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Thermal transport across solid interfaces: Effects of structure, bonding and other imperfections

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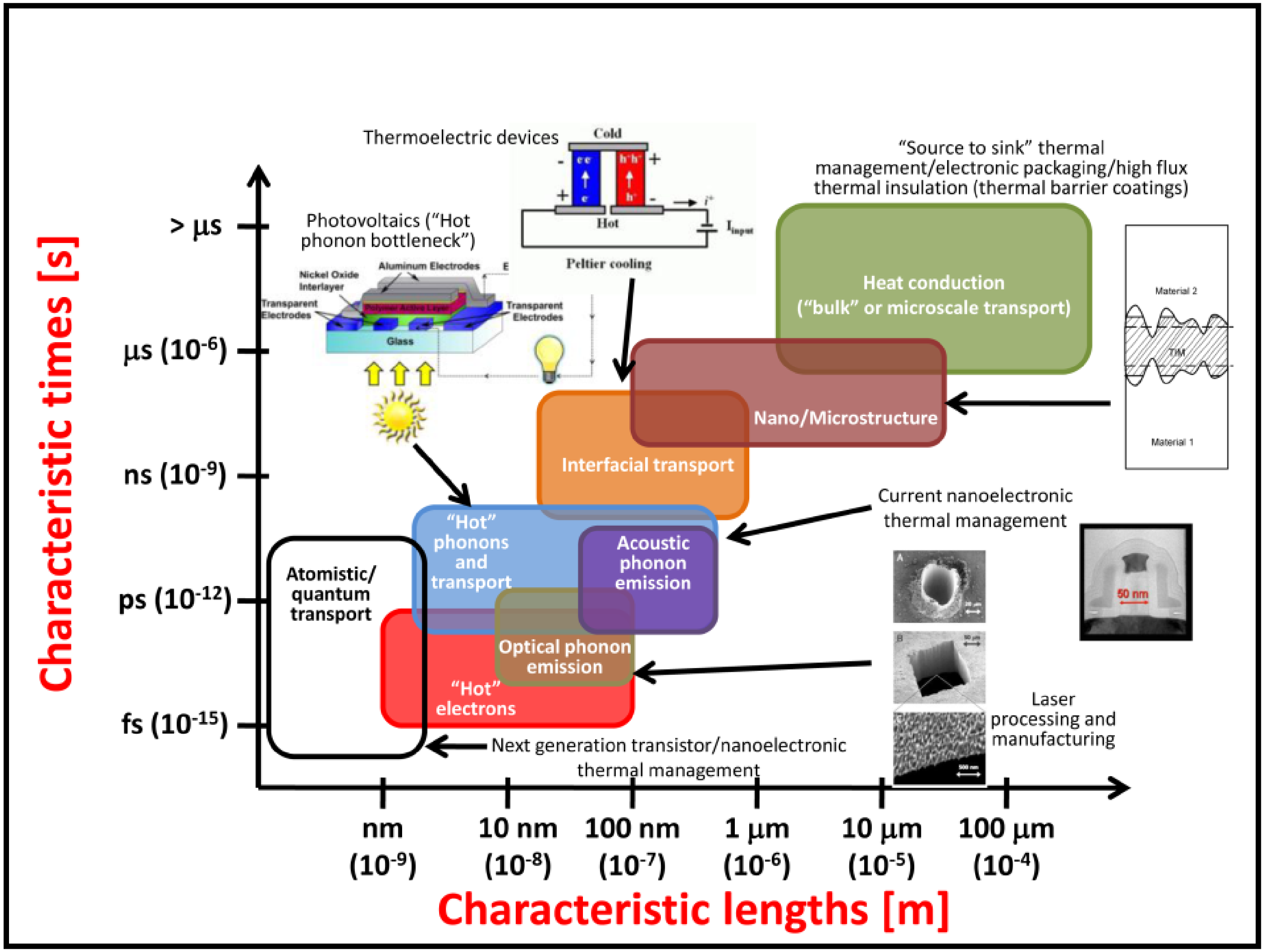
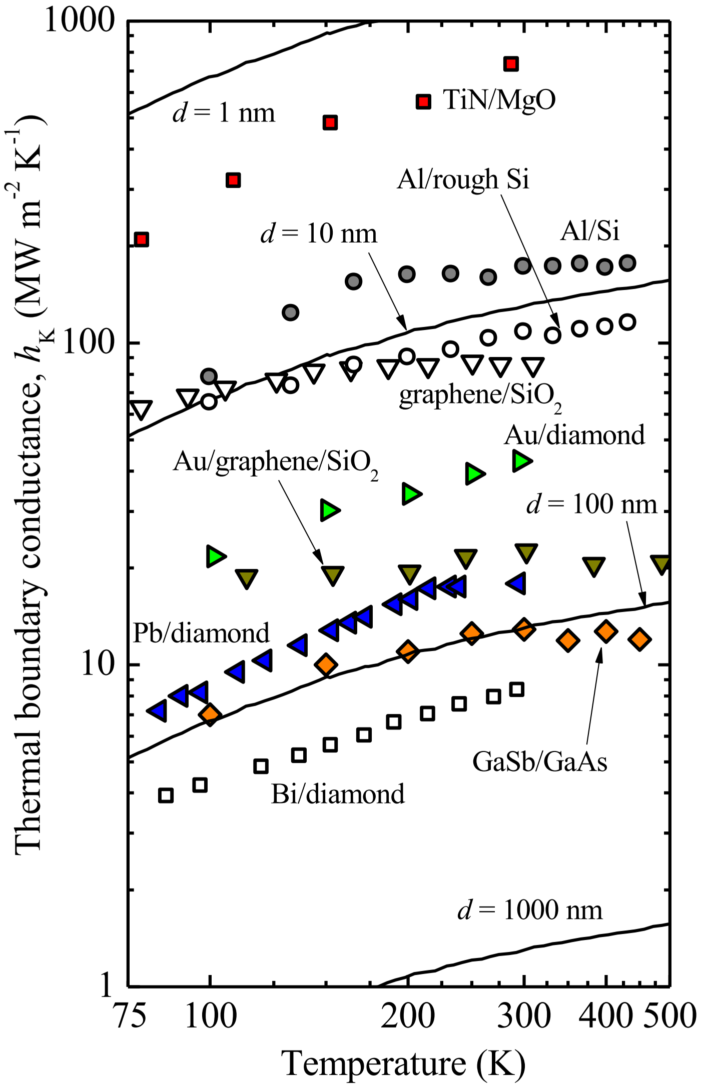
Thermal transport regimes



Thermal boundary conductance



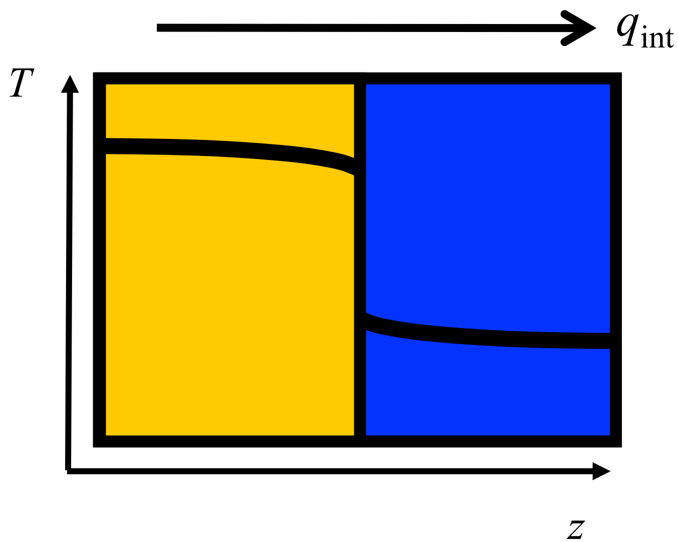
$$h_{K,SiO_2} = \frac{\kappa_{SiO_2}}{d}$$

Thermal boundary conductance

or

Kapitza conductance

$$q_{int} = h_K \Delta T$$



Outline

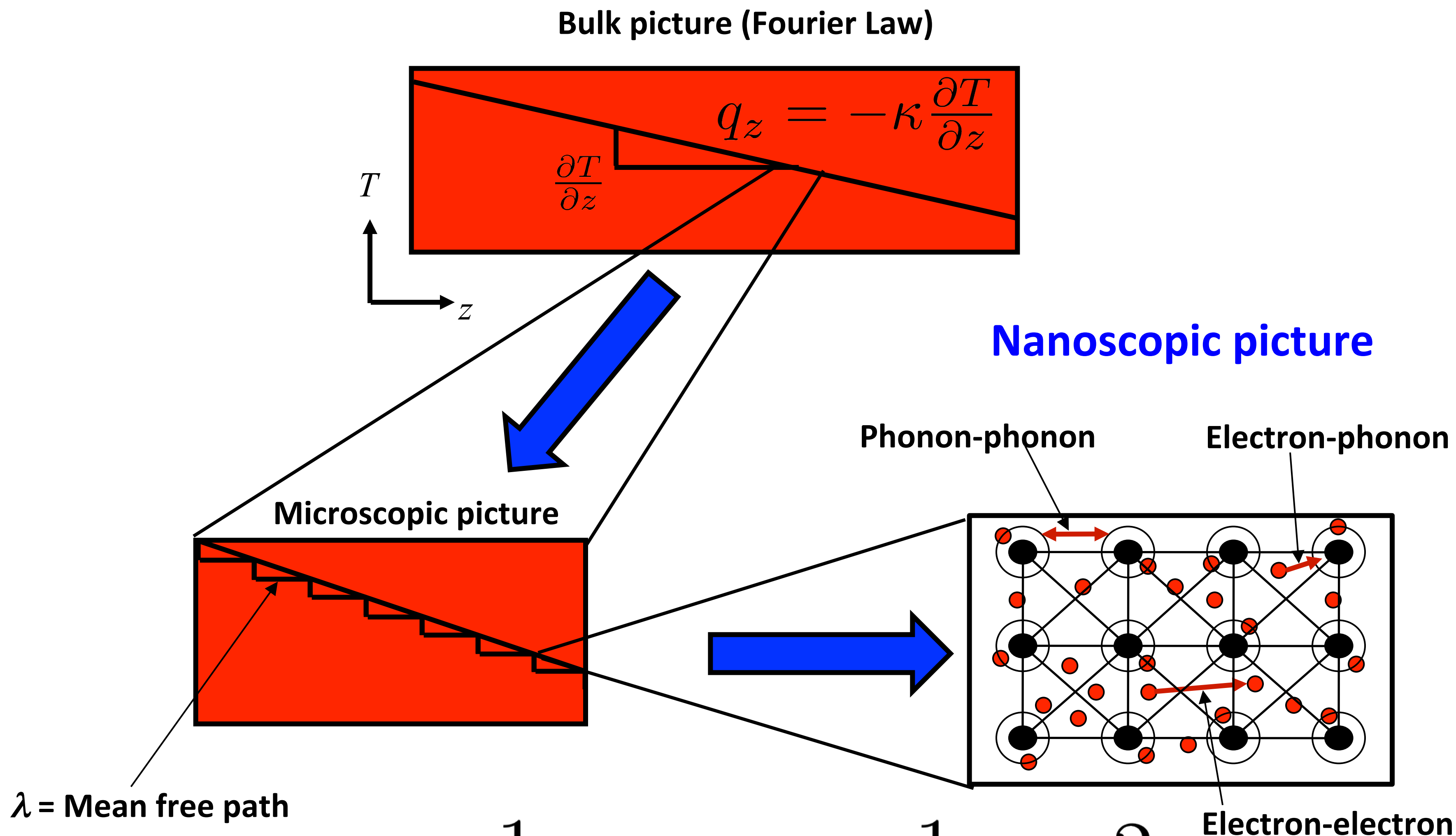
- Measurement of thermal properties on the nanoscale with time domain thermoreflectance

- Effects of geometric roughness on thermal conductance across Al/Si interfaces

- Effects of dislocations on thermal conductance across Al/GaSb and GaSb/GaAs interfaces

