Public Abstract
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Title:Ab Initio Molecular Dynamics Study of Nanoscale Heat Transfer and Energy Conversion

In this thesis, ab initio molecular dynamics simulation based on a plane wave/pseudopotential implementation of density functional theory was adopted to investigate nanoscale heat transfer and energy conversions for semiconductors.
The first one investigates the heat conduction process occurring in Si/Ge superlattices at selected stages from the initial point of nonzero temperature gradient to the final state of thermal equilibrium. The ab initio molecular dynamics simulation was performed to get deep sight into the detailed information of the structural, dynamic and vibrational properties of Si/Ge superlattices. The statistical comparisons of temperature evolution curves were made according to the kinetic theory. The ab initio molecular dynamics simulation outputs in the work shows reasonable thermophysical results of the thermal energy transport process. The radial distribution functions and mean square displacements were calculated and further discussions were made to explain and probe the structural changes relating to the heat transfer phenomenon. Furthermore, the vibrational density of states of the two layers (Si/Ge) were computed and plotted to analyze the contributions of phonons with different frequencies to the heat conduction. Coherent heat conduction of the low frequency phonons was found and their contributions to facilitate heat transfer were confirmed.
The second one studies the thermal energy transportation phenomena spanning from heat conduction of thermal radiation with the modeling of variable gap distances in different thin layer systems. By imposing thermostats to keep constant temperatures of the nanoscale thin layers, the initial thermal non-equilibrium between the neighboring layers was established under the vacuum condition. The ab initio simulations were carried out for different material combinations and interfacial distances of silicon and germanium layers. The results show significant distinctions of heat transfer under different materials and temperatures combinations. Further discussions on the equilibrium time were made to explain the simulation results.
The third one presents an ab initio molecular dynamics study of femtosecond laser processing of germanium is presented in this paper. The method based on the finite temperature density functional theory is adopted to probe the nanostructure change, thermal motion of the atoms, dynamic property of the velocity autocorrelation, and the vibrational density of states. Starting from a cubic system at room temperature (300 K) containing 64 germanium atoms with an ordered arrangement of 1.132 nm in each dimension, the femtosecond laser processing is simulated by imposing the Nose Hoover thermostat to the electronic subsystem lasting for ~100 fs and continuing with microcanonical ensemble simulation of ~200 fs. The simulation results show solid, liquid and gas phases of germanium under adjusted intensities of the femtosecond laser irradiation. We find the irradiated germanium distinguishes from the usual germanium crystal by analyzing their melting and dynamic properties.
As the first work of studying the nanoscale energy transport spanning from heat conduction to thermal radiation and the femtosecond laser material interaction in mechanical engineering, the simulation results highlight the promising application of the first-principles molecular dynamics in thermal engineering. We believe our results and the conclusion drawn will be quite useful in helping to resolving the heat transfer and energy conversion problem during the miniaturization of integrated circuits and molecular electronics.