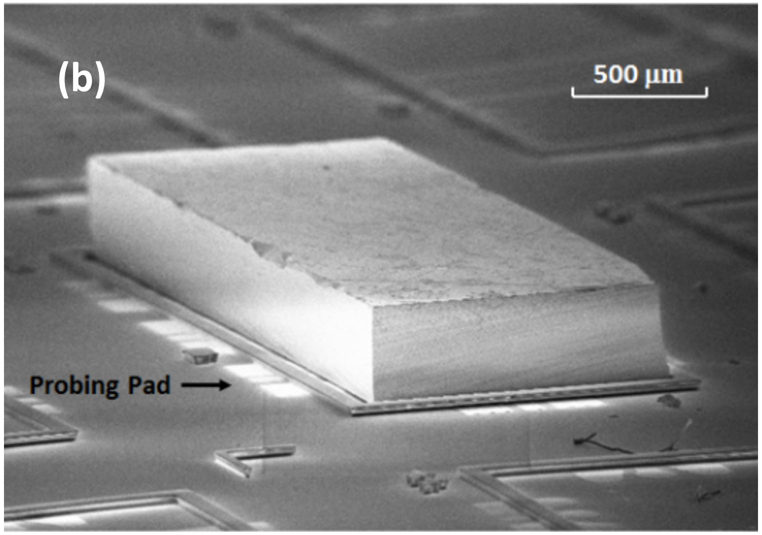
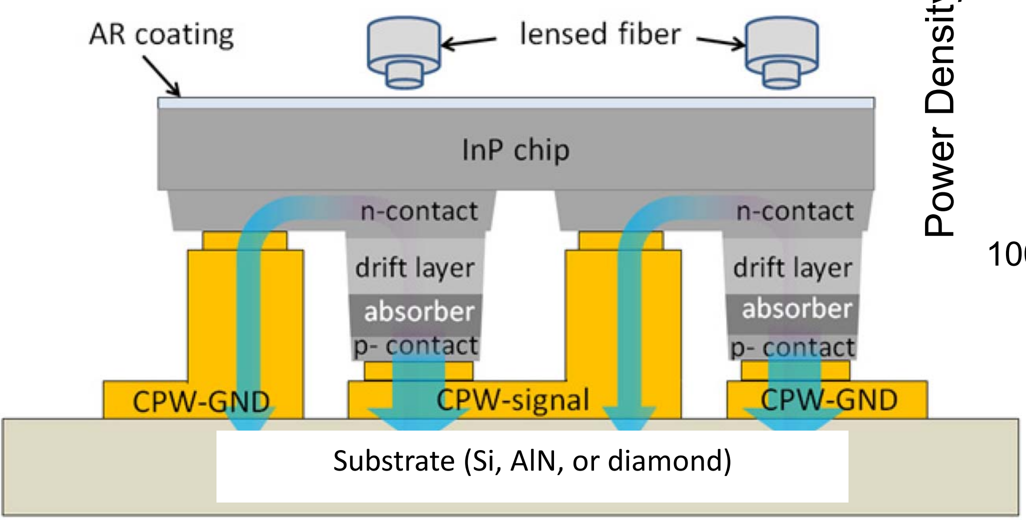
School of Engineering & Applied Science
University of Virginia

Interfacial imperfection effects on the thermal boundary resistance in materials and devices

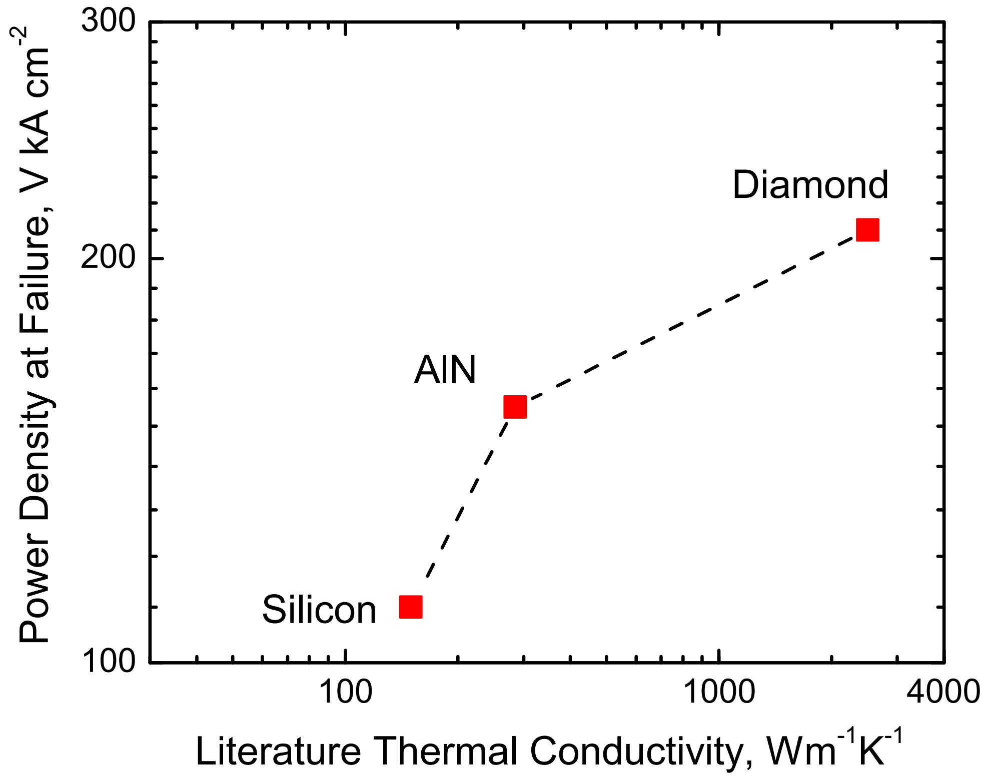
Patrick E. Hopkins
Associate Professor
Dept. Mech. & Aero. Eng.
University of Virginia
phopkins@virginia.edu
patrickehopkins.com

High power device thermal management - traditional





(c)



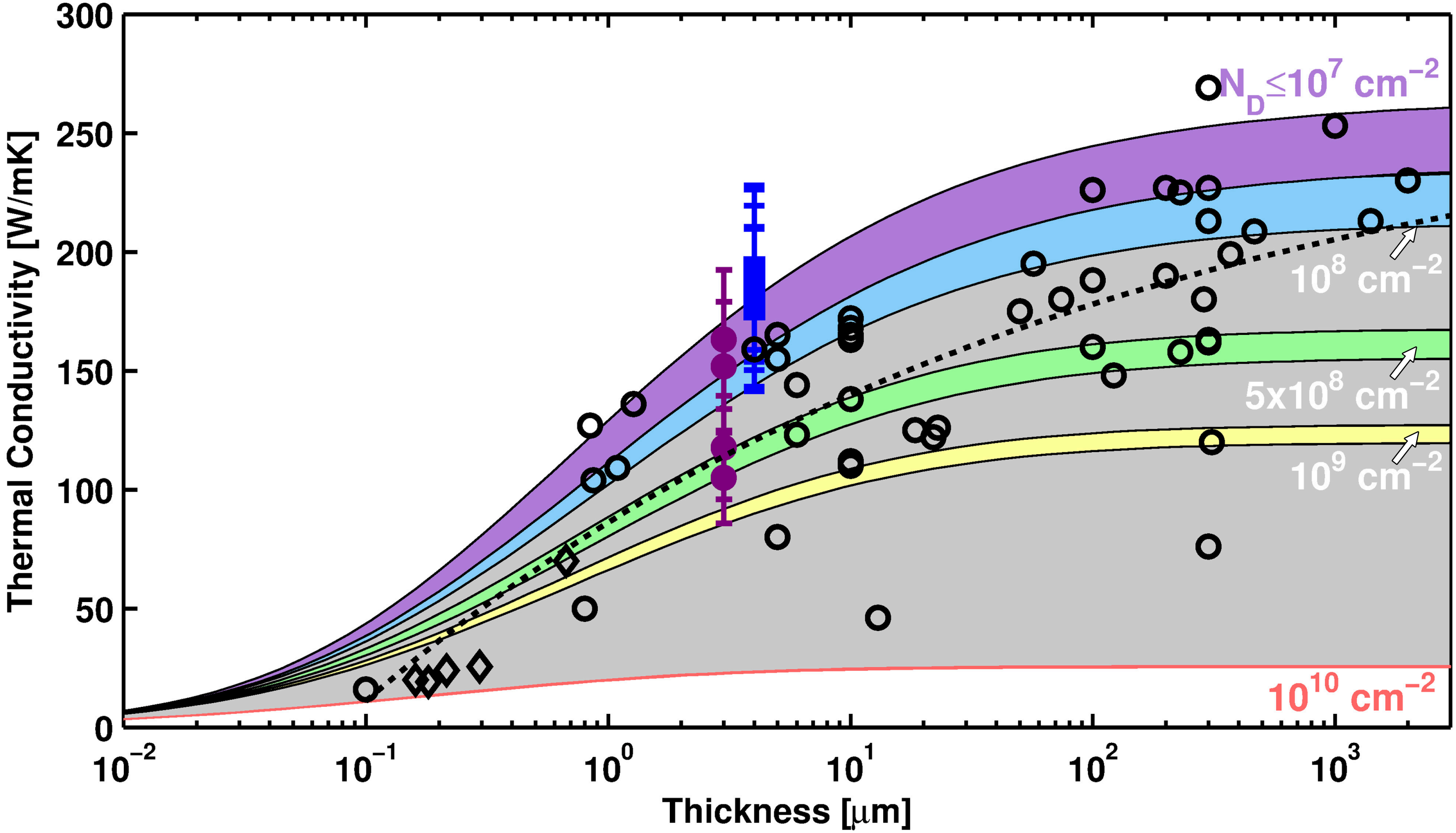
Collaboration with Joe Campbell (UVA)

IEEE Photonics. **5**, 6800307 (2013)

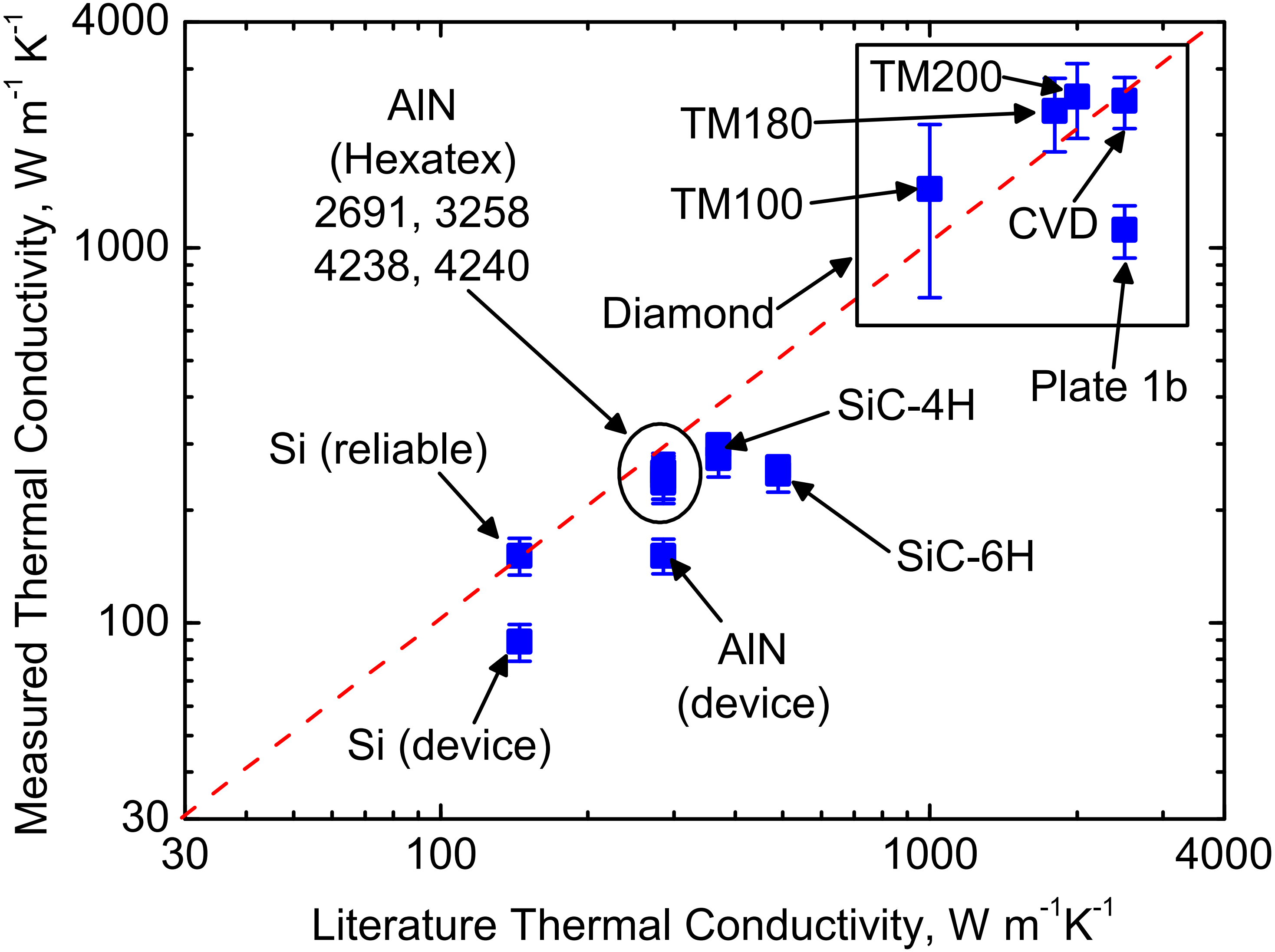
Nanoscopic view: not all materials created equal

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

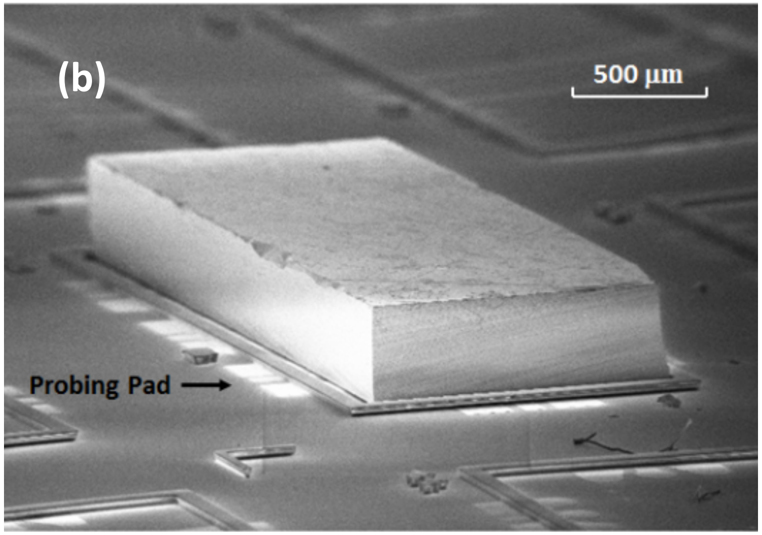
The case of GaN: Collaboration with Thomas Beechem (SNL)
J. Appl. Phys. **120**, 095104

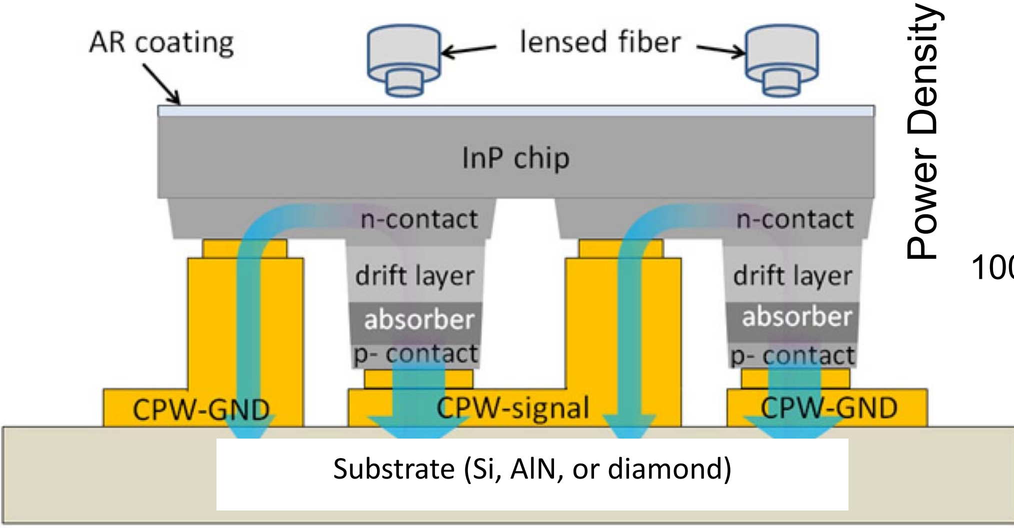


AlN is not AlN is not AlN, and 1 number is always assumed

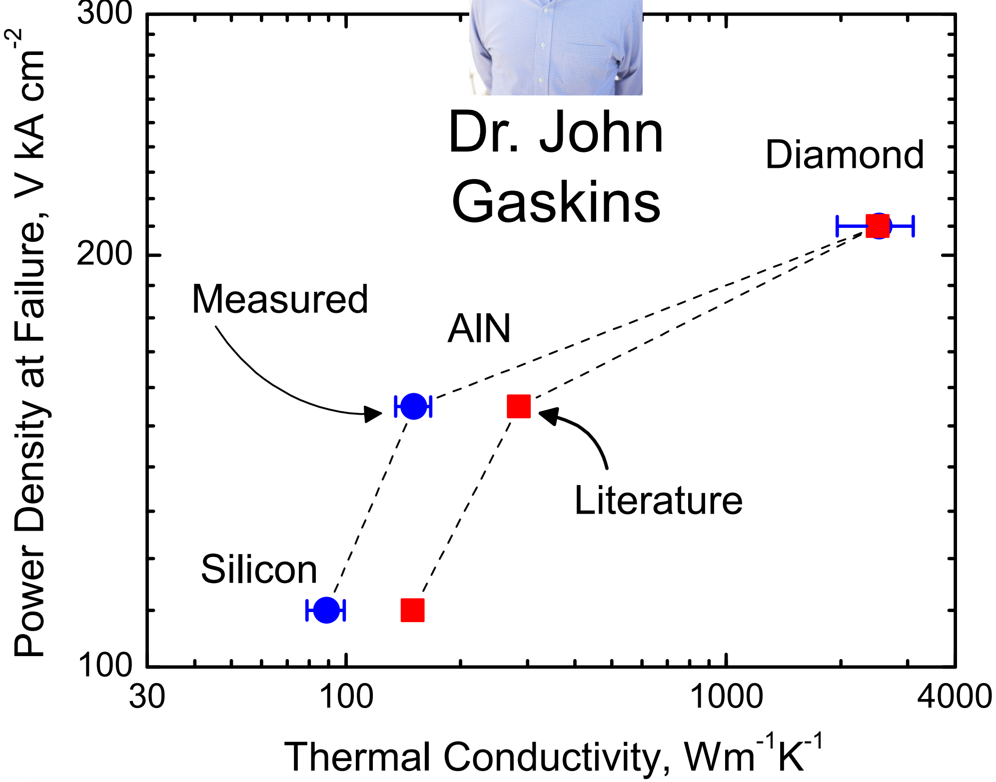


High power device thermal management - traditional





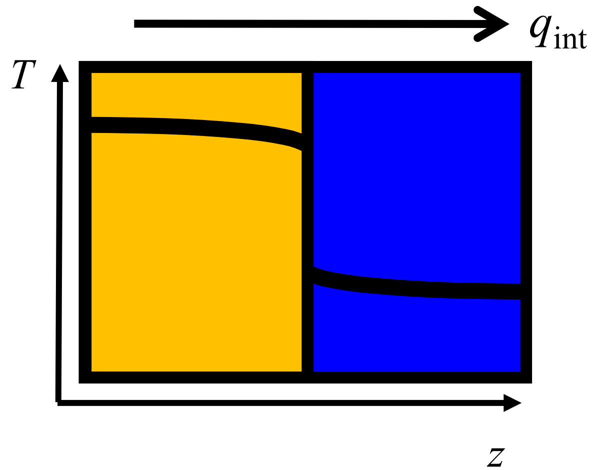
(c)