- Effects of bonding on thermal conductance across graphene interfaces

Thermophysics on the nanoscale



$$\kappa = \frac{1}{3}Cv\lambda = \frac{1}{3}Cv_g^2\tau$$

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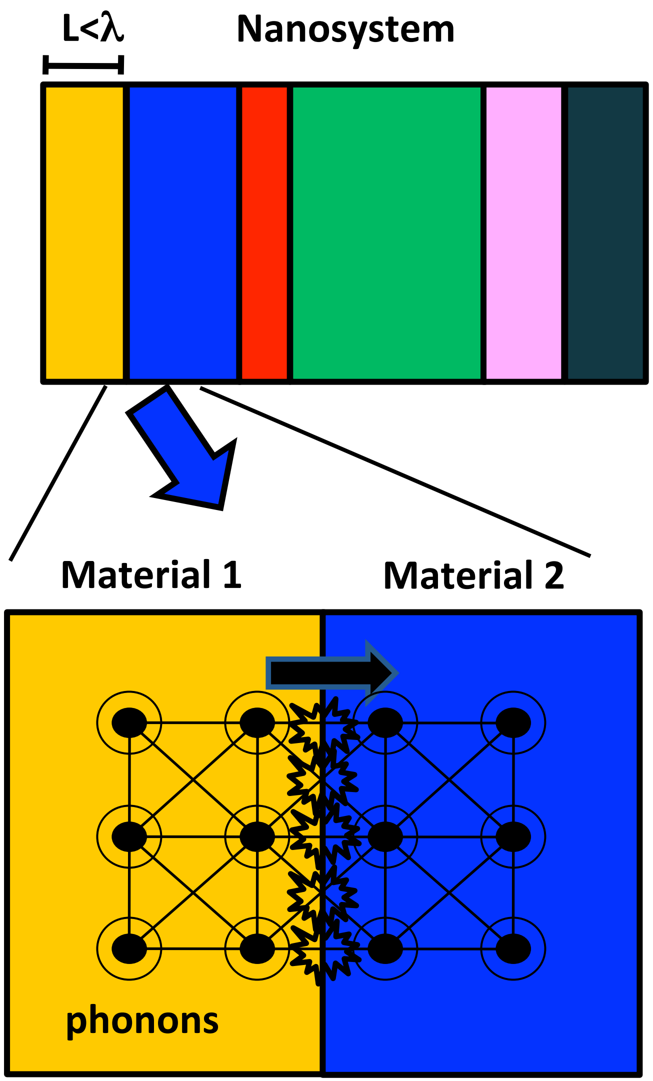
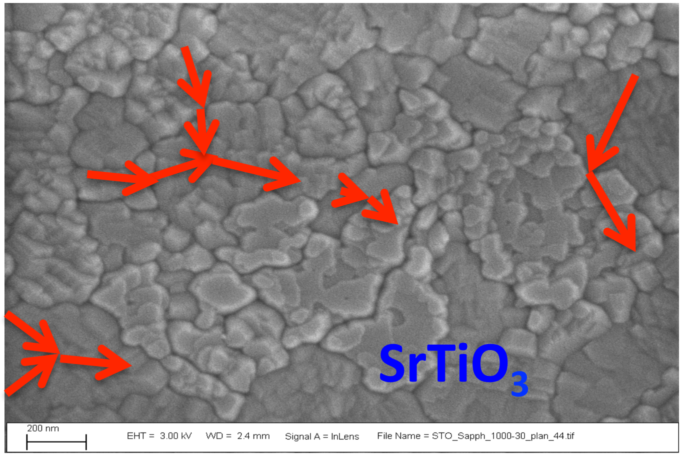
Thermophysics on the nanoscale

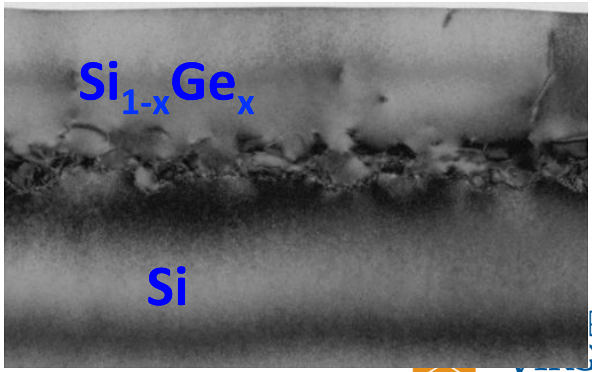
What happens if λ is on the order of L?



e.g. Nanoscale composites and thin films

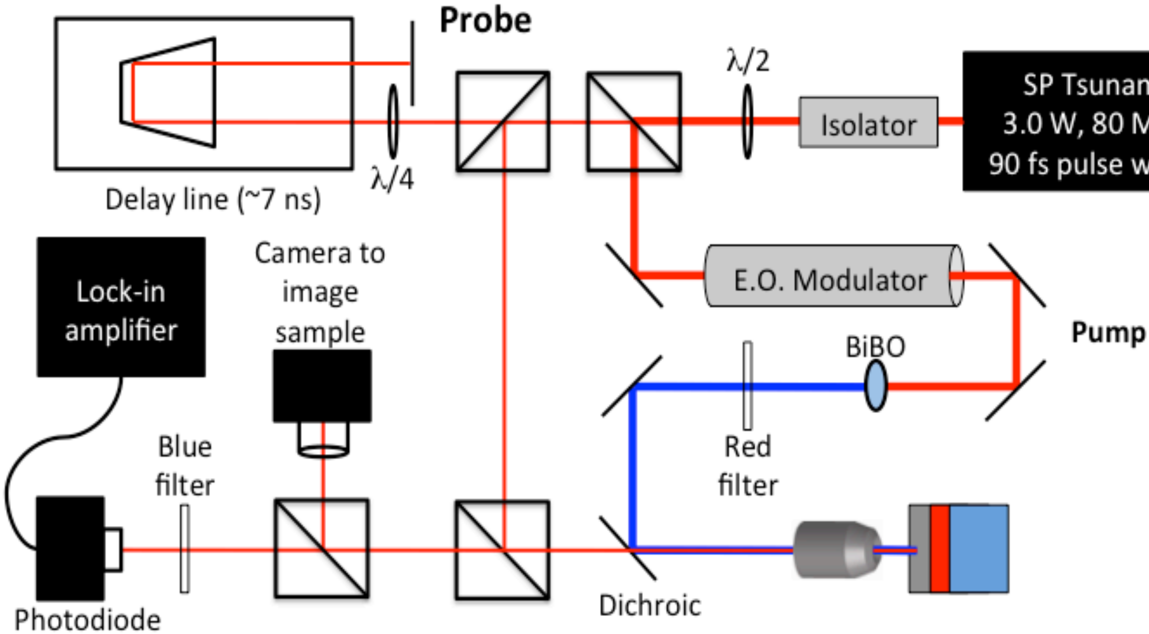
Collaborative work with Jon Ihlefeld at Sandia

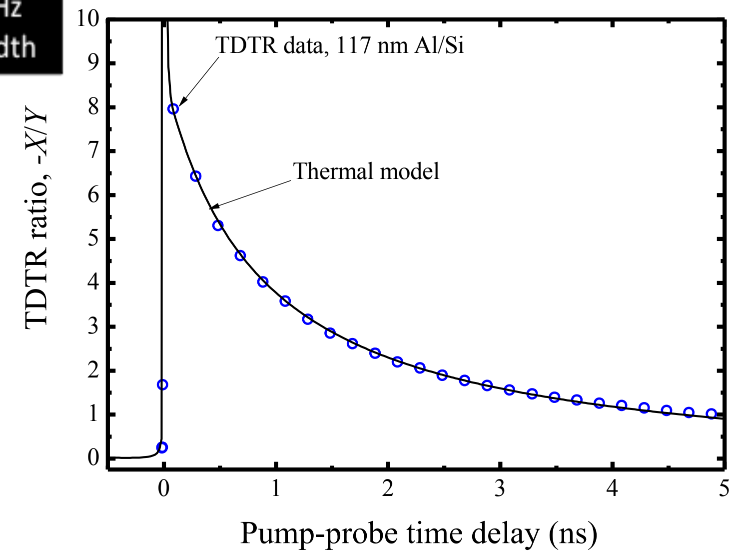


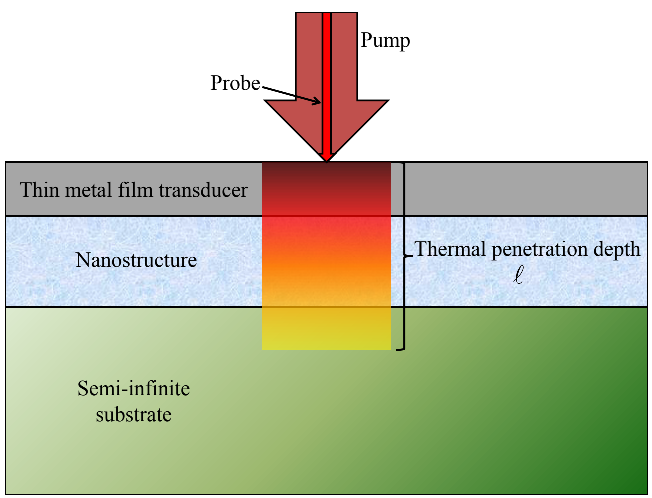


Time Domain ThermoReflectance (TDTR)

Hopkins *et al.*, *J. Heat Trans.* 132, 081302 (2010)







- **Can measure thermal conductivity of thin films and substrates (κ) separately from thermal boundary conductance (h_K)**
- **Nanometer spatial resolution (~10's of nm)**
- **Femtosecond to nanosecond temporal resolution**
- **Noncontact**

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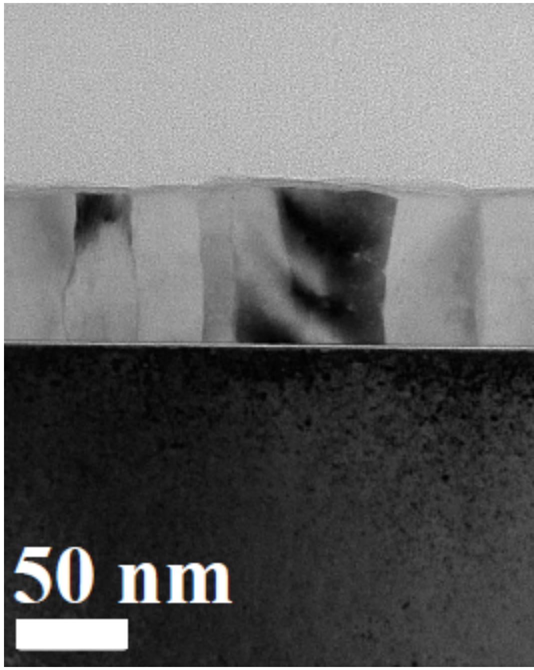
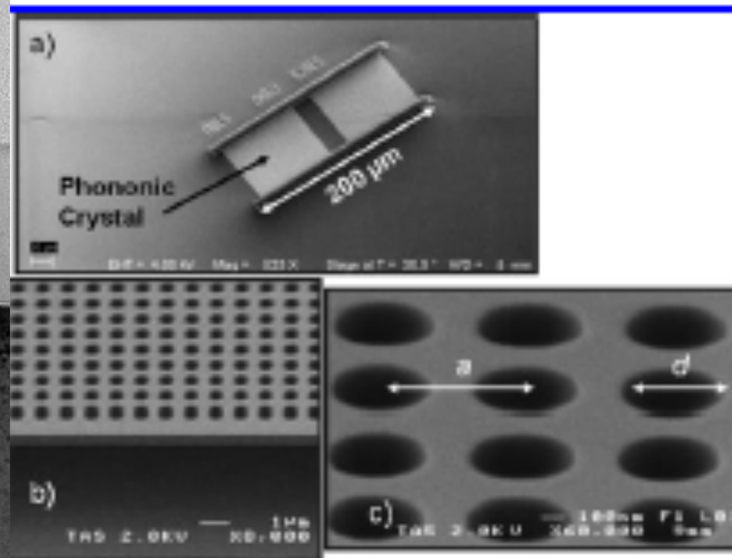
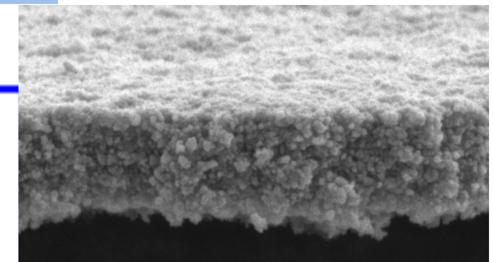
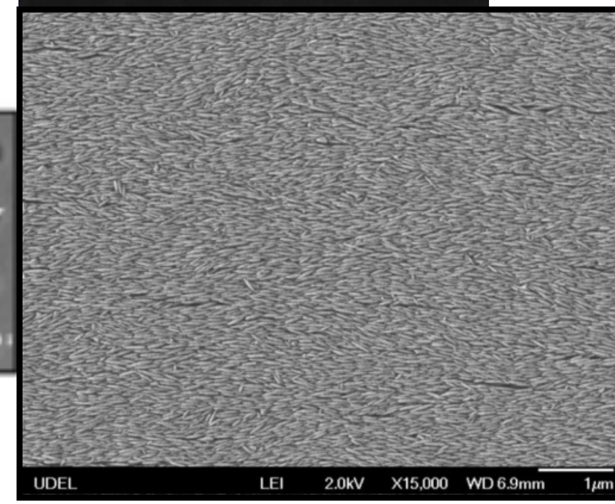
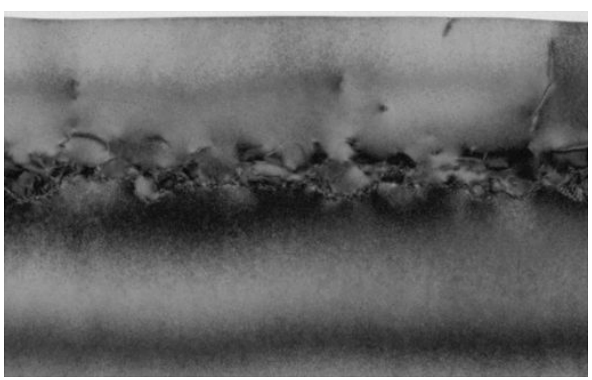
What can we measure with TDTR?











