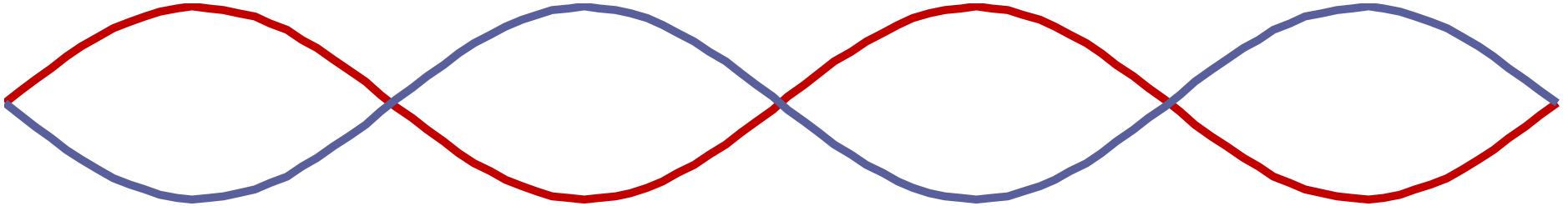
SAND2011-3831C

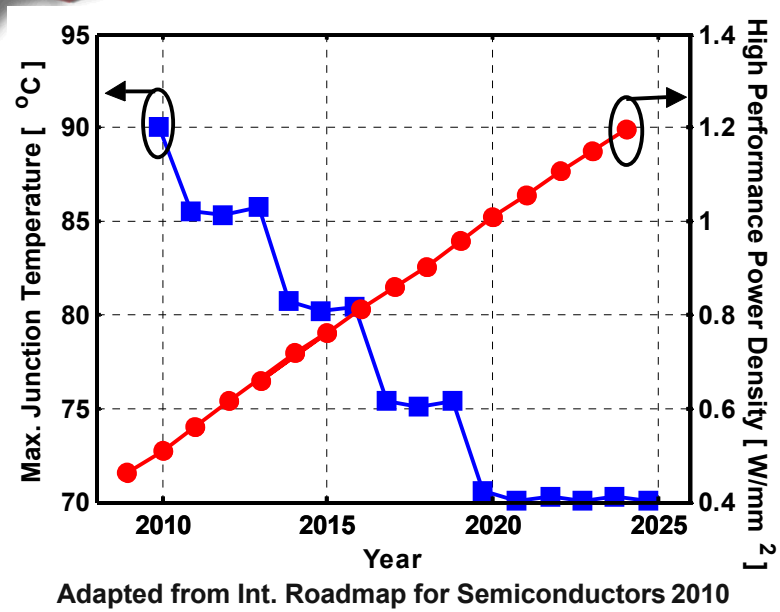
On the Role of Optical Phonons in Thermal Boundary Conductance (TBC)



