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Modifying Thermal Behavior at Interfaces Via Material Manipulation

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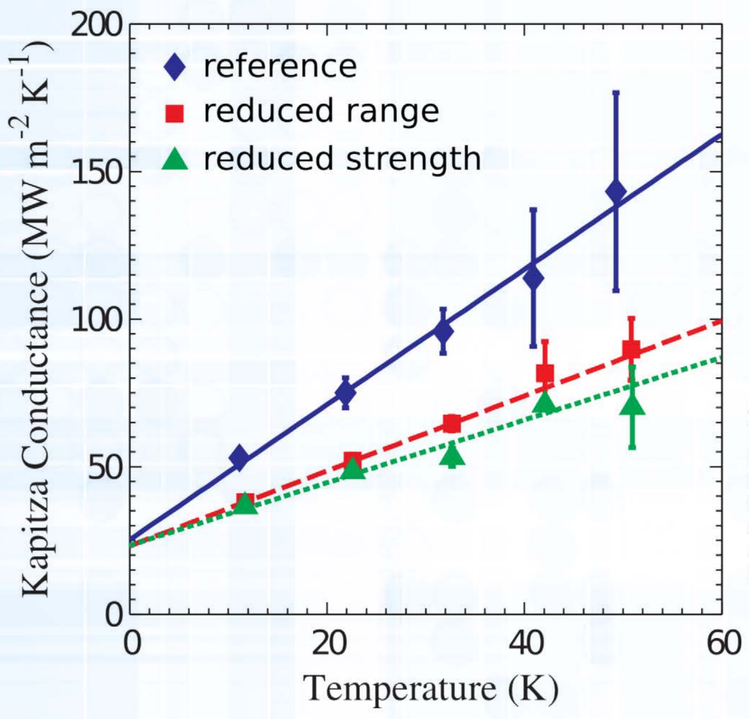
Intent

As devices shrink and are increasingly composed of multilayer and polycrystalline materials, interfaces begin to dominate thermal performance. To date, most models represent the interface strictly in terms of the bulk properties of its adjacent materials. This work was undertaken to investigate the effect of departures from an idealized interface with the goal of improving design models to reduce risk and open design space.

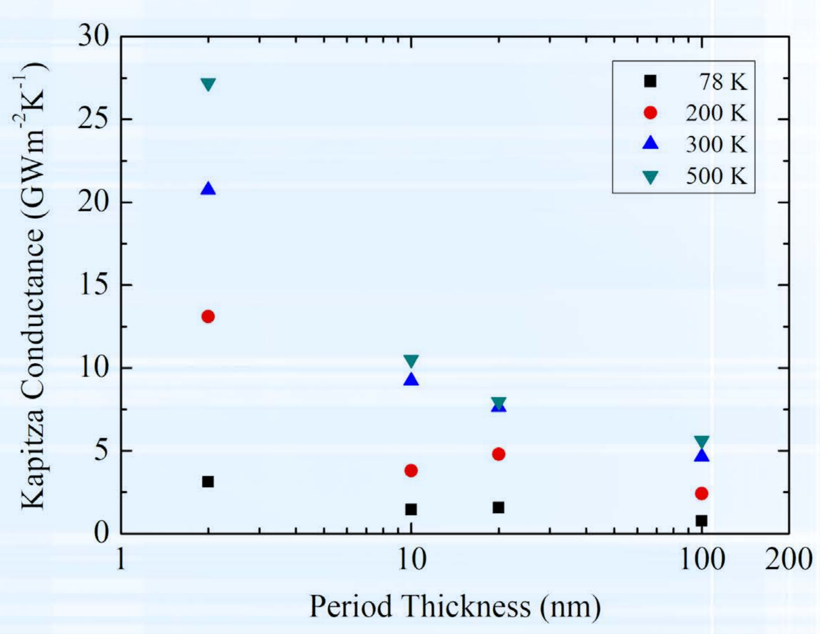
Bonding

- Molecular dynamics study of the effect of cross-species bond:
  - interaction range
  - strength
- Reducing either quantity reduces Kapitza conductance
- Temperature sensitivity also reduced
  - implies inhibition of inelastic transmission



