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ΤΜΗΜΑ ΦΥΣΙΚΗΣ
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Σ Ε Μ Ι Ν Α Ρ Ι Ο

Thermal conductivity of nanostructures and nanostructured materials

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Abstract

Advances in nanofabrication technologies have revolutionized the fabrication of nanostructures and nanostructured materials. Their applications in molecular electronics, quantum computers, actuators, sensors, and molecular machine are rapidly spreading. Their novel functions involve unique mechanical, thermal, and electronic properties. A crucial question is whether or not they efficiently transfer heat current and whether they remain mechanically stable at a given operational temperature. Phonon confinement observed in semiconductor nanowires, superlattices and phononic crystals modifies the phonon velocities, while surface and interfacial scattering increases the thermal resistance. Measuring temperatures and heat fluxes with a nanometer scale resolution is difficult, and such measurements are most often carried out using atomic simulations, which may help in understanding the microscopic phenomena at play. Molecular dynamics (MD) simulations allows the prediction of the thermal transport properties of semiconductors and insulators because in these materials, energy is mainly carried by phonons. Among the MD simulation approaches to calculate the thermal conductivity, there are two main methods: the nonequilibrium (NEMD) method based on forcing a temperature gradient on the system and the equilibrium (EMD) method within the Green-Kubo approach. During this seminar, a number of examples of thermal transport properties obtained by Molecular Dynamics (MD) simulations will be given (nanowires, superlattices, nanoporous materials and nanoinclusions). The common feature of these systems is the small ratio between their characteristic system size and the phonon mean free path, which leads to a ballistic heat transport. Furthermore, when the density of interfaces gets large, the energy transport properties of the materials cannot longer be described solely by the thermal conductivities of the constituents of the material, but depend also on the thermal boundary resistance which measures the transmission of phonons across an interface.