# Study of Kapitza Resistance at Fluid-Solid Interfaces in Planar and Cylindrical Nano-Confinement Systems

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In this work, we study the interfacial thermal resistance or the Kapitza resistance at fluid-solid interfaces with the help of molecular dynamics simulation techniques. We introduce a novel and reliable linear response method to compute the Kapitza resistance at fluid-solid interfaces using equilibrium molecular dynamics (EMD) simulations. The predicted value of Kapitza resistance shows an excellent agreement with the results obtained from both EMD and non-equilibrium molecular dynamics (NEMD) simulations in planar and cylindrical interfaces. Our method is independent of the correlation time compared to Green-Kubo based methods, which only work in short correlation time intervals. We studied the size effect of the Kapitza resistance such as the area of cross-section, width of the water layer and the number of graphene layers in a water-graphene system. It is found that the Kapitza resistance slightly decreases with the addition of graphene layers due to the large phonon mean free path along the graphene cross-plane, whereas the surface area and width of water block do not have any influence. Also, we studied the nano-confinement effect of the Kapitza resistance in a water-carbon nanotube (CNT) interface, in which the water is confined inside the CNT. NEMD methods are not suitable for calculating Kapitza resistance in cylindrical geometry, whereas our EMD method can be used in both planar and cylindrical interfaces. The Kapitza resistance decreases with an increase in CNT diameter and converges to the planar graphene surface value as the number of water molecules per unit surface area approaches the value in the graphene surface and ahigher overlap of the phonon spectrum. A slight increase in the Kapitza resistance with the addition of the number of layers of the CNT wall was observed, whereas the chirality and flow do not have any impact.