- Thermal conductivity of bulk materials
- Thermal conductivity of thin films and superlattices
- Thermal conductivity of suspended films
- Thermal conductivity of nanoparticle films
- Thermal conductivity of porous films
- Thermal boundary conductance across interfaces

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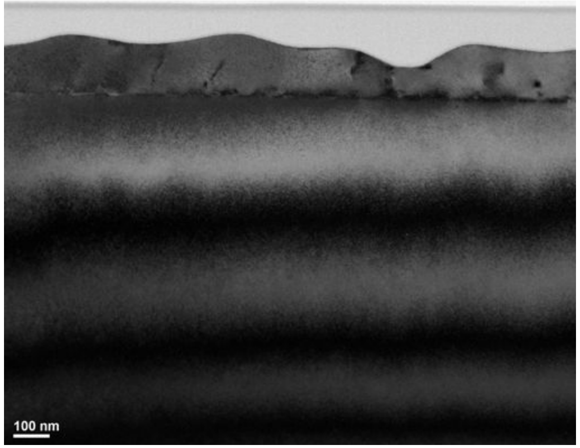
Outline

- Measurement of thermal properties on the nanoscale with time domain thermoreflectance
- Effects of geometric roughness on thermal conductance across Al/Si interfaces
- Effects of dislocations on thermal conductance across Al/GaSb and GaSb/GaAs interfaces
- Effects of bonding on thermal conductance across graphene interfaces

Outline

- **Effects of geometric roughness on thermal conductance across Al/Si interfaces**

- **Collaborators: Jerry Floro (UVa), Leslie Phinney (Sandia)**
- **Hopkins *et al.*, *Phys. Rev. B* 82, 085307 (2010)**
- **Hopkins *et al.*, *Phys. Rev. B* 84, 035438 (2011)**
- **Duda and Hopkins, *Appl. Phys. Lett*. 100, 111602 (2012)**



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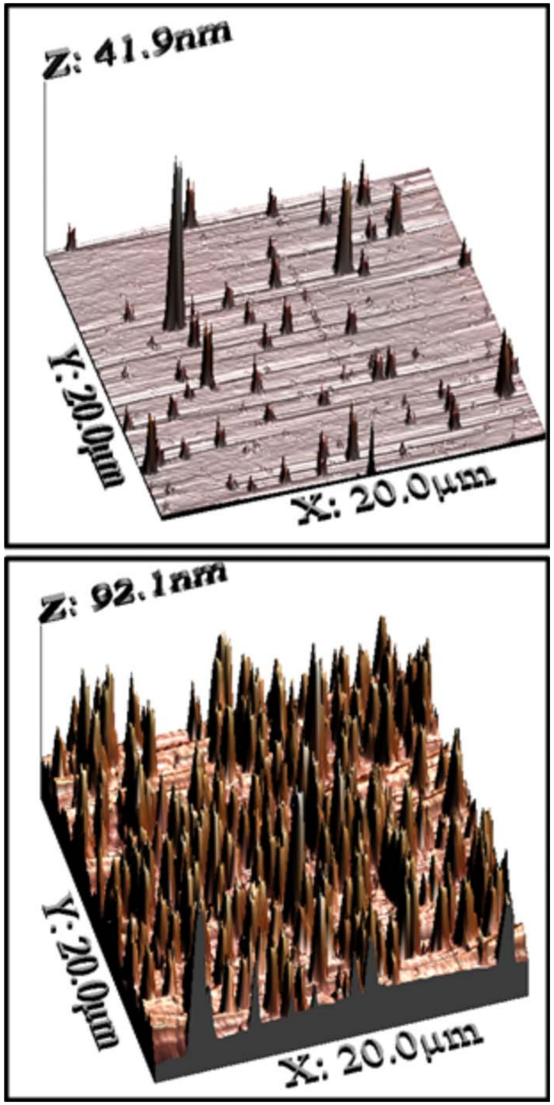
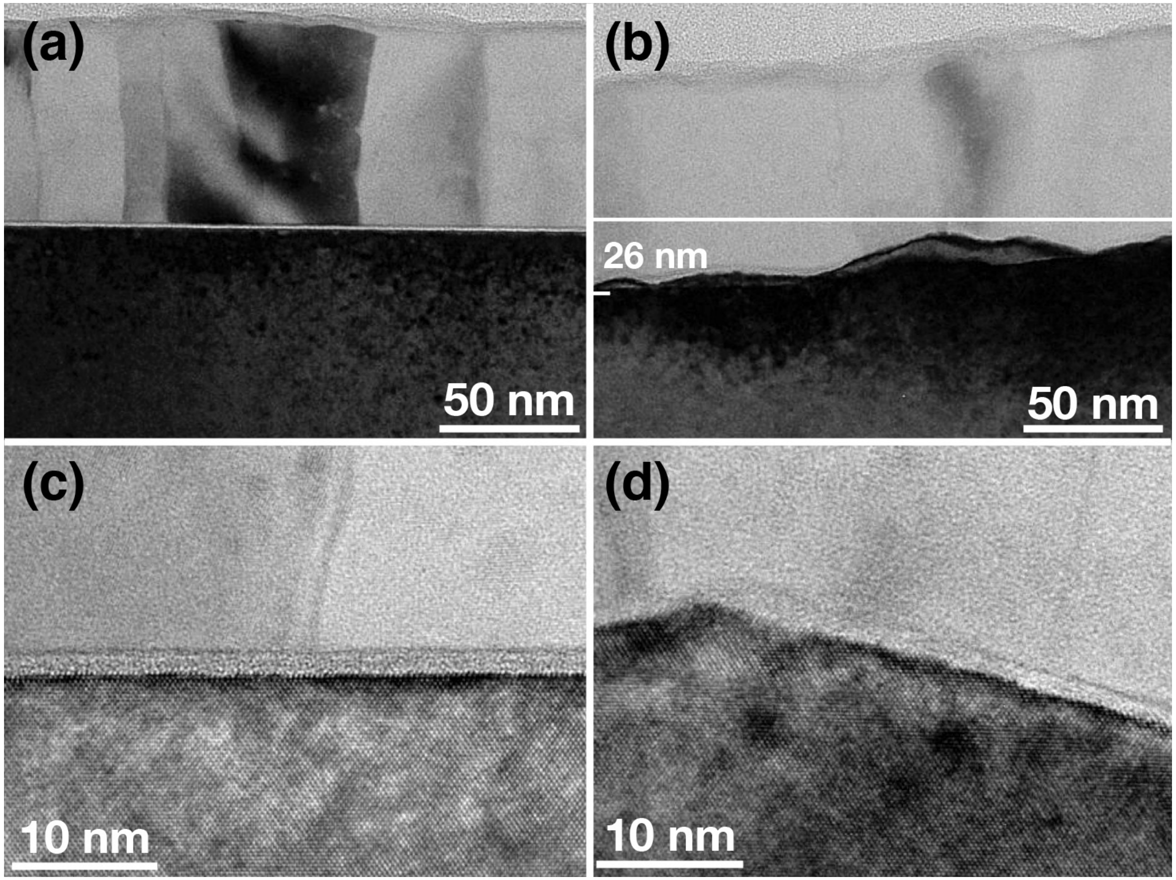
Rough Al/Si interfaces – chemical etching



TMAH processed to change surface roughness



Hopkins *et al.*, *Phys. Rev. B*. 82, 085307 (2010)
Duda and Hopkins, *Appl. Phys. Lett*. 100, 111602 (2012)

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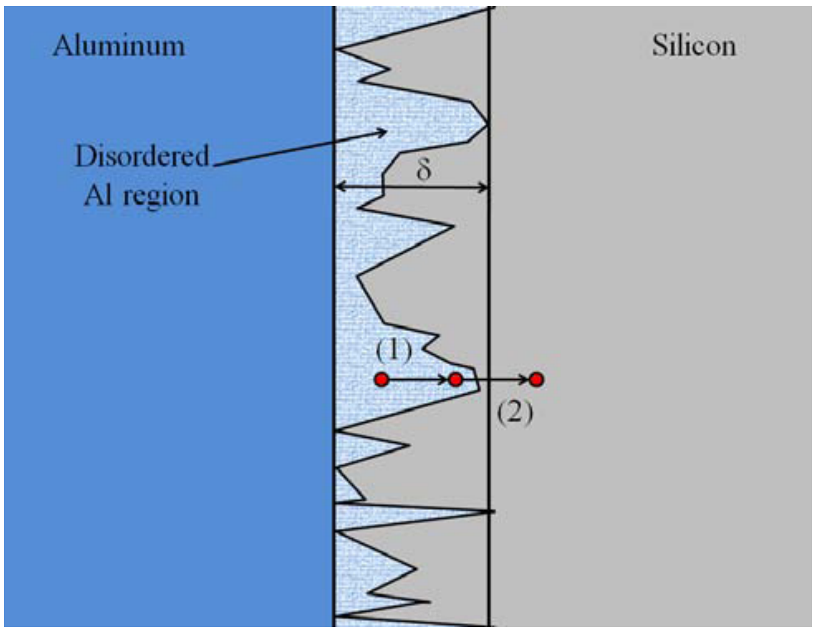
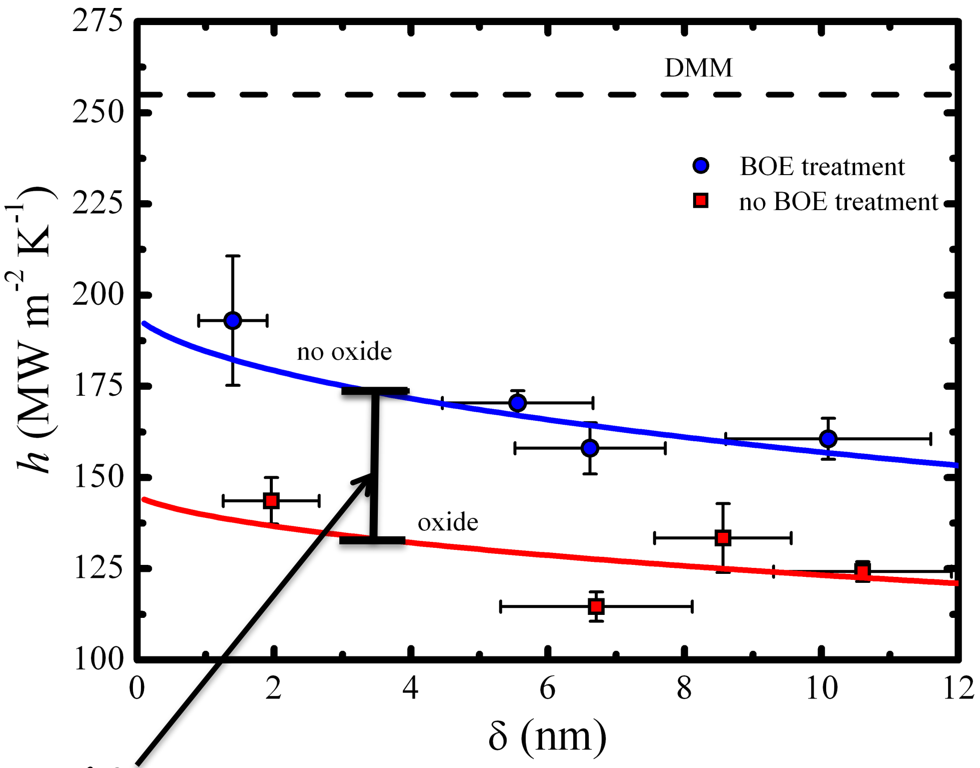
Effects of the oxide layer

Oxide layer acts as a resistor in series with Al/Si





$$\Delta h_{\mathrm{K}} = \frac{\kappa_{\mathrm{SiO_2}}}{\delta}$$

Hopkins *et al.*, *Phys. Rev. B*. 82, 085307 (2010)

