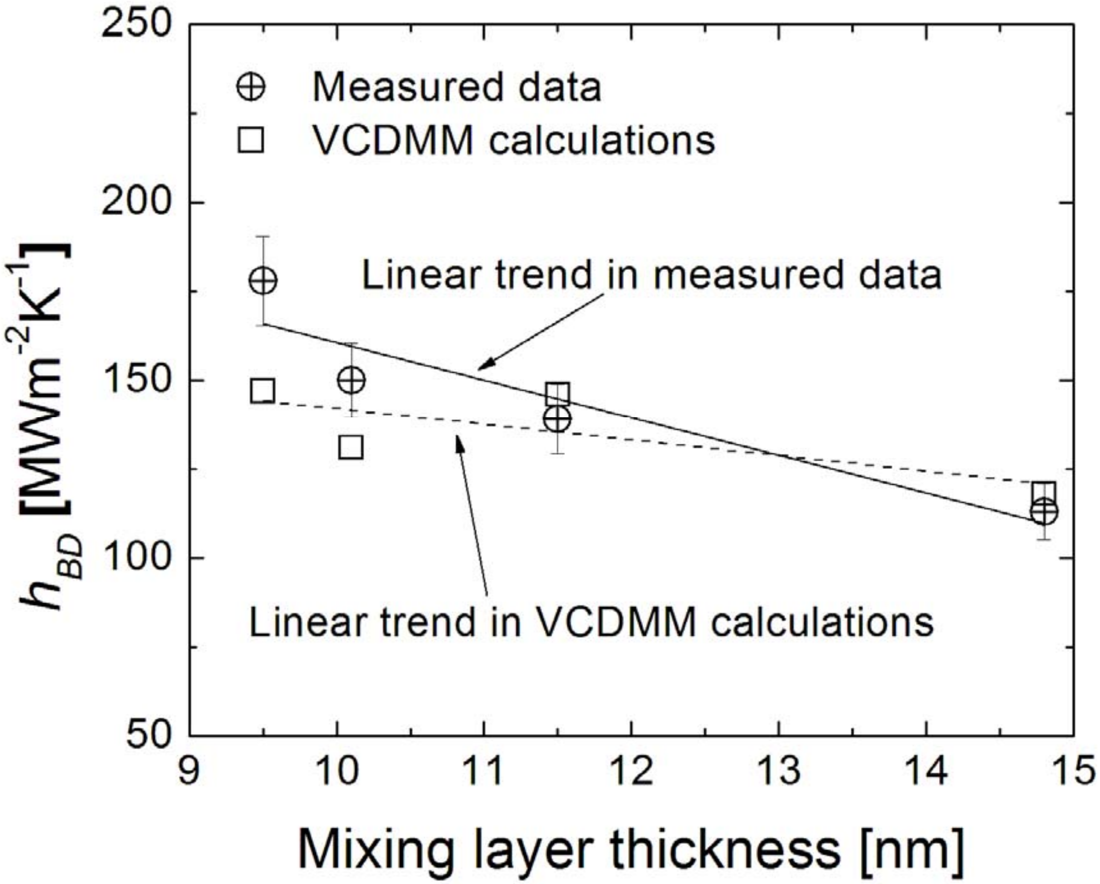


Majumdar and Reddy, APL, 2006

$$R_{ep} = \frac{1}{\sqrt{k_p G}} = \frac{1}{h_{ep}}$$

$$h_{BD} = \left\{ \frac{1}{\sqrt{k_p G}} + \frac{D_{\text{int}}}{\lambda_{\text{int}}} \left[\frac{1}{\sum_j h_{pp,j}^{1\to VC}} + \frac{1}{\sum_j h_{pp,j}^{VC\to 2}} \right] \right\}^{-1}$$