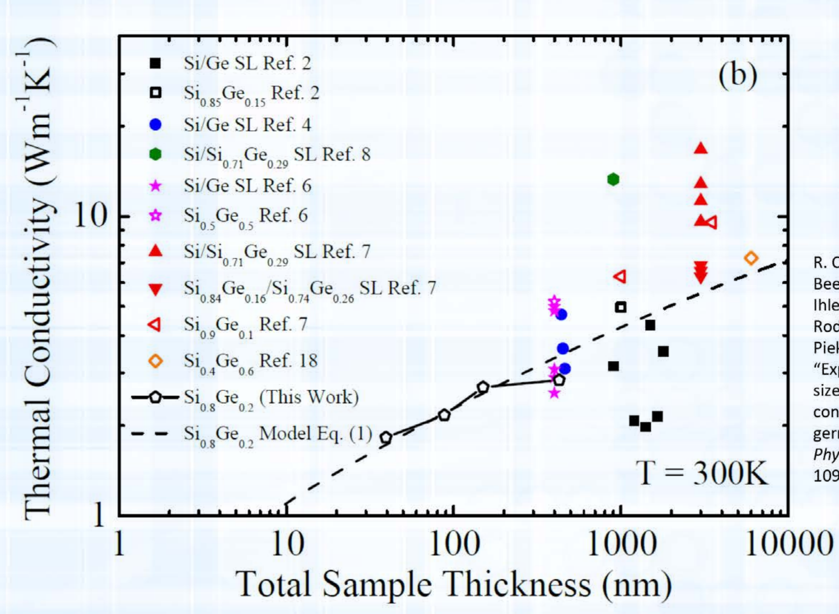
J.C. Duda, T. S. English, E.S. Piekos, W.A. Soffa, L.V. Zhigilei, and P.E. Hopkins. "Implications of cross-species interactions on the temperature dependence of Kapitza conductance." *Physical Review B*, 84:193301 (2011).

Layer Thickness



- Immiscible system (Cu/Nb)
  - Interfaces are sharp
- Kapitza conductance larger for thinner layers
  - Effect increased at higher temperature
  - May be caused by ballistic transport across the layer
  - Model proposed
  - Paper in preparation

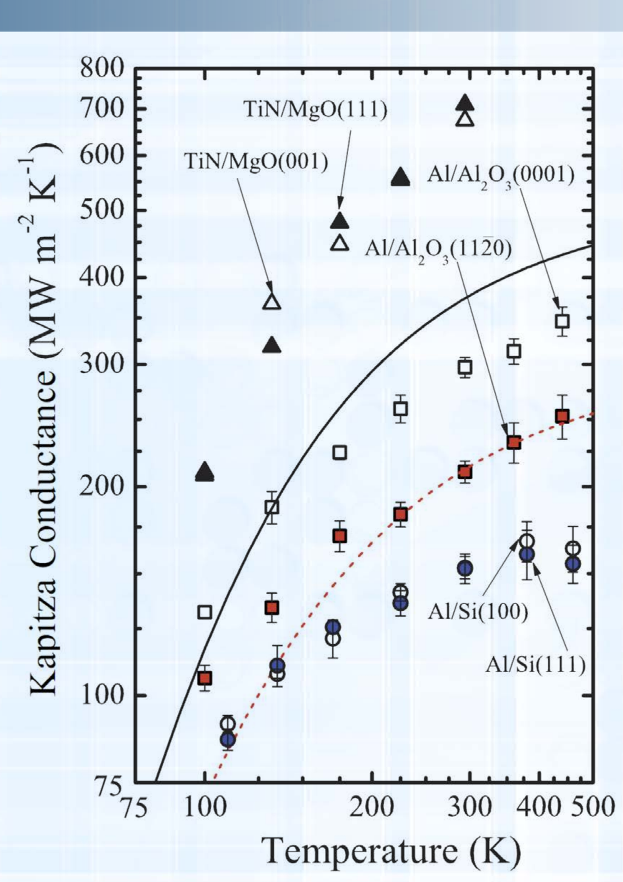
- Kapitza conductance variation in Si / Si_xGe_{1-x} interfaces not resolvable, despite varying dislocation densities
  - but dependence of bulk thermal conductivity on thickness was surprisingly strong
- Alloy scattering shifts dominance to low frequency phonons
  - Increases sensitivity to sample boundaries vs. internal boundaries



R. Cheaito, J.C. Duda, T.E. Beechem, K. Hattar, J.F. Ihlefeld, D.E. Medlin, M.A. Rodriguez, M.J. Campion, E.S. Piekos, P.E. Hopkins, "Experimental investigation of size effects on the thermal conductivity of silicon-germanium alloy thin films," *Physical Review Letters*, 109(19):195901 (2012).

