

High performance computer simulations for understanding the thermoelectric properties of Si/Ge nanowire configurations.(Thushari Jayasekera)

As new technologies and new materials are innovated, scientists tend to focus on smaller and faster devices. When the device size becomes smaller, the circuit density drastically increases, resulting in high heat dissipation in the system, thus thermal management at the nanoscale requires a great attention. We need to better understand the thermoelectric properties in nanoscale devices in order to better manage thermal properties in the system. In-depth understanding of thermal transport properties is not only important for efficient thermoelectric applications, but for efficient thermal management of nano devices. The most interesting electronic and thermal properties arise from nanoscale constrictions with compositional/structural mismatch.

Among several low-dimensional semiconductor nanowires based on Si/Ge/Si-Ge heterojunctions have shown to be potential candidates for nanoelectronic and thermoelectric applications. These nanostructures can be constructed without extended defects, and by controlling the composition; the electronic properties can be engineered. Moreover, since the vibrational modes of such a system are governed primarily by compositional and structural properties, also the thermal transport properties can be engineered by modifications of the device geometry and of the chemical constituents. In this study, we will investigate the effect of controlled doping, defect formation, superlattice and hierarchical nanostructuring in the vibrational modes and thermal transport properties of these systems.

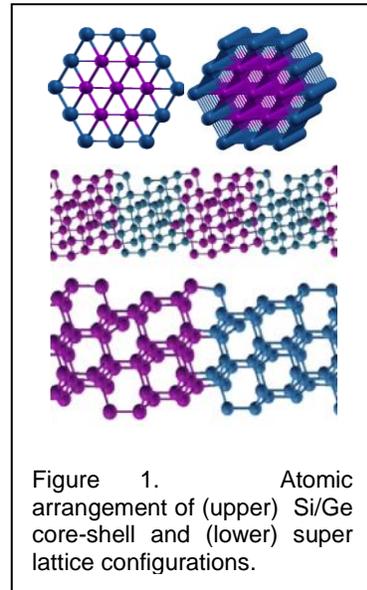


Figure 1. Atomic arrangement of (upper) Si/Ge core-shell and (lower) super lattice configurations.

REU Student will perform high performance computer simulations on different nanowire configurations including core-shell nanowires, interfaces and super lattices as sketched in the Figure 1, in view of finding better thermoelectric materials.

The student will have the opportunity to learn different calculation techniques for understanding nanoscale device performance, high performance computer simulations, which will be helpful in their career irrespective of the future field of interest. The student also will get the opportunity to collaborate with the experimental groups and get the exposure on how to relate the data obtained from the simulations to experimental observations.