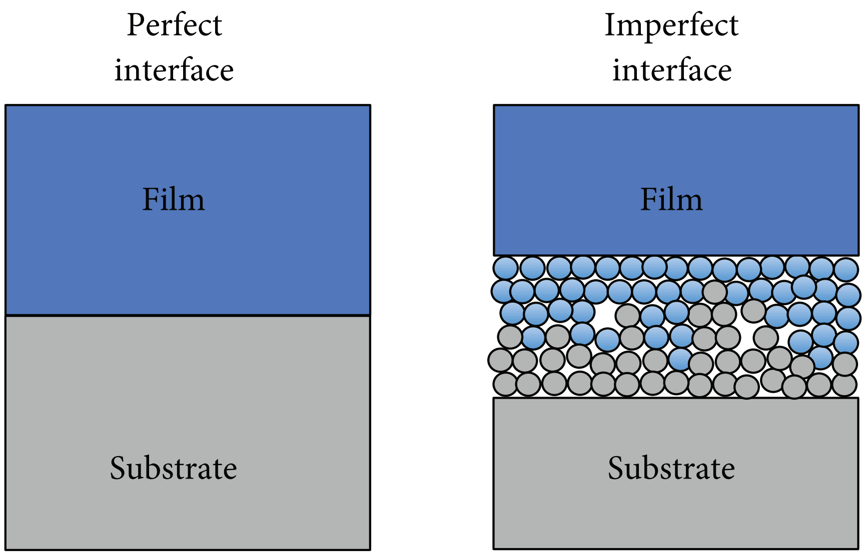
Collaboration with Joe Campbell (UVA)

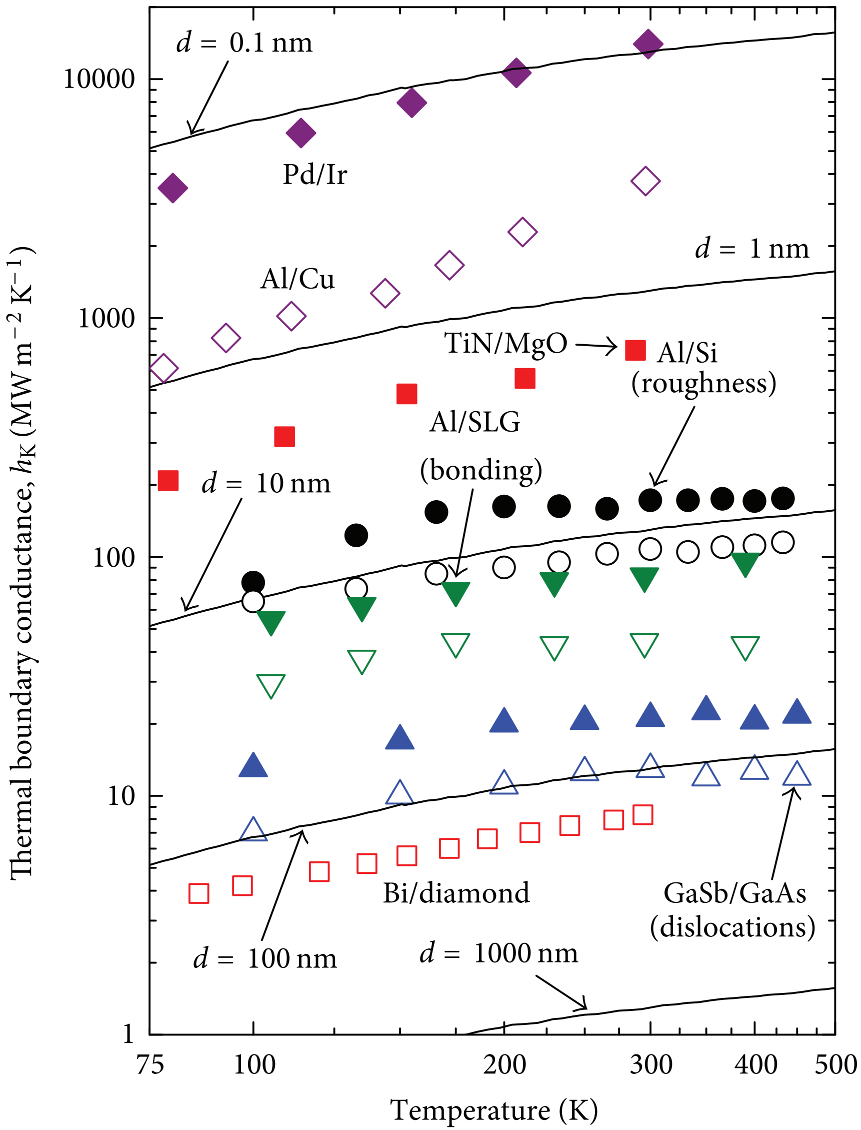
IEEE Photonics. **5**, 6800307 (2013)

Thermal boundary conductance (TBC) – nanoscale issues



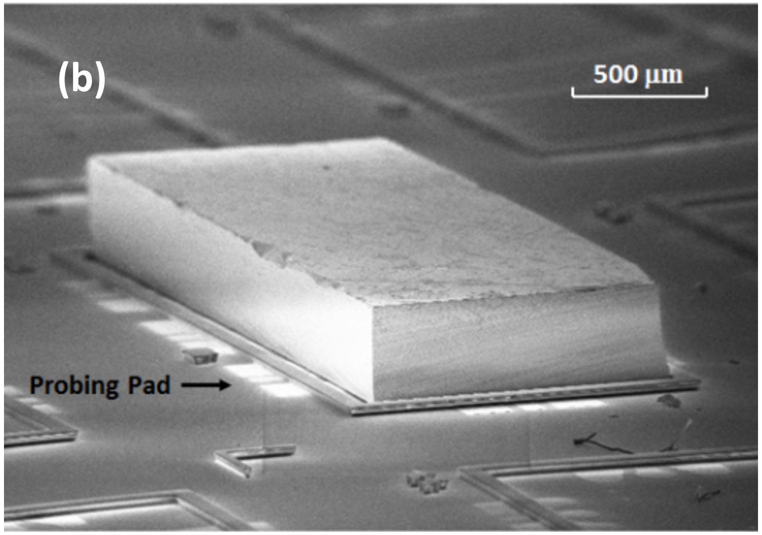
$$q = h_K \Delta T = \Delta T / R_K$$

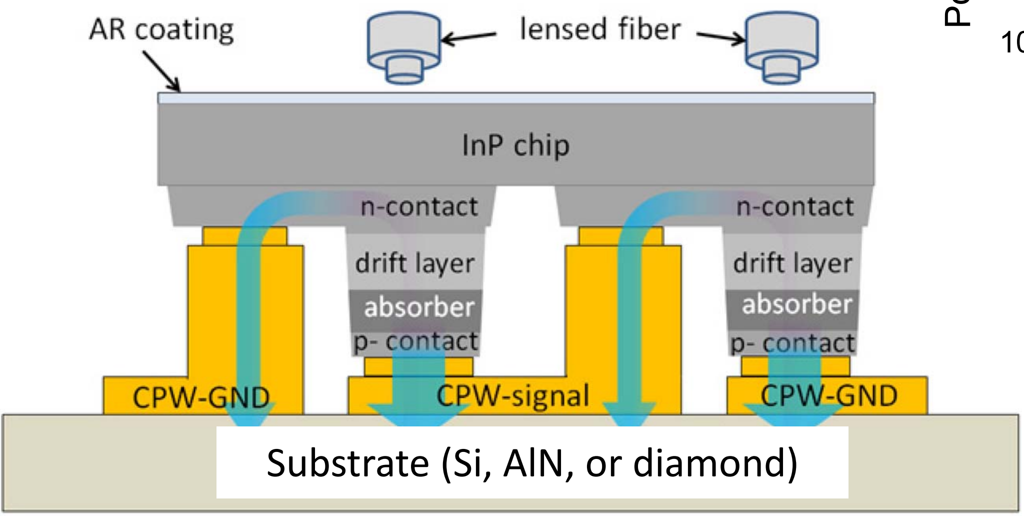




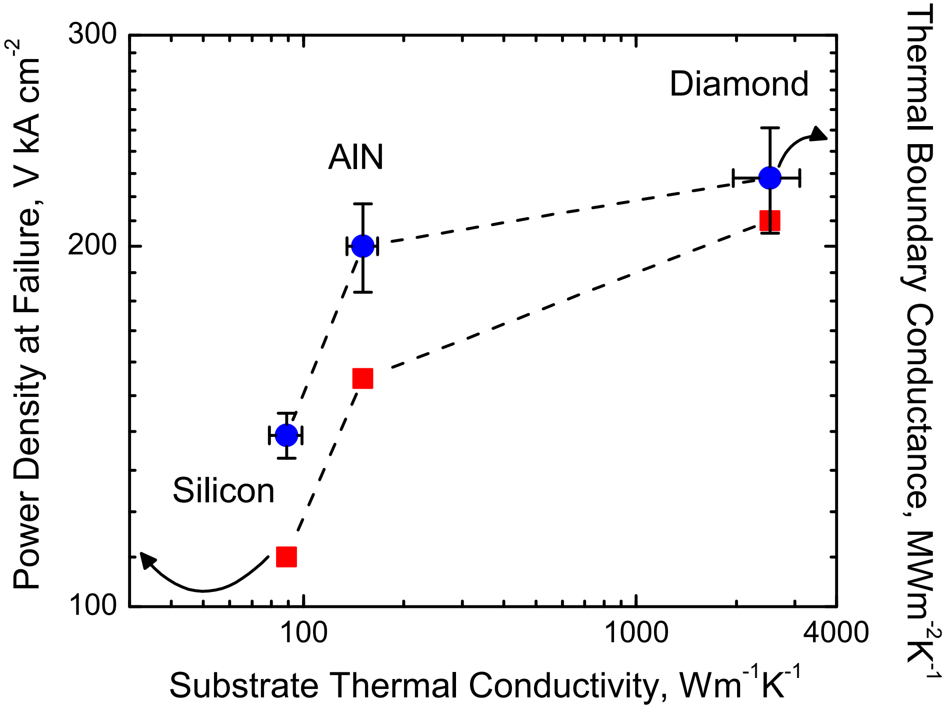
ISRN Mech. Eng. **2013**, 682586

High power device thermal management - nano



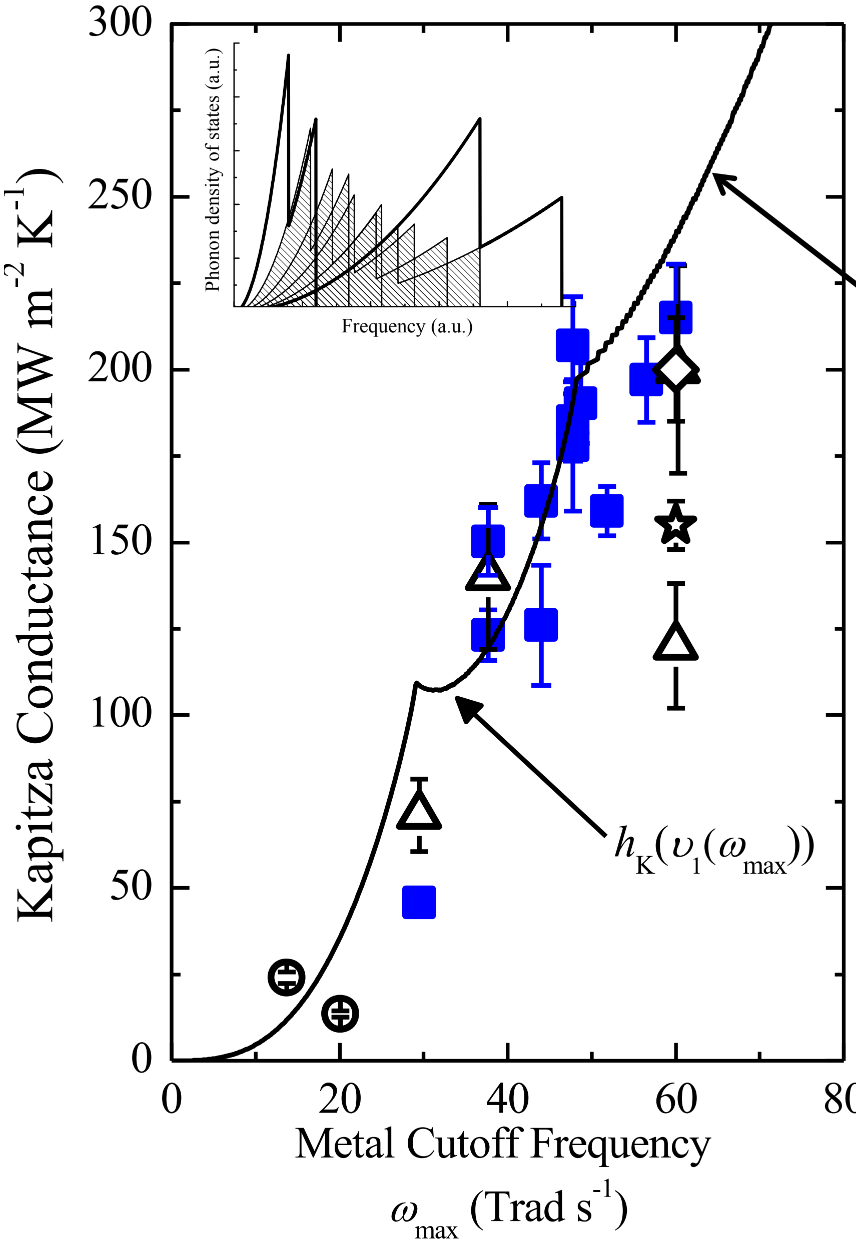


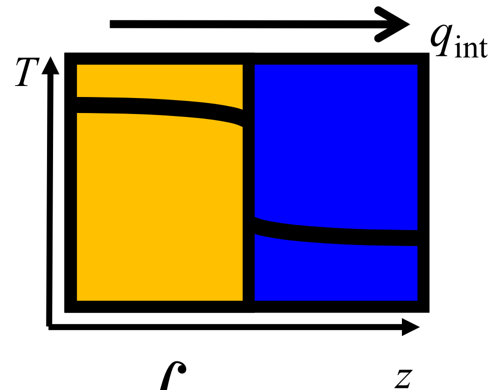
(c)



Contact/heat sink TBC plays direct role in power density
***J. Lightwave Tech.* 35, 4242**

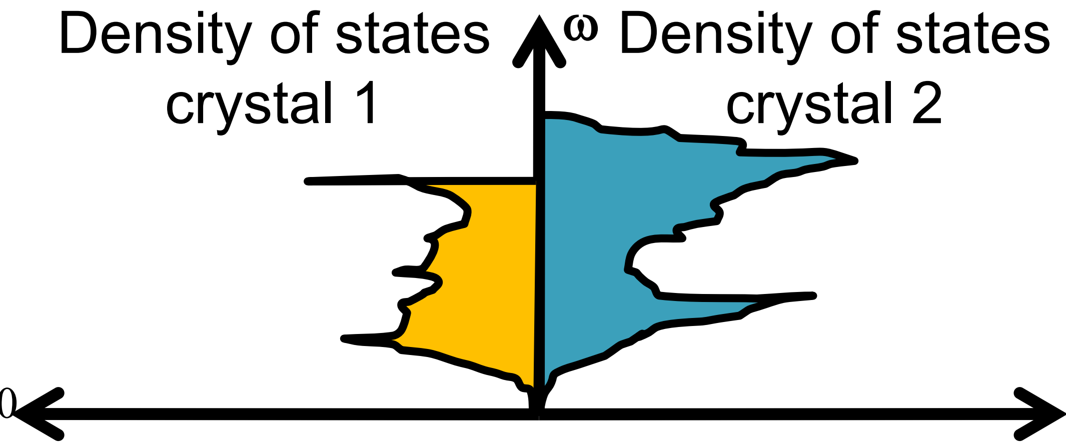
What drives TBC across interfaces? Simple/cubic interfaces





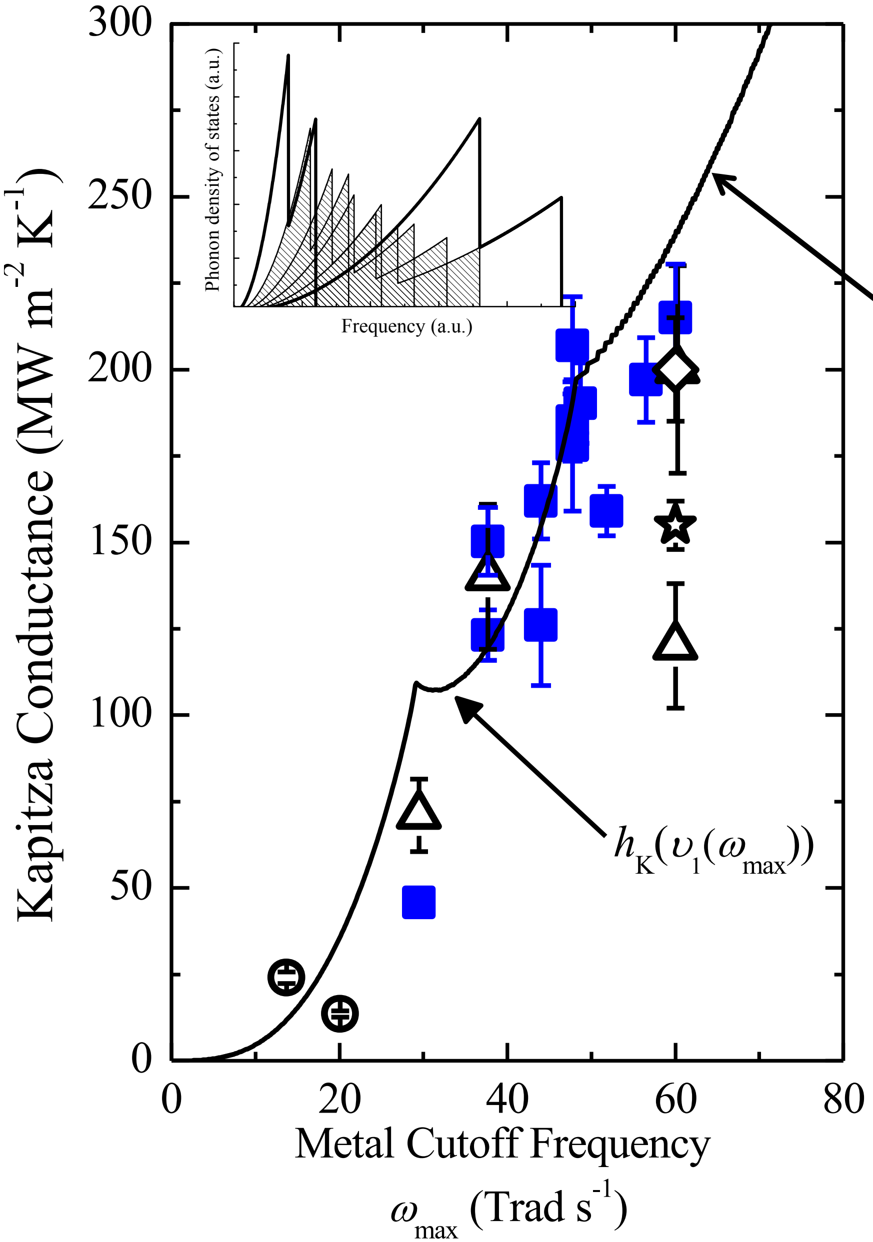
$$h_K \propto \int_\omega C_\omega v_\omega \tau_\omega \, d\omega$$

