

## **Strain Effects on the Thermal Conductivity of Nanostructures**

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Nanostructures such as carbon nanotubes and nanowires have shown great advantages in thermal management and energy harvesting applications due to their particularly high and low thermal conductivity. In practical applications these nanostructures are always under strain either due to external pressure or the mismatch of lattice constant and coefficient of thermal expansion. In this paper, molecular dynamics (MD) simulation is systematically performed to investigate the strain effects on thermal conductivity of carbon and silicon nanostructures, namely, graphene, carbon nanotubes, silicon thin films and nanowires. By fitting the heat current autocorrelation function of the equilibrium MD simulation with a developed method based on frequency dependent thermal conductivity analysis, the memory effects of long acoustic phonons arising from periodic boundary condition can be screened and accurate thermal conductivity can be obtained, which has been considered as a significant challenge in MD simulation for a long time. Using this analysis method, size-independent thermal conductivity from MD simulation of bulk silicon is investigated for validation, which shows good agreement with experimental data of enriched silicon. The simulations are then performed for carbon and silicon nanostructures with different characteristic length under different external strain. The strain is applied by a simple method under periodic boundary condition along the axial direction. Results show that thermal conductivity of carbon and silicon nanostructures can be greatly tuned by changing their external compressive or tensile strains, which can be used for enhancing the performances of nano and micro systems.