Orientation

- Properly executed, the Diffuse Mismatch Model predicts orientation-dependent Kapitza conductance for non-cubic materials
  - Must account for shape and orientation of Brillouin zone
- Measurements confirm theory
  - Aluminum on sapphire (non-cubic) and silicon (cubic) measured for two orientations



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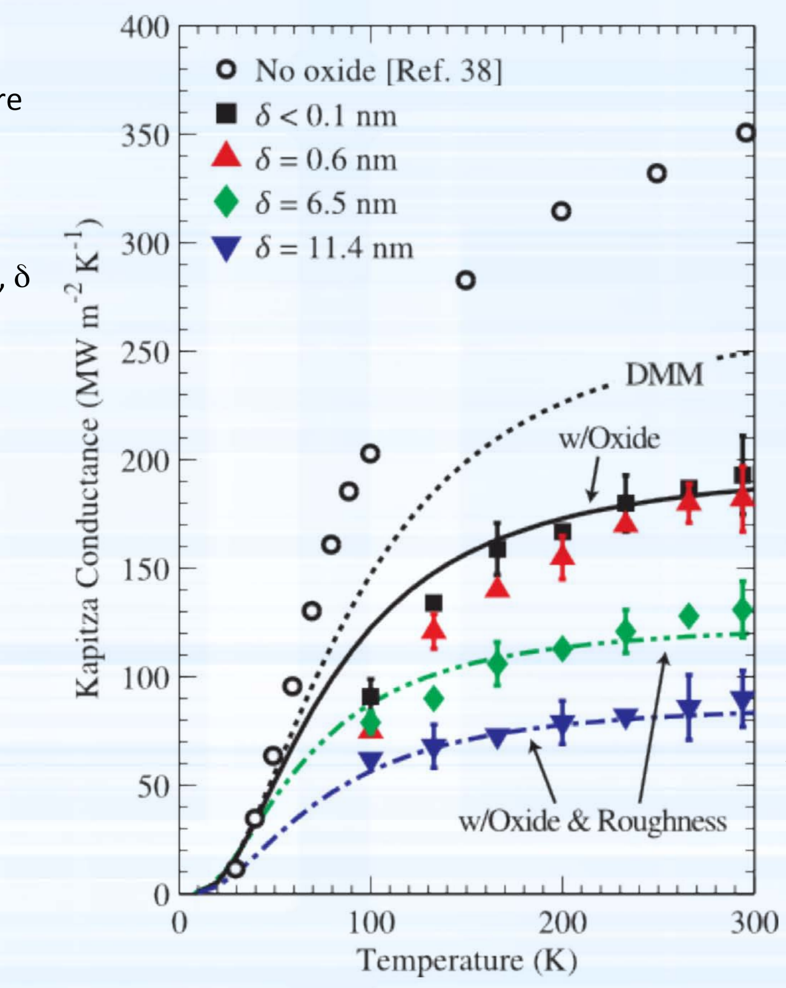
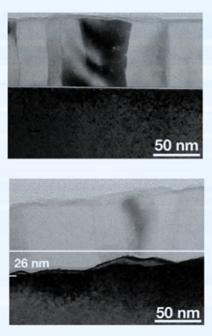
Roughness

- Silicon surface chemically etched before aluminum deposition
  - Timed tetramethyl ammonium hydroxide (TMAH) etch
  - Provides controlled RMS roughness, δ
  - Inexpensive and repeatable
- Diffuse Mismatch Model modified to include roughness effect
  - Native oxide added via a series resistance model