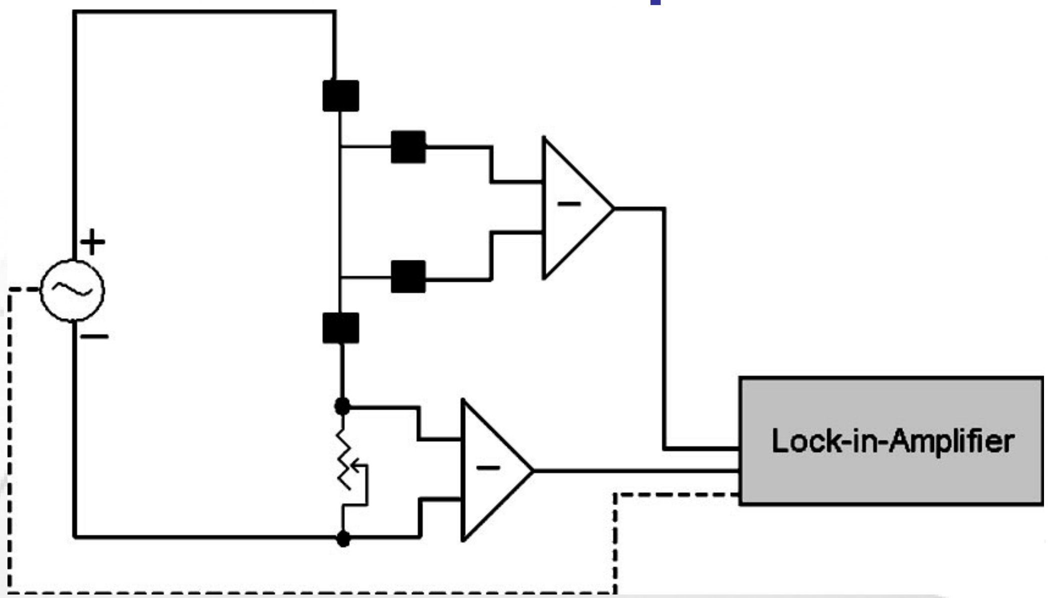
Effects of disorder on h_{BD}

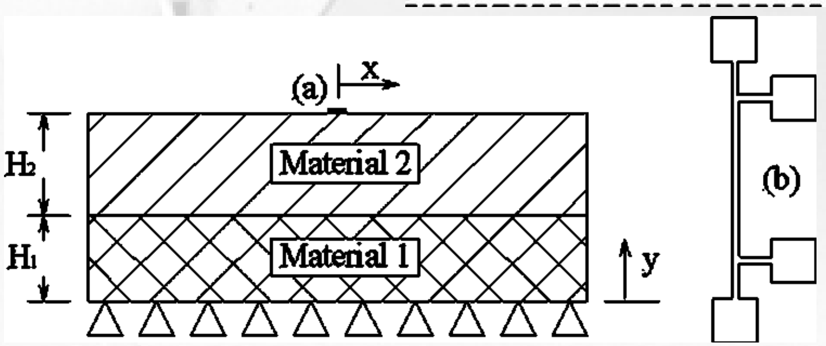


DMM predicts h_{BD} that is almost 8 times larger than that measured on the samples and no dependence on mixing layer thickness or composition.

The VCDMM calculations are within 18% of the measured values and show the same trend with mixing layer thickness as the measurements.

3ω technique

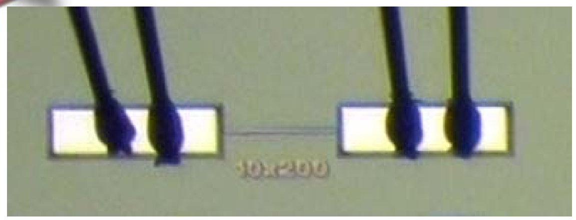


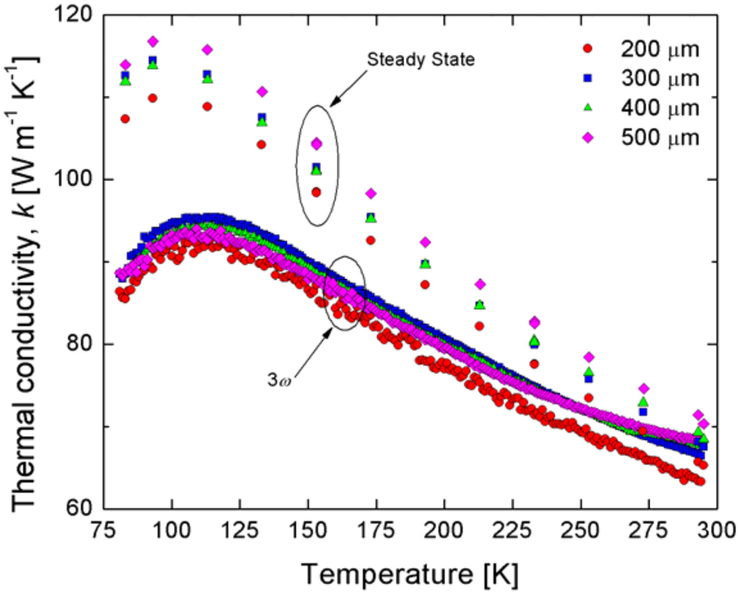


B. W. Olson, S. Graham, and K. Chen, Review of Scientific Instruments **76**, 053901 (2005).

- **Measure thermal conductivity of nanocomposites**
- **Control temperature of sample and subject samples to large temperature variations during measurements**
- **Sensitive to anisotropic area such as structurally variant interfacial regions**

