World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:9, No:01, 2015

Estimation of Thermal Conductivity of Nanofluids Using MD-Stochastic Simulation-Based Approach

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Abstract : The thermal conductivity of a fluid can be significantly enhanced by dispersing nano-sized particles in it, and the resultant fluid is termed as "nanofluid". A theoretical model for estimating the thermal conductivity of a nanofluid has been proposed here. It is based on the mechanism that evenly dispersed nanoparticles within a nanofluid undergo Brownian motion in course of which the nanoparticles repeatedly collide with the heat source. During each collision a rapid heat transfer occurs owing to the solid-solid contact. Molecular dynamics (MD) simulation of the collision of nanoparticles with the heat source has shown that there is a pulse-like pick up of heat by the nanoparticles within 20-100 ps, the extent of which depends not only on thermal conductivity of the nanoparticles, but also on the elastic and other physical properties of the nanoparticle. After the collision the nanoparticles undergo Brownian motion in the base fluid and release the excess heat to the surrounding base fluid within 2-10 ms. The Brownian motion and associated temperature variation of the nanoparticles have been modeled by stochastic analysis. Repeated occurrence of these events by the suspended nanoparticles significantly contributes to the characteristic thermal conductivity of the nanofluids, which has been estimated by the present model for a ethylene glycol based nanofluid containing Cu-nanoparticles of size ranging from 8 to 20 nm, with Gaussian size distribution. The prediction of the present model has shown a reasonable agreement with the experimental data available in literature.

Keywords : brownian dynamics, molecular dynamics, nanofluid, thermal conductivity
Conference Title : ICMME 2015 : International Conference on Metallurgical and Materials Engineering
Conference Location : London, United Kingdom
Conference Dates : January 19-20, 2015