Jithu Paul

Curriculum Vitae

School of Nano Science and Technology
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Education

August 2014–Ongoing — **Master of Technology**, *Nanoscience and Technology*, *School of Nano Science and Technology* , NIT, Calicut.
India

August 2008–May 2012 — **Bachelor of Technology**, *Mechanical Engineering*, TKM College of Engineering, Kollam.
India

Masters Thesis

Title — *Liquid layering and the enhanced thermal conductivity of nanofluids: A molecular dynamics study*

Supervisor (May 2015 - Ongoing) — **Prof. C. B. Sobhan**, *School of Nanoscience and Technology, NIT Calicut*, India.
Affiliate, George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, USA

Description — A molecular dynamics investigation into the anomalous thermal conductivity enhancement of nanofluids. Studied the effect of liquid layering around the nanoparticle with particle size variation at constant volume fraction and its connection with thermal conductivity of the nanofluid. (**More details attached in the last pages**)

Research expertise

- Thermal conductivity calculation of heterogeneous systems using Green - Kubo method.
- Water (TIP3P) and metal oxide (comb3) simulation in molecular dynamics.

Research Interests

- Theoretical work in nanoscale heat transfer based on phonon transport
- Molecular simulations or theoretical works in fluids or colloids

Language Known

English

Computer skills

Molecular dynamics softwares: LAMMPS, Packmol, VMD, Materials Studio

Teaching experience

June 2012–July 2014: Faculty in Mechanical Engineering, A. W. H Engineering College, Calicut, India

Achievement

- Full credits (SGPA 10) for M-Tech project in 3rd Semester

Publications

- *Jithu Paul, A. K. Madhu, U. B. Jayadeep, C. B. Sobhan ; Liquid layering and the enhanced thermal conductivity of nanofluids: a molecular dynamics study, Proceedings of the ASME Summer Heat Transfer Conference 2016, SHTC2016, July 10-14, 2016, Washington DC, USA (Accepted)*
- *Jithu Paul, A. K. Madhu, U. B. Jayadeep, C. B. Sobhan ; An investigation into the fundamental mechanisms of anomalous enhancement in thermal transport in nanofluids. (In preparation)*

References

Project Guide: **Prof. C. B. Sobhan**, *School of Nano Science and Technology*, NIT calicut, Kerala, pin : 673601, India, **email id : csobhan@nitc.ac.in**. http://nitc.ac.in/index.php/?url=users/view/57/27/3

Class Tutor: **Mr. Shijo Thomas**, *School of Nano Science and Technology NIT calicut*, Kerala, pin : 673601, India, **email id : shijo@nitc.ac.in**, http://nitc.ac.in/index.php/?url=users/view/213/27/3.

Details of work done so far and significance of the scientific contribution

The work explores thermal conductivity enhancement of nanofluides at very small nanoparticle sizes and its connection with liquid layer forms at the surface of the nanoparticle. From many years ago itself, it was observed the anomalous thermo - physical properties exibited by colloidal suspensions of nano sized particles in a base fluid more commonly known as nanofluids. This anomalous behaviour was an interesting problem for many researchers as its very high potential for heat management with the scope of using lesser pumping power. Among the various thermo - physical properties one of the most discussed one was thermal conductivity. Various models have been suggested to explain the often anomalous enhancement of thermal conductivity. Liquid layering around the nanoparticle was one of the reasons attributed to the enhancement of thermal properties of the nanofluid. Although many researchers proposed liquid layering has no significant role in thermal conductivity enhancement, always there was a scope where the suface area and radius of curvature of the particle become minimum. We can expect a huge influence of liquid layering at this domain. Also most of the studies was experimental and the particle sizes they used was above 30nm. To study layering effect more fundamentally at small particle size range I selected classical molecular dynamics simulation using LAMMPS software as the tool. I could obtain exponential increase in thermal conductivity enhancement below 5nm particle size at constant volume fraction, proving the high heat transfer capability of very small sized nanoparticles even with a very small volume fraction of the nanofluid. The influence of liquid layering on thermal conductivity has been investigated in two stages, in the first stage the effect of the particle size on the extent of liquid layering around the nanoparticle has been investigated with the help of radial distribution function by simulating copper nanoparticle, suspended in liquid argon. In the second stage the exact source of thermal conductivity enhancement variation with reduction in particle size was studied by splitting the heat flux equation in the Green- Kubo equation.