Thomas Beechem
John Duda
Patrick Hopkins
Pam Norris

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

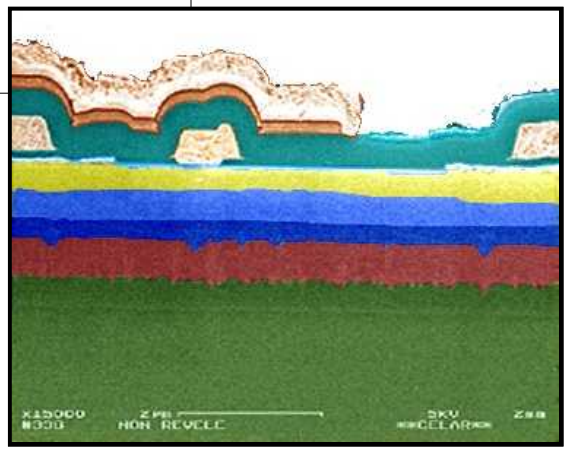
The Interface Effect

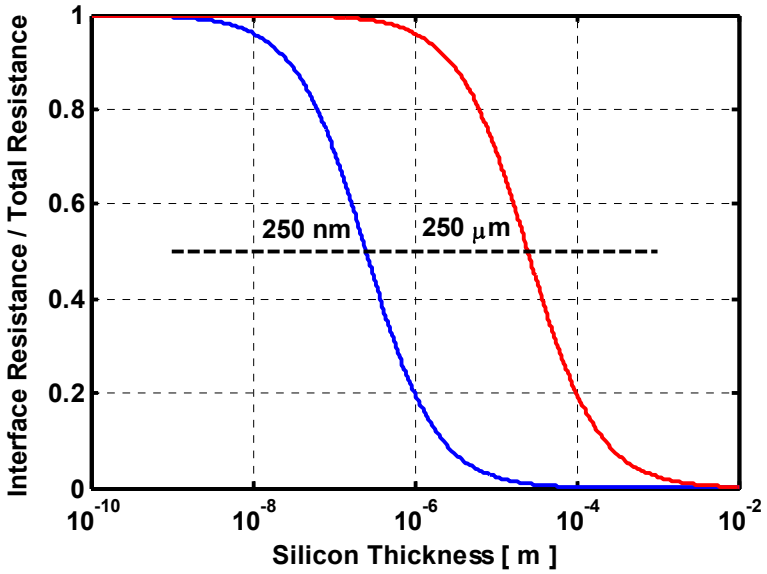


Adapted from Int. Roadmap for Semiconductors 2010

The image cannot be displayed. Your computer may not have enough memory to open the image, or the image may have been corrupted. Restart your computer, and then open the file again. If the red x still appears, you may have to delete the image and then insert it again.