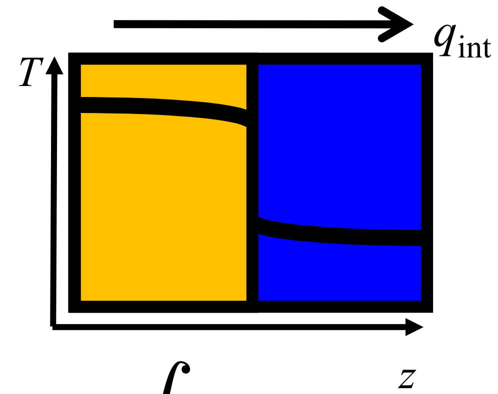
<u>Diffuse Mismatch Model for metal/Si</u>



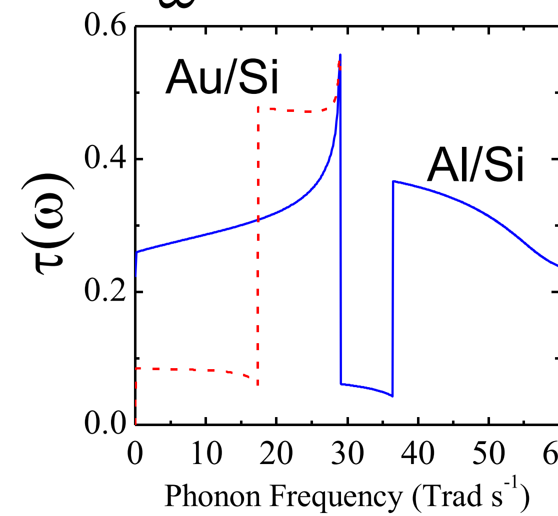
PRB **91**, 035432 (2015)

What drives TBC across interfaces? Simple/cubic interfaces



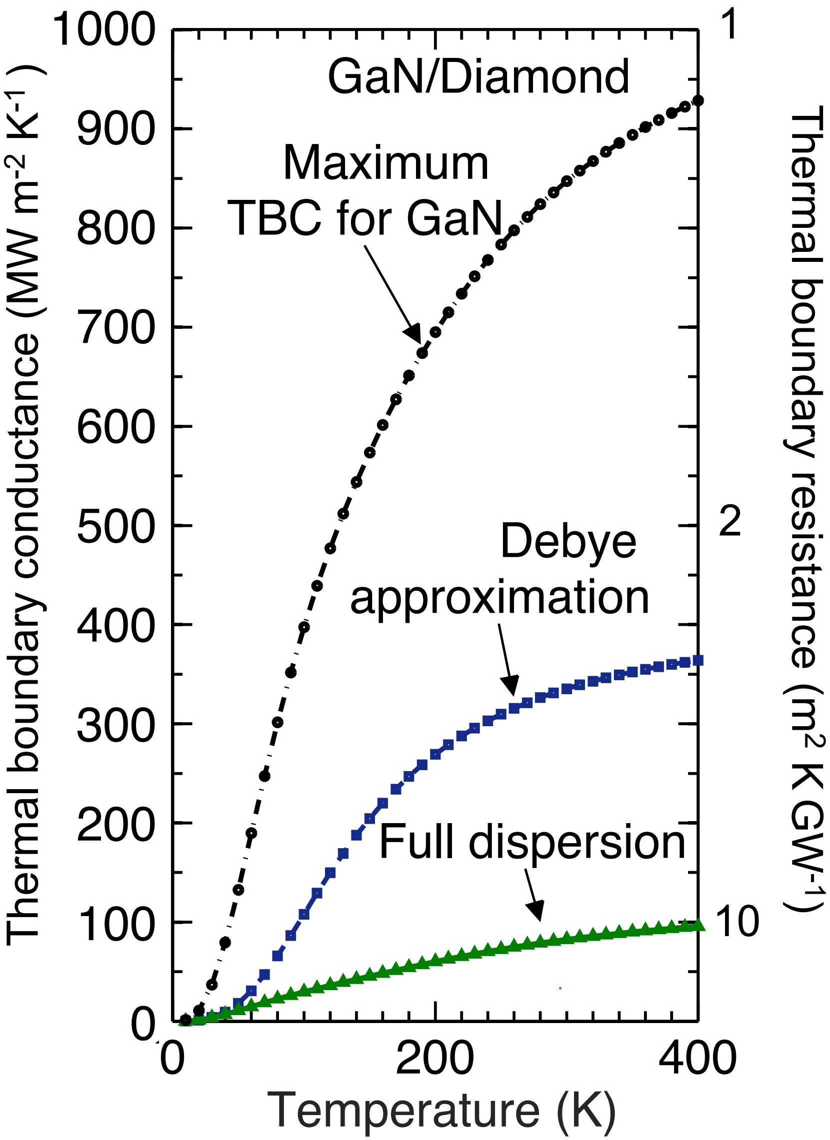


$$h_K \propto \int_\omega C_\omega \upsilon_\omega \tau_\omega \, d\omega$$



PRB **91**, 035432 (2015)

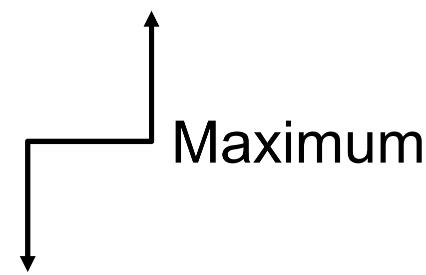
Simple predictions break down for complex materials



Reasonable goals/limits for TBC/TBR should consider reasonable approximation of material properties

Is a "maximum TBC reasonable"?

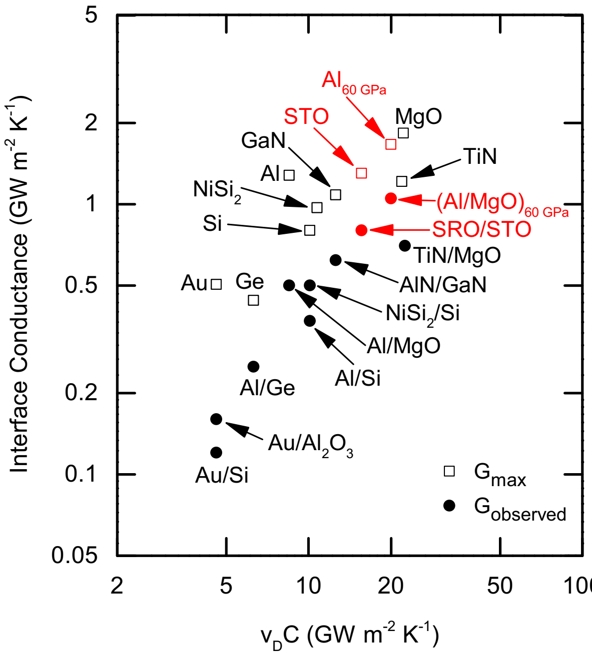
$$h_{\mathrm{K}} \propto \int_{\omega} C_{\omega} v_{\omega} \tau_{\omega} \, \mathrm{d}\omega$$



$$\tau_{\omega} = 1$$

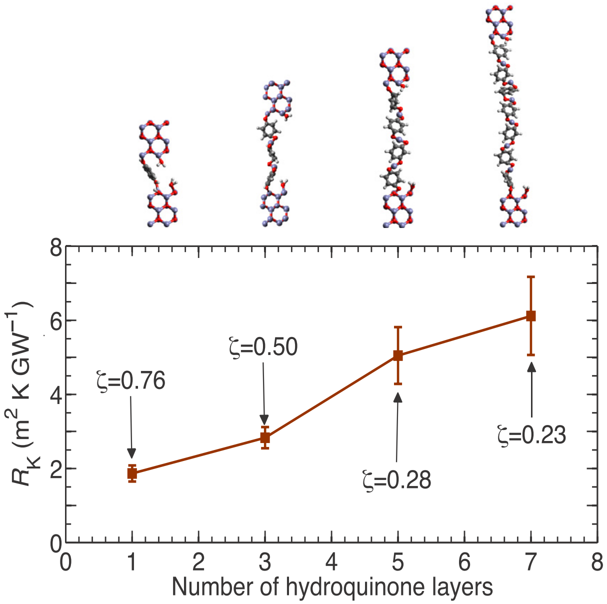
Achieving maximum TBC

- All vibrational energy trans. across the interface
- Perfect interface (lattice matched, no imperfections)
- Well matched phonon spectra



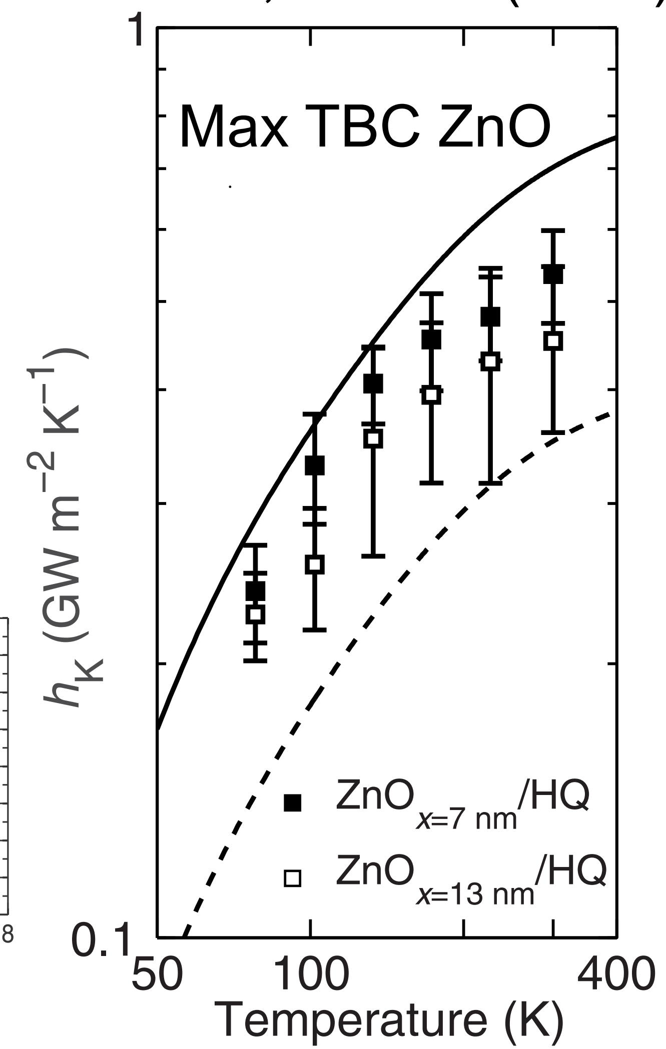
Wilson and Cahill, *PRB* **91**, 115414 (2015)

Dr. Ashutosh Giri

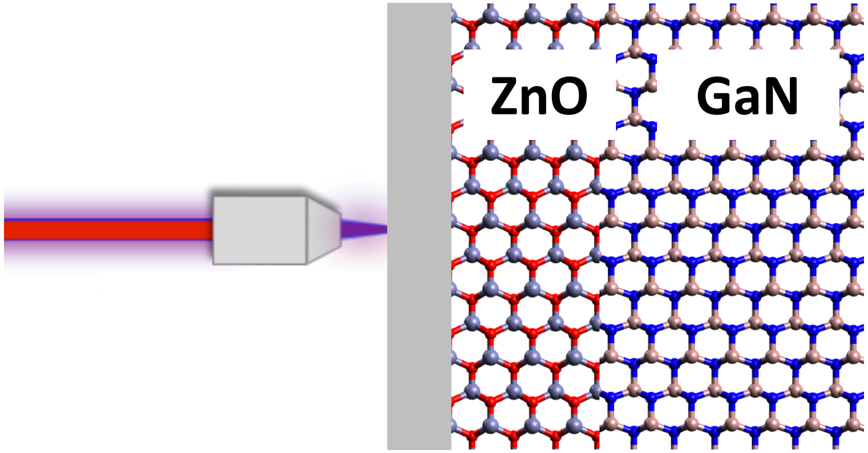


Derived TBC from ZnO/HQ/ZnO SL

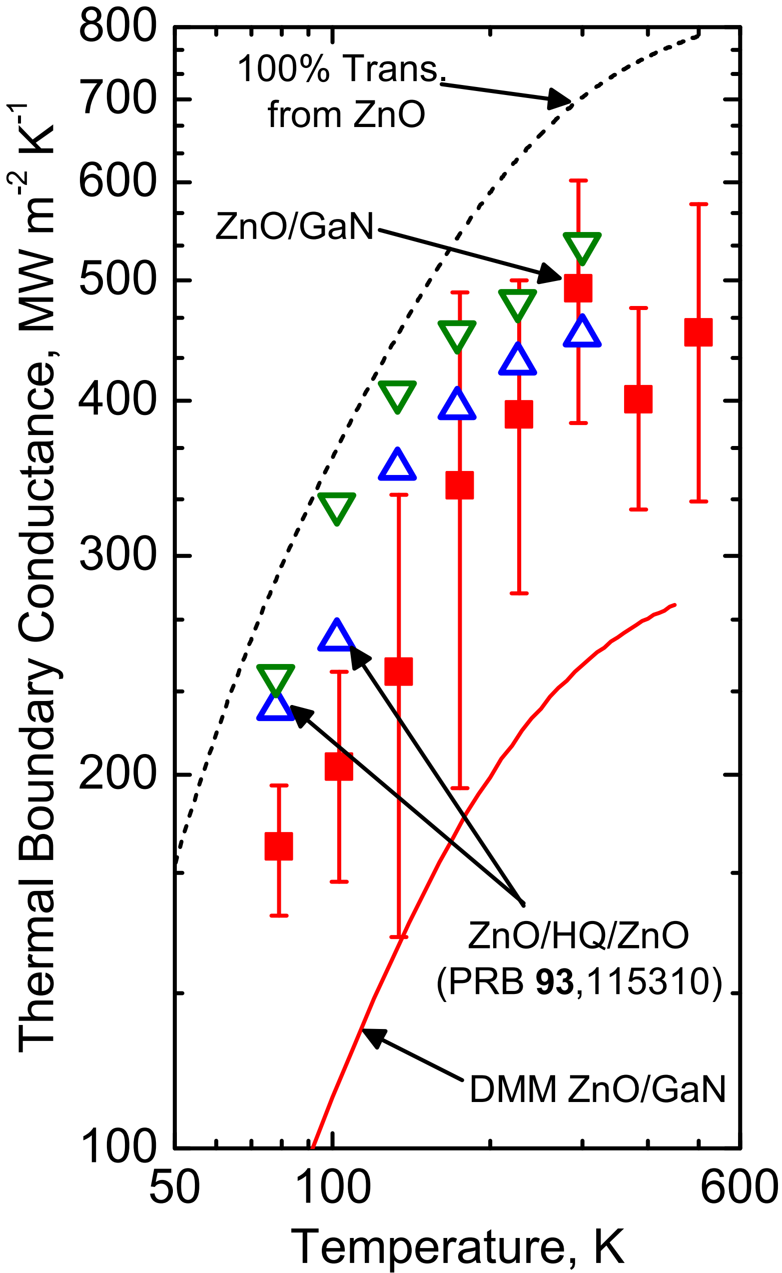
PRB **94**, 115310 (2016)



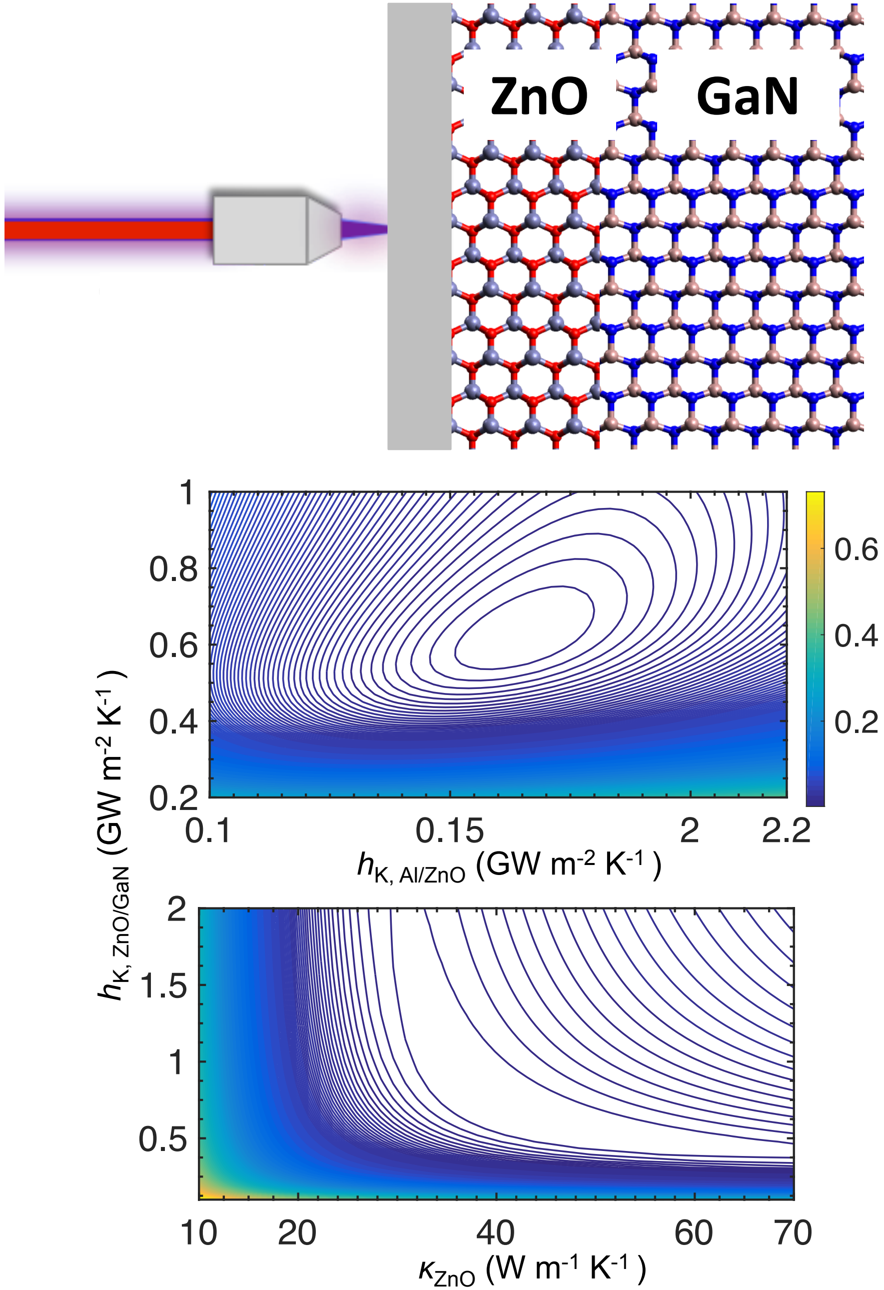
Maximum TBC at non-metal/non-metal isolated interface?