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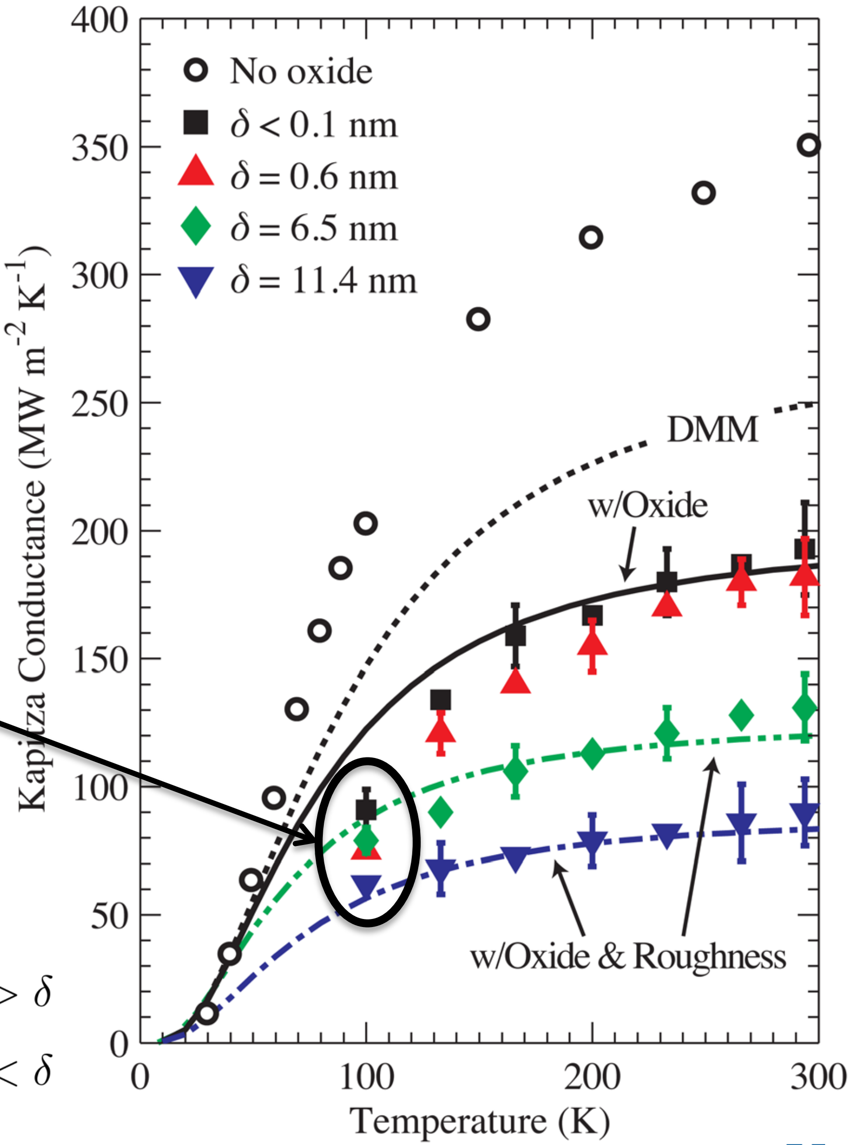
Temperature trends at rough interfaces



Convergence of h_K – selected phonon transmission and scattering

$$h_K = \begin{cases} h_{DMM} & \lambda > \delta \\ h_{DMM}\left(\exp\left[-\left(\frac{4\pi\beta}{\lambda}\right)\delta\right]\right) & \lambda < \delta \end{cases}$$

Duda and Hopkins, *Appl. Phys. Lett*. 100, 111602 (2012)

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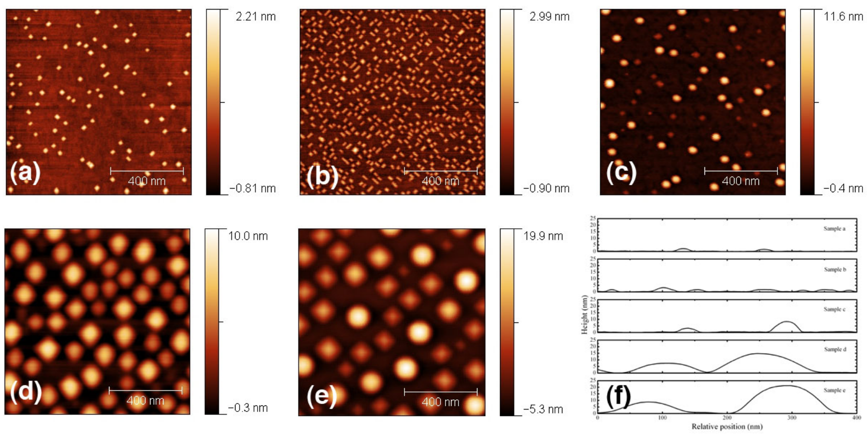
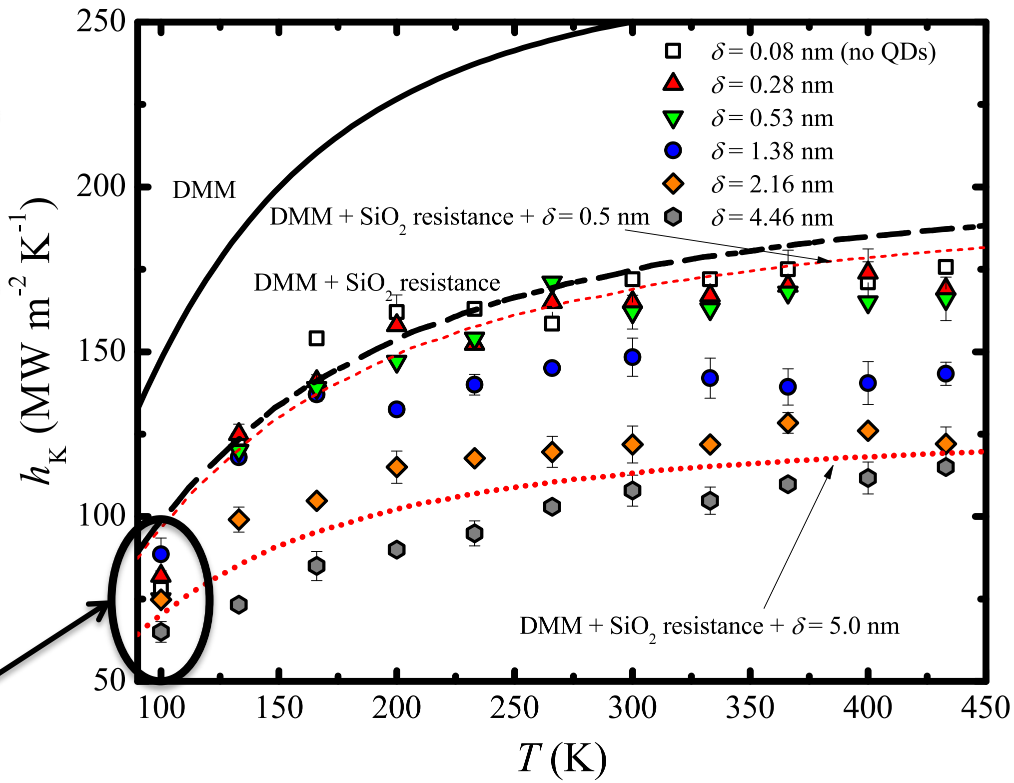
Rough Al/Si interfaces – quantum dots

Jerry Floro's group @ U.Va. (floro@virginia.edu)





Convergence of h_K – selected phonon transmission and scattering (SAME AS CHEMICALLY ROUGH INTERFACES)

$$h_K = \begin{cases} h_{DMM} & \lambda > \delta \\ h_{DMM}\left(\exp\left[-\left(\frac{4\pi\beta}{\lambda}\right)\delta\right]\right) & \lambda < \delta \end{cases}$$

Hopkins *et al.*, *Phys. Rev. B* 84, 035438 (2011)

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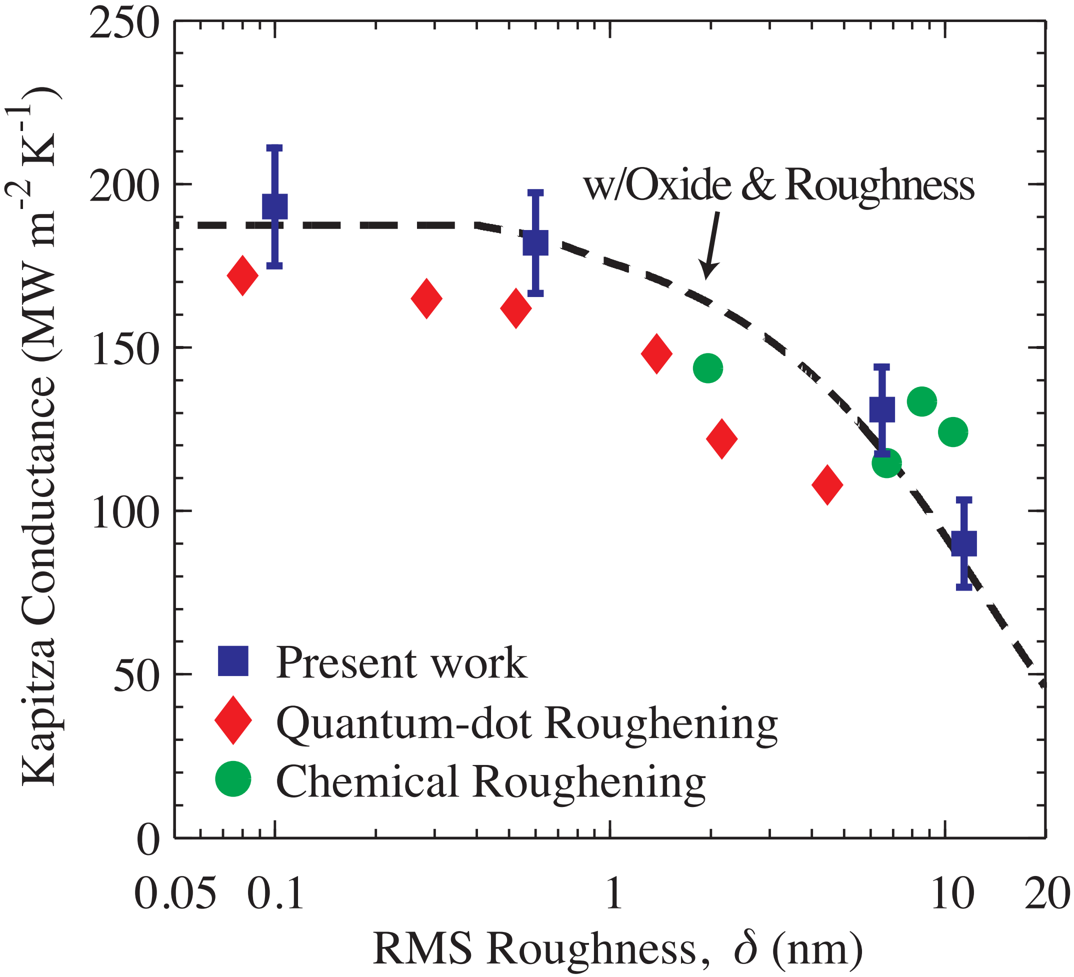
Roughness as a "knob" for thermal control

$$h_K = \begin{cases} h_{DMM} & \lambda > \delta \\ h_{DMM}\left(\exp\left[-\left(\frac{4\pi\beta}{\lambda}\right)\delta\right]\right) & \lambda < \delta \end{cases}$$



Duda and Hopkins, *Appl. Phys. Lett*. 100, 111602 (2012)

Outline

•Effects of geometric roughness on thermal conductance across Al/Si interfaces

•Roughness can be used to control thermal conductance across interfaces by selectively "filtering" certain phonon wavelengths

•Collaborators: John Duda (Postdoc), Jerry Floro (UVa), Leslie Phinney (Sandia)

•Hopkins *et al.*, *Phys. Rev. B* 82, 085307 (2010)

•Hopkins *et al.*, *Phys. Rev. B* 84, 035438 (2011)

•Duda and Hopkins, *Appl. Phys. Lett*. 100, 111602 (2012)

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Outline

- **Measurement of thermal properties on the nanoscale with time domain thermoreflectance**

- **Effects of geometric roughness on thermal conductance across Al/Si interfaces**

- **Effects of dislocations on thermal conductance across Al/GaSb and GaSb/GaAs interfaces**

- **Effects of bonding on thermal conductance across graphene interfaces**

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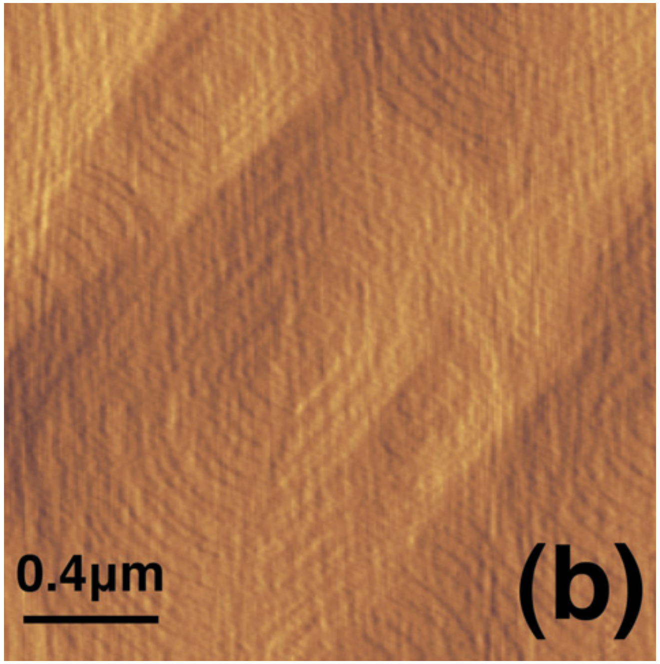
Outline