Cross section of Ipad CPU from

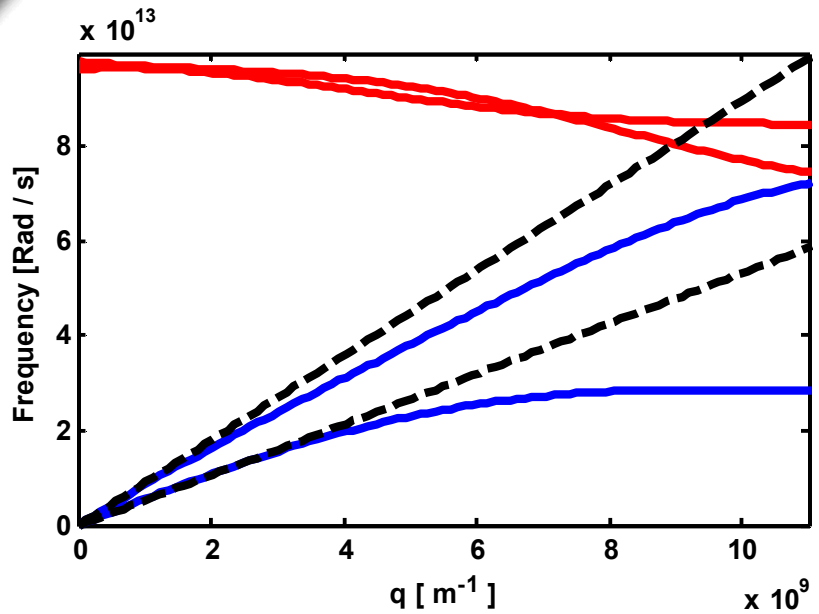


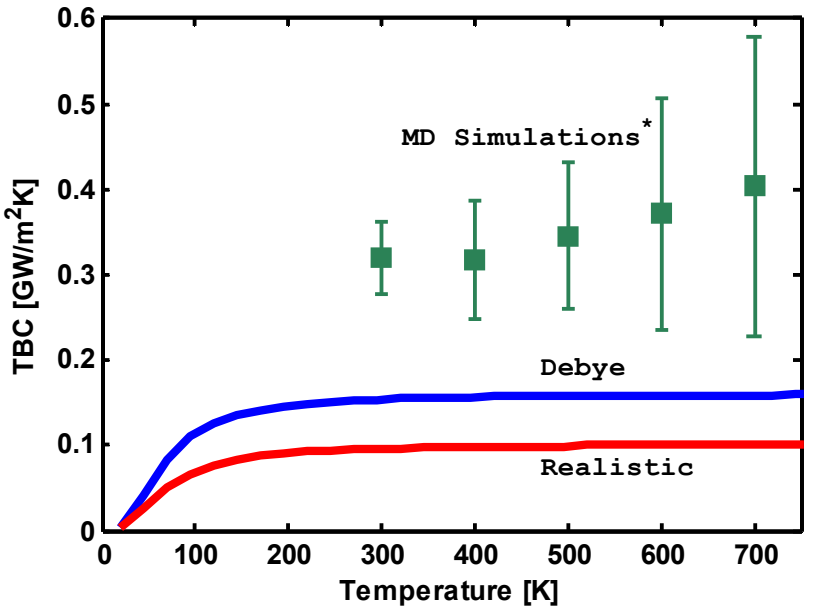


Takeaway: **Interfacial transport plays a role.**

Sandia National Laboratories

Debye & the DMM





- DMM's 2 main assumptions
  - Diffuse scattering
  - Debye solid

- Using a more realistic dispersion, leads to lower correlation with MD predictions.

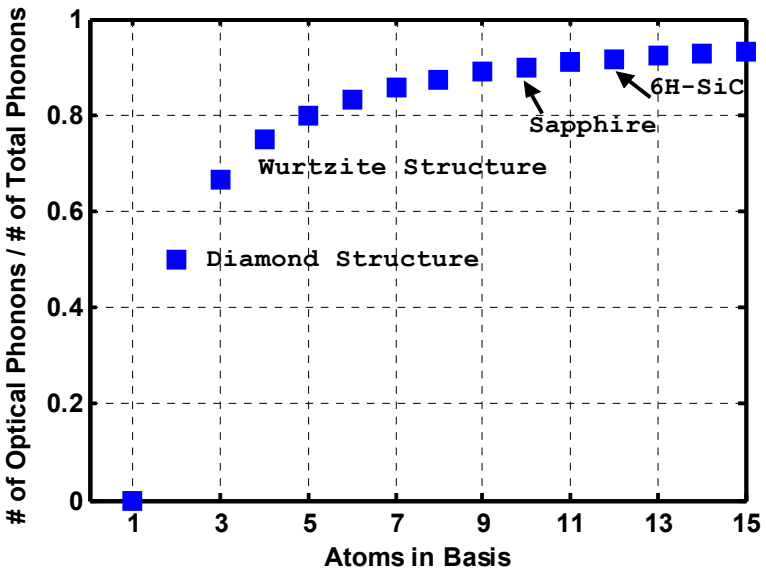
Takeaway: Does Debye approximation compensate for the removal of the optical phonons (OP's)?

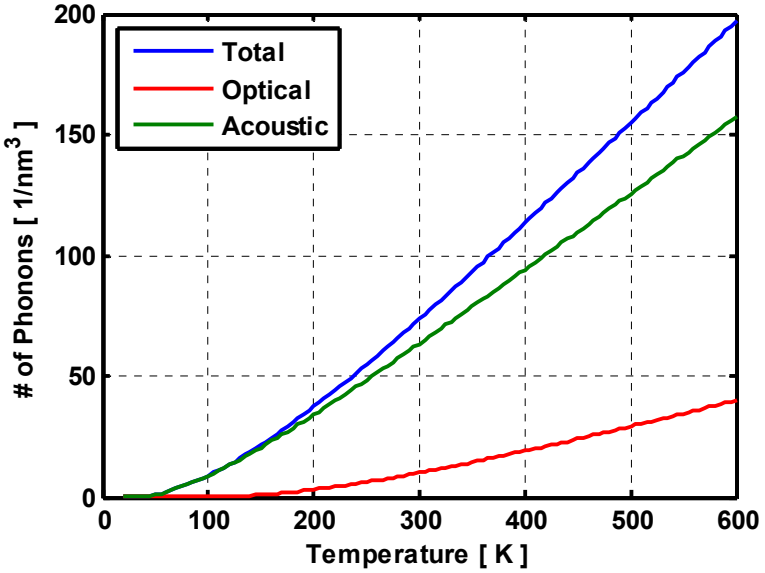
*MD Simulations: Landry and McGaughey PRB 2009

Sandia National Laboratories

Optical Phonons & Semiconductors

- 3p-3 adds up fast.
  - Wurtzite: 75 % of phonons are optical modes.
- Optical modes ignored because:
  - They are “frozen out”
  - The move slow.

