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Effects of temperature and anharmonicity at single interfaces: evidence from experiments

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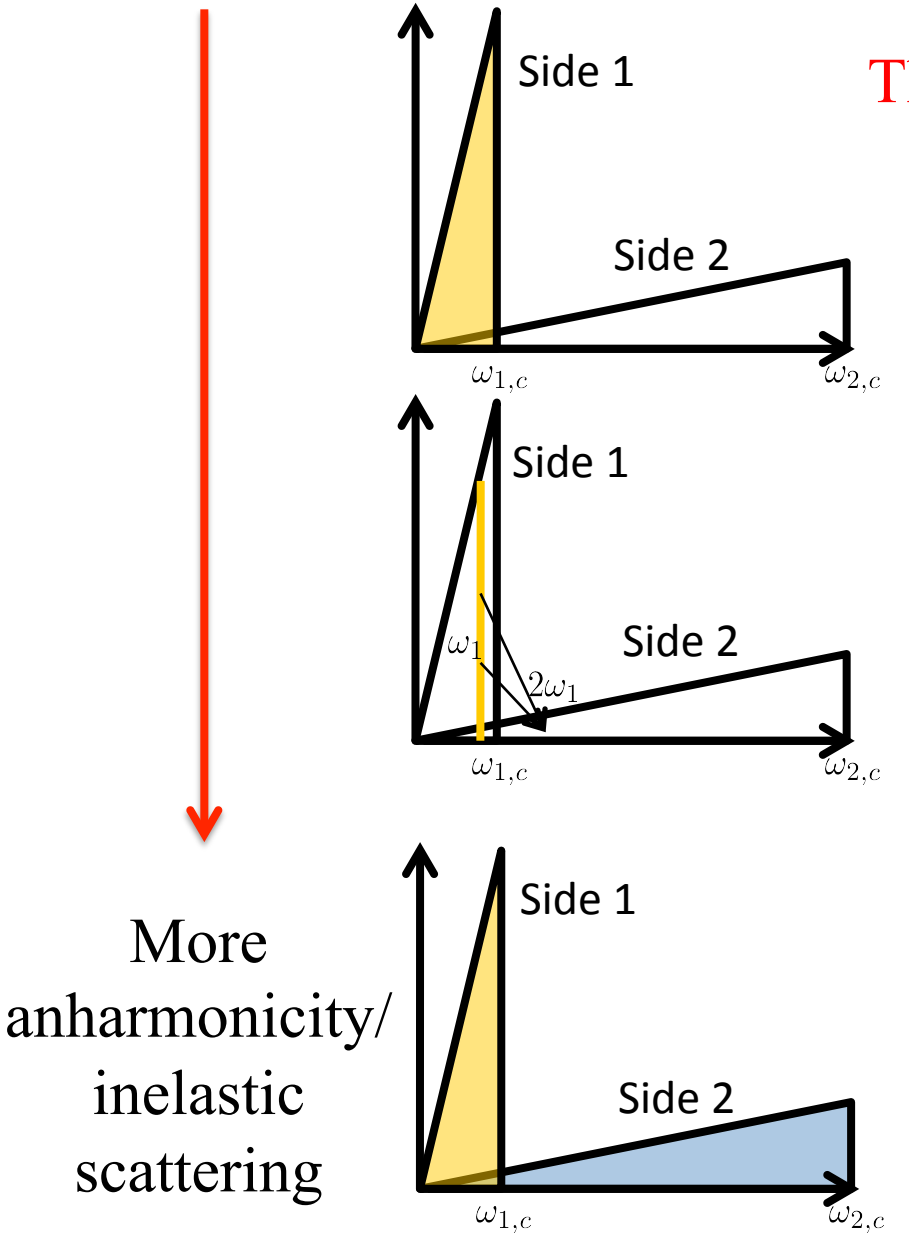
The density of states picture



More anharmonicity/ inelastic scattering

The traditional "elastic" picture (DMM)

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

Selected inelastic scattering

Hopkins, *J. Appl. Phys.* 106, 013528 (2009)

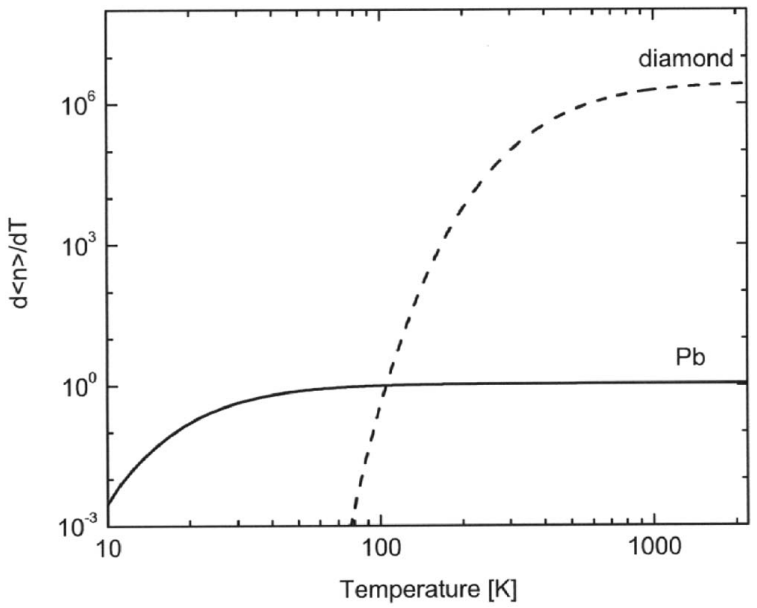
Hopkins, Duda, Norris, *J. Heat Trans.* 133, 062401 (2011)

Maximum transmission (MTM)

Dames and Chen, *J. Appl. Phys.* 95, 682 (2004)

