

Thermal transport behavior in silicon nanostructures has become more important due to the application of these promising nanostructures in the engineering of next-generation nanoelectronic devices. In this presentation, the study in which molecular dynamics simulations are performed to evaluate the thermal transport in silicon nanostructures are described. In addition, the effects of various types of defects, impurities and strain are explored in tuning the thermal conductivity of the mentioned kinds of nanostructures. At the first stage, non-equilibrium molecular dynamics simulation is carried out to assess the interfacial thermal conductance of six different types of constructed grain boundaries in the silicene nanoribbons. In the following stage, a continuous polycrystalline model is designed based on the results of molecular dynamics and the effective thermal conductivity of the polycrystalline sample is obtained by the finite element method. Moreover, the effects of factors such as the grain size and tensile strain on the effective thermal conductivity of polycrystalline film are examined. The results indicate that the thermal conductivity of polycrystalline silicene changes from 4.9 to 40.5 W/mk for the grain sizes of 2 to 1000 nm. In a separate part, the thermal conductivity of silicene nanotubes with different lengths and diameters is investigated. Additionally, the effects of chirality, grain boundary, strain, vacancy defect, and temperature on the thermal conductivity are explored. The results indicate that the thermal conductivity of silicene nanotubes is one order of magnitude lower than that of bulk silicon and possesses a strong dependence on the length. Besides, silicene nanotubes consisting of the grain boundary exhibit nearly 30% lower thermal conductivity compared with pristine ones. The underlying mechanism is demonstrated by calculating the phonon power spectral density. Eventually, considering the widespread application of silicon nanowires in the design of nanoelectronic devices and the importance of heat management in these devices, the effect of impurity and axial-torsion on the thermal conductivity of silicon nanowires is evaluated. Additionally, thermal rectification in telescopic silicon nanowires is examined. The results present that at the interface of two nanowires with different diameters, a significant thermal boundary resistance occurs and the asymmetric systems are created whose thermal conduction is depending on the temperature gradient. This effect, which is called thermal rectification, plays an important role in the design of complex thermal systems.