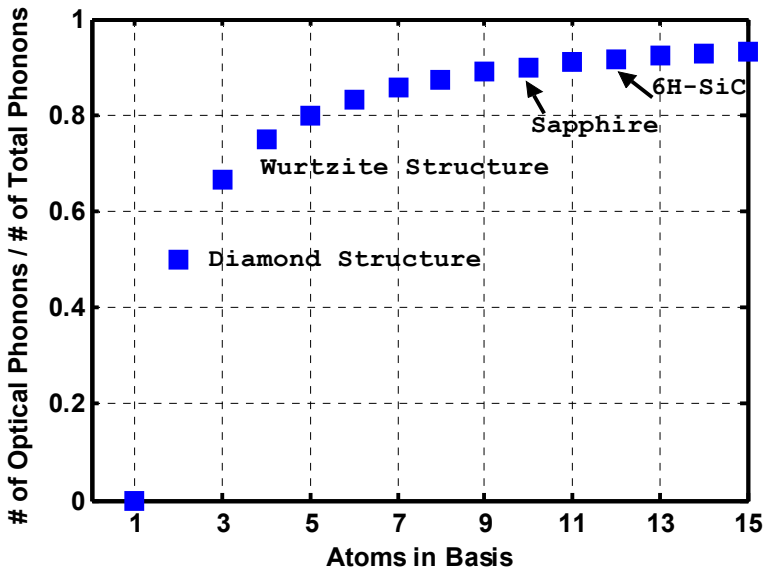


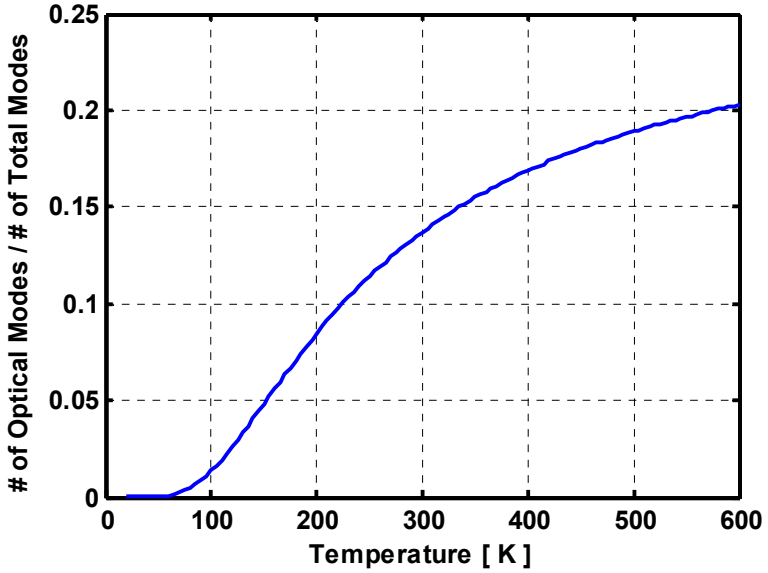


Sandia National Laboratories

Optical Phonons & Semiconductors

- 3p-3 adds up fast.
  - Wurtzite: 75 % of phonons are optical modes.
- Optical modes ignored because:
  - They are “frozen out”
  - The move slow.