Temperature dependence - anharmonicity

Hopkins and Norris, *Nano. Micro. Thermophys. Eng.* **11**, 247 (2007)



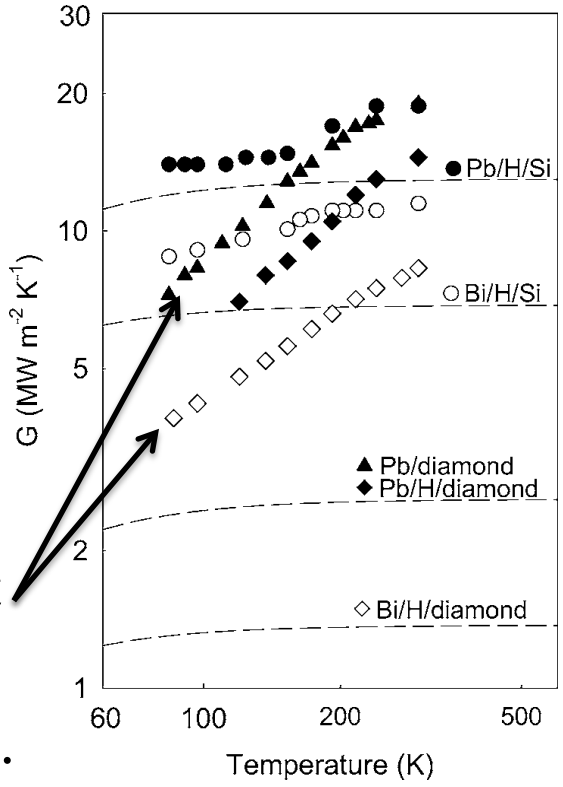
Pb temperature trends = elastic

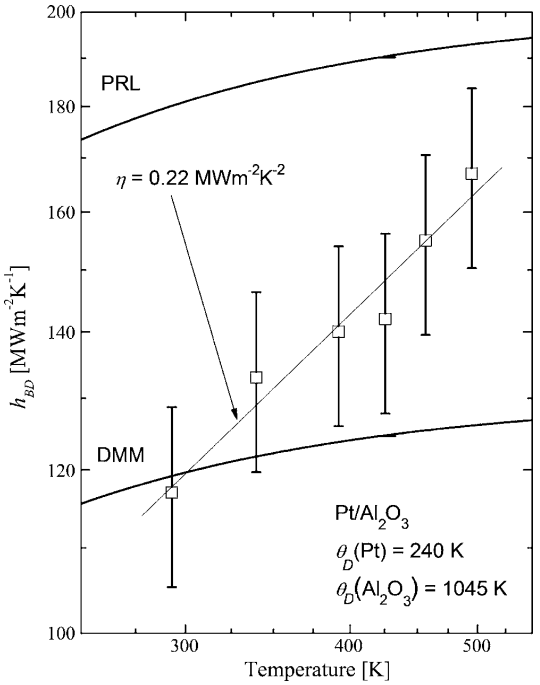
Diamond temperature trends = inelastic

How do temperature trends change relative to Debye temperatures?

Evidence of inelastic scattering – look at temperature trends

Electrons? Probably not during ep equilibrium…





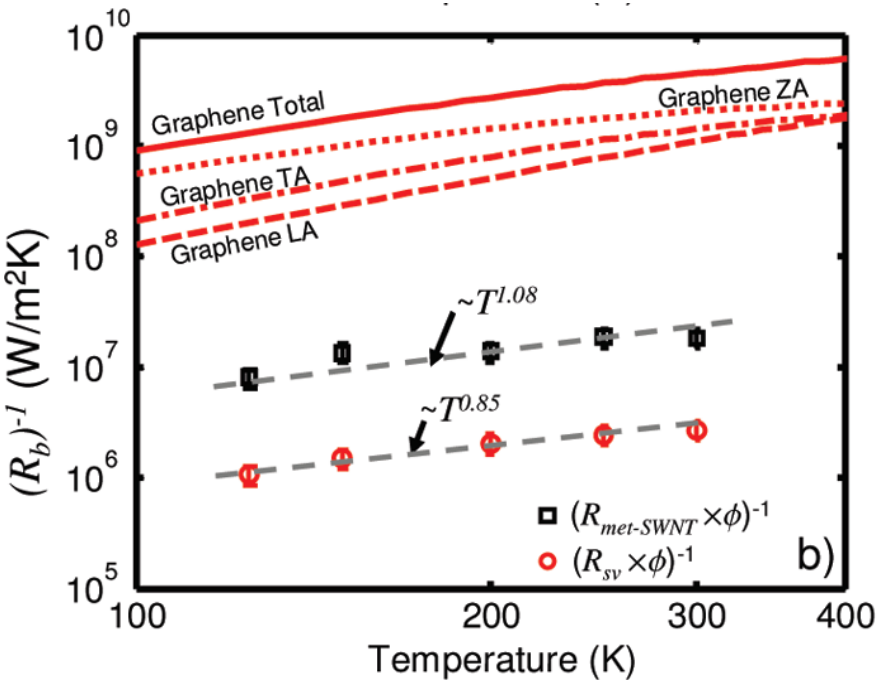
Lyeo and Cahill, *Phys. Rev. B* **73**, 144301 (2006)

Hopkins, Norris and Stevens, *J. Heat Trans.* **130**, 022401 (2008)

What has been observed beyond the simple metal/bulk non-metal substrate picture?

