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Phonon Thermal Transport in Thin Films Simulated by Molecular Dynamics

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Abstract

Advances in the nanotechnology industry have created the urgent need to develop accurate methodologies to model heat transport in devices with features in the nanometer range. New, not fully understood thermal transport phenomena arise as a consequence of the miniaturization of the device features into nanometer scale. The thermal properties of thin films and multilayers differ from those of the bulk material; the scattering of energy carriers (phonons) with boundaries, among other factors, drastically alters thermal conductivity. However, thermal properties of thin films are not fully understood. In this project, thermal properties of thin films and multilayers by means of molecular dynamics simulations will be studied. The objective is to predict and understand thermal properties of nano-materials composed of thin films used in semiconductors and data storage technologies.