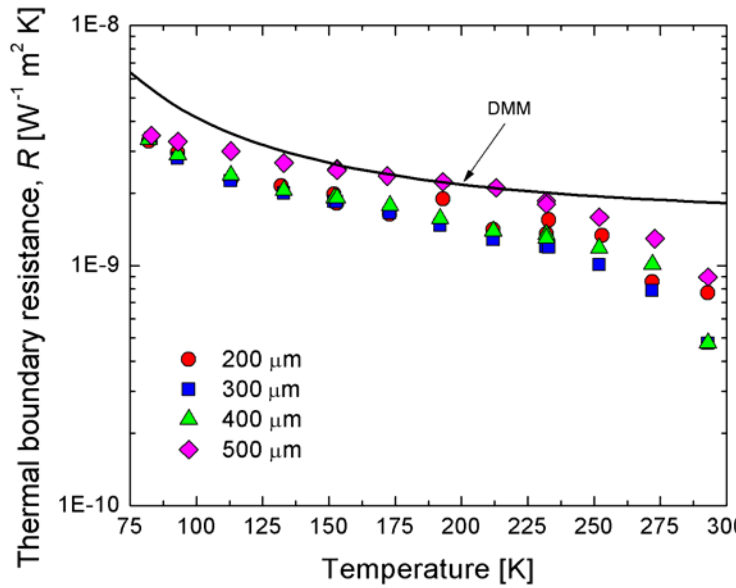
3ω technique for h_{BD}





Study at SNL Albuquerque during Summer 2007 by Hopkins and Phinney

TBR at contact pad-P4 interface



Hopkins and Phinney, **MNHT2008-52293** (2008)

Hopkins and Phinney, Submitted to the Journal of Heat Transfer

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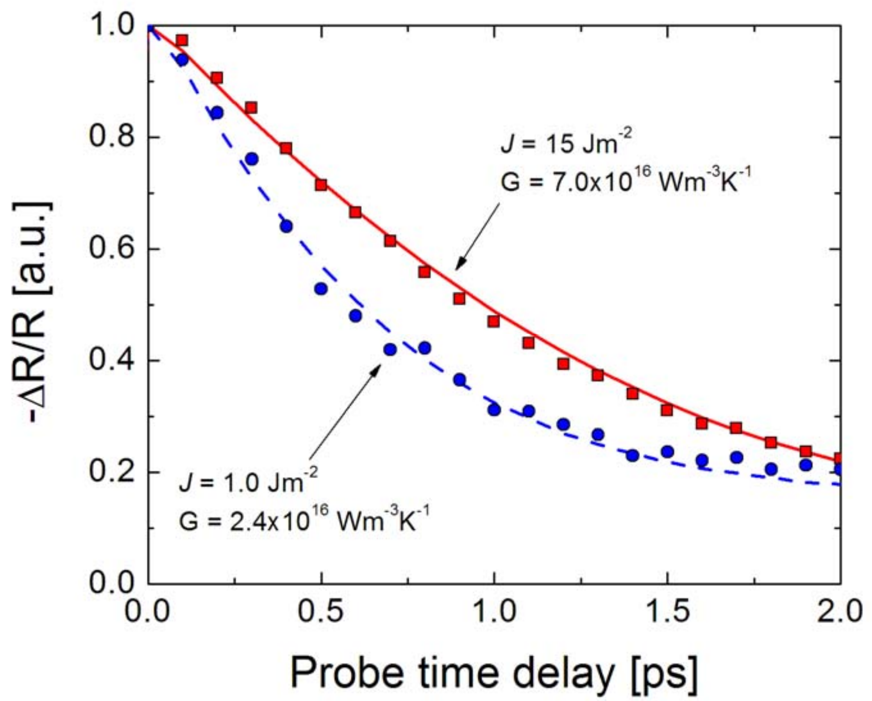
UPTTR

