Molecular Level Investigation of Nanoscale Interface Thermal Resistance

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The performance and reliability of Micro and Nano Electro Mechanical Systems (MEMS and NEMS) strongly depend on molecular level understanding of the heat and mass transport in nano-scale. For instance, the latten heat generated in these MEMS and NEMS needs to be removed by the heat transport either to the ambient or to a coolant. In such cases, the understanding of interface thermal resistance (ITR) observed between nano-scale device components and surrounding/confined fluid, as well as between suspended nano-particles and fluid medium in nano-fluidics coolants plays a critical role. In this presentation, we will focus on my molecular dynamics (MD) studies on nanoscale heat transfer. We target to characterize ITR for simple and complex liquid/solid couples. First, a phenomenological model which can predict the ITR as a function of the wall temperature will be introduced for Argon/Silver and Argon/Graphite interfaces. Analytical solutions employing this model as the coefficient of a Navier-type temperature jump boundary condition result in successful predictions of temperature distribution in nano-channels as thin as 5nm. Next, we will focus on Water/Silicon system. The wetting behavior of a pure silicon surface is studied with Water nano-droplets to properly tune the interaction parameters to recover the correct wetting behavior measured by experiments. Resultant ITR values are found to be in good agreement with the experimental measurements on hydrophobic surfaces. Further characterizations will be made on temperature and pressure dependence of ITR. Developing models for temperature jump boundary condition provide effective engineering solutions for nanoscale heat transfer problems.