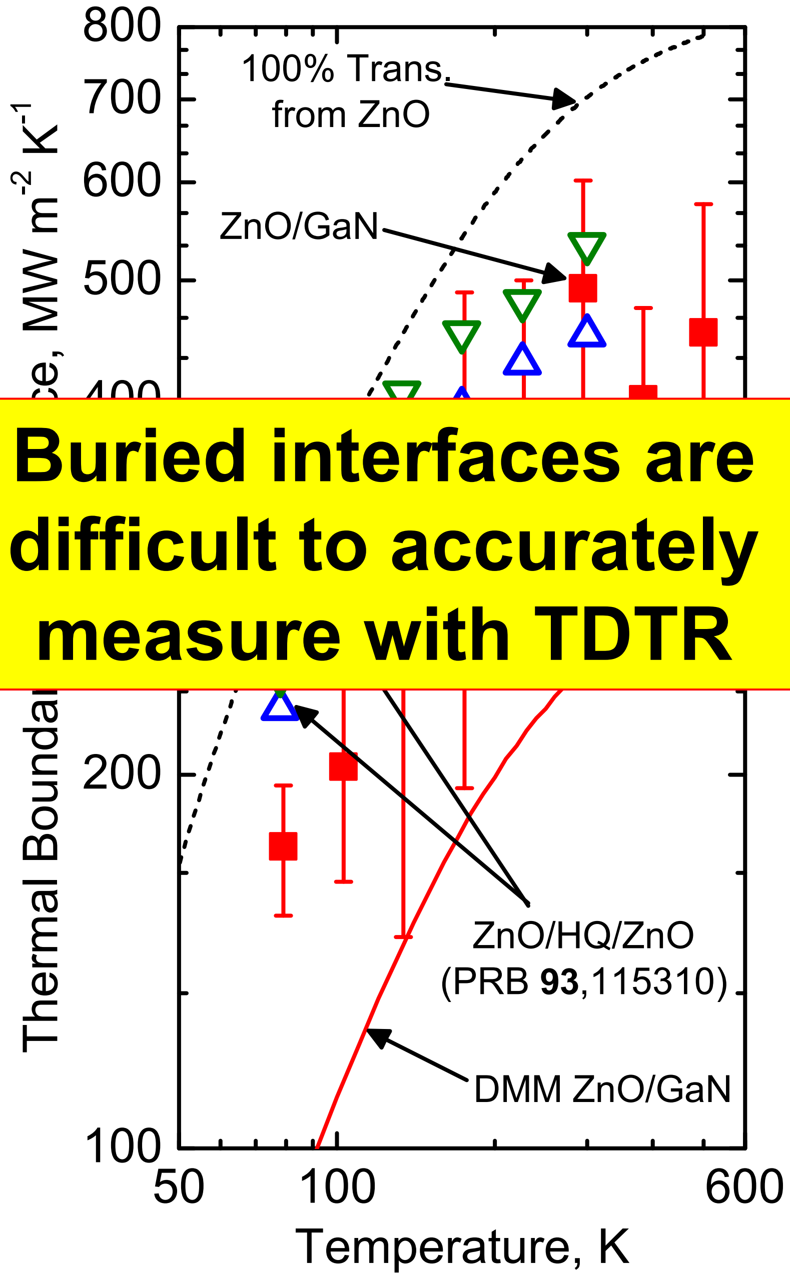


- Highest TBC measured at single insulator/insulator interface of crystalline materials
- Can not be fully explained by phonon mismatch
- Note: large uncertainties due to signals being dominated by Al/ZnO resistance



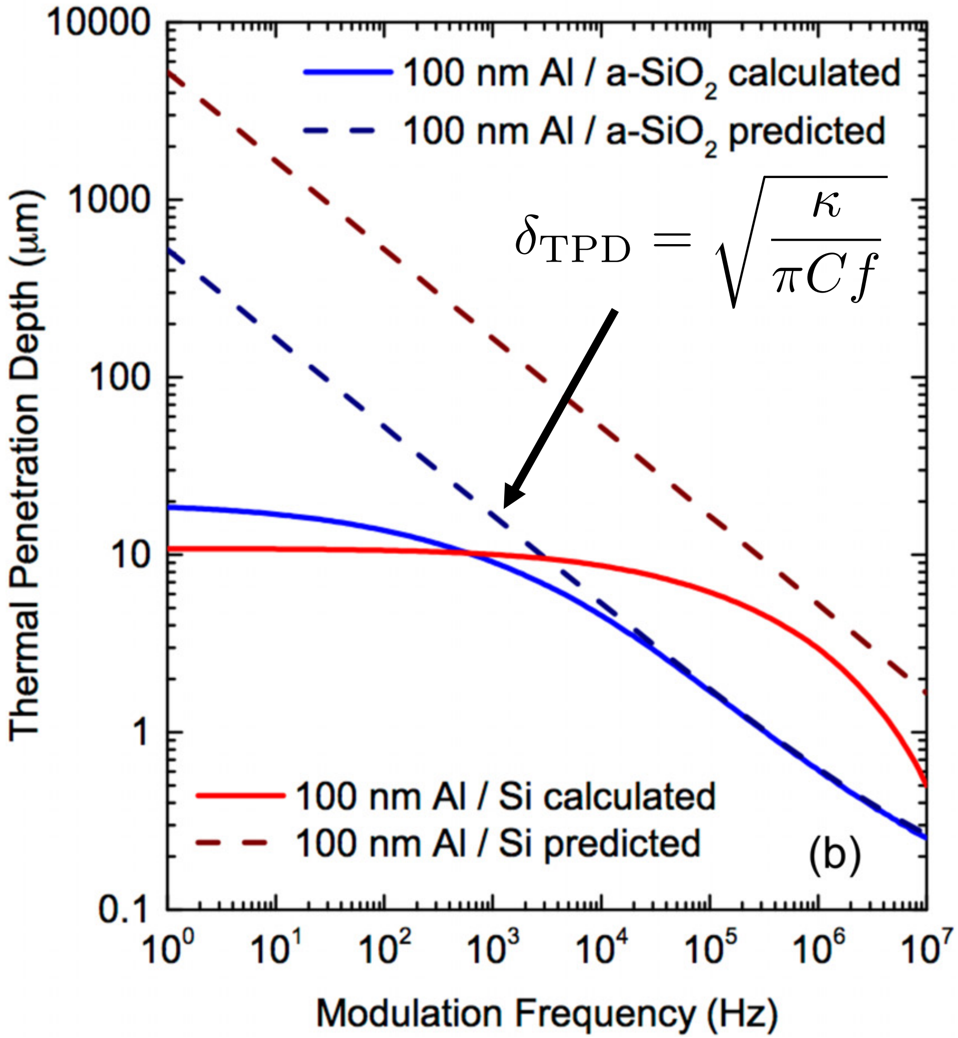
Side note: what can TDTR actually measure???



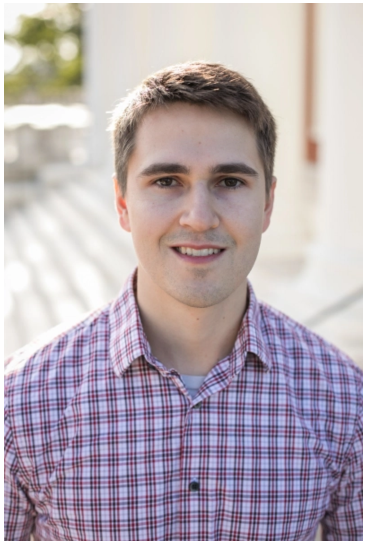


Buried interfaces are difficult to accurately measure with TDTR

Side note: what can TDTR actually measure???



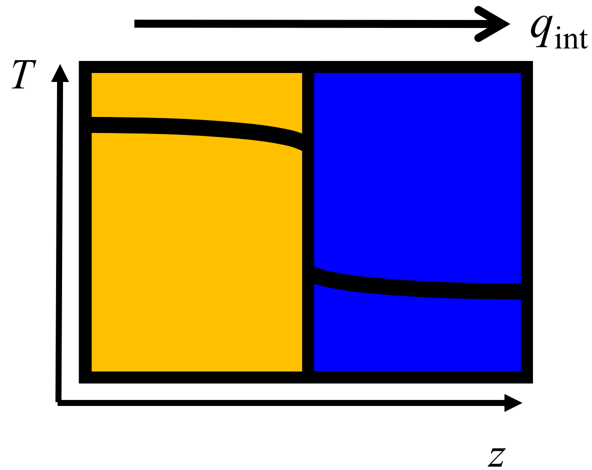
Braun and Hopkins
JAP **121**, 175107 (2017)



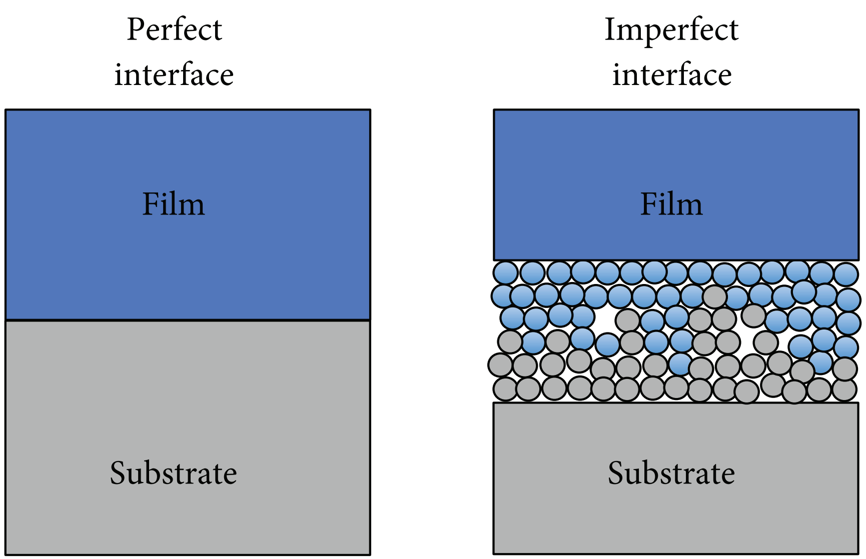
Jeff Braun

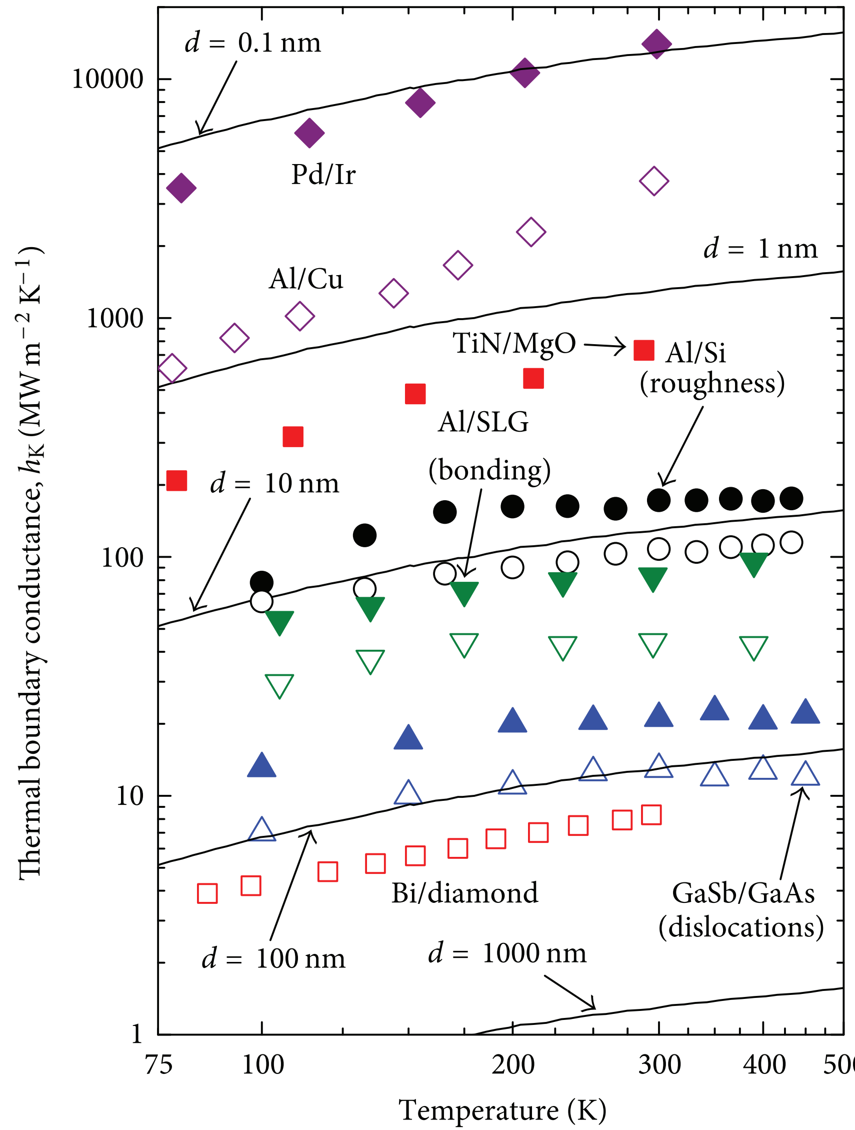
TDTR does not measure as "deep" as we think it does!

What about imperfect interfaces?



