Temperature Dependence of Thermal Boundary Conductance at FCC Embedded Atom Metal Interfaces: a Molecular Dynamics Approach

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Properties of nanoscale devices become increasingly dependent on interfaces as device dimensions continue to decrease. Thermal boundary conductance (TBC) is a property that must be considered in the thermal management of nanoscale devices. Recent molecular dynamics simulations (MDS) and experimental results suggest there is some thermal transport mechanism that is dependent on temperature in the classical limit. Such a realization would suggest inelastic scattering at the interface becomes a dominant transport mechanism at high temperatures. Currently used models such as the diffuse mismatch model (DMM) do not account for inelastic scattering and hence, do not predict a temperature dependence of TBC well above the Debye temperature. This temperature dependence would deem current models inadequate in predicting TBC at high temperatures and significantly affect the development of future models. Temperature effects on the thermal boundary conductance are investigated in a non-equilibrium molecular dynamics (NEMD) simulation. An embedded atom method (EAM) is employed, which is well suited for simulating the properties of face-centered cubic (FCC) metals such as copper and gold. An interfacial boundary is constructed between two materials in the computational cell. Heat is added to the material on one side of the boundary and removed from the other. In this way, a non-equilibrium heat flux is allowed to develop across the interface. The temperature profile of the computational cell is calculated and the conductance across the boundary can be derived from Fourier's law of heat conduction. Preliminary results suggest strong linear temperature dependence at temperatures well above the Debye temperature. This may imply revisions to existing models are necessary in the high temperature limit.