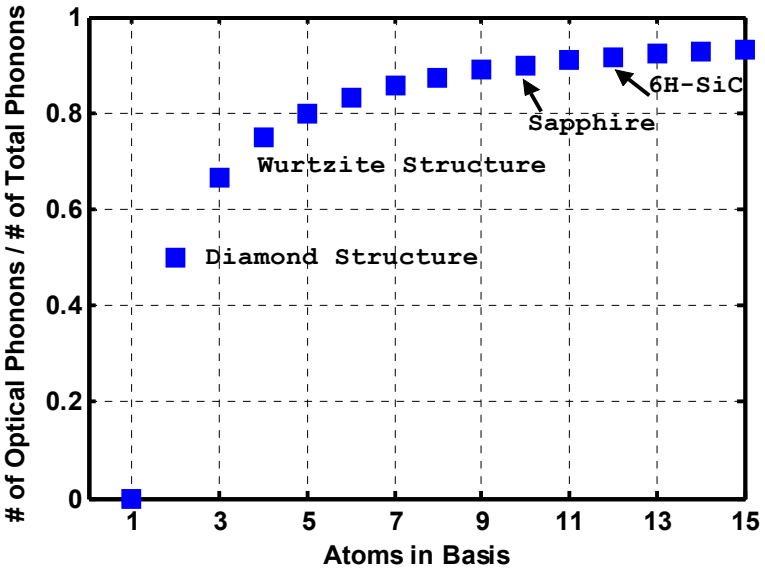


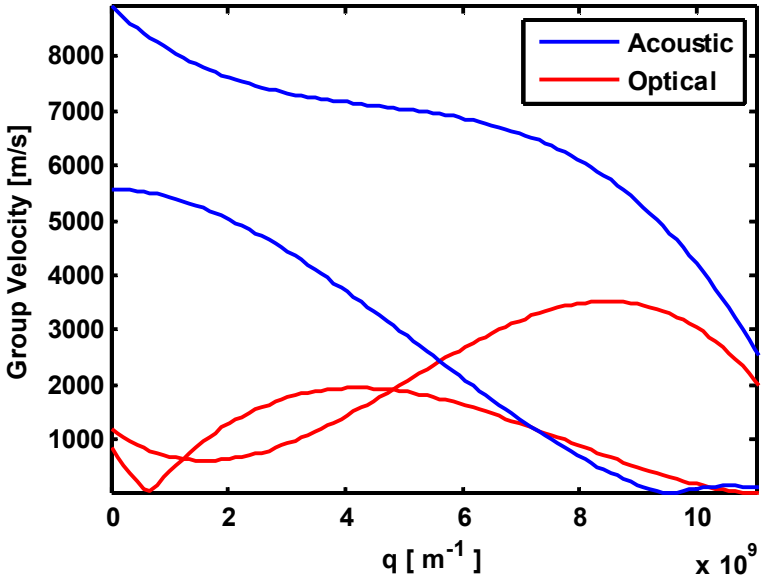


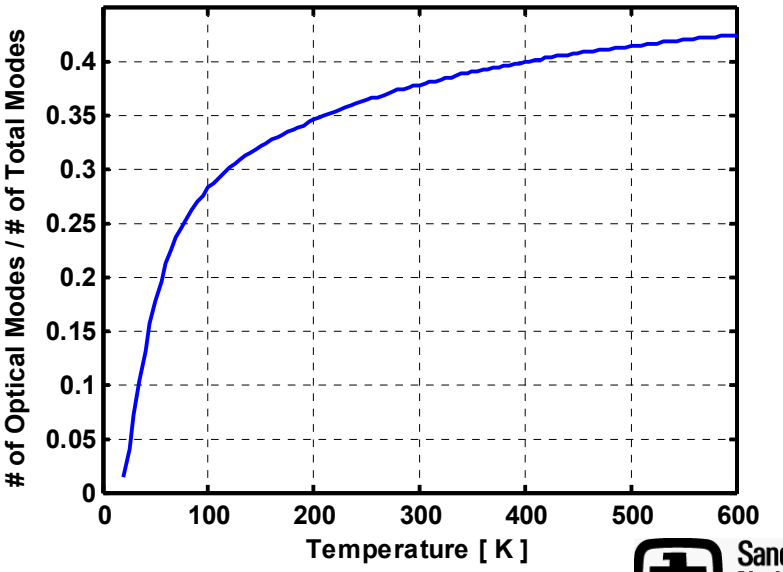
Sandia National Laboratories

Optical Phonons & Semiconductors

- 3p-3 adds up fast.
  - Wurtzite: 75 % of phonons are optical modes.
- Optical modes ignored because:
  - They are “frozen out”
  - The move slow.

