Title: Molecular dynamics simulation study on thermal conduction of CNT-Cu/Al composites with new MEAM potentials between C and Cu/Al

Carbon nanotubes (CNTs) have a promising potential thermal management application in micro/nano-electromechanical system (MEMS/NEMS) due to high thermal conductivity. CNTs-reinforced Cu/Al (CNT-Cu/Al) composites are attractive to meet the requirement of high thermal performance materials applied in many areas, such as aerospace, automotive and electronic packaging. In this research, molecular dynamics (MD) simulation is used to study the thermal conduction of CNT-Cu/Al composites. Before the simulation is conducted, new modified embedded atom method (MEAM) potentials, which are important for MD simulation, are developed for Cu-C and Al-C binary system and are validated to correctly predict physical properties, such as cohesive energy, lattice constants, surface energy and institutional energy. Then two temperature model along with nonequilibrium molecular dynamics method (TTM-MD) is used to study the thermal conductivity of CNT-Cu/Al composites. Two temperature model can consider the electrons consideration, which can play a crucial part for calculating metal-based composites. Compared to MD method with just phonons consideration, TTM-MD includes electron-electron interactions, electron-phonon coupling and phonon-phonon interactions. The resultant thermal conductivity of CNT-Cu/Al composites by TTM-MD is much higher than that of pure Cu/Al and simulation results from MD methods. It proves that TTM-MD is reliable to calculate thermal conduction of metal-based materials and shows huge potential application of CNT-Cu/Al composites of high thermal conduction. Simulation results also show that the orientation of embedded CNT in metal matrix can significantly influence the thermal conductivity of CNT-Cu/Al composites. Interfacial thermal resistance between CNT and Cu/Al substrate are then calculated. Factors including the direction of heat flow, temperature dependence and CNT engagement as well as the metal crystal orientation on the resultant interfacial thermal resistance are investigated. Thermal rectification can be observed due to change of heat flow. Internal metal nanowire filling ratio and the crystal structures of metal substrate are found all significantly affecting the resultant interfacial thermal resistance.

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The public is welcome to attend.