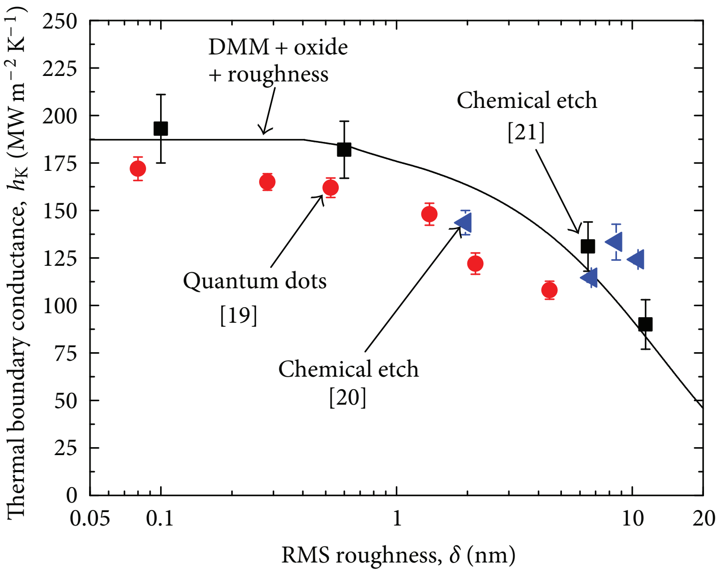
$$q = h_K \Delta T = \Delta T / R_K$$

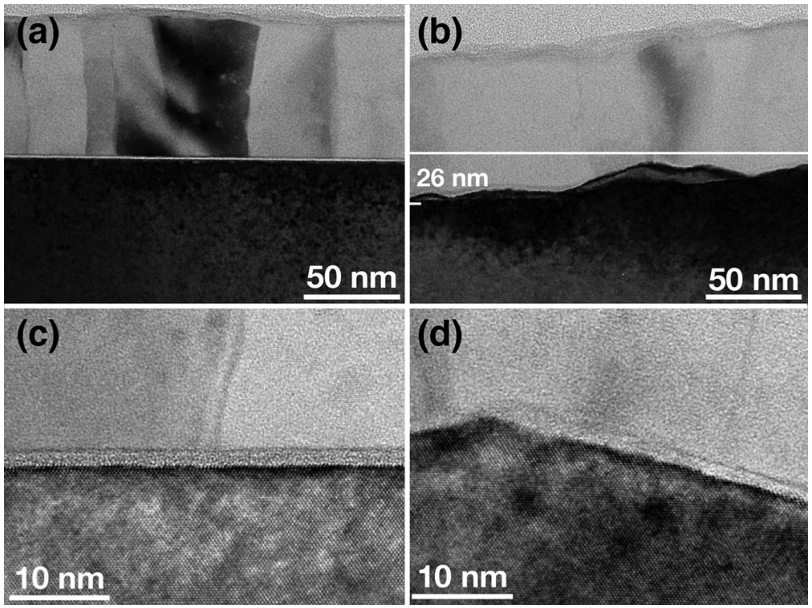


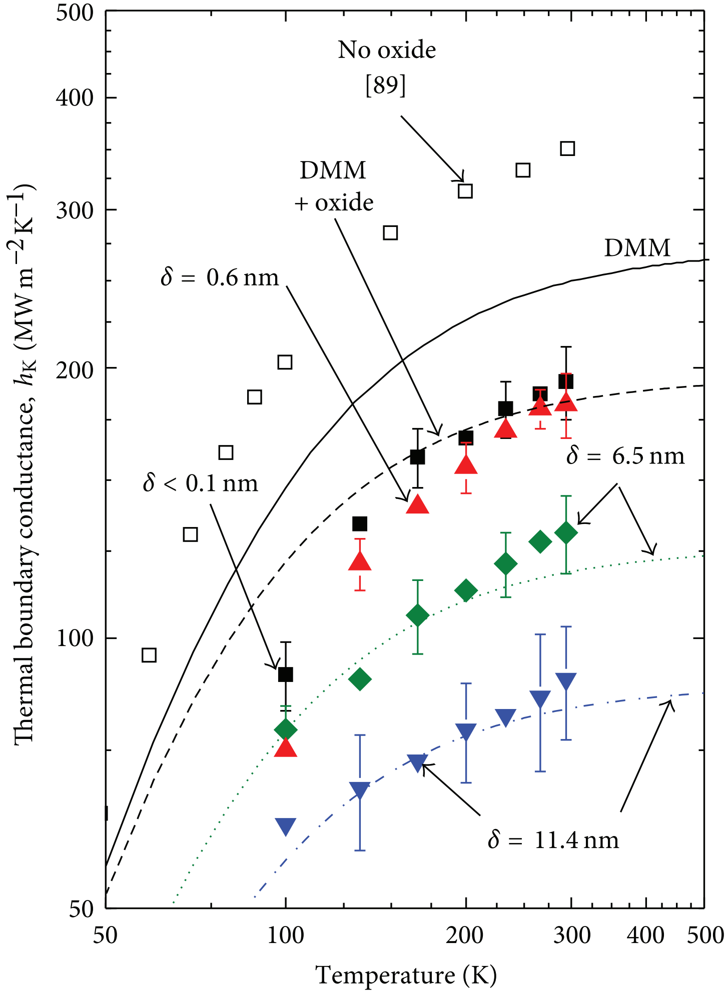


ISRN Mech. Eng. **2013**, 682586

Geometric roughness – Al/Si interfaces

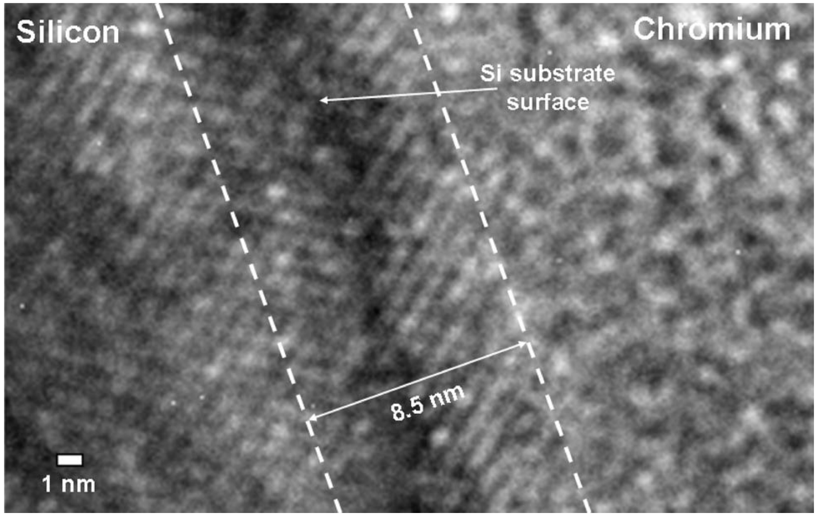


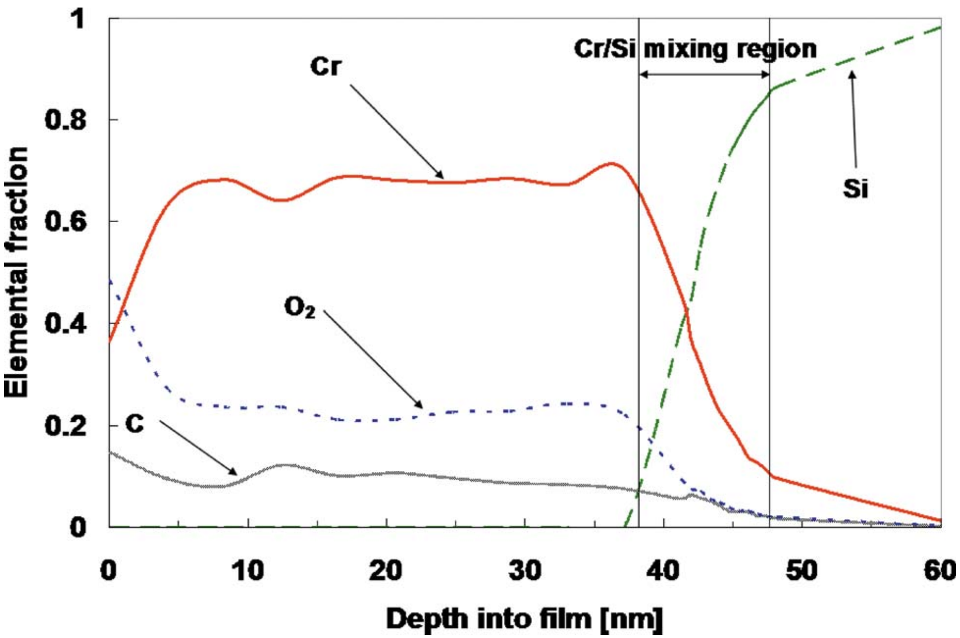




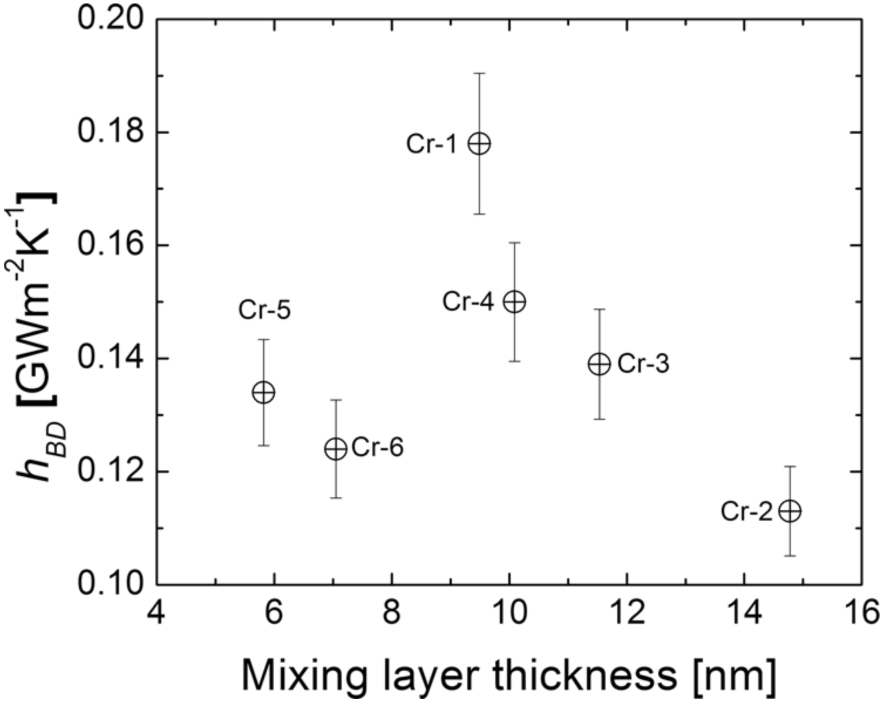
PRB **82**, 085307 (2010)
PRB **84**, 035438 (2011)
APL **100**, 111602 (2012)

Atomic interdiffusion – Cr/Si interfaces



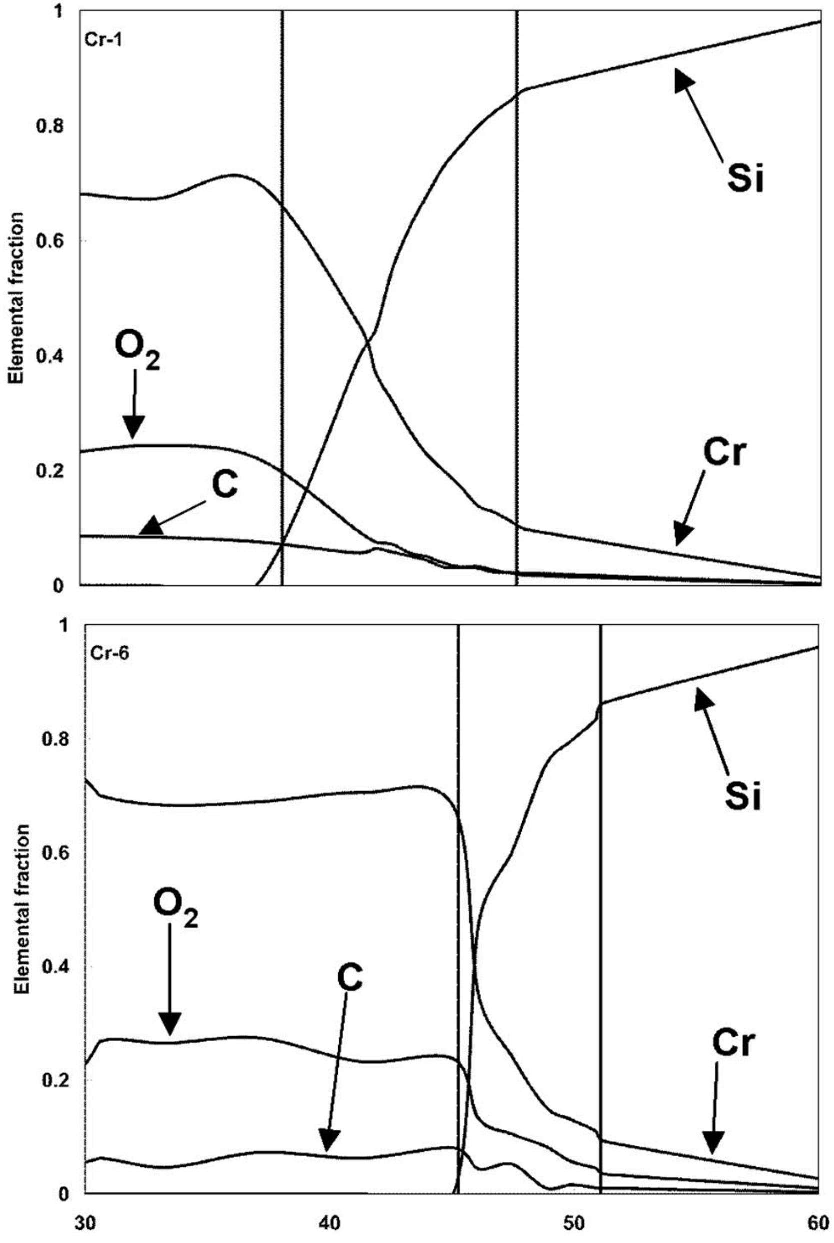


Thickness of mixing layer or elemental spatial gradient?

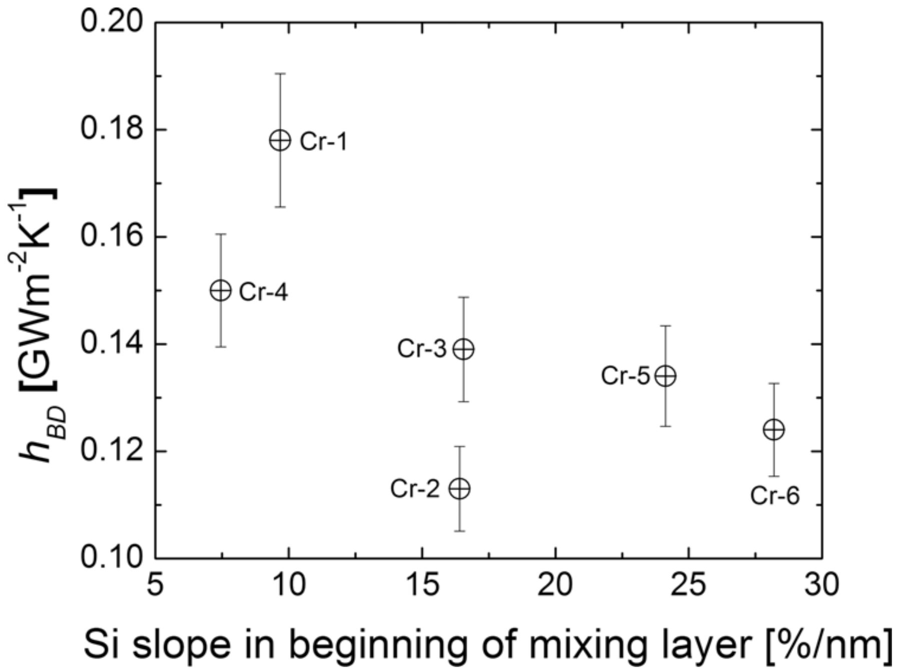


Collab. w/ S. Graham (Ga Tech)
APL **90**, 054104 (2007)
J. Heat Trans. **130**, 062402 (2008)

Atomic interdiffusion – Cr/Si interfaces



Thickness of mixing layer or **elemental spatial gradient?**

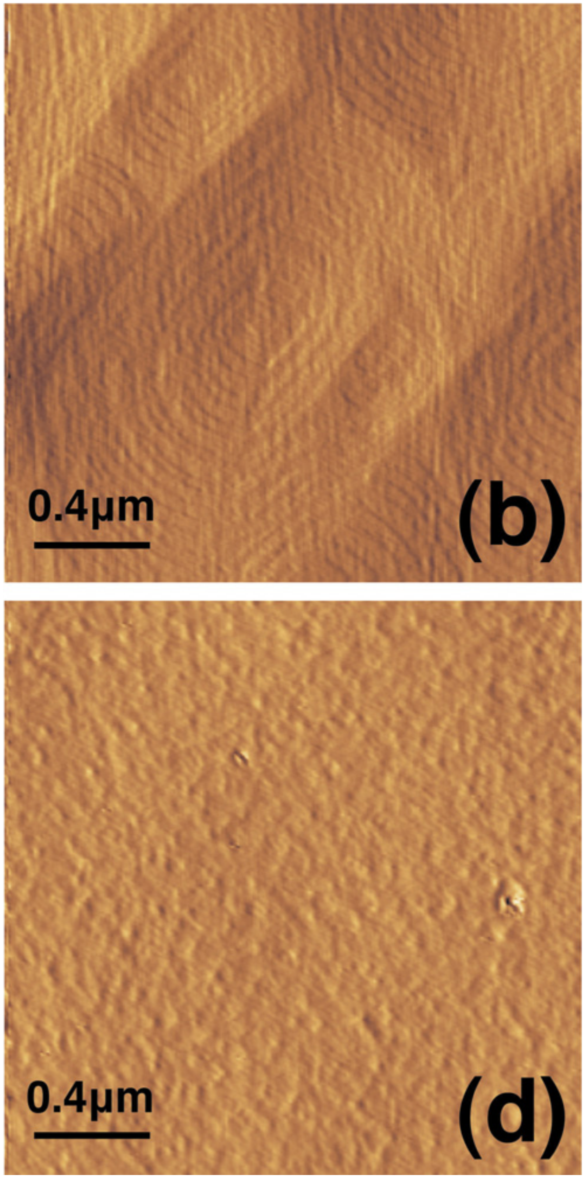


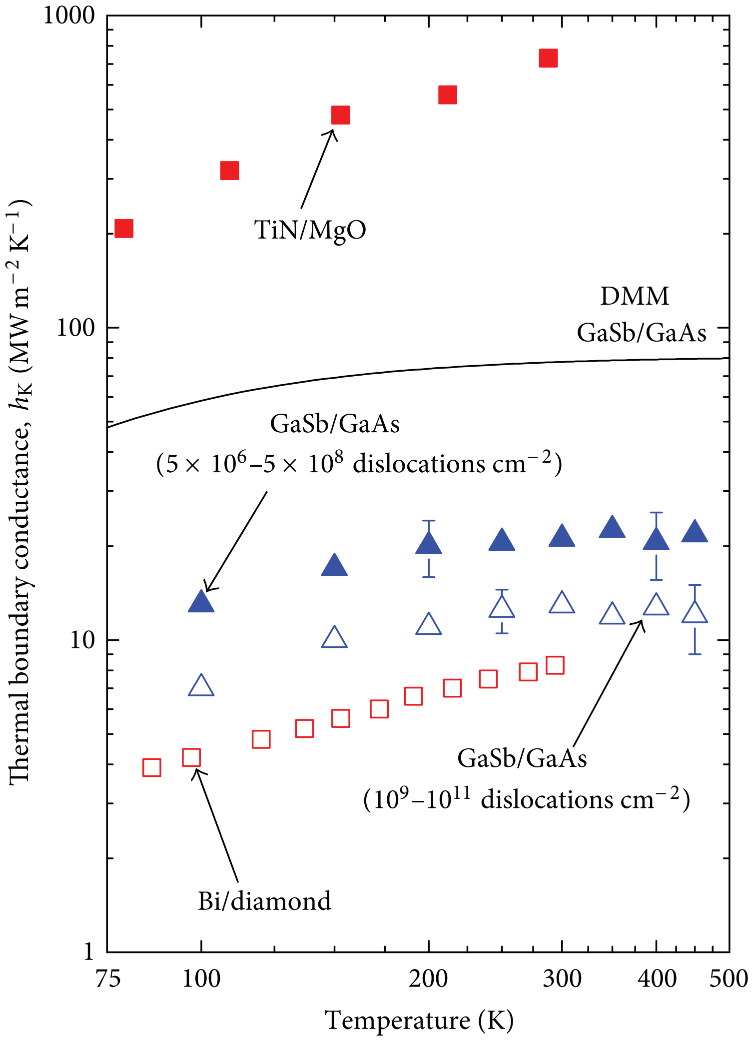
Collab. w/ S. Graham (Ga Tech)

APL **90**, 054104 (2007)

J. Heat Trans. **130**, 062402 (2008)

Dislocation density – GaSb/GaAs interfaces

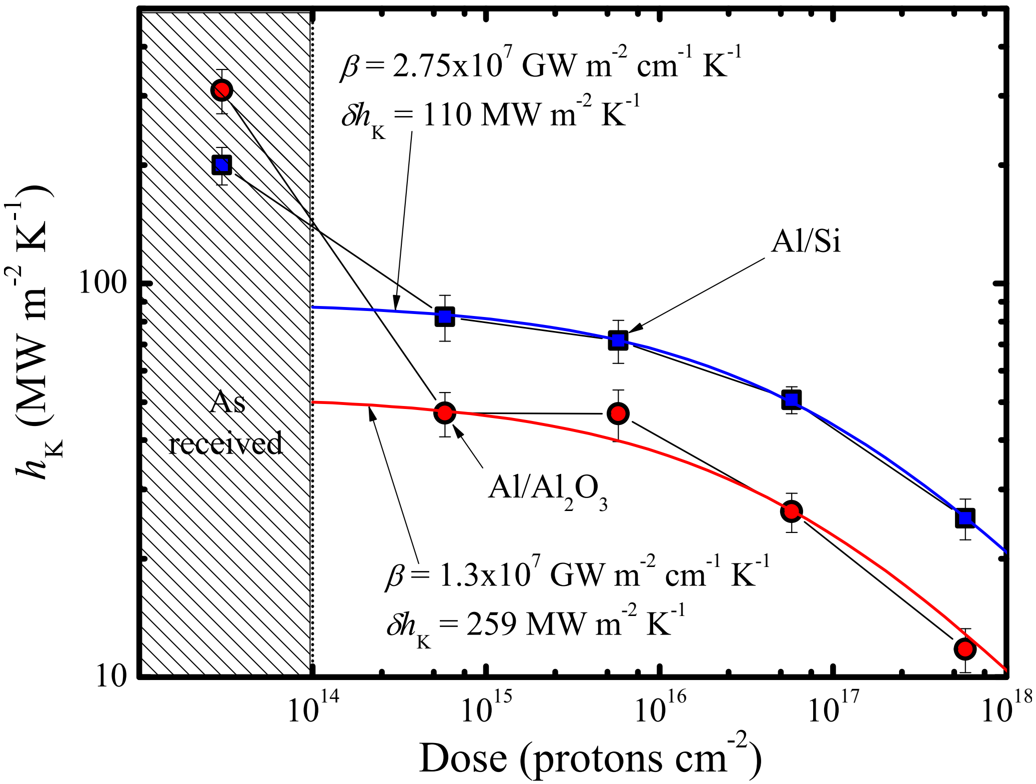


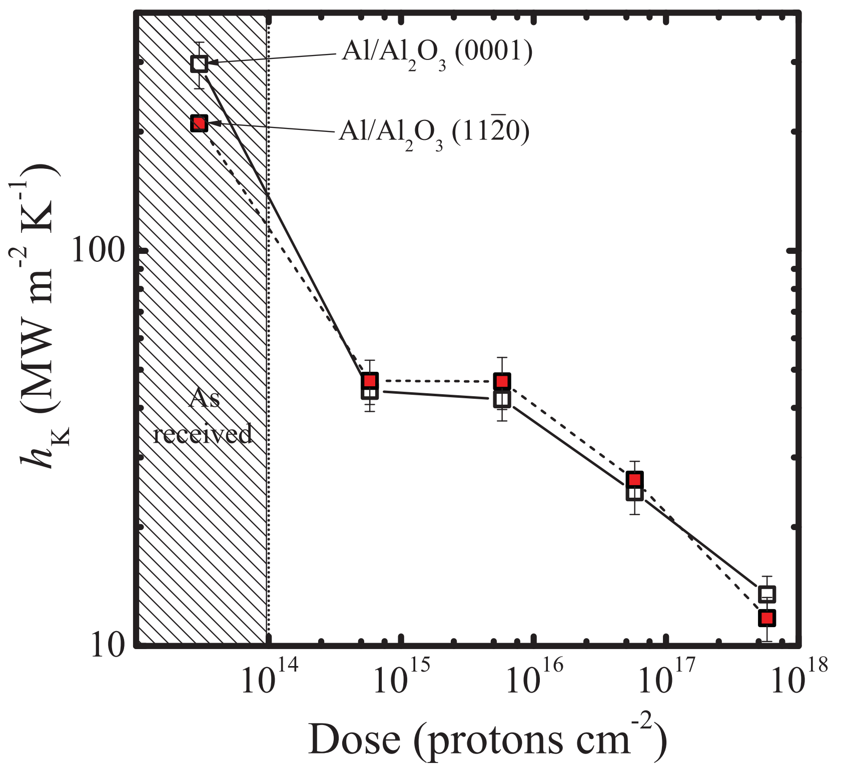


Collab. w/ G. Balakrishnan (UNM)
APL **98**, 161913 (2011)

Disordered layers (native oxides, amorphous layers, "junk")

Thin amorphous carbonaceous layer built up at surface during ion irradiation from contamination from vacuum pumps





Ion irradiation @ SNL by Dr. Khalid Hattar

APL **98**, 231901 (2011)

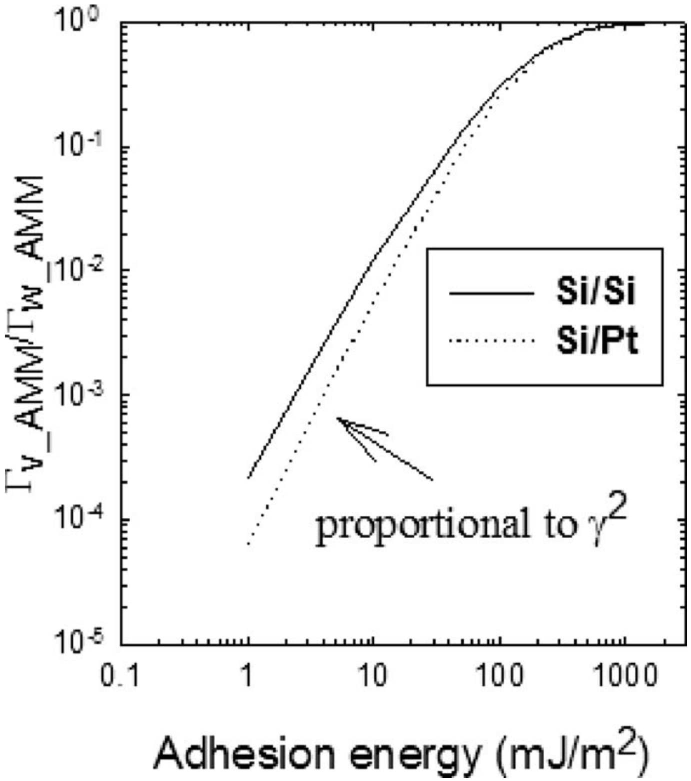
PRB **84**, 125408 (2011)

APL **101**, 099903 (2012)

So how does one increase TBC? Bonding (Analytical)

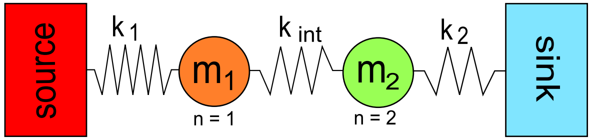
Weakly bonded interfaces offer additional resistance beyond that offered by the intrinsic mismatch…..so increase the bonding!