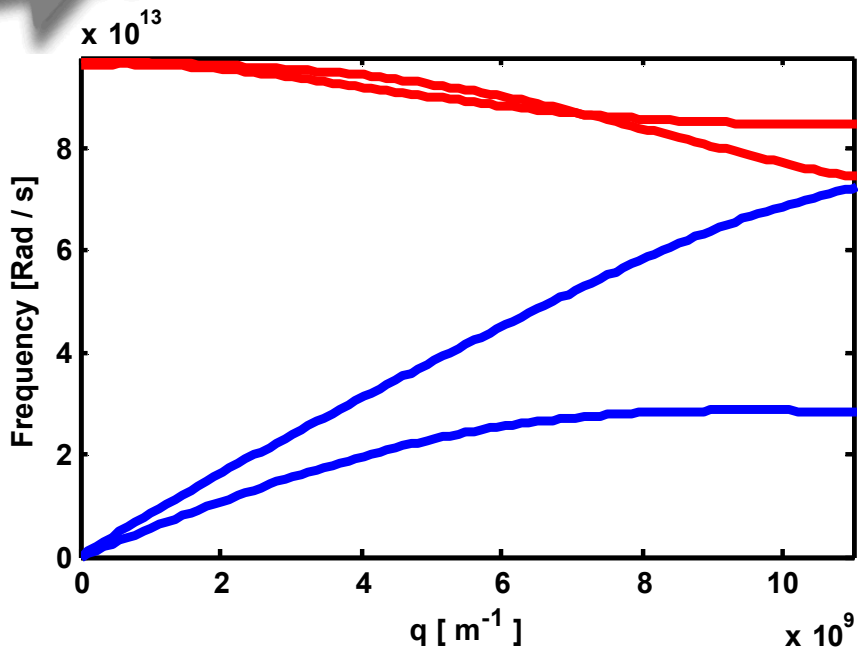






Sandia National Laboratories

DMM Modifications for OPs



- Departures from DMM
  - Isotropic dispersion of direction perpendicular to interface
- Fit previously calculated dispersions using 4th order polynomials.

$$h_{BD}^{1-2} = \frac{1}{8\pi^2} \sum_j \int_{q_1} \hbar\omega_{j,1}(q) q_{j,1}^2 \left| v_{j,1}\left(q_{j,1}\right) \right| \frac{df_o}{dT} \zeta^{1-2} dq_1$$

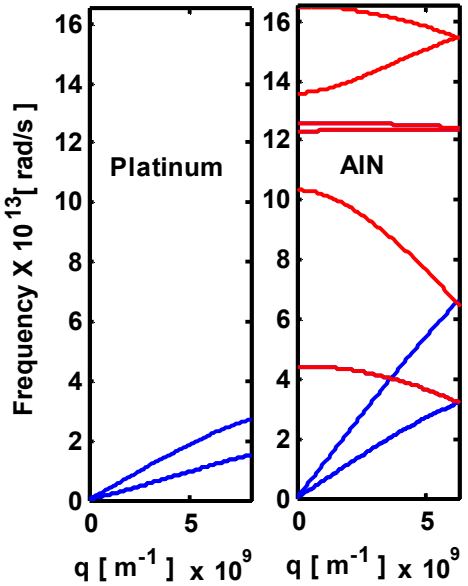
- Scattering assumptions utilized to calculate transmission ratio, ζ
  - Limit of Elastic scattering
  - Limit of Elastic + Inelastic scattering (Termed: Inelastic)