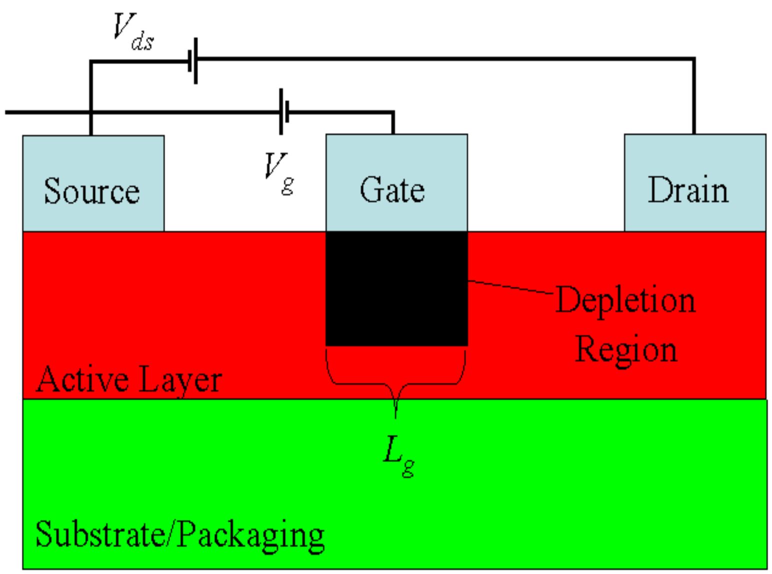


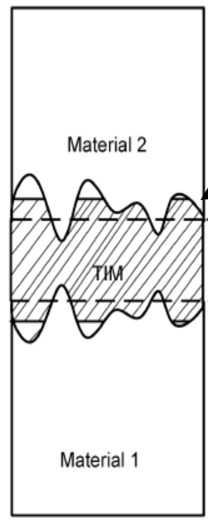
Different e-p equilibration curves for different fluences

Hopkins and Norris, Applied Surface Science, 253, 6289 (2007)

- **Measure electron-phonon scattering**
- **Vary incident laser flux**
- **Heat sample to examine effects of allowable phonon frequencies**
- **Electron-phonon relaxation measurements sensitive to interfacial disorder in ultrathin films**

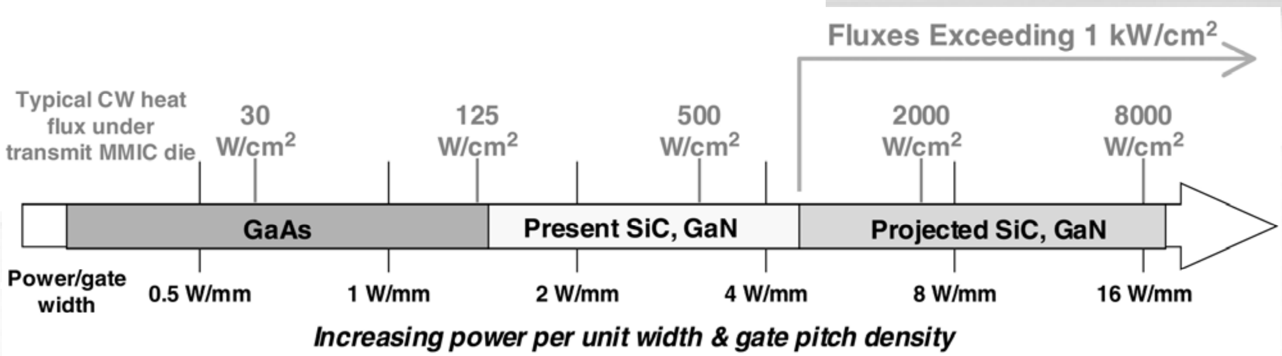
Electron and Phonon Scattering Effects on Thermal Transport in Microelectronic Applications





Structural disorder around device/TIM

How does this disorder effect electron and phonon thermal transport?



Smith, A. N. and Calame, J. P., International Journal of Thermophysics, 25, 409 (2004).