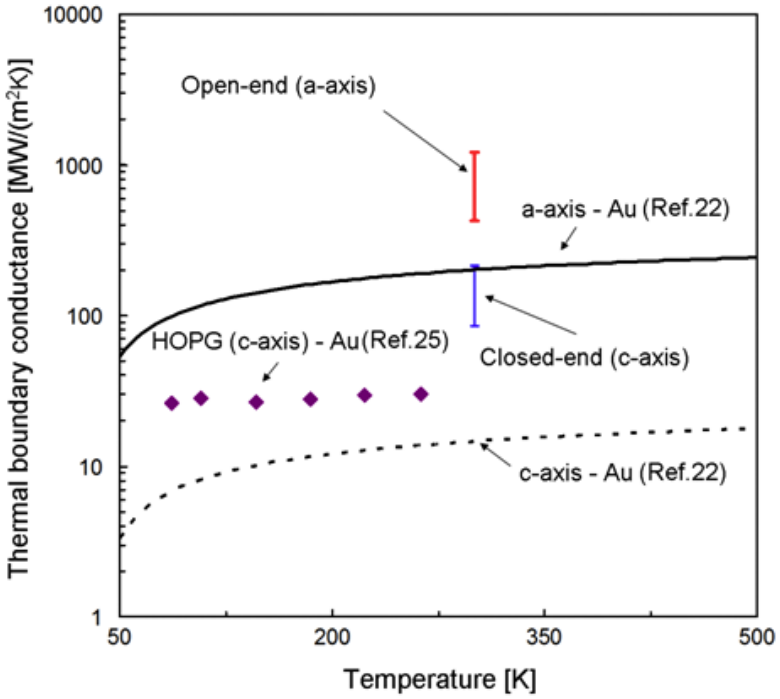
Metal/carbon nanotubes

Metal/SWCNT film



Panzer *et al*., *Nano Lett.* **10**, 2395 (2010)

Metal/individual SWCNT



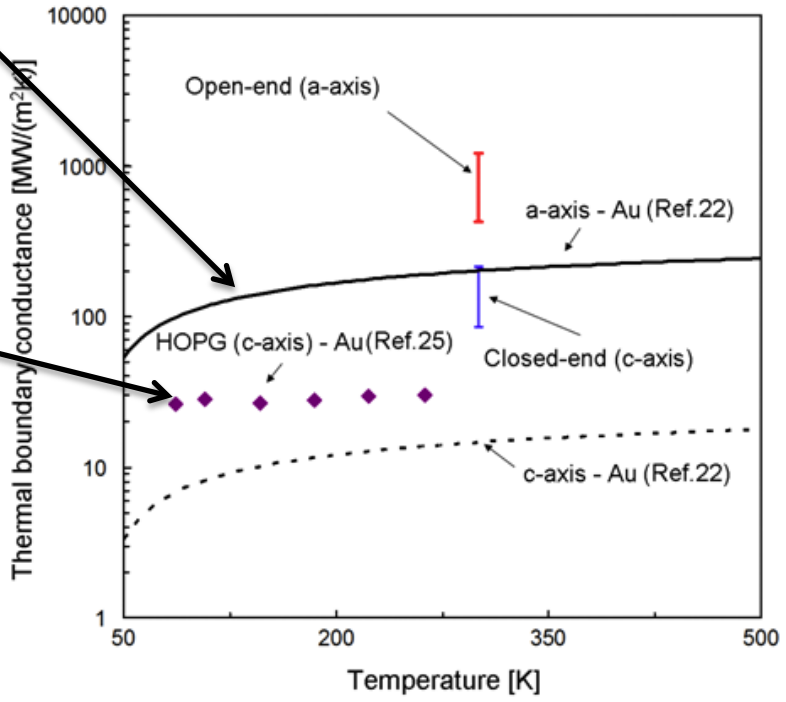
Hirotani *et al*., *Nanotech.* **22**, 315702 (2011)

Metal/carbon nanotubes

Duda *et al.*, *Appl. Phys. Lett.* 95, 031912 (2009)
(note: Theory)

Schmidt *et al.*, *J. Appl. Phys.* 107, 104907 (2010)

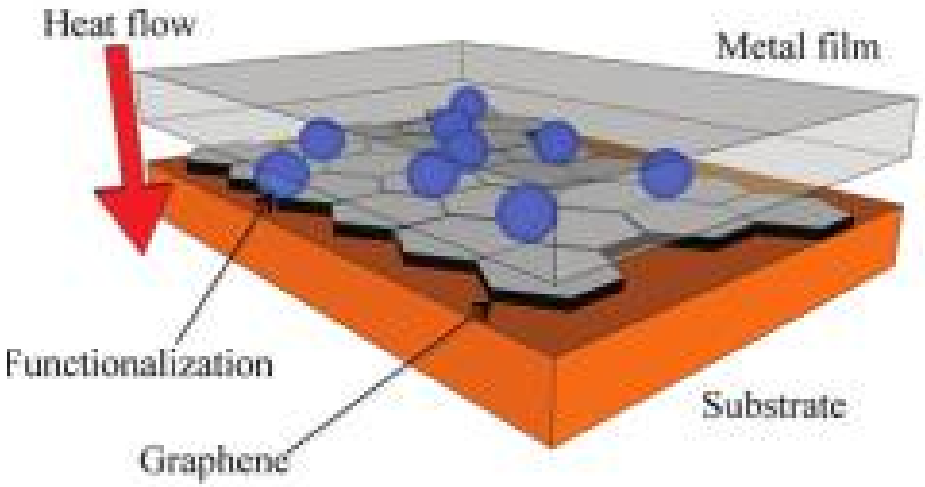
Metal/individual SWCNT



Can the interfacial bond enhance inelastic scattering, or does it just add elastic modes?