•Effects of dislocations on thermal conductance across Al/ GaSb and GaSb/GaAs interfaces

•Collaborators: Ganesh Balakrishnan (UNM)

•Hopkins *et al.*, *Appl. Phys. Lett.* 98, 161913 (2011)



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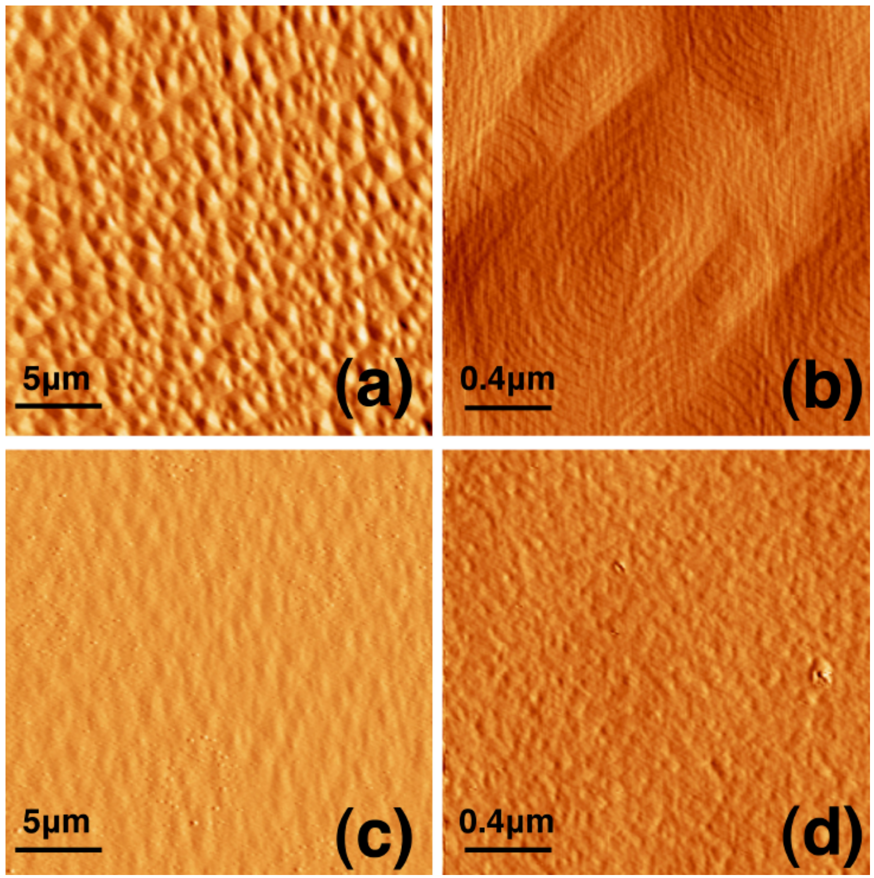
Epitaxial GaSb growth on GaAs

Ganesh Balakrishnan's group @ U. New Mexico (gunny@unm.edu)

Non-IMF

δ = 2.3 nm
~10^{10} dislocations/cm2



IMF
Reduced threading and screw dislocations

δ = 1.7 nm
~10^{7} dislocations/cm^2

Huang, *et al.*, *Appl. Phys. Lett.* 88, 131911 (2006)
Jallipalli, *et al.*, *Nanoscale Res. Lett.* 4, 1458 (2009)
Huang, *et al.*, *J. Appl. Phys.* 105, 103104 (2009)

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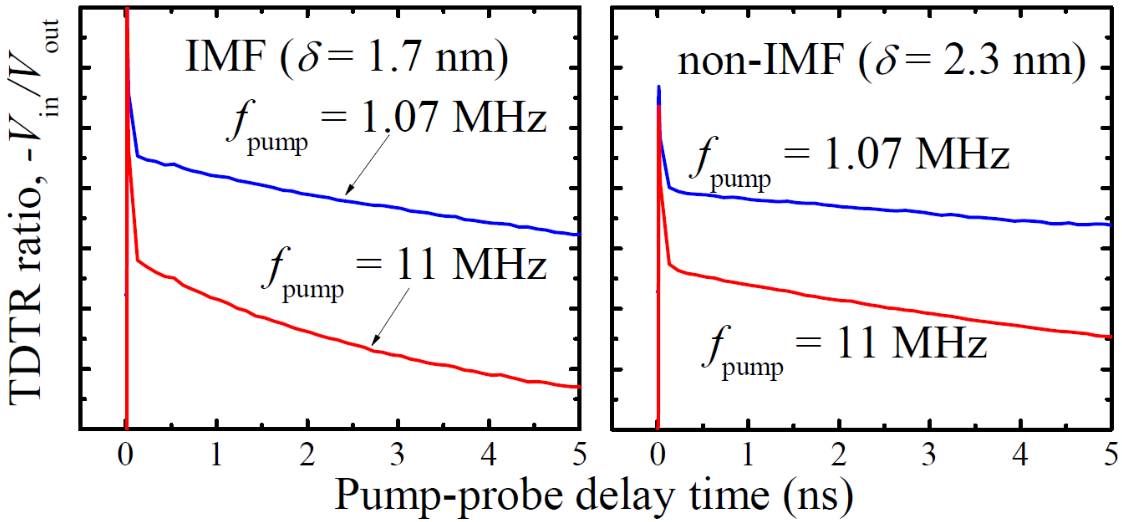
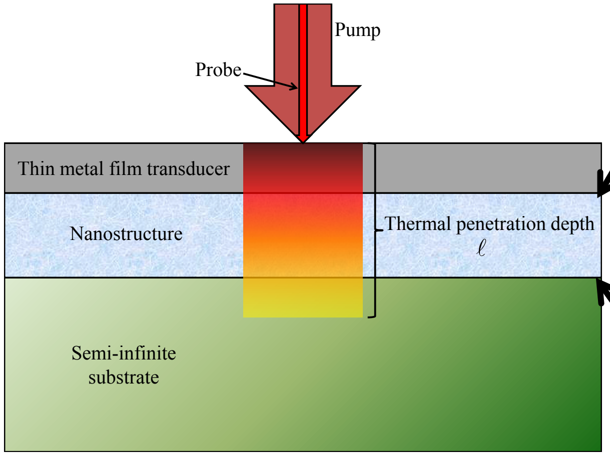
“Depth profiling” with TDTR



Increase how “deep” you probe in TDTR by decreasing the frequency



***h*$_K$ – Al/GaSb (*f* = 11 MHz)**

$$\ell \approx \sqrt{\frac{\kappa}{\pi C f_{\text{pump}}}}$$

***h*$_K$ – GaSb/GaAs (*f* = 1.07 MHz)**

Hopkins *et al.*, *Appl. Phys. Lett*. 98, 161913 (2011)

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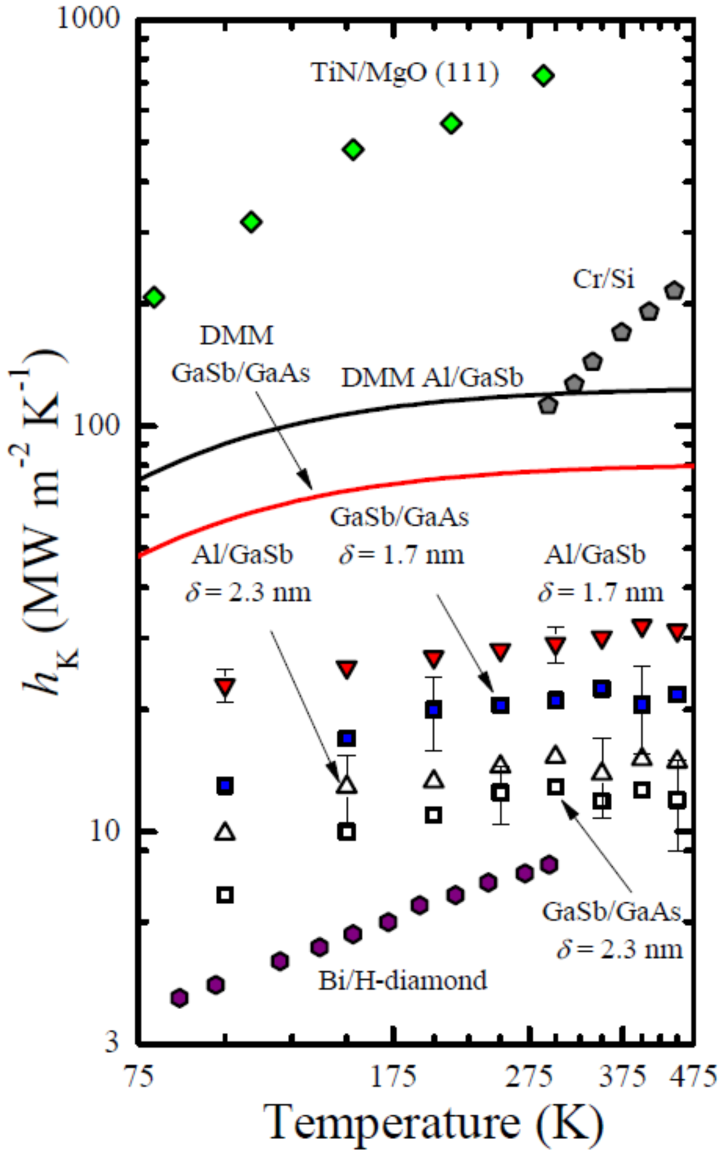
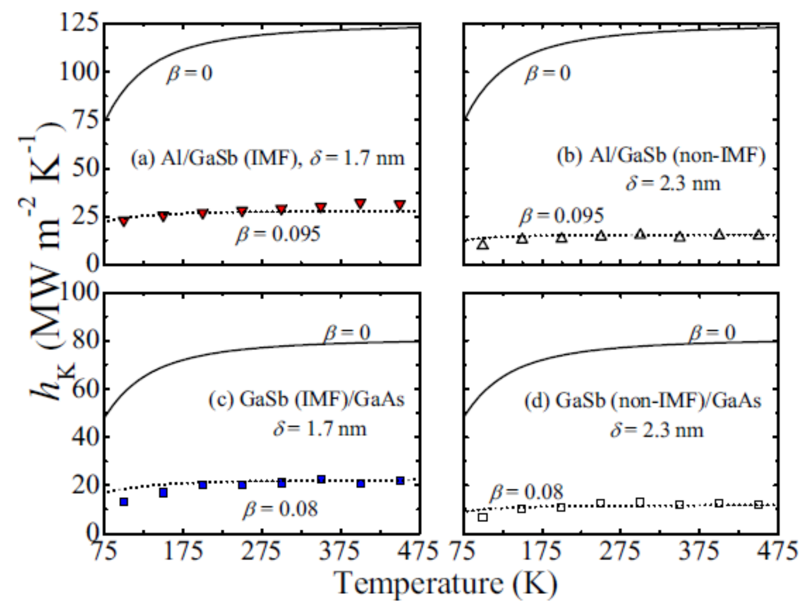
Interfacial dislocation effects on h_K



$$h_K = \begin{cases} h_{DMM} & \lambda > \delta \\ h_{DMM}\left(\exp\left[-\left(\frac{4\pi\beta}{\lambda}\right)\delta\right]\right) & \lambda < \delta \end{cases}$$



10^3 change in dislocation density only changes thermal conductance across dislocation dense interfaces by a factor of ~2

Hopkins *et al.*, *Appl. Phys. Lett*. 98, 161913 (2011)

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Outline

- **Effects of dislocations on thermal conductance across Al/GaSb and GaSb/GaAs interfaces**

- **10^3 change in dislocation density changes thermal conductance by ~2 at dislocation dense interfaces.**

- **Collaborators: Ganesh Balakrishnan (UNM)**
- **Hopkins *et al.*, *Appl. Phys. Lett.* 98, 161913 (2011)**

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Outline

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- **Effects of bonding on thermal conductance across graphene interfaces**