It is very important to ensure whether there is any structural change happens in the liquid region that surrounding the nanoparticle before proceeding into the work. The idea was to make different shells around the nanoparticle and then plotting the radial distribution function of the liquid Ar atoms in these shells. The result was exciting, very clear solid like behavior obtained in these spherical shells upto an radial extent. In the first stage to study the dependance of extent of liquid layering with the particle size, the method used is by taking seven different systems of Cu nanoparticle and Ar basefluid of same volume fraction but different particle sizes and to repeat the procedure of plotting RDF of different shells surrounding the particle for each case. As expected, the liquid layer thickness was highly influenced by paricle size in the small size domain, the layering thickness increased with reduction in particle size below a particular particle size, above that thickness was almost constant. The next step was to study the thermal conductivity of these seven cases, expecting there should be a same trend in thermal conductivity also because of the reason that liquid layer should have a higher thermal conductivity than base fluid. Green – Kubo method had chosen to calculate thermal conductivity of the system, as it is an equilibrium approach.

For heterogeneous system like nanofluid the most challenging part in the simulation was the addition of partial enthalpy term in the heat flux equation which is not provided in the softwares like LAMMPS. The thermal conductivity of each case calculated and the result was as expected, qualitatively thermal conductivity was similar to layering thickness in each case (different particle sizes). *(Jithu Paul, A. K. Madhu, U. B. Jayadeep, C. B. Sobhan ; Liquid layering and the enhanced thermal conductivity of nanofluids: a molecular dynamics study, Proceedings of the ASME Summer Heat Transfer Conference 2016, SHTC2016, July 10-14, 2016, Washington DC, USA (Accepted)*

In the second stage the fundamental side of thermal conductivity enhancement at this domain was explored by cross examining the Green – Kubo equation. The exact source from where this enhancement comes from when reducing the particle size at constant volume fraction is examined by splitting each component in the heat flux equation. The heat flux equation in the Green – Kubo formula is a summation of Kinetic, potential, collision and enthalpy terms of different species (Ar and Cu). The heat current correlation function for each term has been separatily calculated . The first splitting was through the species summation and the observation was 90% of thermal conductivity enhancement coming from Ar-Ar autocorrelation and it was quantitatively and qualitatively very similar to total thermal conductivity. From this effect we can predict that the reason responsible for thermal conductivity enhancement in our size domain is that some effect happening in Ar-Ar interaction. Then the focus goes on Ar-Ar interactions, where we can again split it into its kinetic, potential, collision and enthalpy terms. There will be four autocorrelations and twelve cross correlations. All correlations are plotted for the seven cases we have, and the finding was only one cross correlation is responsible for the qualitative nature of thermal conductivity enhancement with particle size. The component is kinetic – potential cross correlation in the Ar liquid. This cross correlation increases with decrease in particle size, below a particular nanoparticle size and its having a negative value closer to zero above that nanoparticle size. This increase in cross correlation of kinetic and potential part in Ar is explained as the interplay between the Kapitza resistance and liquid layering. It leads to the same conclusion that we made earlier that liquid layering is the major factor responsible for thermal conductivity enhancement of nanofluids for small nanoparticles less than 5nm. *(Jithu Paul, A. K. Madhu, U. B. Jayadeep, C. B. Sobhan ; An investigation into the fundamental mechanisms of anomalous enhancement in thermal transport in nanofluids at lower nanoparticle sizes. (In preparation)*

The next attemt is to extend these results into water - metal oxide nanofluid system. Water created using packmol software and CuO nanoparticle created in material studio software and applied charges using discover module. Both are combined in packmol and converted into datafile using LAMMPS software. For water applied TIP3P model and CuO used comb3 potential. The simulations are under progress.