Hirotani *et al.*, *Nanotech.* **22**, 315702 (2011)

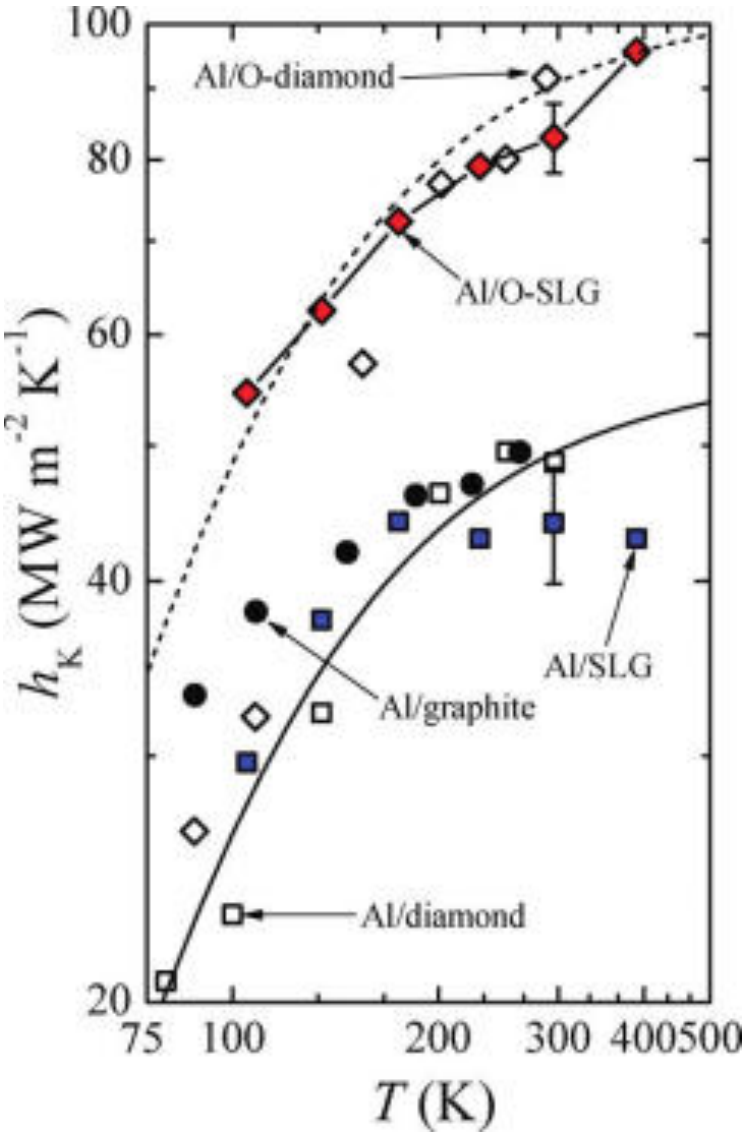
Bonding vs. anharmonicity: graphene, graphite and diamond



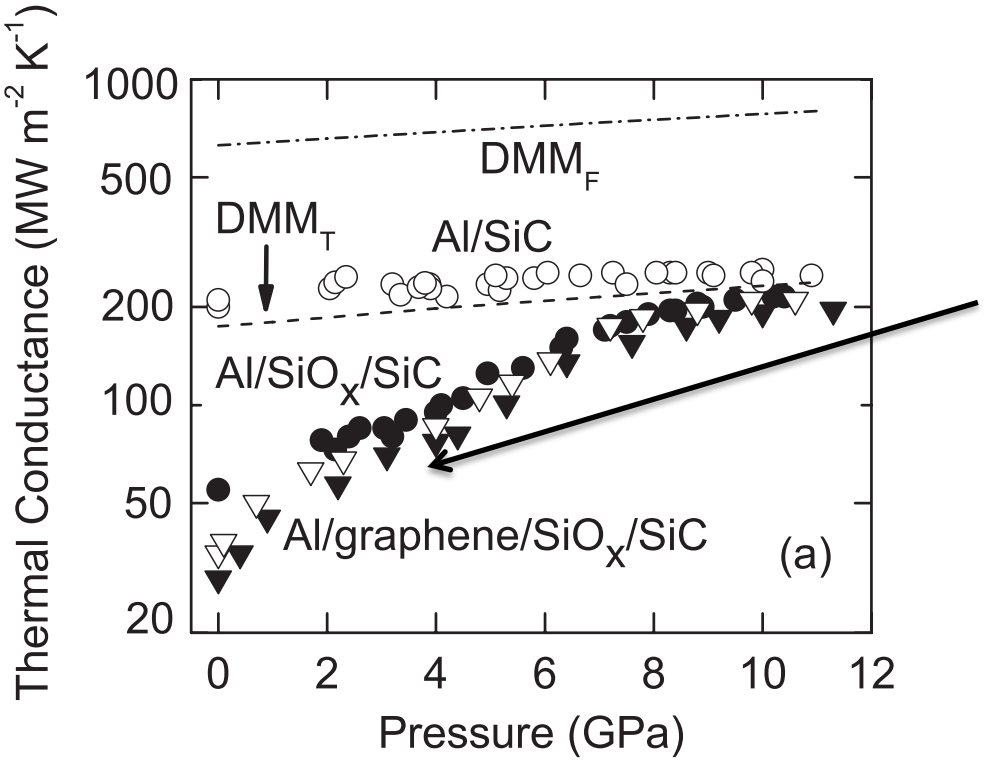
Graphene: Hopkins *et al*., *Nano Lett.* **12**, 590 (2012)

Graphite: Schmidt *et al. J. Appl. Phys.* **107**, 104907 (2010)

Diamond: Collins *et al*. *Appl. Phys. Lett.* **97**, 083102 (2010)



Bonding vs. anharmonicity: can pressure lend insight?