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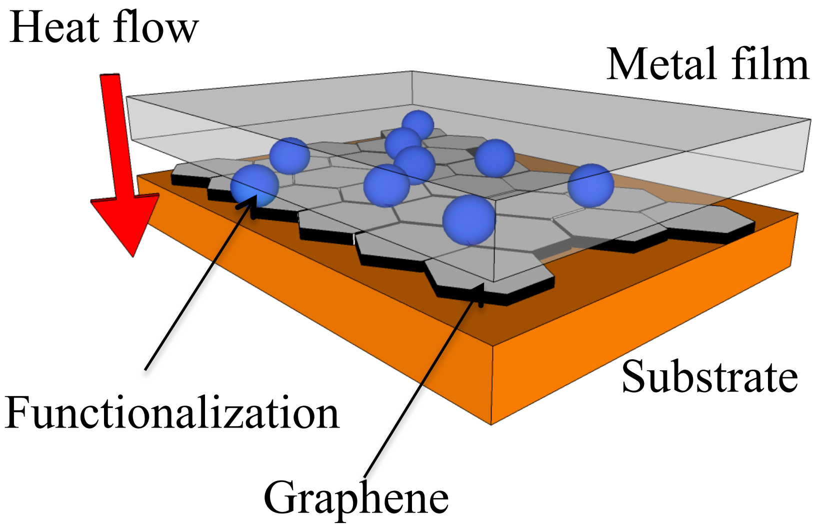
Outline

- **Effects of bonding on thermal conductance across graphene interfaces**

- **Collaborators: Scott Walton (NRL)**
- **Hopkins *et al.*, *Nano Lett.* 12, 590 (2012)**
- **Duda *et al.*, *Phys. Rev. B* 84, 193301 (2011)**



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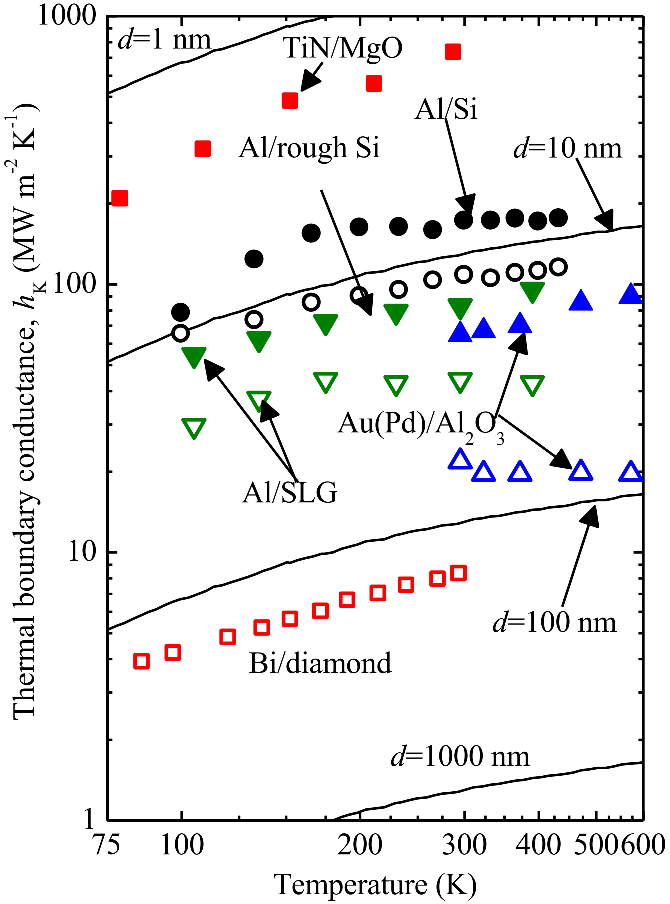
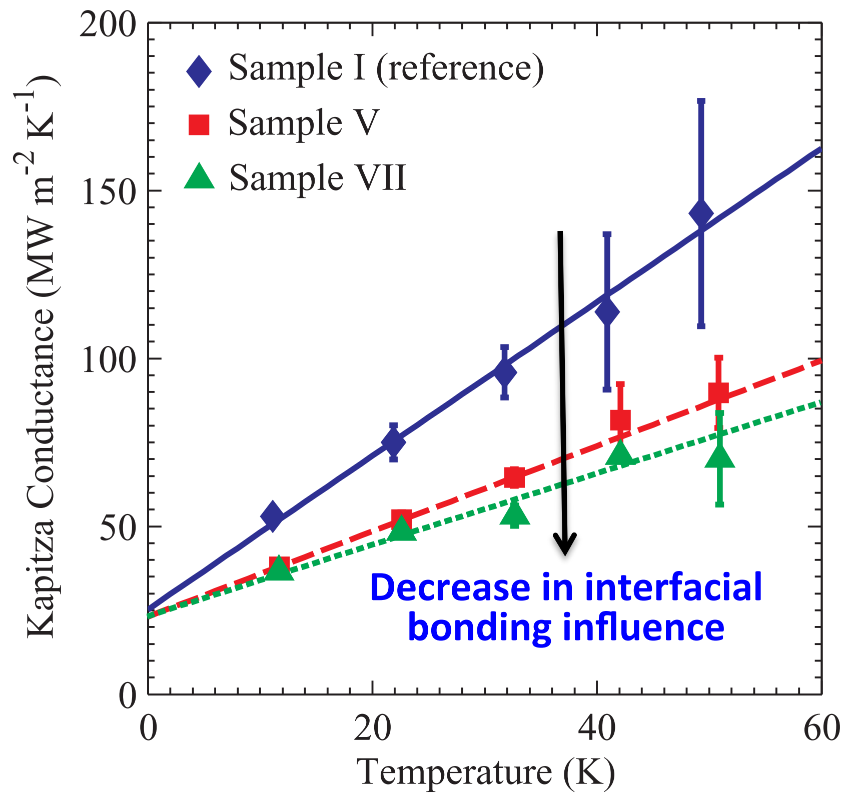
Bonding/transport relationships of TBC





Hopkins *et al.*, *Nano. Lett.* 12, 590 (2012)
Oh *et al.*, *Adv. Mat.* 23, 5028 (2011)

Duda *et al. Phys. Rev. B* 84, 193301 (2011)

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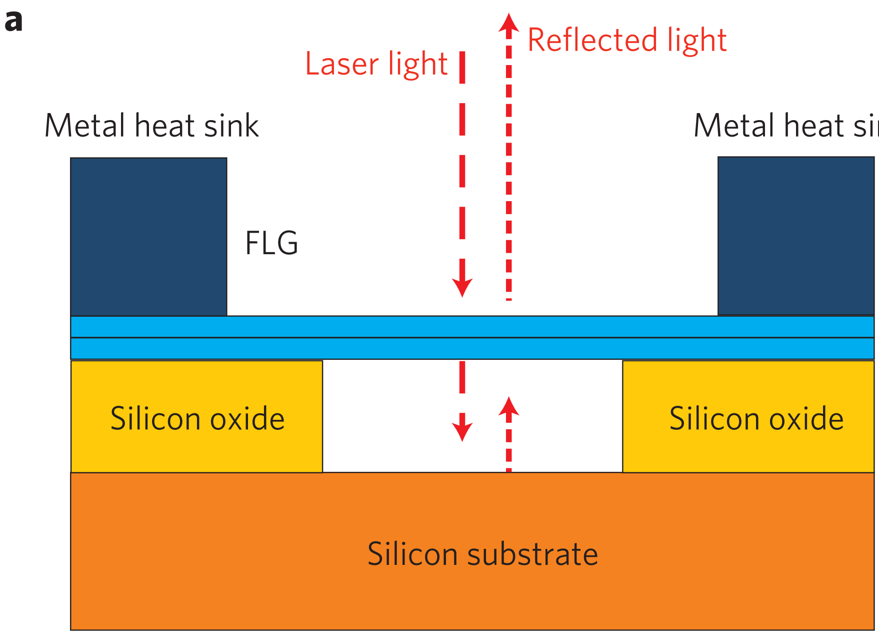
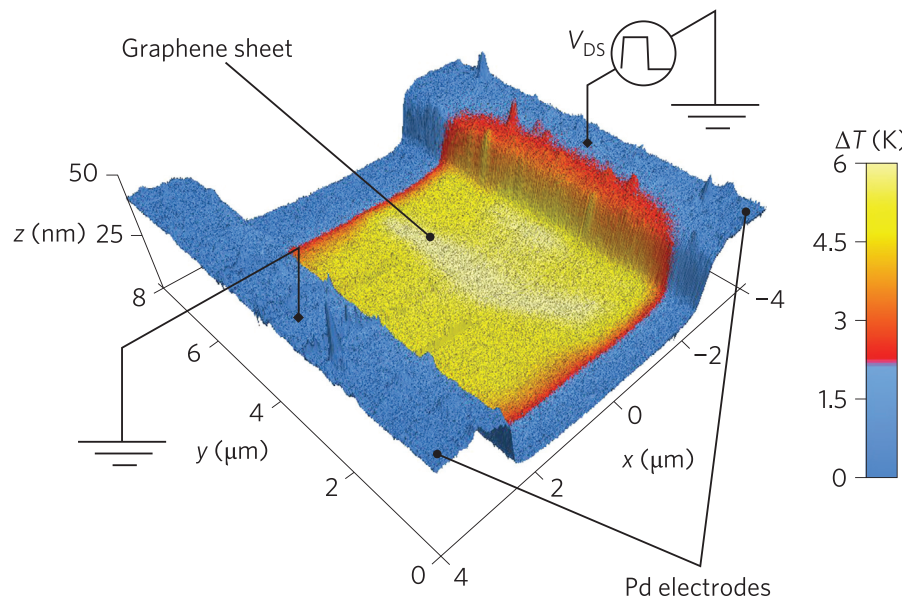
Bonding at graphene contacts



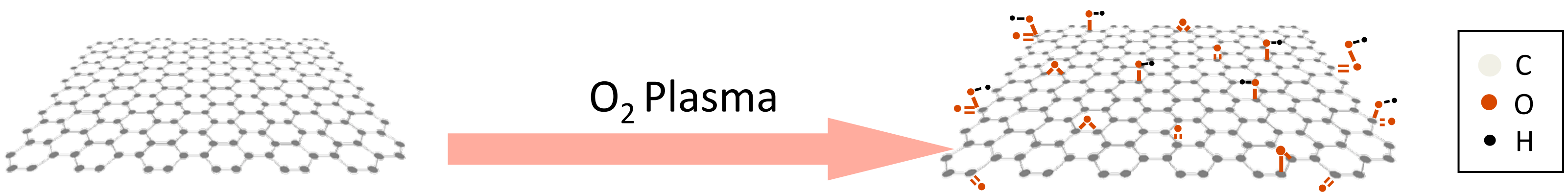


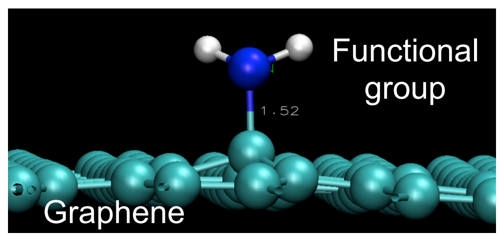
Ghosh *et al*. *Nat. Mat.* 9, 555 (2010)

Grosse *et al*. *Nat. Nano*. 6, 287 (2011)

Manipulating bonds at graphene contacts

Scott Walton
Naval Research Laboratories
scott.walton@nrl.navy.gov





- **Functional groups can't be washed off – covalently bound groups**
- **Functionalization is reversible after anneal – doesn't disrupt graphene**

Baraket *et al*. *Appl. Phys. Lett*. v. 96, 231501 (2010)

