Thermal Conductivities of Semiconducting Nanostructures
ALEXANDER ROBILLARD, RALF MEYER, Laurentian University — The thermal properties of semiconductors, much like their electrical properties, are of great interest due to their applications in science and industry. In particular, nanostructured materials such as nanowires and nanolattices can exhibit unique thermal properties which can be used in areas such as energy harvesting, thermoelectric materials and computer components. In order to assess the thermal properties of these types of structures, molecular dynamics simulations of silicon and germanium nanostuctures have been performed using reverse non-equilibrium molecular dynamics. This method creates an artificial heat flow by interchange of momenta, which allows the measurement of an induced temperature gradient and therefore a value for the thermal conductivity. Results are presented from simulations of nanowires and nanoparticles, and more complex structures built from nanowires and nanoparticles. The temperature profile induced on these structures is presented and their thermal characteristics are examined.

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