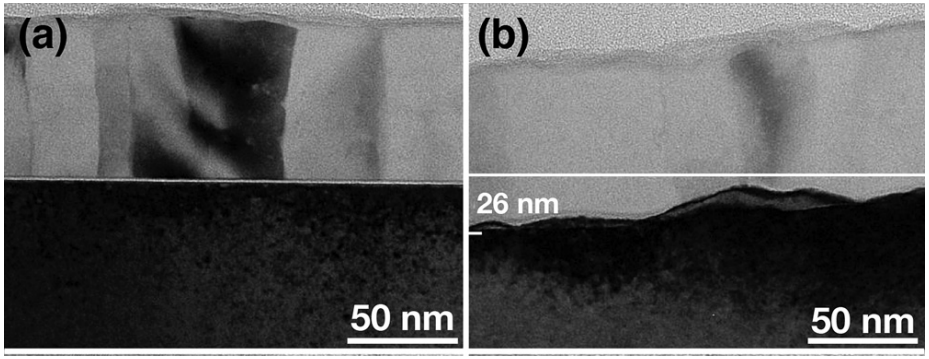
Hsieh *et al.*, *Phys. Rev. B,* **84**, 184107 (2011)

All the "action" is for the weak bond, no further change with the strong bonds. TBC scales linearly.

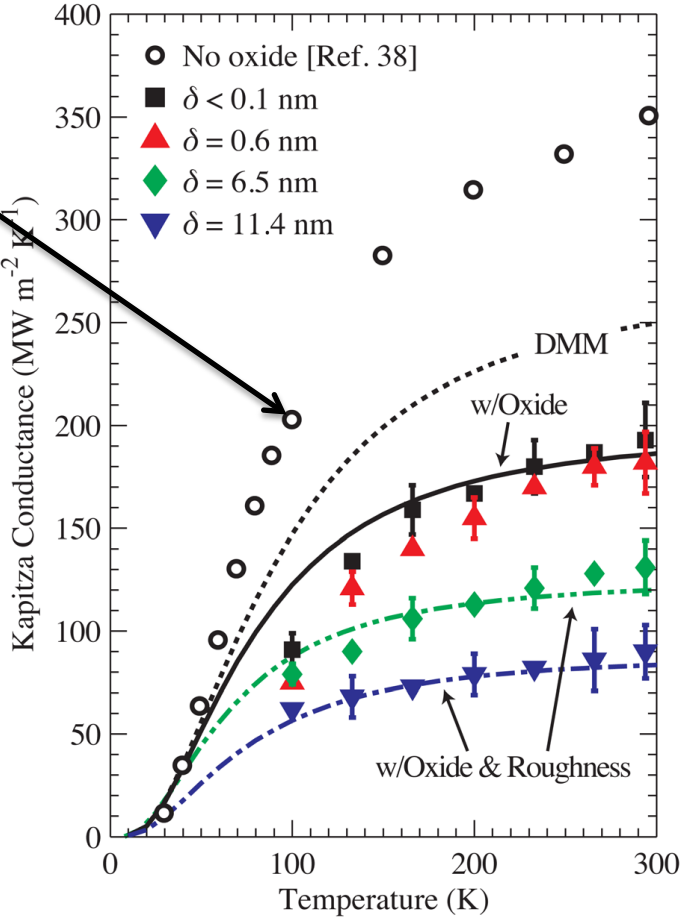
Jury is still out. Need more work on this topic, both experimental and computational

Anharmonicity vs. disorder?

Data from: Minnich *et al*. *Phys. Rev. Lett*. **107**, 095901 (2011)



- Rough interfaces "flatten out" temperature trends
- Removal of oxide increases change with temperature

