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The effect of defect on the thermal conductivity of γ –GNTs: A molecular dynamics simulation

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Abstract:

In this study, we used the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code for investigating the effect of defect on the thermal conductivity of gamma-graphene nanotube (γ –GNT) which have one acetylenic linkages length. The adaptive intermolecular reactive empirical bond order (AIREBO) potential was used to describe the interaction among carbon atoms. Periodic boundary condition applied along the nanotubes axes, Also the systems were equilibrated in the canonical ensemble (NVT; constant number of atoms, temperature and pressure)during 100ps. Following equilibration,gradient temperature along nanotube axis was implemented in the two ends of nanotube with cold and hot slabs with 300 and 360K respectively. After steady state, the thermal conductivity of the γ –GNT was computed using Non-equilibrium molecular dynamics (NEMD) and finally calculated by Fourier's law after measuring heat flux along the tube axis during 200ps.The results show that ideal γ –GNTs have low thermal conductivity compare to CNTs in the same conditions. Moreover, applying vacancy defects from 0.5% to 4% to γ –GNTs are indicated that thermal conductivity decreases and approaches to constant value with increasing defects concentration when the γ –GNT length is constant.

Biography:

Jamal davoodi is a proffeser and coctor of philosophy at University of Zanjan. I am interested in to investigate thermal and mechanical properties of nano-structure by molecular dynamics simulation technique.

Speaker Publications:

1. "Molecular Dynamics Simulation of Diamond Nano Layer Growth on Diamond substrate by Physical Vapor Deposition"
2. "Size and shape dependent thermal properties of rutile TiO 2 nanoparticles: a molecular dynamics simulation study"
3. "Influence of point and linear defects on thermal and mechanical properties of germanium nanowire: A molecular dynamics study"
4. "Separation-Based Adsorption of H2 from Binary Mixtures inside Single, Double, Triple Walled Boron-Nitride Nanotubes: A Grand-Canonical Monte-Carlo Study"
5. "Indirect exchange interaction between magnetic impurities in one-dimensional gapped helical states"

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