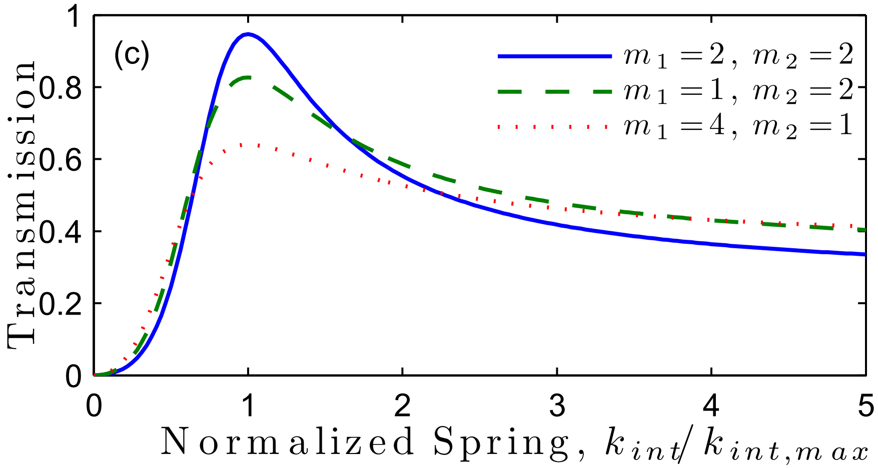
Acoustic mismatch model



Prasher
APL **94**, 041905 (2009)

Nonequilibrium Green's Functions

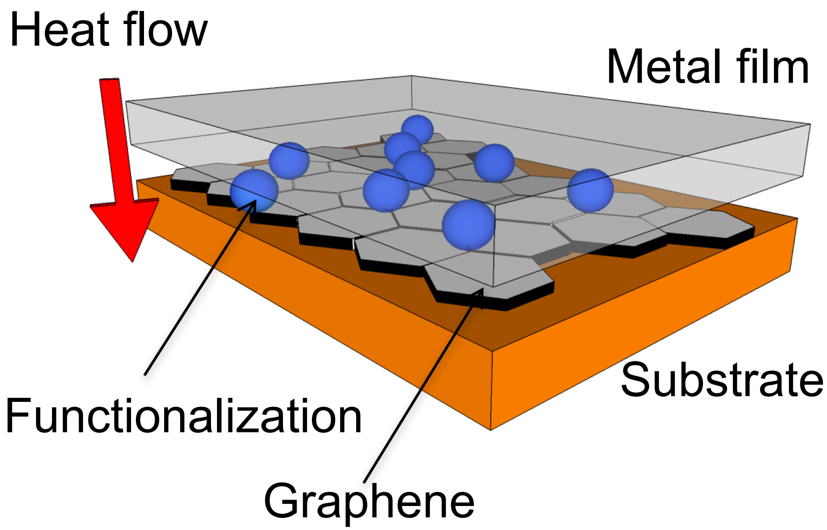


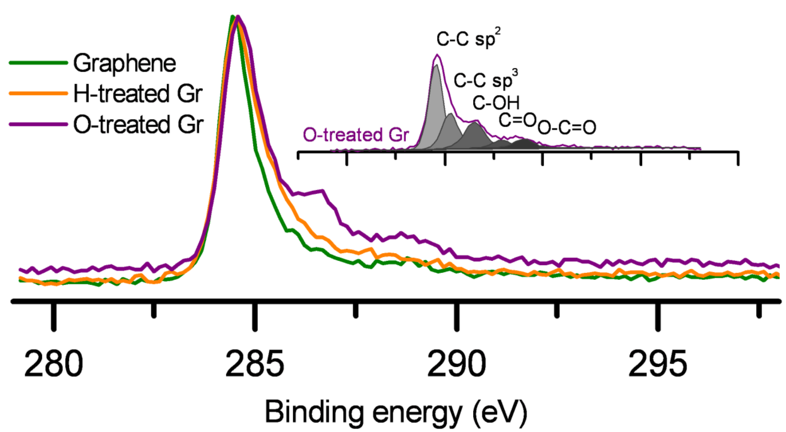


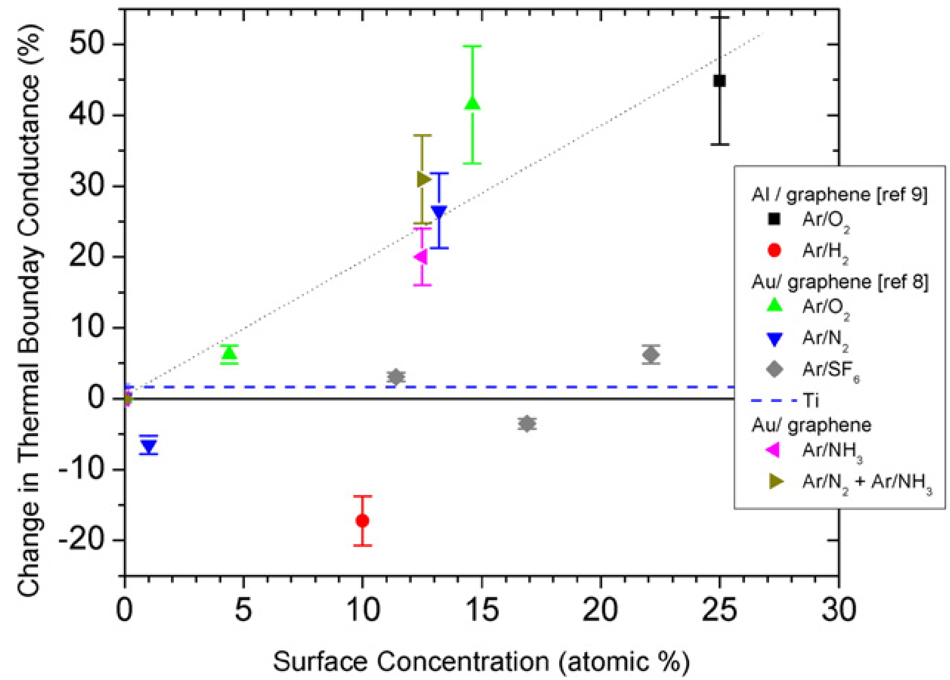
JAP **113**, 013516 (2013)

So how does one increase TBC? Bonding (Experimental)

Adsorbed atoms to change chemistry of graphene surface and bonding at metal/graphene interfaces



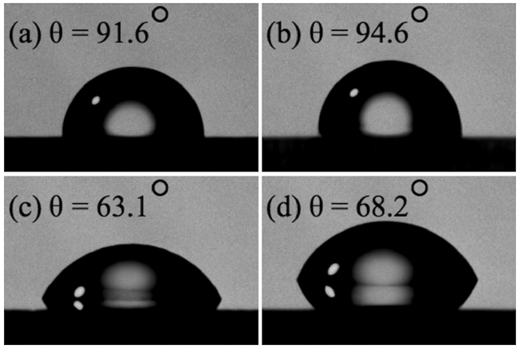


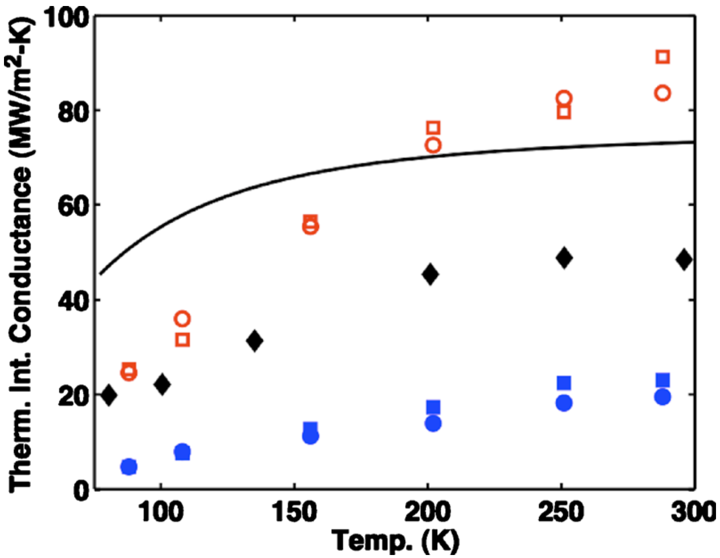


Nano Lett. **12**, 590 (2012)
Nano Lett. **15**, 4876 (2015)
Surf. Coat. & Tech. **314**, 148 (2017)

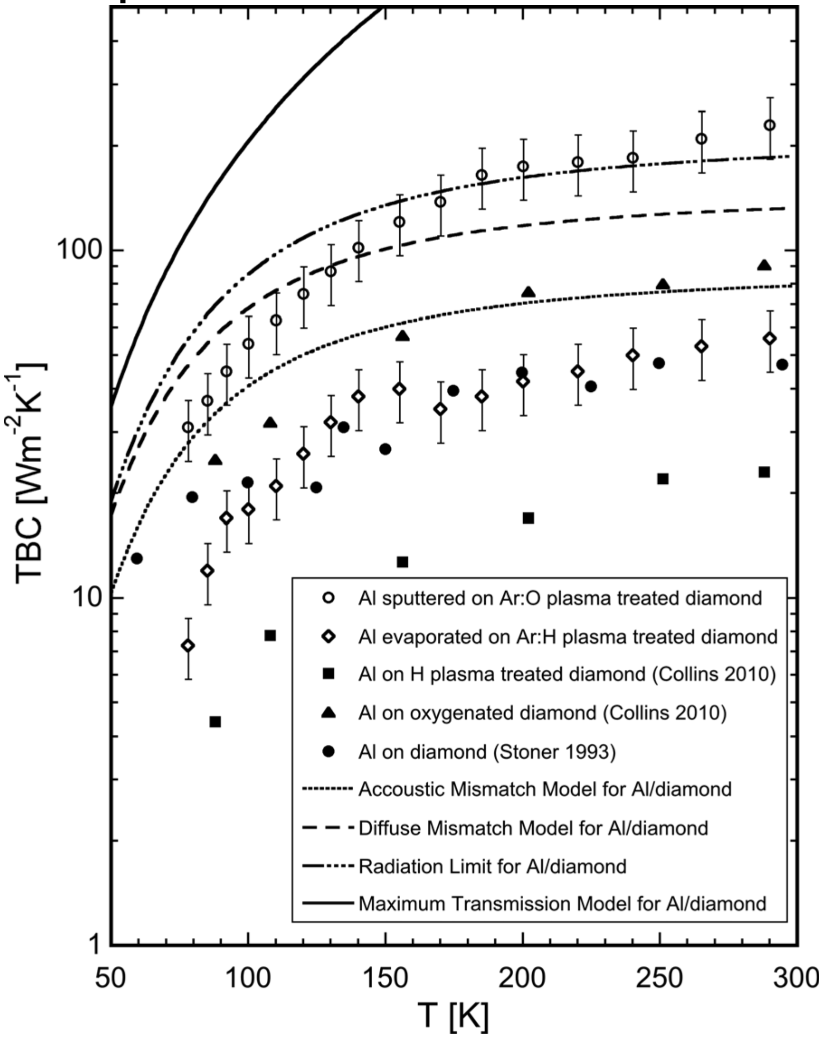
So how does one increase TBC? Bonding (Experimental)

Surface termination of diamond to improve metal/diamond TBC



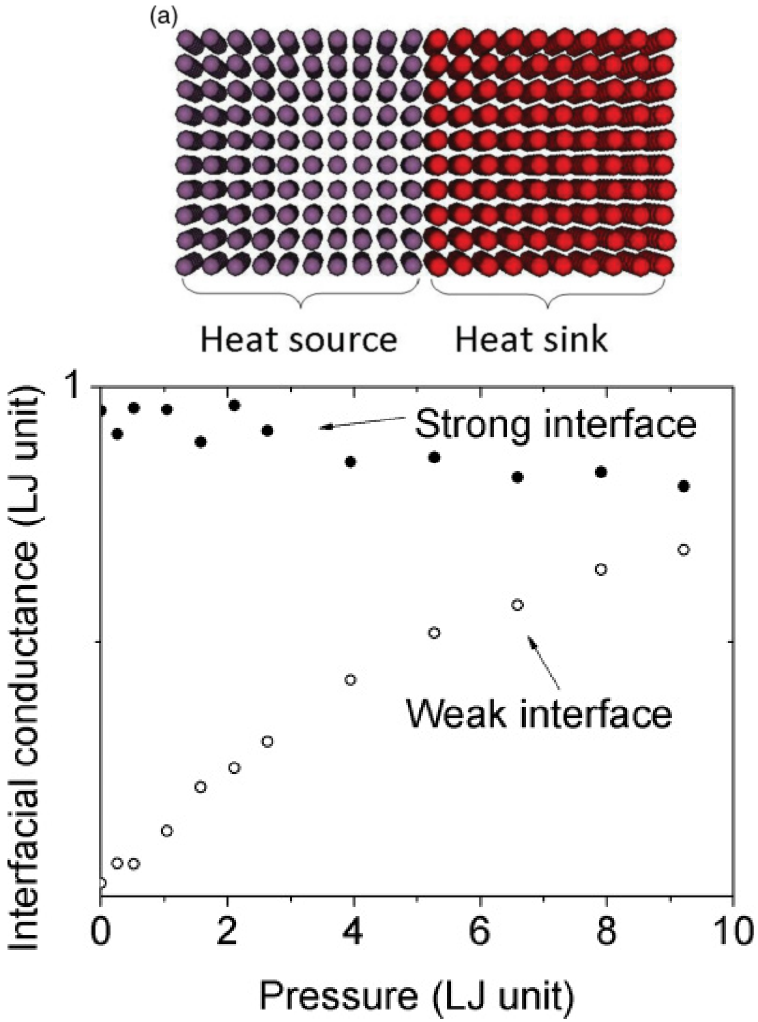


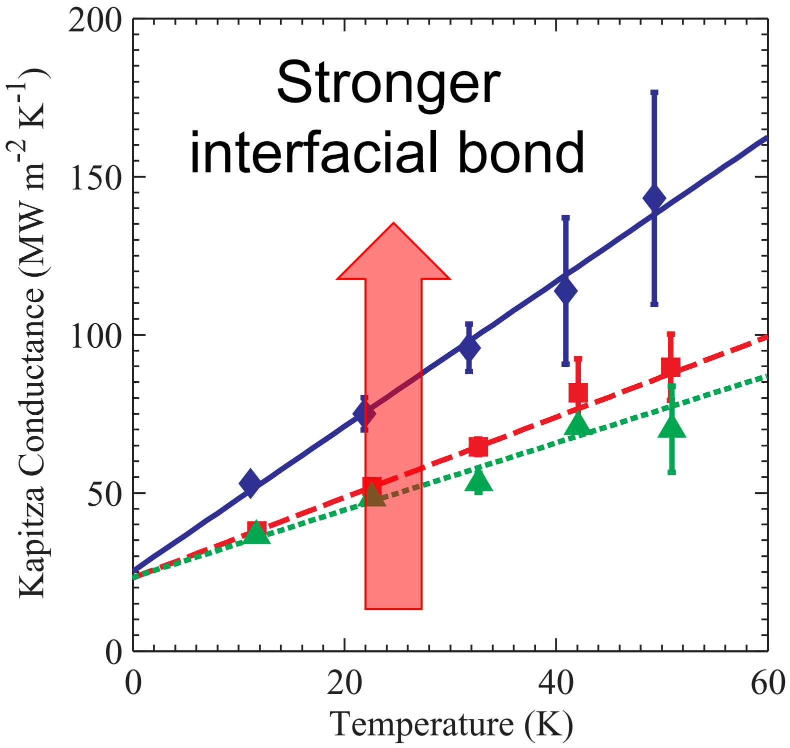
Collins and Chen
APL **97**, 083102 (2010)



Monachon and Weber
JAP **113**, 183504 (2013)

So how does one increase TBC? Bonding (Computational)





Keblinski group
PRB **84**, 195432 (2011)

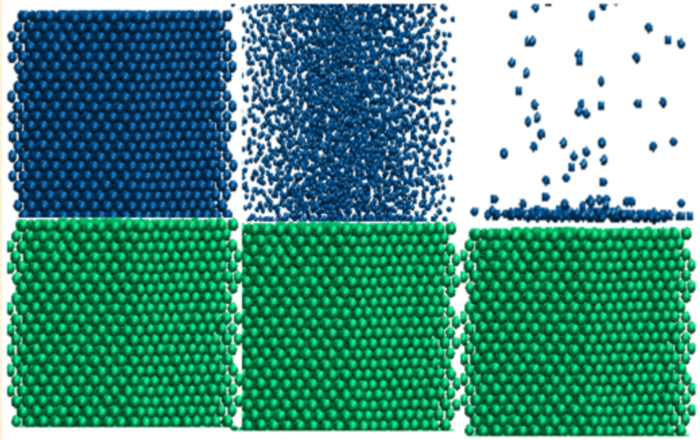
PRB **84**, 193301 (2011)

So *why* does bonding increase TBC ?(Computational)