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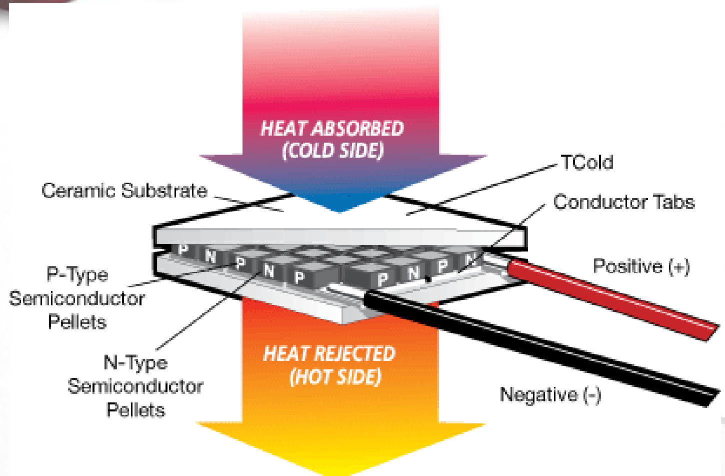
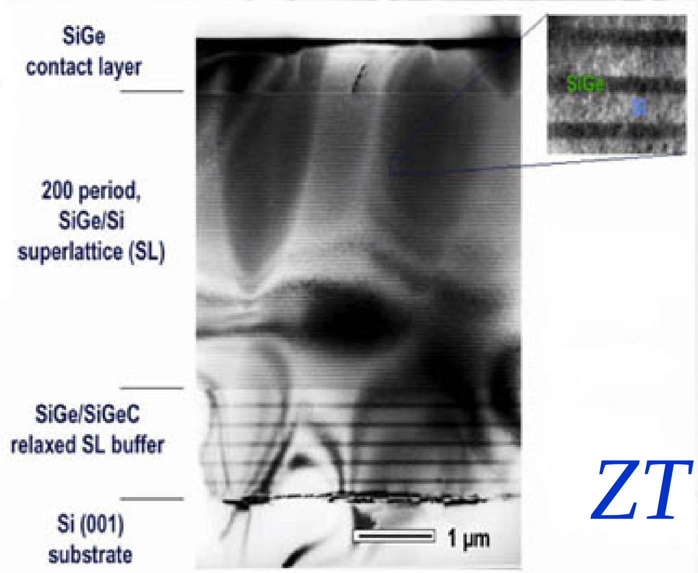
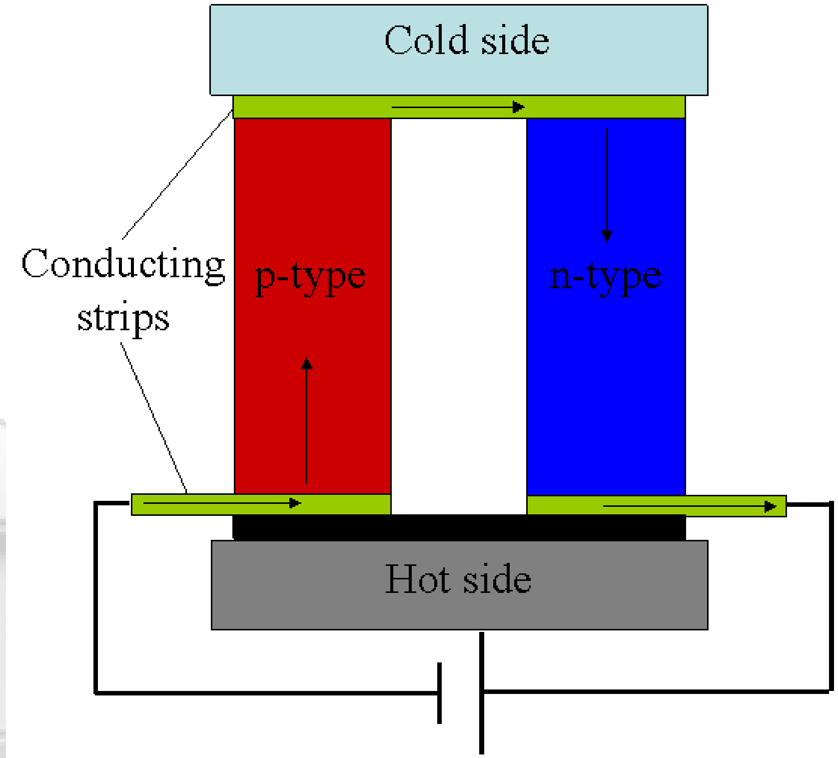
Thermoelectrics







$$ZT = \frac{S^2 \sigma T}{k}$$

ZT = figure of merit
S = Seebeck coefficient
σ = electrical conductivity
k = thermal conductivity
T = temperature

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