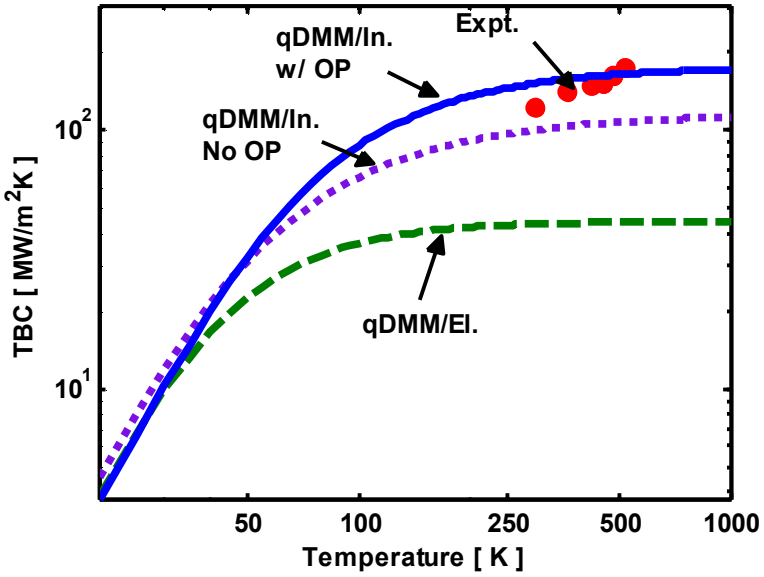
*Full Details: Duda, Beechem, Hopkins, Smoyer, Norris. JAP 2010.

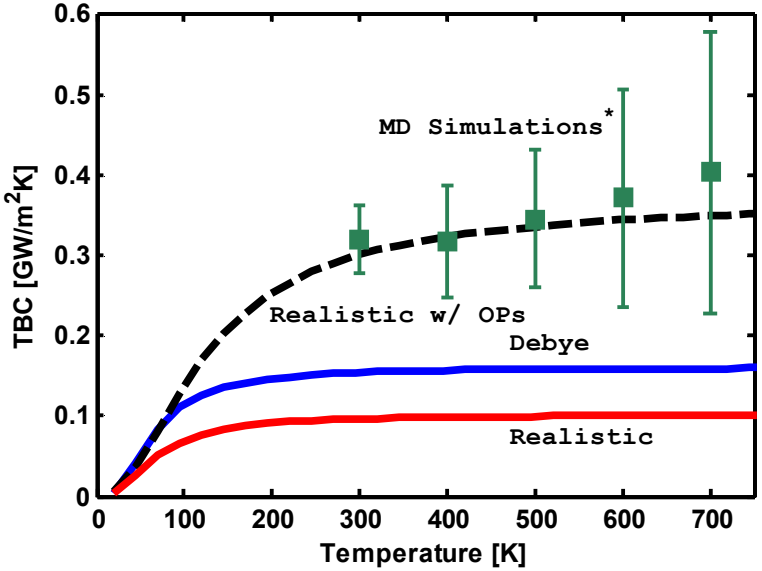
Sandia National Laboratories

Optical Modes in the Inelastic Limit

- Optical phonons most likely to contribute when all scattering modes contribute.
- For Pt/AlN, optical phonons contribute 28 % in inelastic limit.