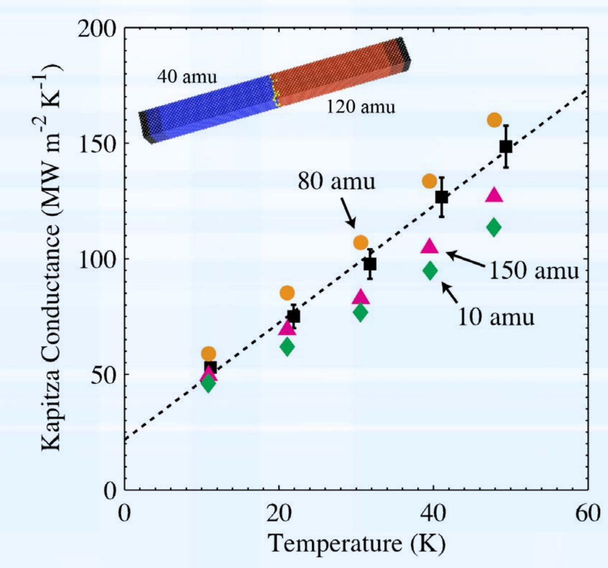




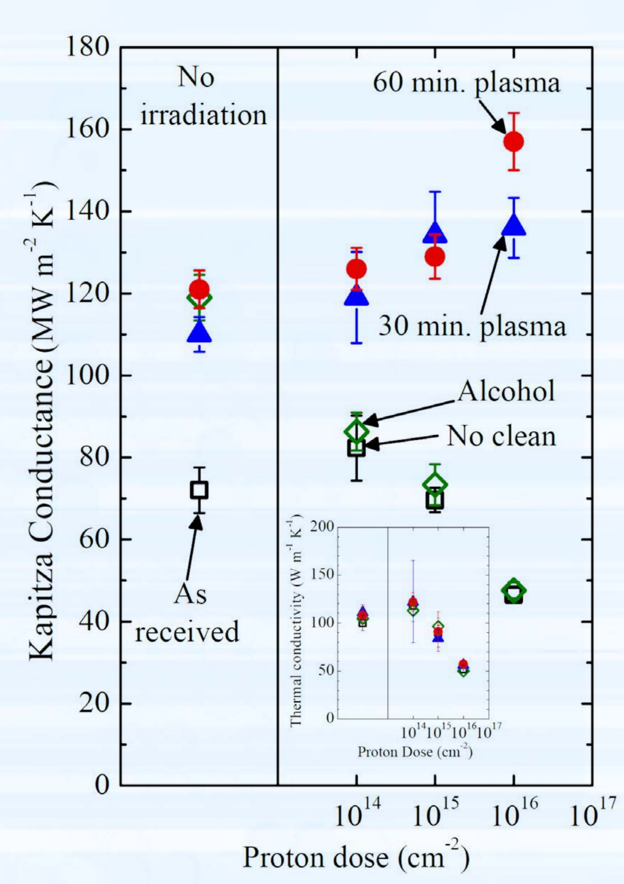
J.C. Duda and P.E. Hopkins. "Systematically controlling Kapitza conductance via chemical etching." *Applied Physics Letters*, 100(11): 111602 (2012)

Mixing

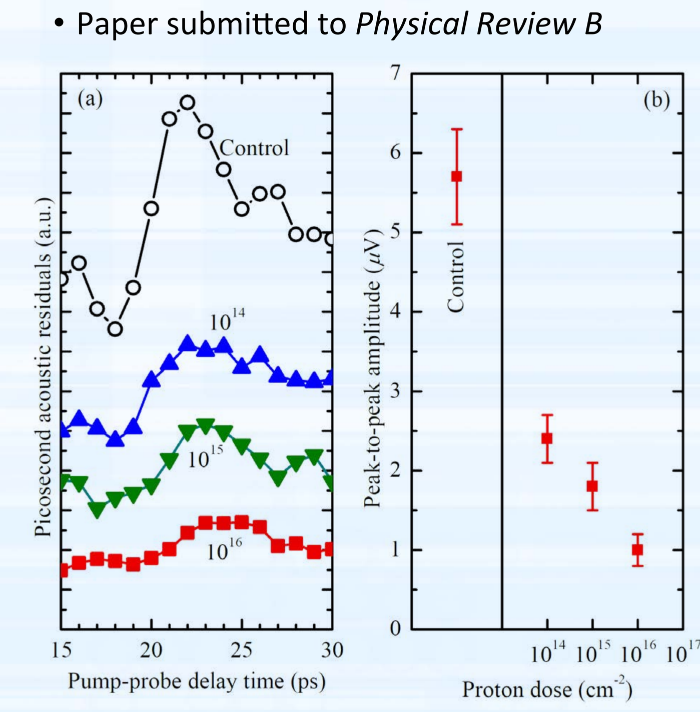
- Molecular dynamics study with inclusions placed near interface
  - Substitutional atoms
  - Identical potential
  - Varied mass, number, and distribution
- Kapitza conductance reduced for atoms heavier or lighter than both bulk materials
- Kapitza conductance *increased* for masses between those of bulk materials



J.C. Duda, T.S. English, E.S. Piekos, T.E. Beechem, T.W. Kenny, and P. E. Hopkins, "Bidirectionally tuning Kapitza conductance through the inclusion of substitutional impurities," *Journal of Applied Physics*, 112(7):073519 (2012).



- Increased TBC via proton irradiation of silicon through native oxide
- Oxygen driven into substrate
  - Observed same trend after stripping the oxide, so change was not in oxide itself
- Picosecond acoustic signature shows decreasing reflected wave amplitude with dose
  - Implies "softening" of transition
- Paper submitted to *Physical Review B*



Key Points

- Departure from an ideal interface usually impedes transport – *but not always*.
- While we have successfully introduced the studied effects into interface models, the generality of these additions, as well as their interaction with each other, remain open questions.

Additional Publications

- N.Q. Le, J.C. Duda, T.S. English, P. E. Hopkins, T.E. Beechem, and P.M. Norris. "Strategies for tuning phonon transport in multilayered structures using a mismatch-based particle model." *J. Appl. Phys.*, 111:084310 (2012).
- P.E. Hopkins, K. Hattar, T.E. Beechem, J.F. Ihlefeld, D.L. Medlin, E.S. Piekos, "Reduction in thermal boundary conductance due to proton implantation in silicon and sapphire." *Appl. Phys. Lett.* 98, 231901 (2011).

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