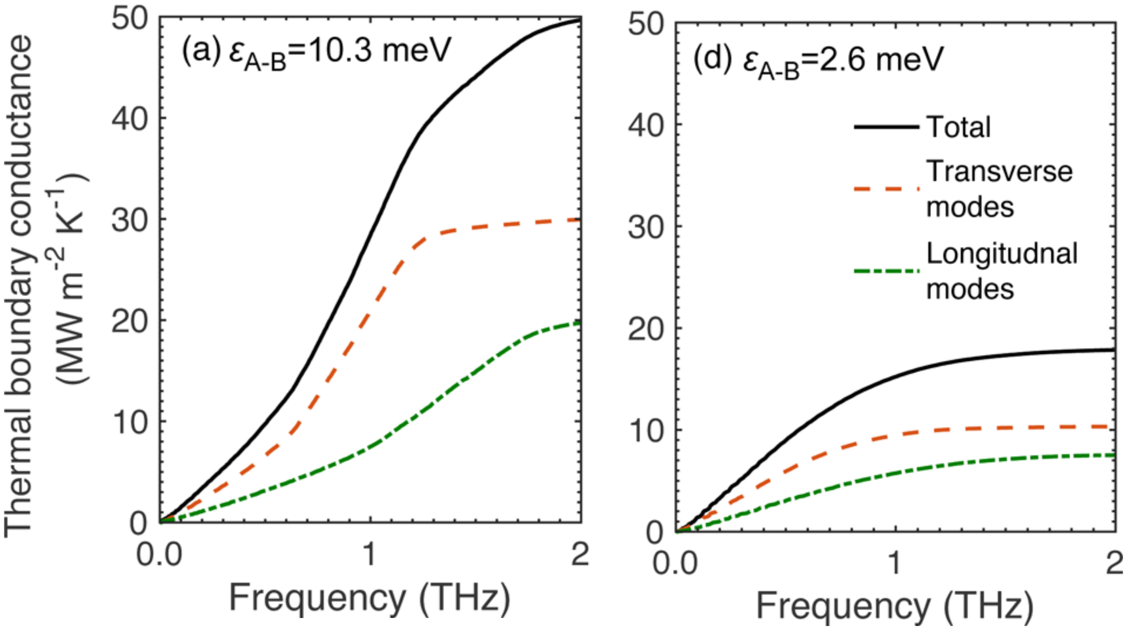
Dr. Ashutosh Giri

Bonding contributions in solid, liquid and gas systems
Seminal works by Keblinski: *J. Chem. Phys.* **118**, 337; *PRL* **102**, 156101; *APL* **99**, 073112; *PRB* **84**, 184107; *PRB* **84**, 195432; *Ind. Eng. Chem. Res.* **51**, 1767; *PRE* **87**, 022119; *IJHMT* **78**, 161

Bonding increases contribution of transverse modes in solid/solid, solid/liquid, and solid/gas systems

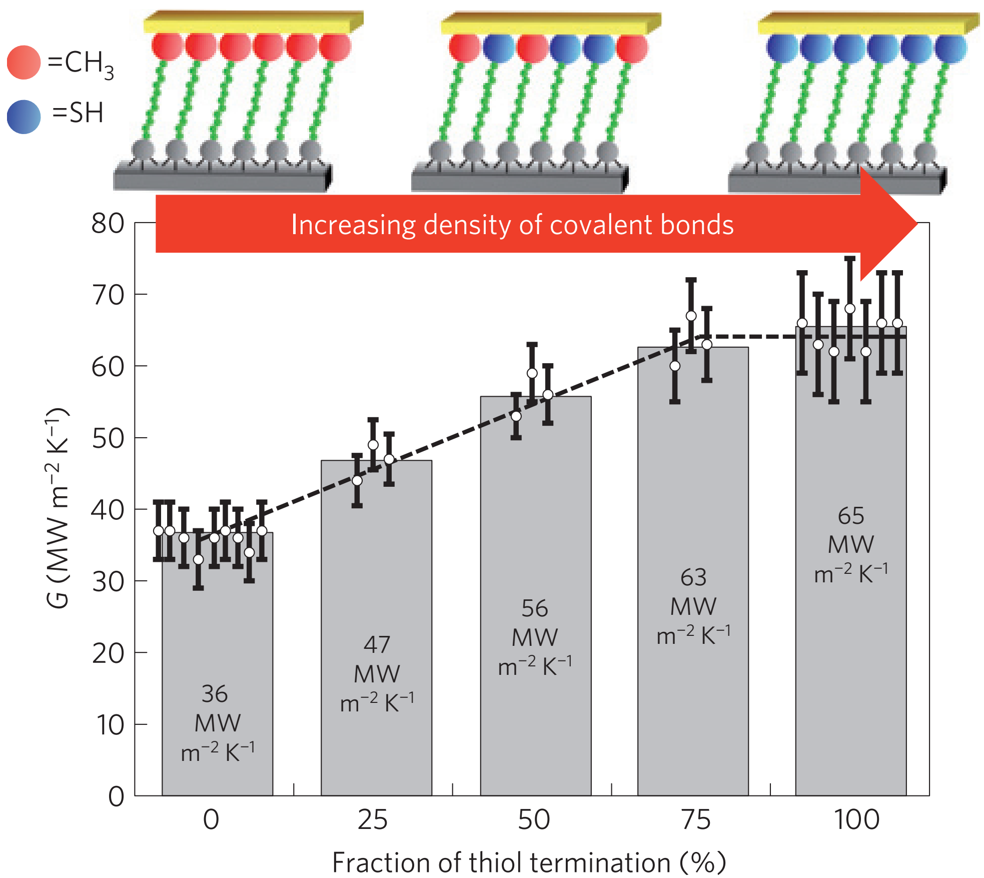


J. Phys. Chem. C **120**, 24847 (2016)

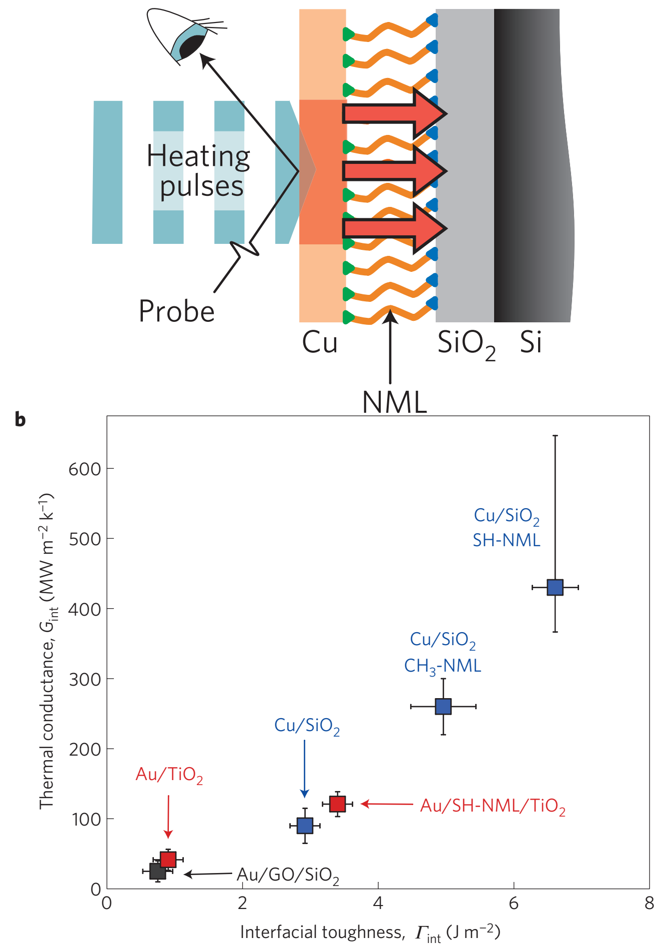


So how does one increase TBC? Bonding with a “thin film”

Molecular monolayer films to improve bonding between film and substrate



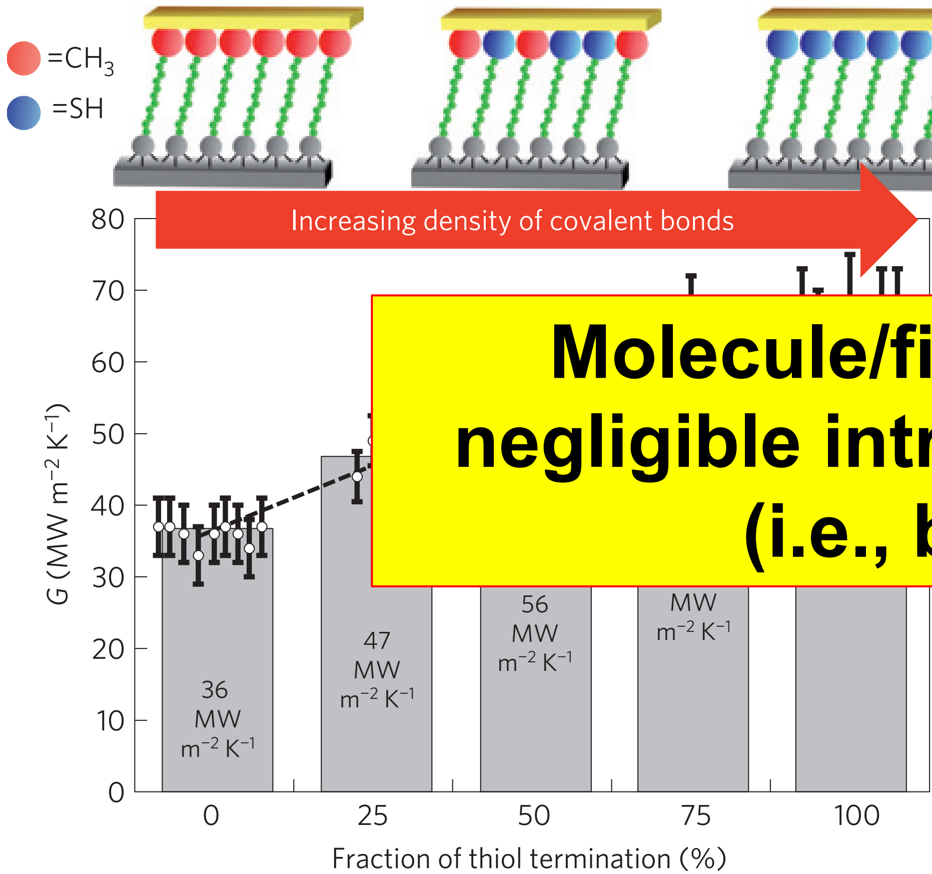
Nat. Mat. **11**, 502 (2012)

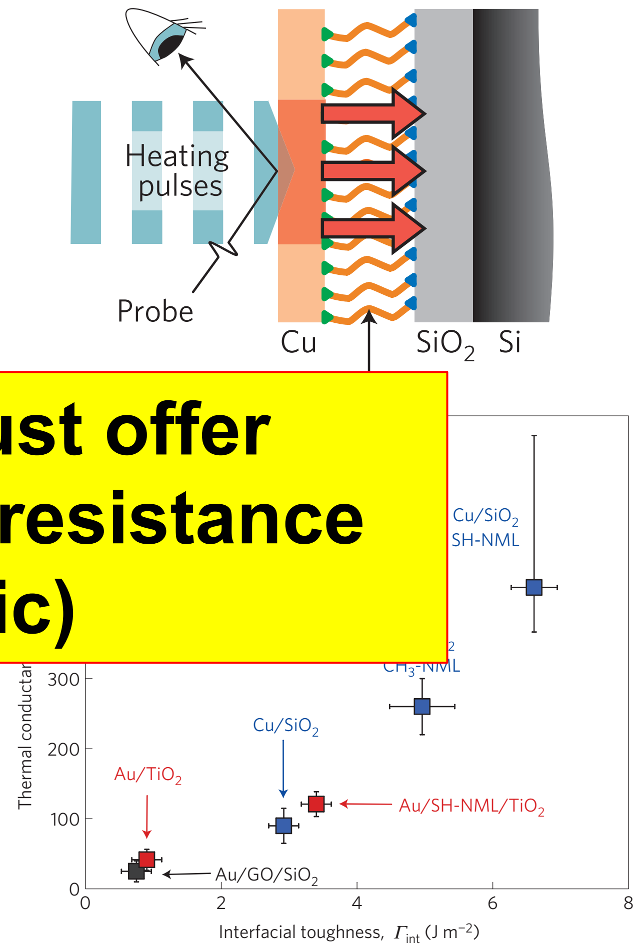


Nat. Mat. **12**, 118 (2013)

So how does one increase TBC? Bonding with a "thin film"

Molecular monolayer films to improve bonding between film and substrate





Molecule/film must offer negligible intrinsic resistance (i.e., ballistic)

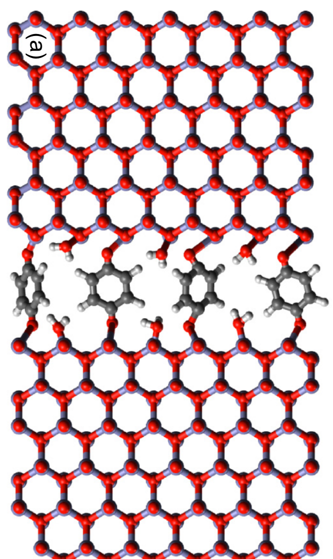
Nat. Mat. **11**, 502 (2012)

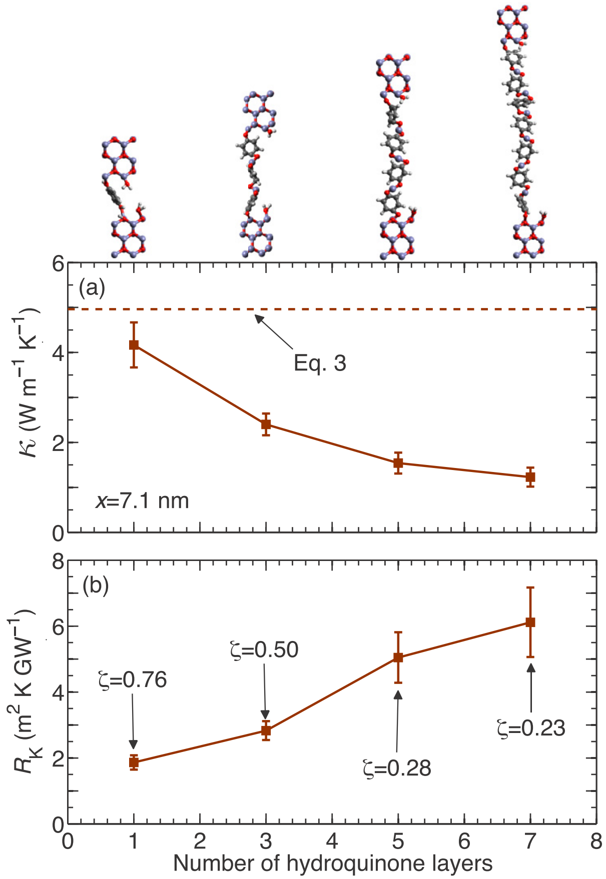
Nat. Mat. **12**, 118 (2013)

Defects vs. bonding: the interplay and engineering

When molecules get too long/large, intrinsic scattering can reduce TBC

Dr. Ashutosh Giri



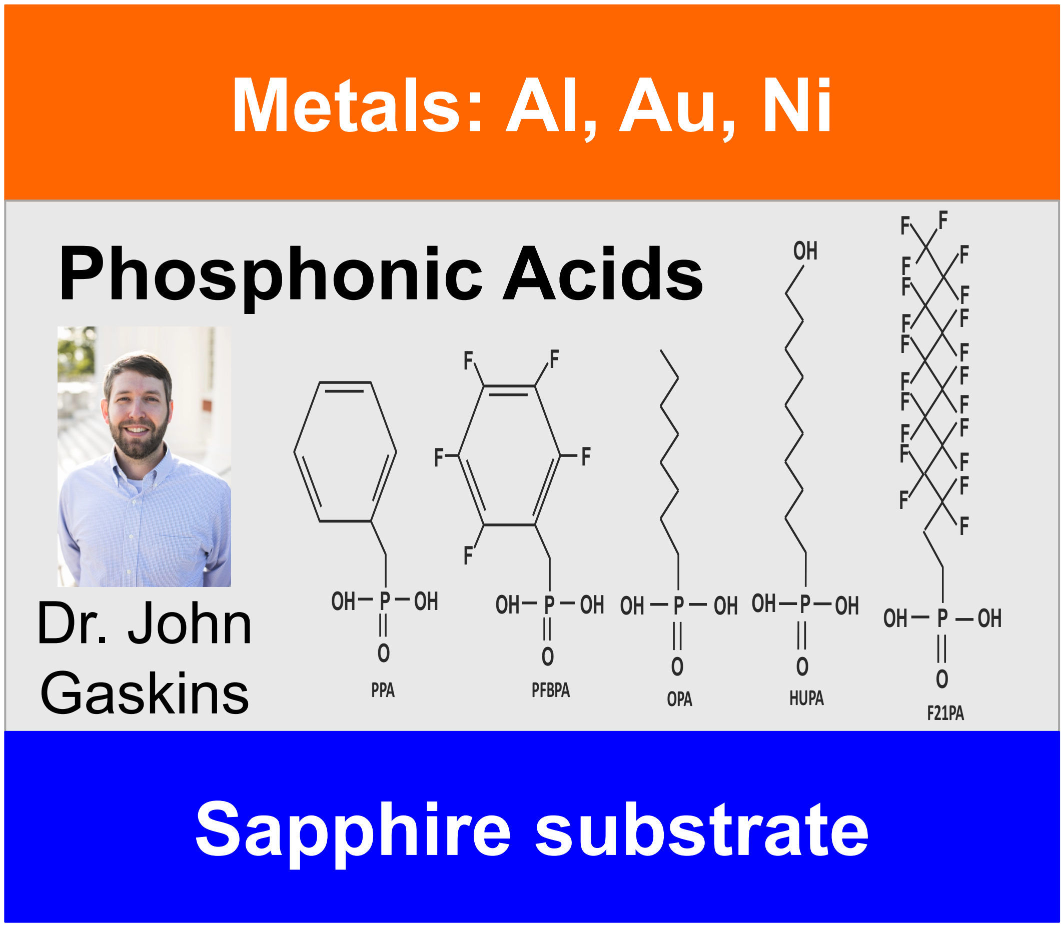


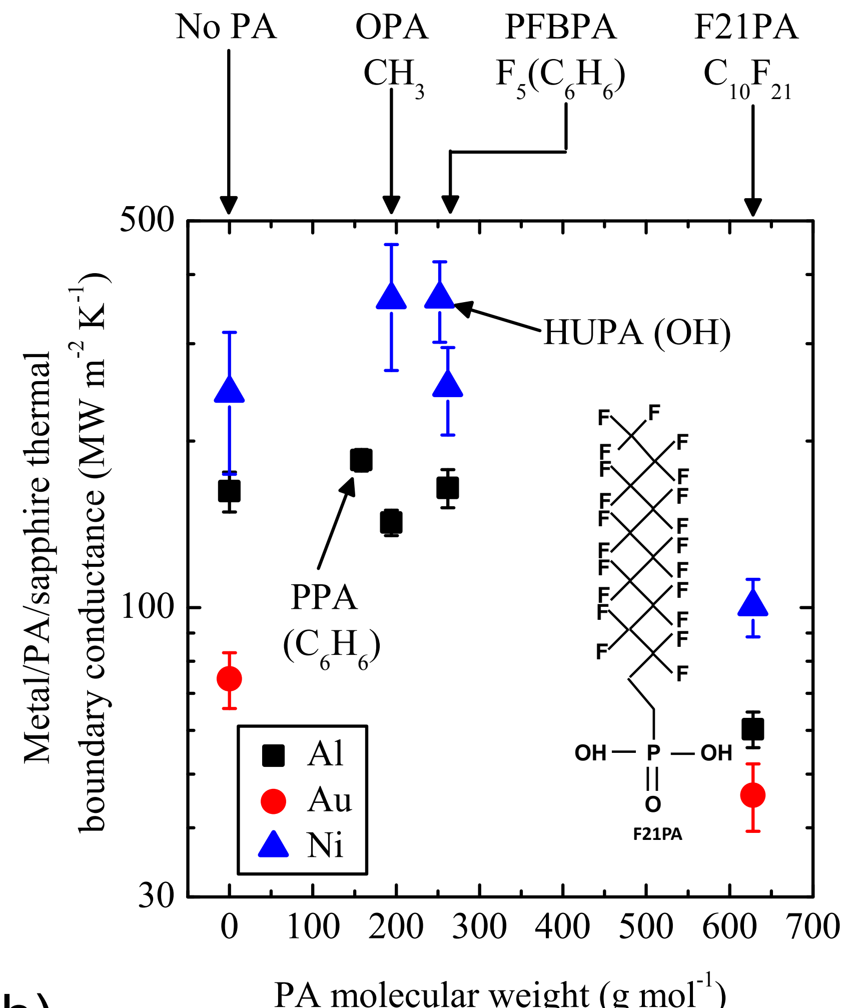
Derived from ZnO/HQ/ZnO SL

PRB **94**, 115310 (2016)