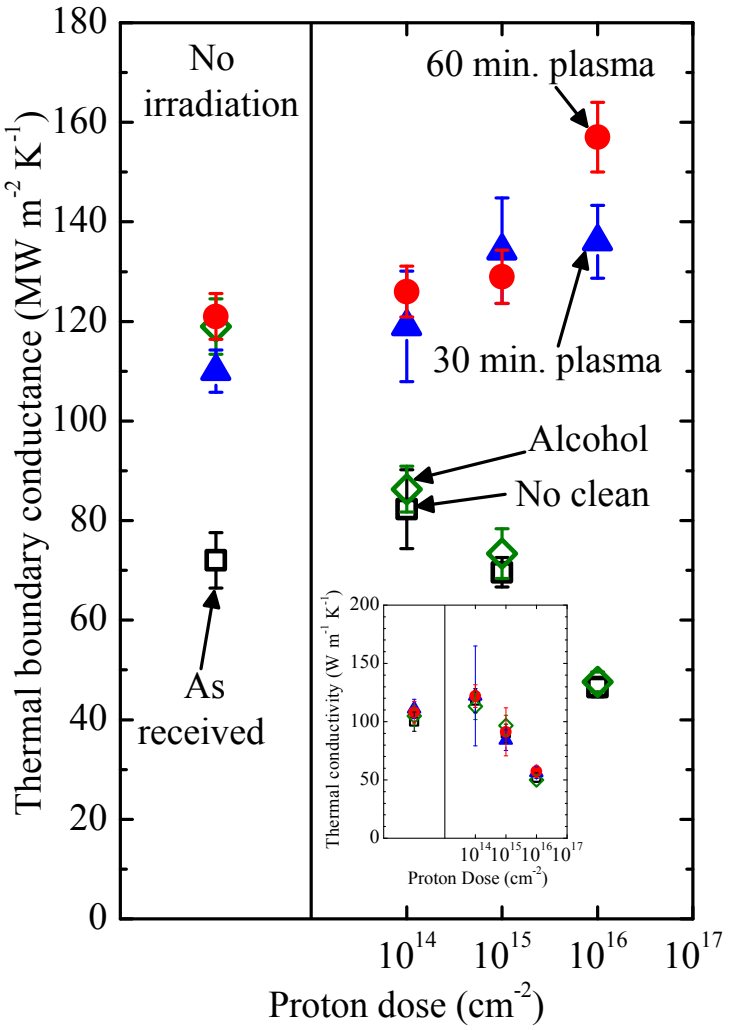


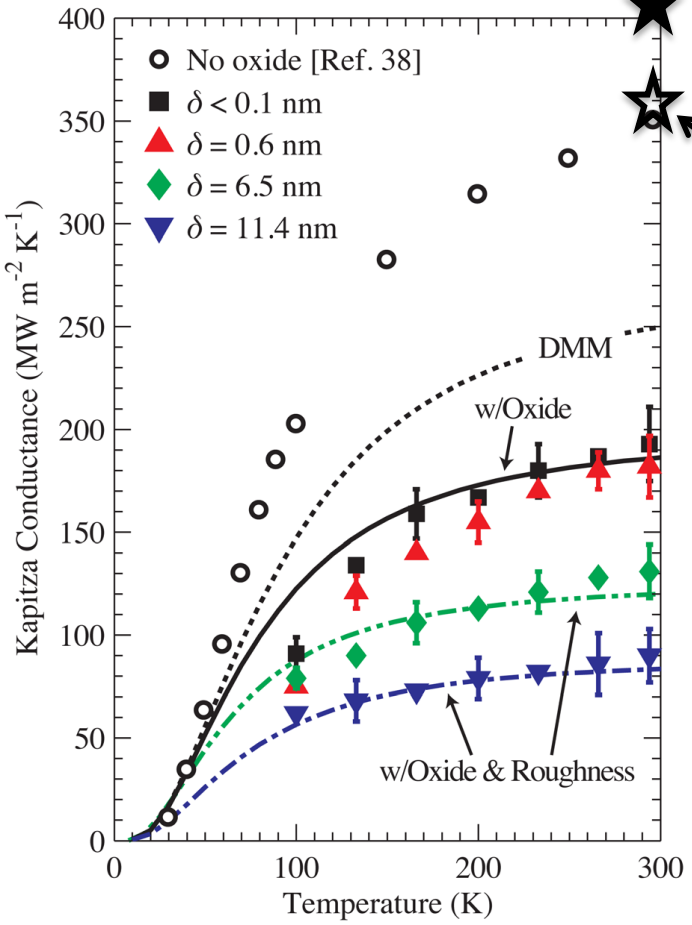
Duda and Hopkins, *Appl. Phys. Lett.* **100**, 111602 (2012)

Can disorder increase TBC/anharmonicity?

Gorham *et al. under review*

Ion mixing increases TBC





Ion mixing, no oxide (Gorham)

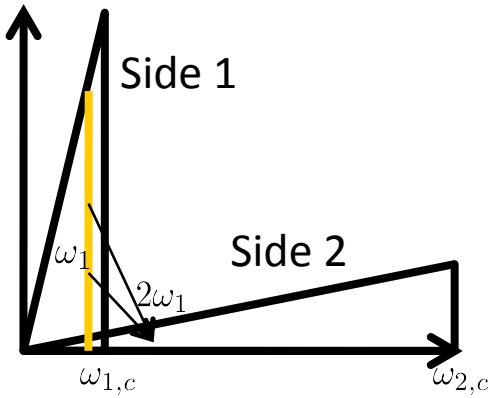
No ion mixing, no oxide (Gorham)

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

Theoretical developments

Let's switch gears and talk about pen and paper theoretical developments

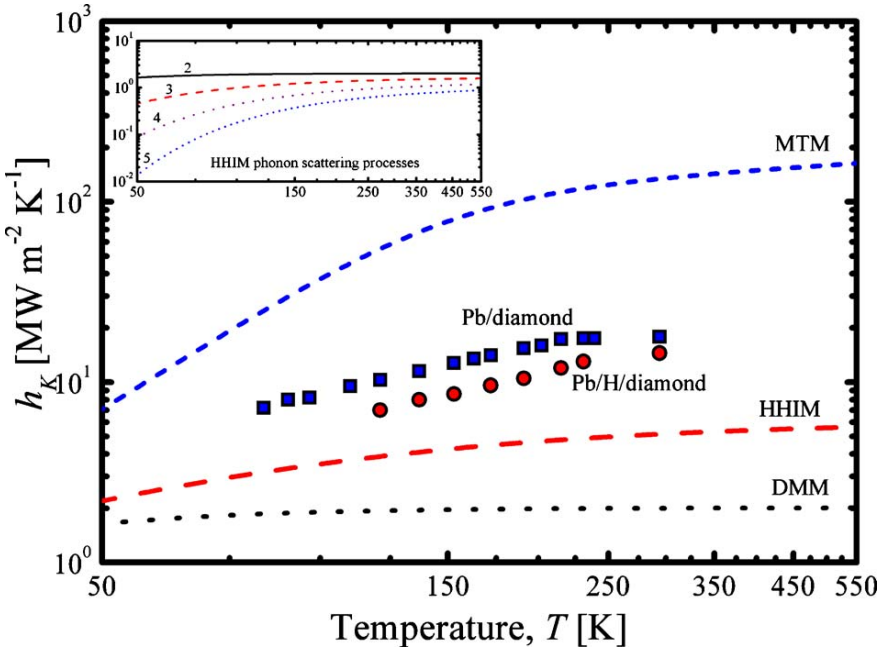
Can we model this (back to the beginning)

