Introduction
A computational algorithm is developed and applied to calculate sub-continuum thermal transport in structures containing semiconductor-gas interfaces. The computational method is attractive in the mesoscopic regime where a solution of the Boltzmann equation is necessary and must incorporate simultaneously the transport properties of the solid and gas heat carriers.

Governing Equations & Gas-Phonon Coupling

- Gas -
  Boltzmann kinetic equation for the velocity distribution function of gas molecules, \( f \):
  \[ \mathbf{v} \cdot \nabla (f) = (\xi_l - f) / \tau \]
  \[ 1 / \tau = \frac{3}{2} \mu / p \]

- Solid -
  Boltzmann transport equation for the energy density of phonons, \( \epsilon'' \):
  \[ \mathbf{v}_g \cdot \nabla (\epsilon'') = (\epsilon'' - \epsilon''') / \tau \]
  \[ \tau = 3k_{ph} / (C_v v_g) \]

Applications

Interfacial thermal resistance

Temperature jump across interfaces severely limits heat transfer in MEMS.

Detailed computations of phonon-gas interactions can quantify thermal pathways.

Gas Conduction Across Nanometer Contacts

At the nanometer scale, the excessive thermal constriction resistance of point contacts may be mediated by thermal transport through gas.

For contacts at the nanometer scale, the gas gap becomes the primary conduction pathway (80%).

Thermal Transpiration-based Kn Pumps

Thermo-molecular pressure difference (TMPD), \( \gamma \)

\[ P_2 / P_1 = \left( \frac{T_2}{T_1} \right)^{\gamma} \]

Conclusions

As surface-to-volume ratios increase, transport across gas-solid interfaces becomes important and interactions amongst heat carriers must be accounted for in many nano-scale applications. The BTE provides an attractive framework within which to integrate transport modeling in gases and solids.