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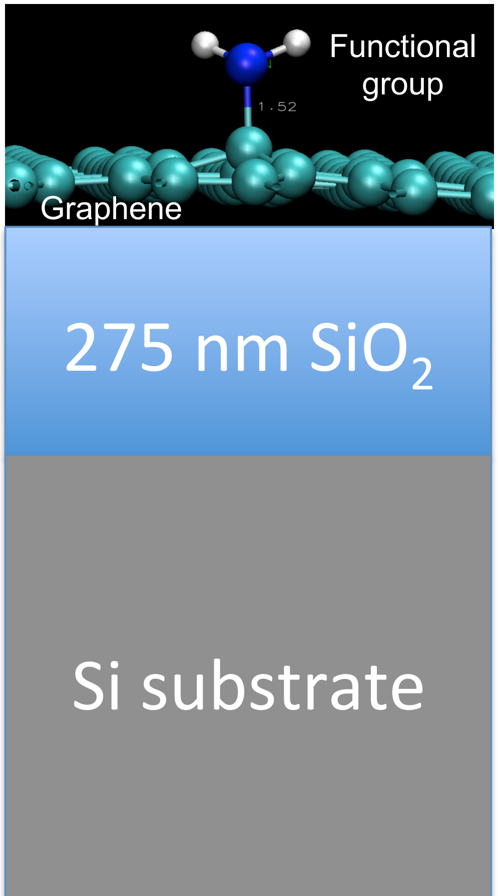
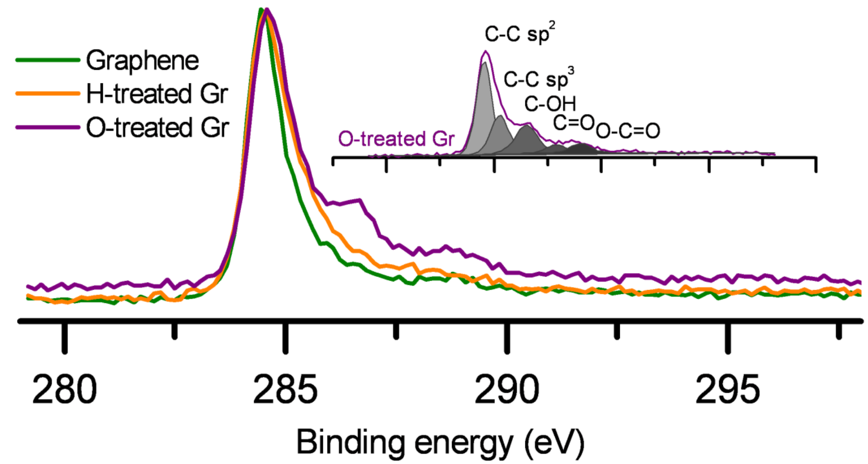
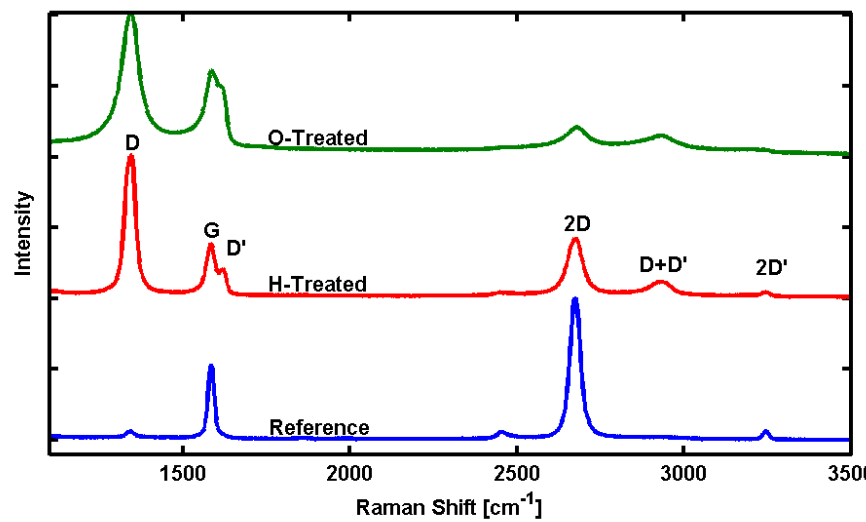
H- and O- functionalized graphene



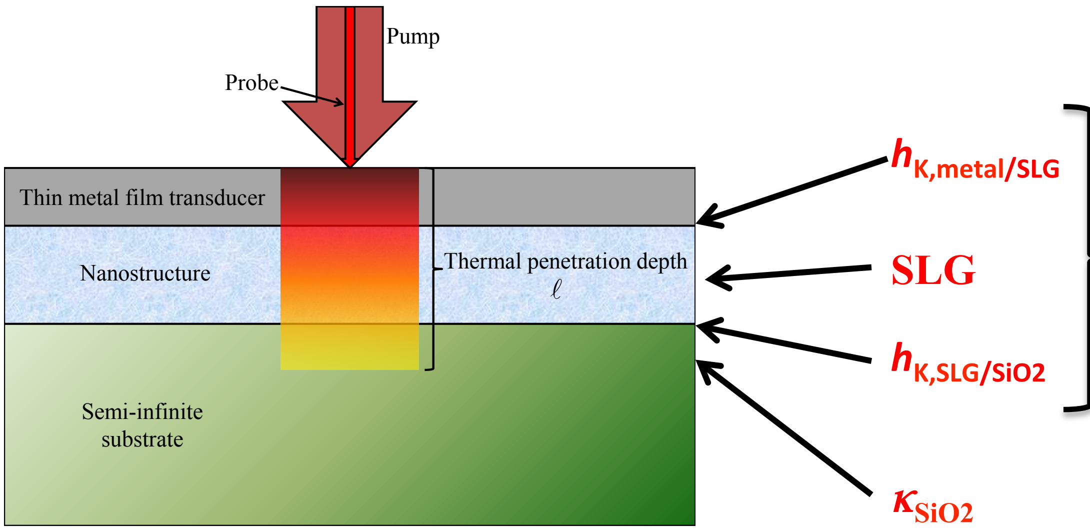
XPS - Scott Walton (NRL)



Raman - Thomas Beechem (Sandia)



Time Domain ThermoReflectance (TDTR)



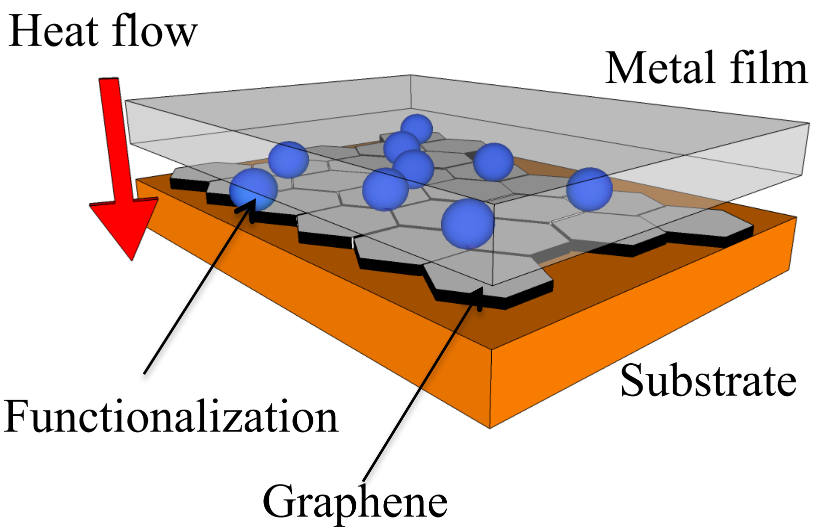
$$h_{\mathrm{K,Al\rightarrow SiO_2}} = \left(\frac{1}{h_{\mathrm{K,Al/SLG}}} + \frac{1}{h_{\mathrm{K,SLG/SiO_2}}} \right)^{-1}$$

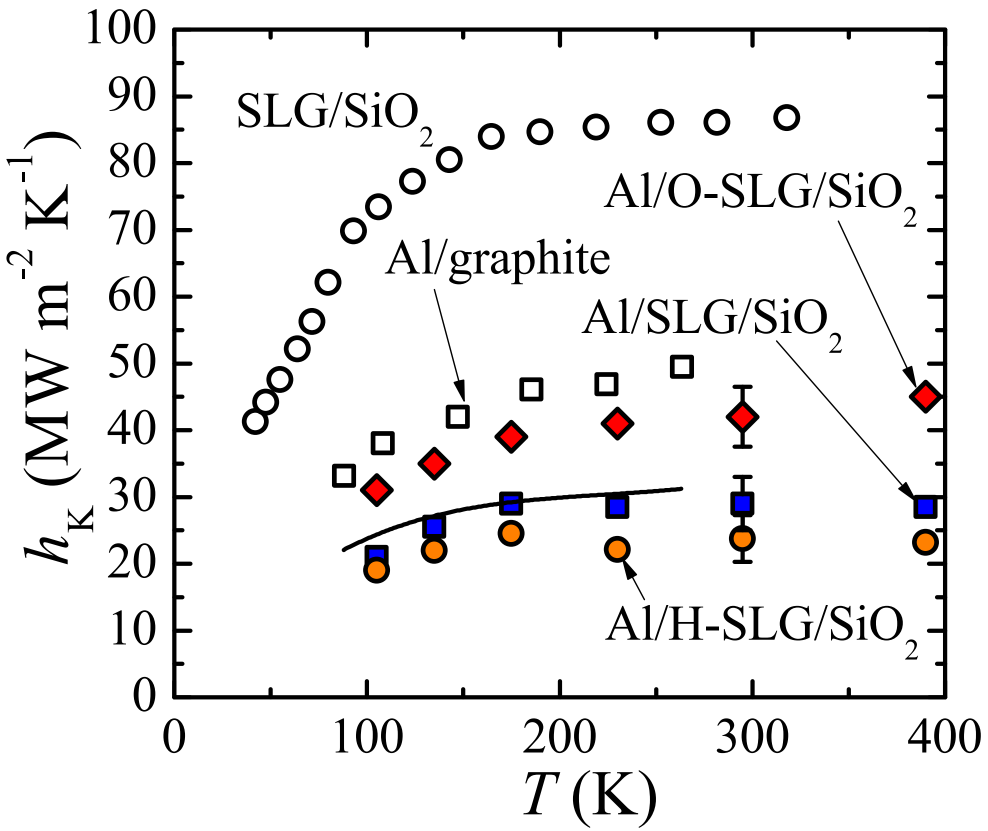
- **SLG/SiO_2 thermal boundary conductance characterized by Chen *et al*.**

  Chen, Jang, Bao, Lau, and Dames, *Appl. Phys. Lett.* 95, 161910 (2009)

- **Functionalization is reversible after anneal – doesn't disrupt graphene**

Al/SLG/SiO_2 conductance





- **Hydrogen functionalization only slightly decreases conductance**
- **Oxygen leads to notable increase in conductance**
- **Line represents series resistor model of Al/graphite (Schmidt *et al*.) and SLG/SiO_2 (Chen *et al*.)**

Schmidt, Collins, Minnich, and Chen, *J. Appl. Phys.* 107, 104907 (2010)

Al/SLG conductance

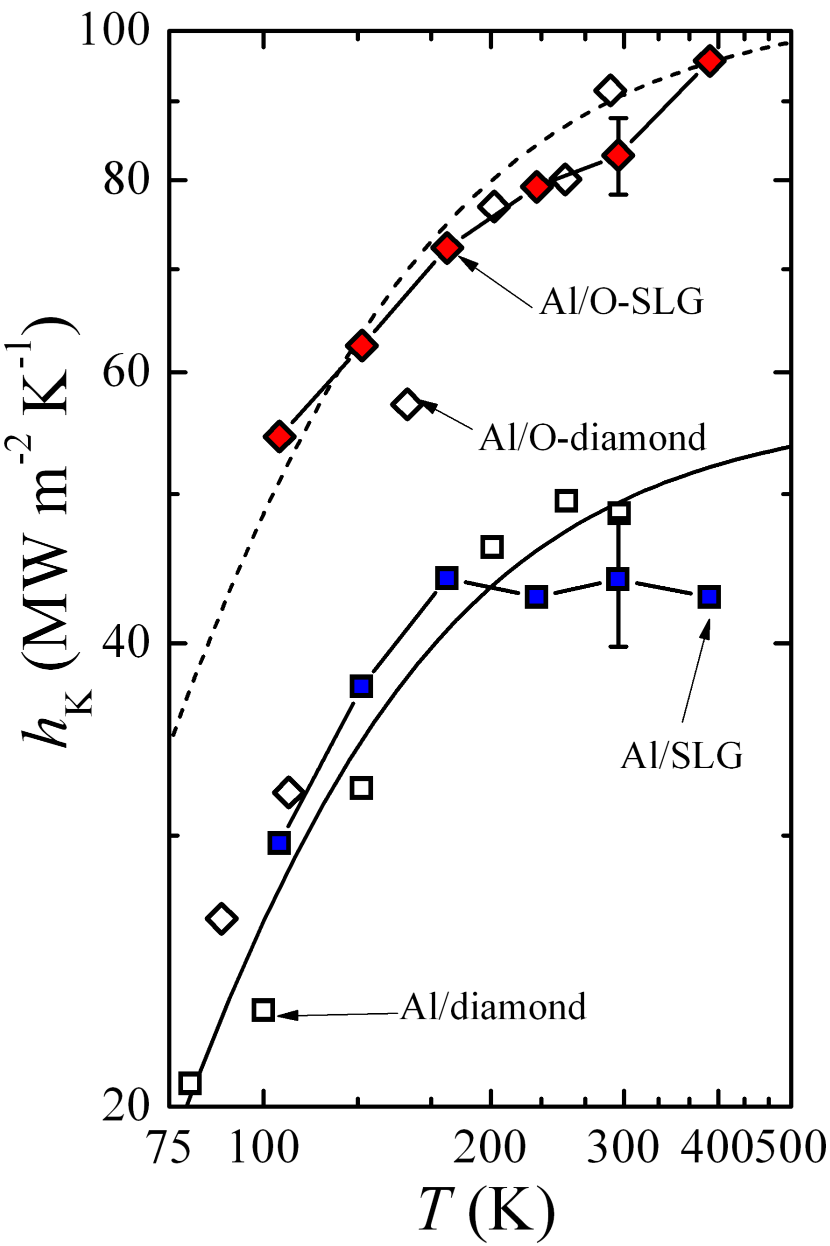
DMM for metal/SLG
(modify DMM for graphite)

$$q_{\mathrm{SLG}} = \frac{1}{8\pi a} \sum_j \int_{k,SLG} \hbar\omega_j(k)\, k f v_{2,j}(k)\, \mathrm{d}k$$