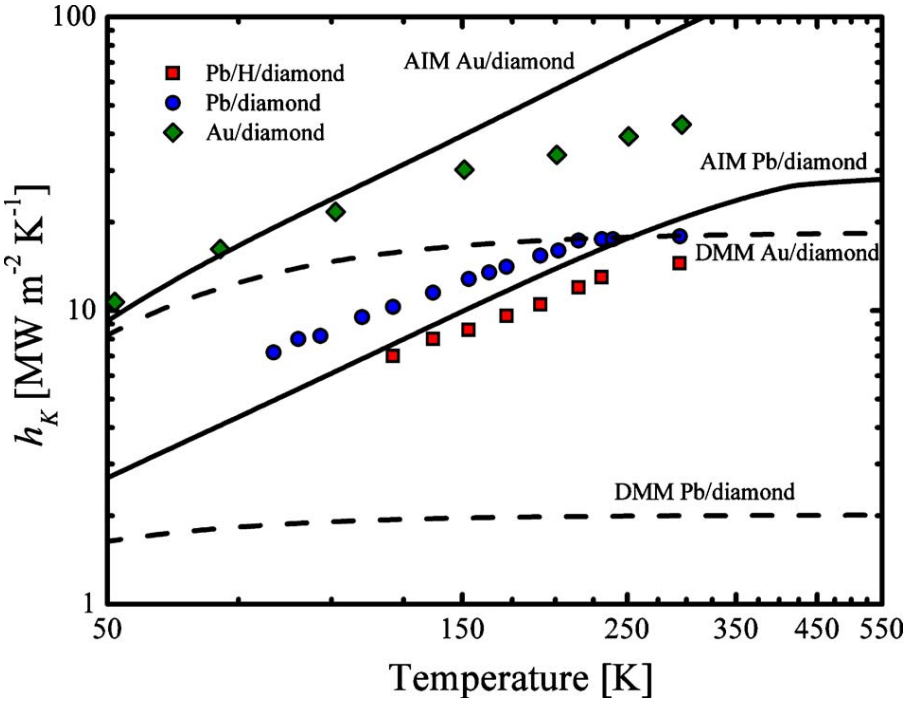


Selected inelastic scattering (higher harmonic)

Hopkins, *J. Appl. Phys.* 106, 013528 (2009)

Hopkins, Duda, Norris, *J. Heat Trans.* 133, 062401 (2011)





Question: what is the most probable interaction? What are the interaction probability/phonon transition probabilities at interfaces?

What about in the classical limit? Can we model MD?

On the Linear Temperature Dependence of Phonon Thermal Boundary Conductance in the Classical Limit

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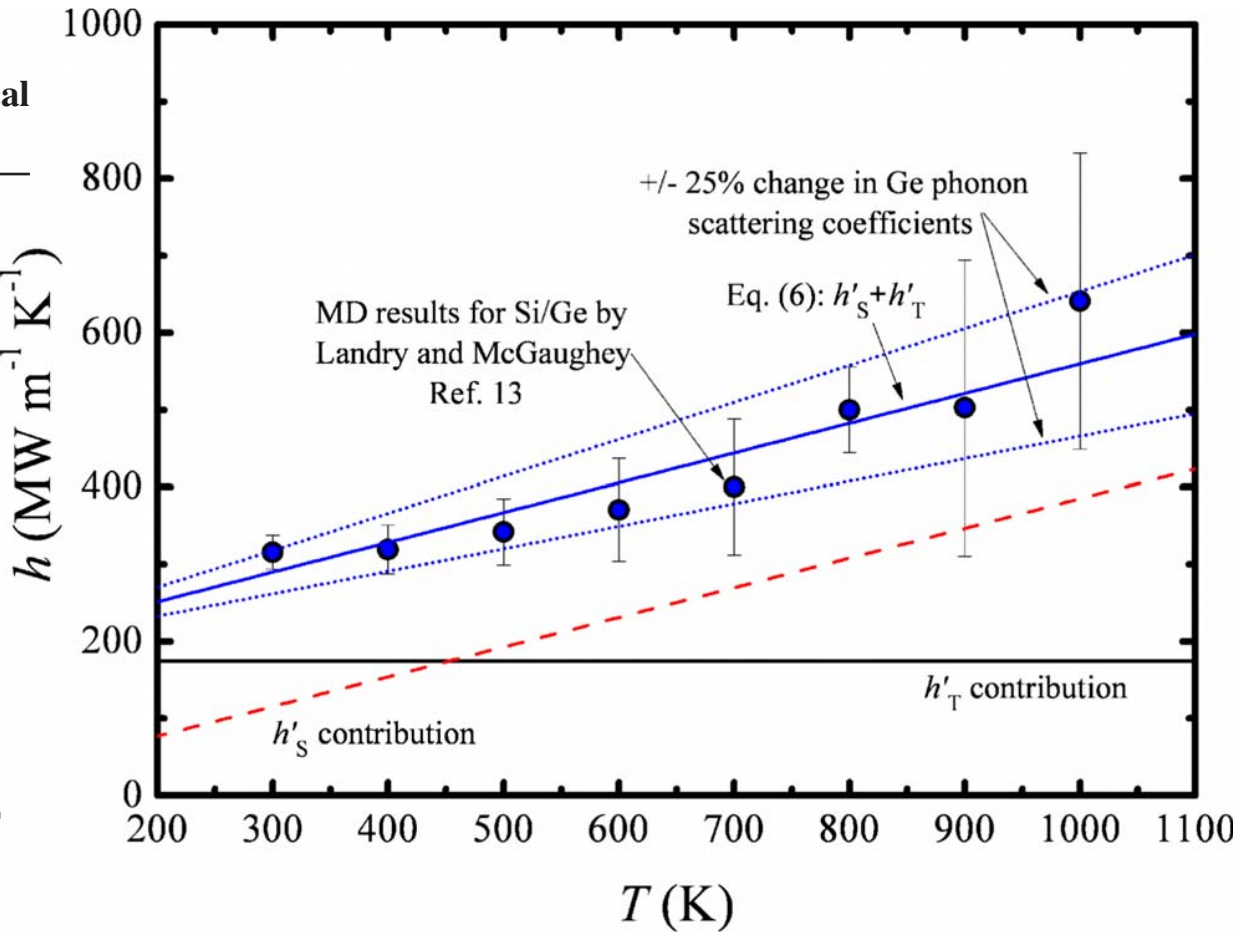
Journal of Heat Transfer

