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Discrete Lattice Modeling of Atomistic Locations in the Interfaces Between Nanomaterials

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Summary

Interfacial region between two nanomaterials can be treated as a separate material since its atomistic structure and characteristics are different than the two materials on its either side. The mechanical as well as electronic properties of composite materials are sensitive to the interfaces. For industrial application of the nanomaterial systems, it is vital to model and measure the discrete atomistic locations in the interface during operating conditions. As the dimensions of nanomaterial systems shrink, the role of interfaces become increasingly important. Because of its nanothickness, the conventional characterization and design parameters like elastic constants, stress and strains are not reliable for interfaces. These parameters are defined for the continuum model of materials in which atoms are assumed to be smeared into a continuum of matter. Mathematically the parameters are expressed in terms of derivatives of certain functions which cannot be defined in discrete spaces. Even the conventional representation of electronic and phonon band structure is not precisely defined for finite and disordered assembly of atoms. The interatomic distance in most semiconductors is about 0.5 nanometer. The continuum model therefore totally breaks down for interfaces that may be only a few nanometers thick.

In order to model the mechanical as well as electronic properties of composites, it is necessary to model the atomistic locations in the interface. Modeling atomistic structure of interfaces is particularly challenging because of its coupling with other materials on its both sides and its disordered lattice structure. I will describe a method based upon the use of lattice Green's function and molecular dynamics for precise modeling of nanomaterial interfaces. The method is applied to model the interfaces between metal/carbon nanotubes and metal/graphene interfaces. Both nanotubes and graphene are potential materials for interconnects in the new generation solid state devices. In addition, the method is also applied to interfaces in strained Si/Ge systems that are used in sub-nanometer transistors. Numerical results for the atomistic locations in these interfaces