Adjust v_2 to match data

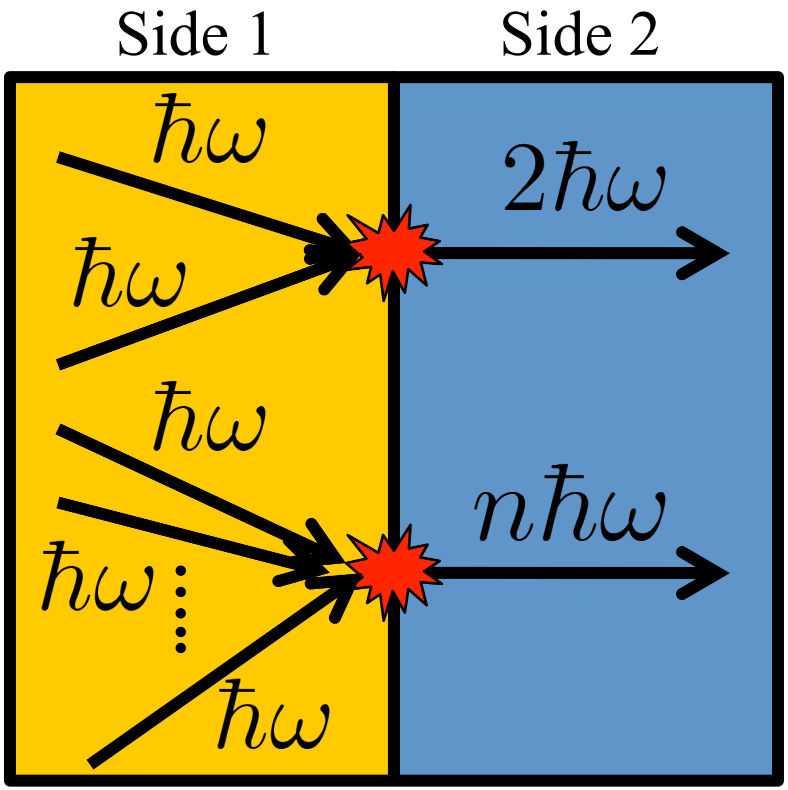
$$\frac{v_{\mathrm{O-SLG}}}{v_{\mathrm{SLG}}} \approx 2 \qquad v \propto \sqrt{K}$$

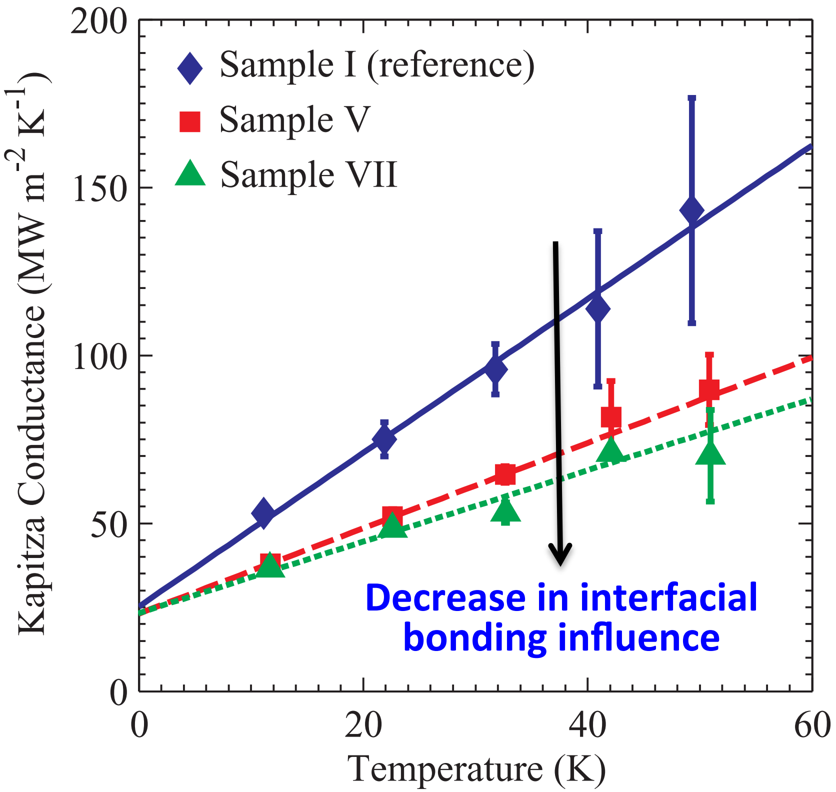
$$\frac{K_{\mathrm{O-SLG}}}{K_{\mathrm{SLG}}} \approx \sqrt{2} = 1.4 = 40\,\%\,\text{increase}$$



Realistic dispersion in DMM
Duda *et al.*, *J. Appl. Phys.* 108, 073515 (2010)
DMM for graphite
Duda *et al.*, *Appl. Phys. Lett.* 95, 031912 (2009)
Diamond data
Collins and Chen, *Appl. Phys. Lett.* 97, 183102 (2011)

Inelastic scattering at interface?





Duda *et al. Phys. Rev. B* 84, 193301 (2011)

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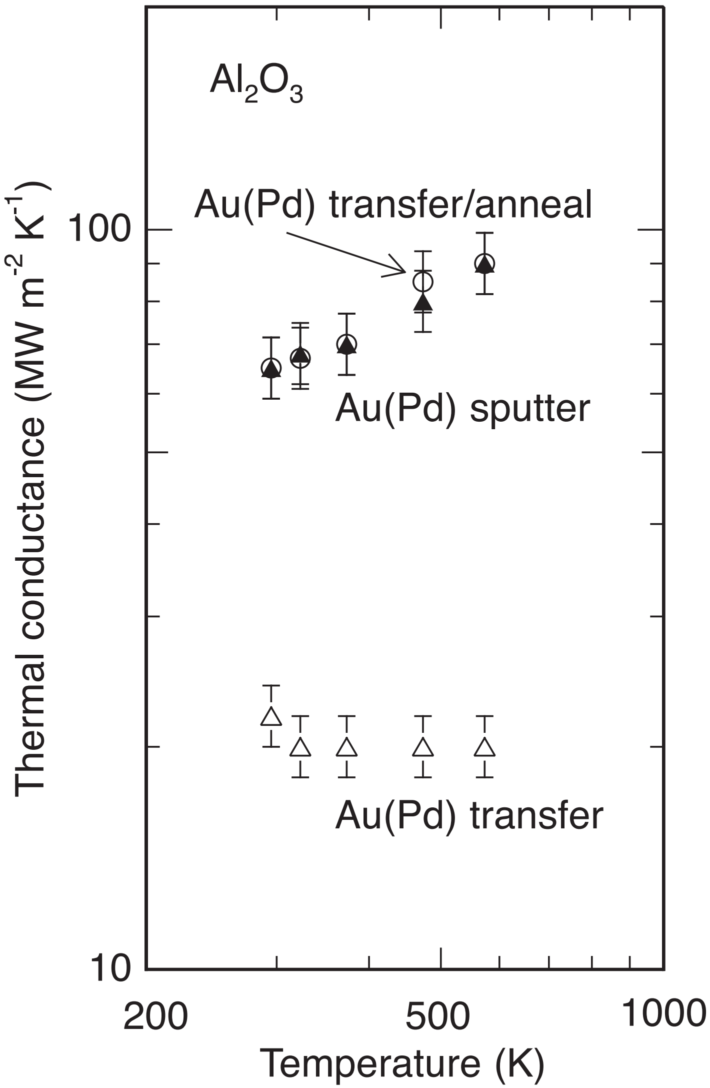
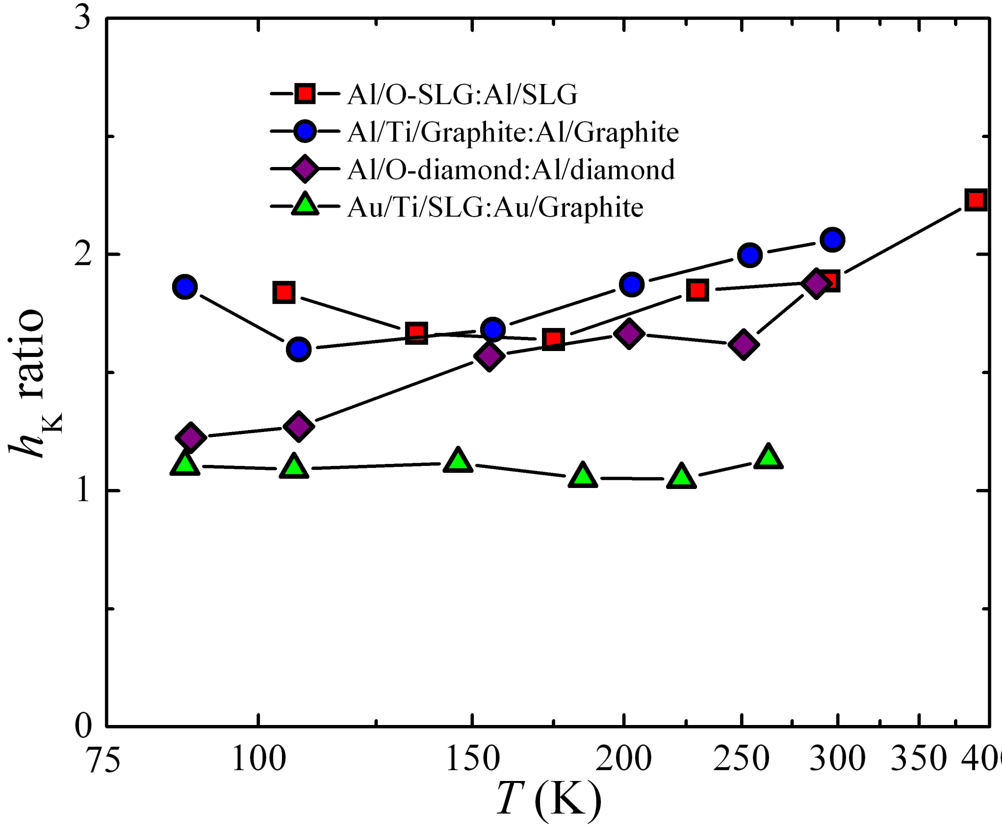
Inelastic scattering at interface?



Oh *et al*., *Adv. Mat.* 23, 5028 (2011)



Hopkins *et al*. *Nano Lett*. 12, 590 (2012)

UNIVERSITY *of* VIRGINIA ENGINEERING *Developing Leaders of Innovation* 175 years

Outline

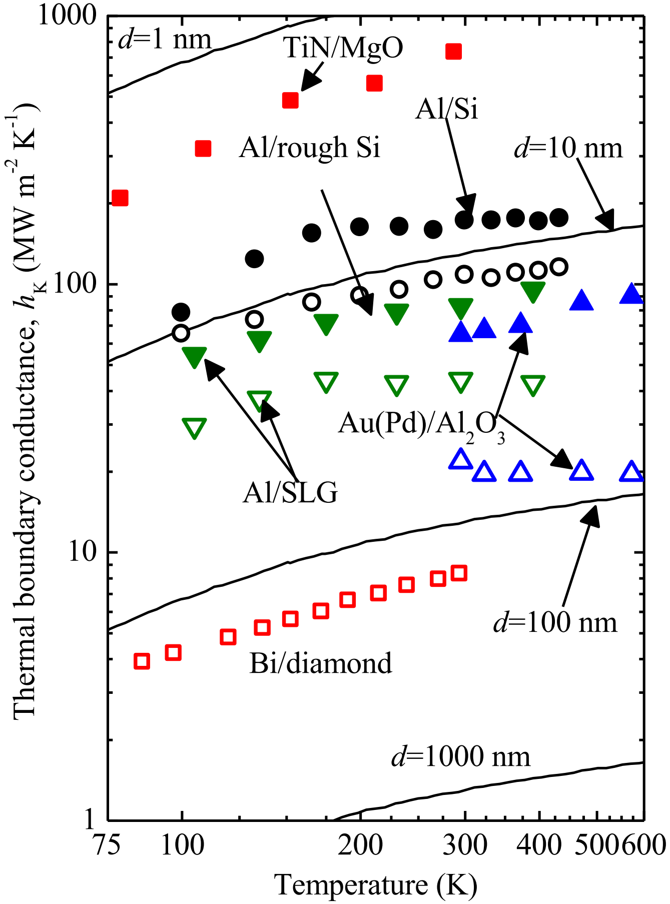
- **Effects of bonding on thermal conductance across graphene interfaces**

- **Plasma functionalization offers a unique way to manipulate the bonding and change phonon scattering at graphene contacts**

- **Collaborators: Scott Walton (NRL)**
- **Hopkins *et al.*, *Nano Lett.* 12, 590 (2012)**
- **Duda *et al.*, *Phys. Rev. B* 84, 193301 (2011)**

Summary

Interfacial quality and bonding can affect thermal conductance



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