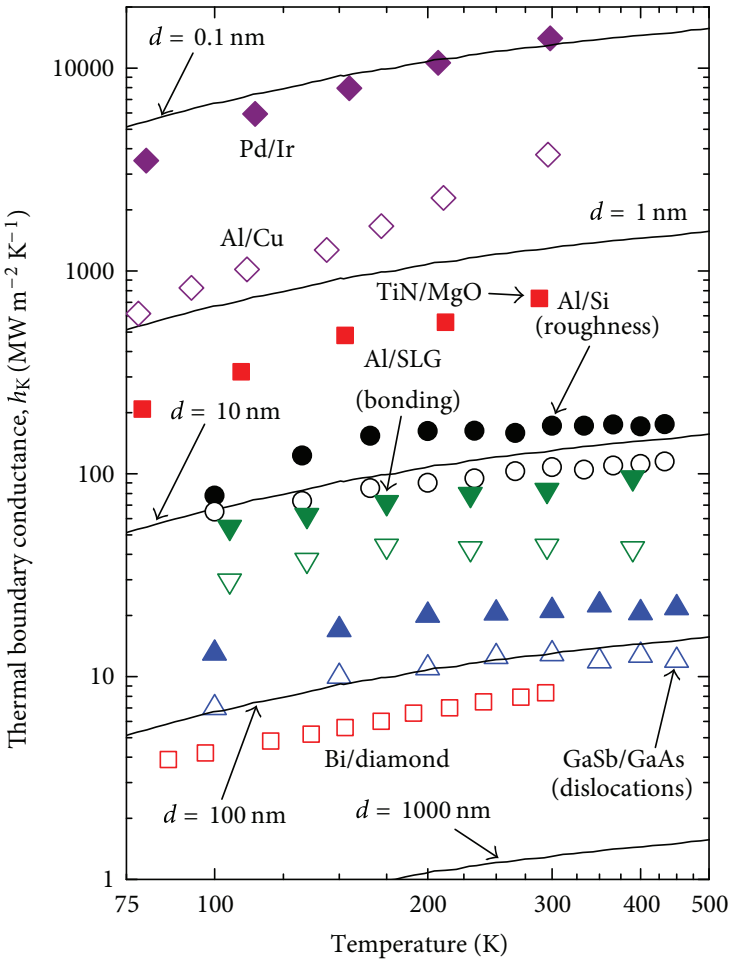
JULY 2011, Vol. 133 / **074501-1**



Phonons emitted across interface are scattered based on other material: linear T dependence comes from UMKLAPP SCATTERING TIME – this needs to be explored in more detail….

Challenges – can we push the extremes with anharmonicity?

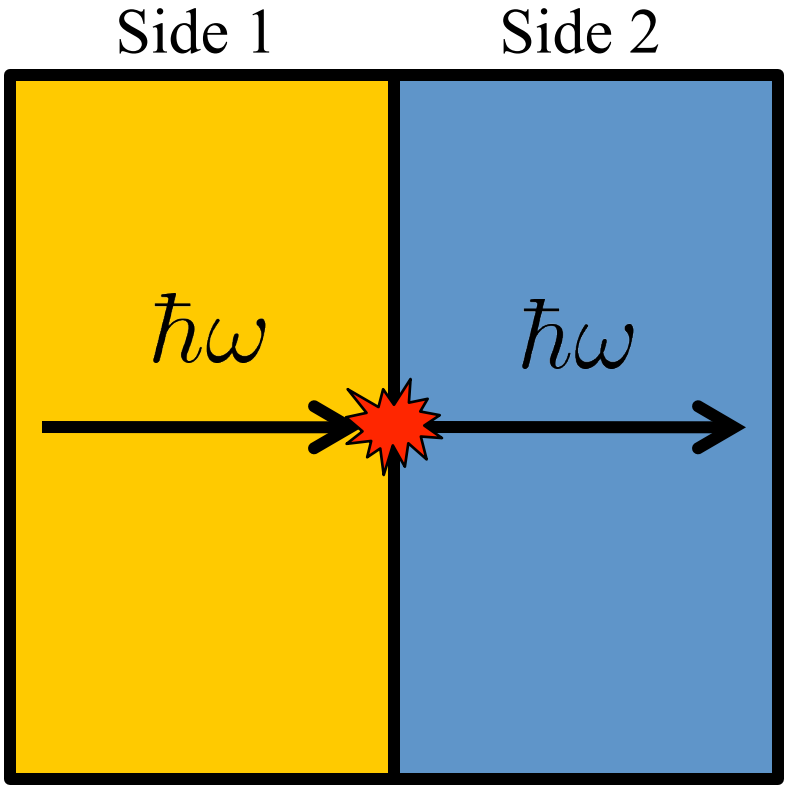
- Interplay between bonding and anharmonicity: what are the roles of 2 and "n-phonon" processes?
- Inelastic scattering vs. disorder: how do interfacial "imperfections" affect the anharmonic processes
- Can we understand anharmonicity from a "bonding" perspective with simulations? How big is "n" in a realistic picture (could n>3 actually exist?)
- BOTH materials are in classical limit: Can we bridge experiments with MD?



Hopkins, *ISRN Mechanical Engineering* **2013**, 682586 (2013)

Interfacial phonon processes

Two phonon scattering (elastic)



"n" phonon scattering (inelastic)