Defects vs. bonding: the interplay and engineering

When molecules get too long/large, intrinsic scattering can reduce TBC





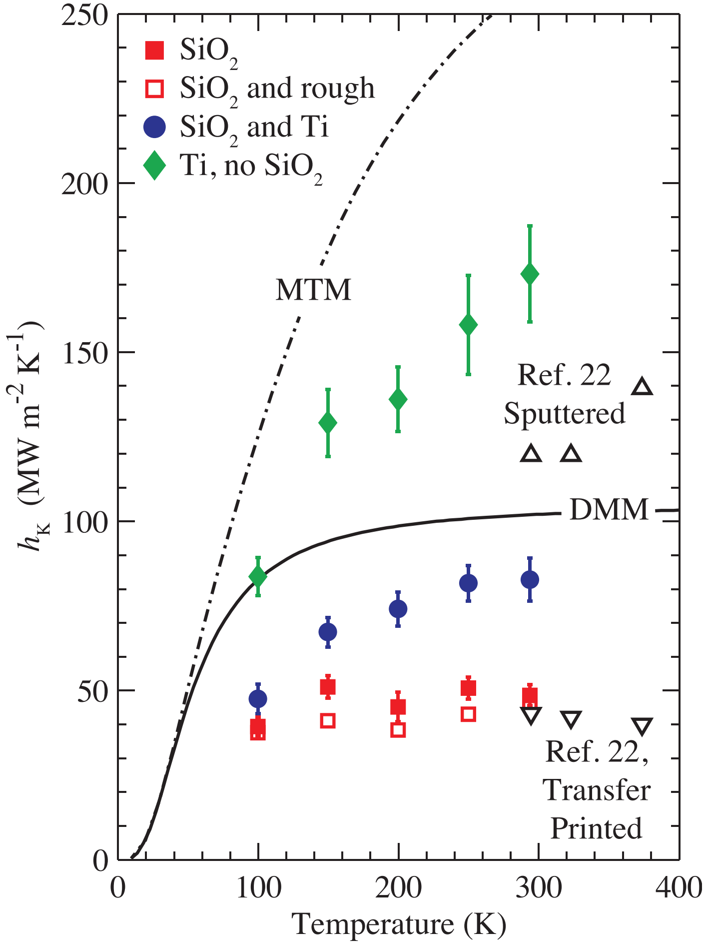
Collaboration with Sam Graham (Ga Tech)

J. Phys. Chem. C **119**, 20931 (2015)

Defects vs. bonding: the interplay and engineering

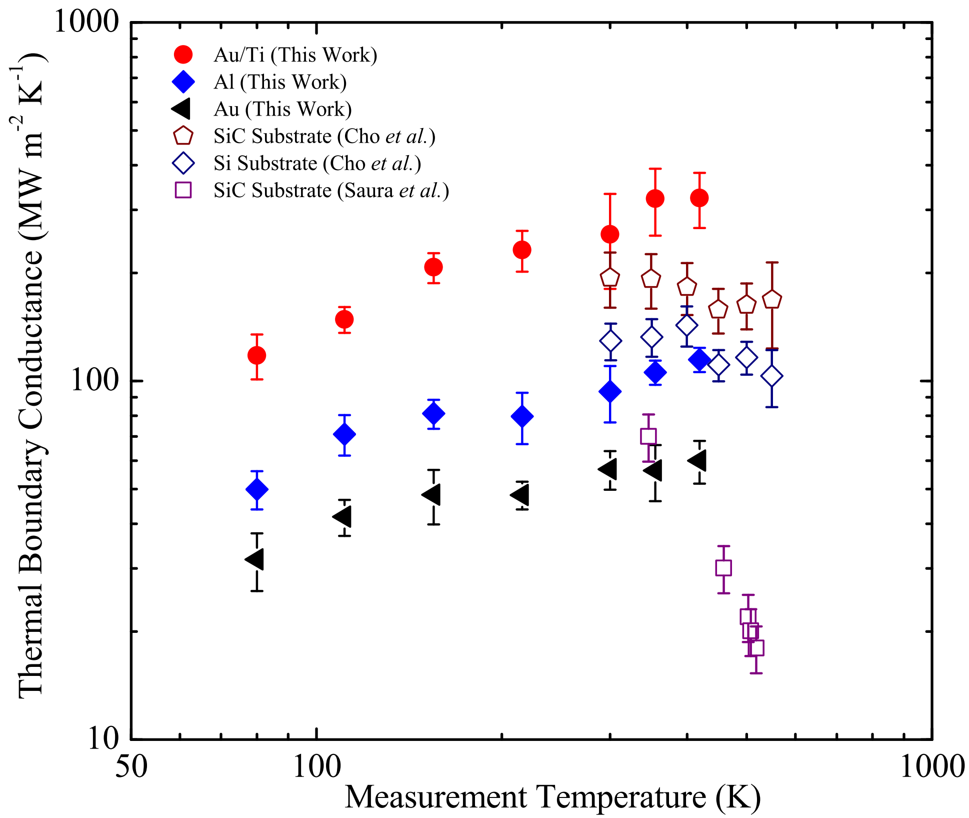
So how about adhesion layers?

Au/Si TBC
Ti adhesion layer



APL **102**, 081902 (2013)

Metal/GaN TBC
Ti adhesion layer for Au

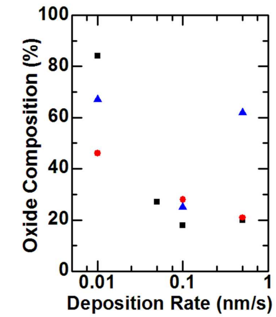


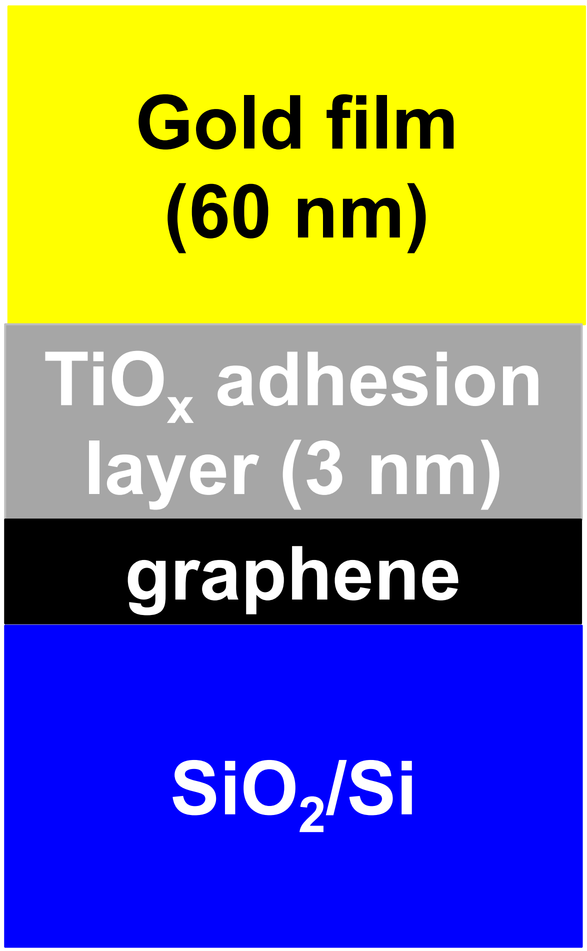
APL **105**, 203502 (2014)

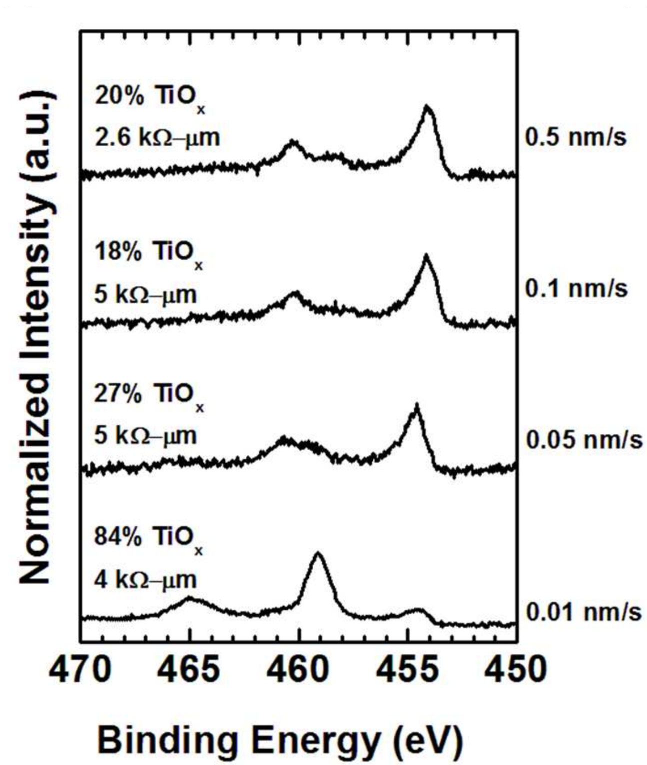
Defects vs. bonding: the interplay and engineering

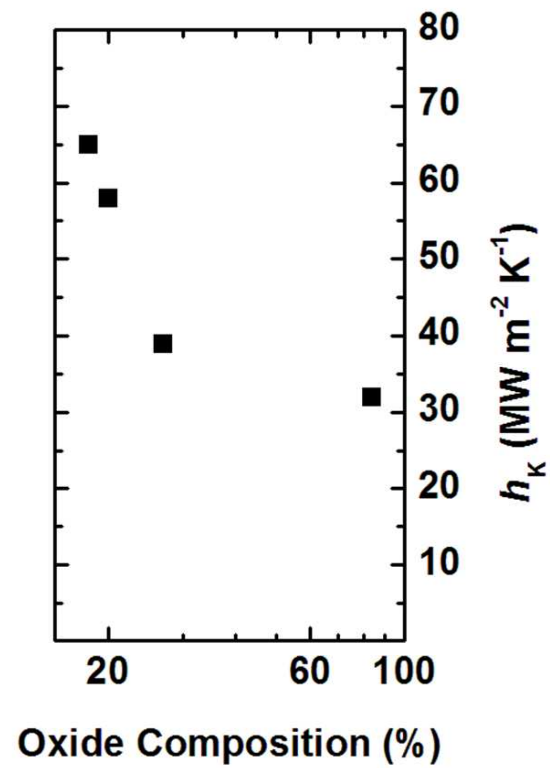
But what do we know about Ti adhesion layers??

More like TiO_x unless deposited under UHV







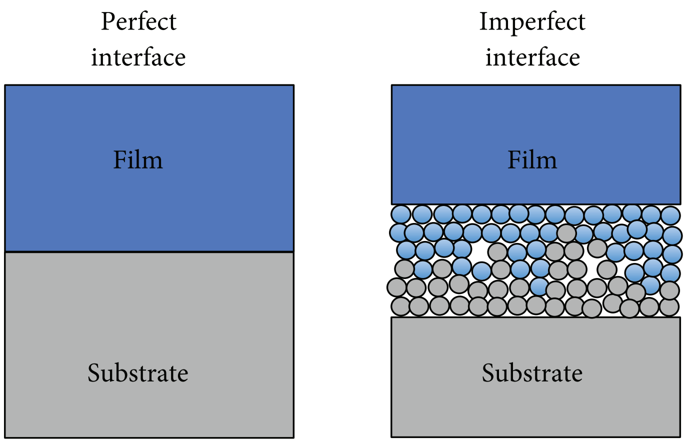


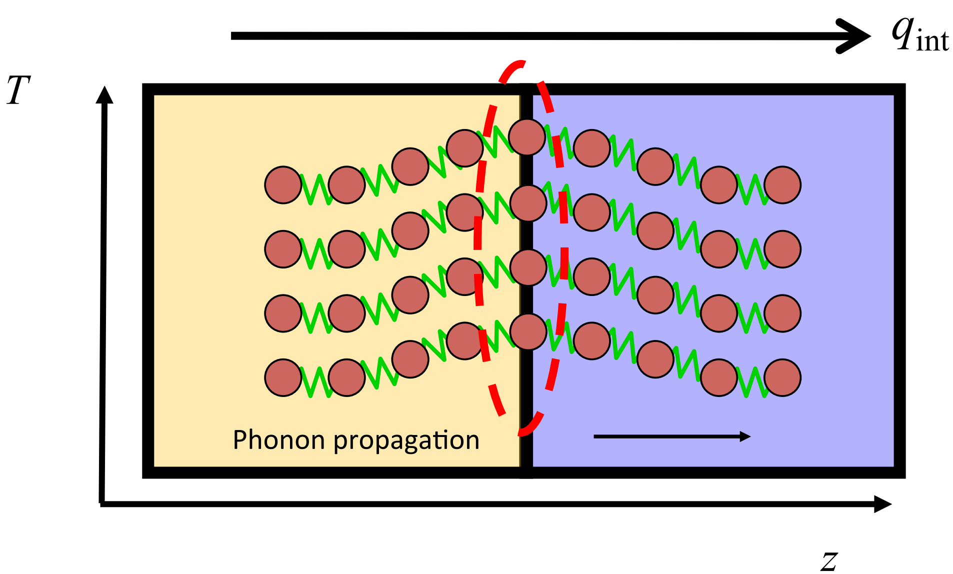
Collaboration with Stephen McDonnell (UVA)

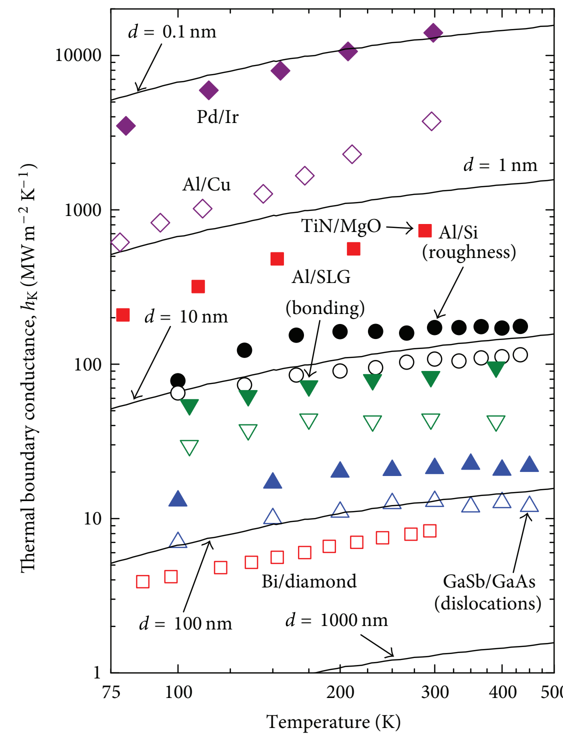
manuscript current under review

Summary

All characteristics at an interface that could impact the the local "masses and springs" impact thermal boundary conductance

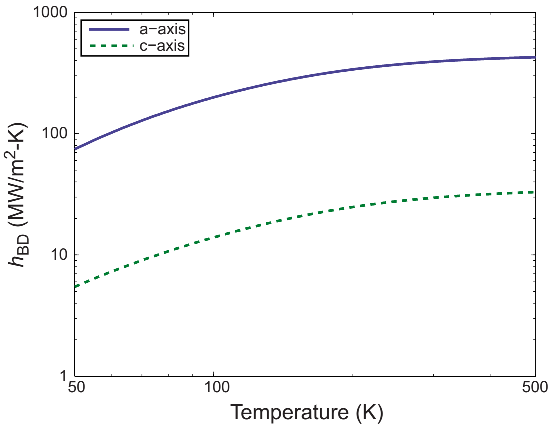




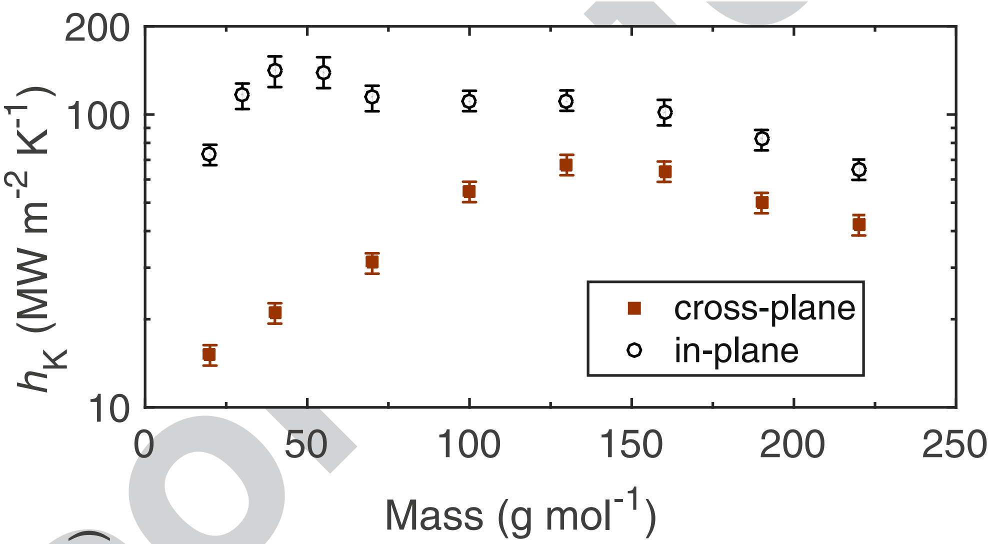


Anisotropy matters

Predicted TBC across Al/graphite interface

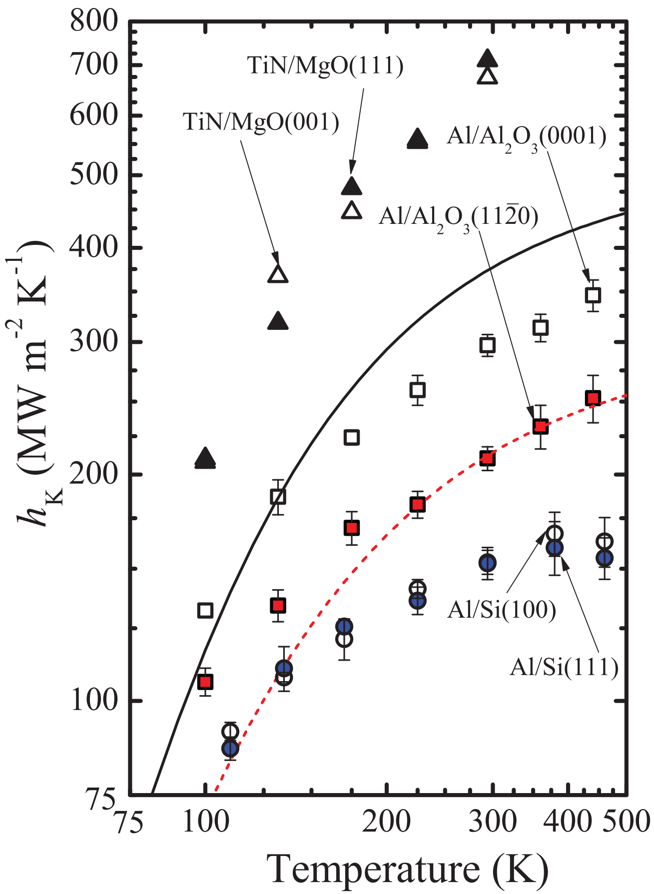


APL **95**, 031902 (2009)



Giri and Hopkins, *Sci. Rep.* (to appear)

Metal/substrate TBC with different substrate orientations



PRB **84**, 125408 (2015)