ABSTRACT

Nanofluids often exhibit significantly higher thermal conductivity compared to the base fluid. It has been shown by earlier researchers that heat exchange between a heat source and nanoparticles, which frequently collide with the heat source, significantly contributes to the enhancement of the thermal conductivity. Contributions of the phononic and electronic modes of heat exchange between a heat source and colliding nanoparticles to the enhanced thermal conductivity have been investigated for the first time, through multi-scale modeling. For this, the nano-scale heat exchange between a nanoparticle and heat source has been modeled using both classical molecular dynamics (MD) and meso-continuum approaches. At a higher length scale, where large numbers of nanoparticles are moving in a fluid and frequently colliding with the heat source, a stochastic model based on the theory of Brownian motion described the movement and the thermal state of the nanoparticles. The model shows that for smaller particle sizes (<10 nm), the prediction of thermal pickup due to phonon transfer made by MD simulation was significantly higher than that predicted by the meso-continuum approach. However, with the increase in the particle size the prediction of the meso-continuum simulation approaches that of the atomistic simulation. For nanoparticles having sizes greater than ~15 nm, the thermal pickup in a collision is not appreciable if the electronic component of thermal conductivity is not taken into account. The present model predicted 72% enhancement in thermal conductivity of water for an addition of 0.1 vol.% Ag nanoparticles of the size range of 4-40 nm, while experimental data in literature for similar Ag-nanofluid gave ~119% enhancement.

For a better assessment of the performance of the present theoretical model, an aqueous Ag-nanofluid with a narrow size distribution of nanoparticles has been synthesized by a one-step method involving direct chemical reduction of silver nitrate ($AgNO_3$) using sodium borohydride ($NaBH_4$), in presence of polyvinylpyrrolidone (PVP) surfactant. The experimentally measured narrow particle size distribution, when fed to the present model, predicts 10.1% enhancement in thermal conductivity, which manifests a good agreement with the experimentally measured thermal conductivity enhancement (12.3%).

The effect of bulk stoichiometry and surface composition of nano-dispersoids on the stability and thermal conductivity of a nickel aluminide (NiAl) intermetallic dispersed aqueous nanofluids have also been studied using dispersoids synthesized through mechanical alloying (MA) of stoichiometric ($Ni_{50}Al_{50}$) and non-stoichiometric ($Ni_{40}Al_{60}$ and $Ni_{65}Al_{35}$) compositions. The higher free-Ni content on the surface of non-stoichiometric Ni-rich NiAl dispersoids of $Ni_{65}Al_{35}$ composition seems to promote better surfactant-nanoparticles interaction, which, in turn, leads to the longer stability of aqueous nanofluid as compared to other NiAl nano-dispersoids.

Keywords: Nanofluids; Thermal conductivity enhancement; Brownian motion; Molecular dynamics; Meso-continuum model; Stability