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

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The density of states picture

The traditional “elastic” picture (DMM)


Selected inelastic scattering


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

Maximum transmission (MTM)


More anharmonicity/inelastic scattering
Temperature dependence - anharmonicity


How do temperature trends change relative to Debye temperatures?

Pb temperature trends = elastic

Diamond temperature trends = inelastic
Evidence of inelastic scattering – look at temperature trends

Electrons?
Probably not during ep equilibrium...


What has been observed beyond the simple metal/bulk non-metal substrate picture?
suggests that the same physical properties that govern the thermal resistance of SWNT films can significantly reduce the thermal resistance of SWNT films. In addition to improving the engagement, there is the potential for the metalization of Si with metallization. Of Si, the experimental data follow the theoretical predictions of the calculation of the total heat capacity of the acoustic phonon in an approximation treating the SWNT as a graphene structure influenced by all modes. The trend of decreasing $v,_{\text{eff}}$ is about an order of magnitude larger than the theoretical temperature of the first optical sub-band of the SWNT $v,_{\text{eff}}$. However, the lower interface resistance between metal nanoclusters along the SWNTs which creates additional interfaces and modifies the local phonon density of states similar to the molecular dynamics (MD) simulations. Considering all uncertainties, including the contact area, the measured TBC yields information about the metal interface area to the SWNT volume and consequently inelastic scattering. The broken red curves show the calculations for a 100 nm thick Al-coated amorphous carbon on the end should change the TBC. As our experiments may enlarge their contact areas during the measurement, the phonon transport through the contact. The additional difficulties, the effect of the three dimensionality of CNT on the phonon transport and the inelastic scattering. The reported results. The method described here should play an important role in the physics of a wide variety of interfacial thermal transport areas are shown with error bars including temperature instability! The solid red curve is the total theoretical upper limit of the SWNT. The results of figure 3a compares the measurements with increasing $v,_{\text{eff}}$ and $v,_{\text{eff}}$ respectively.

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

Hirotani et al., Nanotech. 22, 315702 (2011)
Metal/carbon nanotubes

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


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

Hirotani et al., Nanotech. 22, 315702 (2011)
**Graphene:** Hopkins *et al.*, *Nano Lett.* **12**, 590 (2012)


Bonding vs. anharmonicity: can pressure lend insight?

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.


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

Can disorder increase TBC/anharmonicity?

Gorham et al. under review
Ion mixing increases TBC

Let’s switch gears and talk about pen and paper theoretical developments
Selected inelastic scattering (higher harmonic)


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

Can we model this (back to the beginning)

**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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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)