- Inelastic limit for Si/Ge
  - 40% contribution of optical phonons

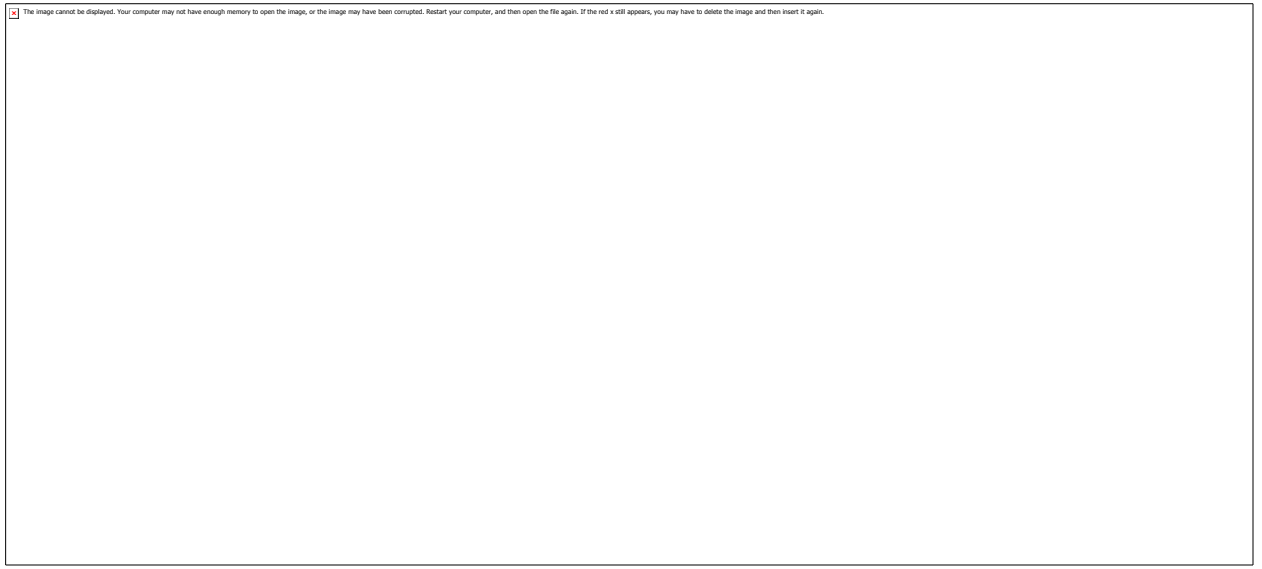
Question: **Is this contribution only an effect of the upper, inelastic, limit?**

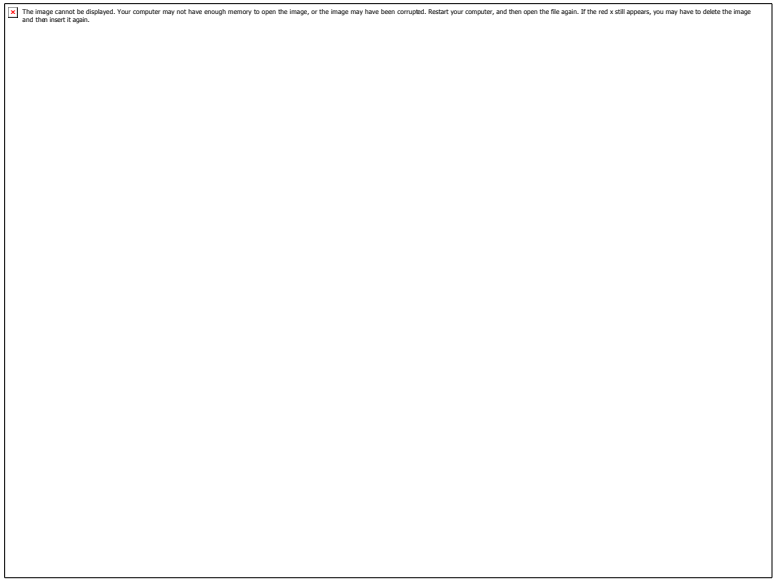
*MD Simulations: Landry and McGaughey PRB 2009 *Expt: Hopkins et al. J. Heat Trans. 2008.

Sandia National Laboratories

Optical Modes in Elastic Limit

- Elastic test case:
  - 91% of modes optical variety.
- >70% of TBC carried by optical modes at T>300K





- Optical phonon contribution is significant even for systems without high numbers of basis.

Takeaway: Optical Phonons must be considered in TBC calculations.

Sandia National Laboratories

Post-Doctoral Opening at Sandia ABQ

Position Title: ***Raman Spectroscopy for Thermal Property Characterization***

Focus: **Combine CW Raman principles with ultrafast techniques to produce new methods to measure basic heat transport properties and physics.**

Timeframe: **Position Open Now**

Go to: ***http://www.sandia.gov/careers/search-openings.html***

Search: **Posting ID # 637411**

Sandia National Laboratories