

Materials Science and Technology Division

“Computational Analysis of Thermodynamic and Mechanical Properties of Nano-Materials”

Huijuan Zhao
University of Illinois, Urbana-Champaign

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Abstract:

Current research in nano-technology has led to advances in design and fabrication of nano-electro-mechanical systems (NEMS). The design, optimization and fabrication of NEMS for various applications can be accelerated by developing accurate physical theories, and computational design tools. For NEMS devices, nano-scale effects, such as quantum effects, surface effects, material defects become significant. Classical theories and bulk material properties based on the continuum assumption may not be directly applicable for nano-scale devices. Accurate and efficient computational models and systematic study of material properties at nano-scale are among the many challenges currently facing the nanotechnology community.

In this work, the top-down quasi-continuum approach for multi-scale analysis of silicon nanostructures is extended at finite temperature. The quasi-continuum method employs the classical continuum mechanics framework and the constitutive relations are extracted from the atomistic description. For finite temperature solid systems under isothermal conditions, the constitutive relation is determined by using the Helmholtz free energy density. In this work, five different quasi-harmonic models are investigated to calculate the Helmholtz free energy density and the material properties of silicon and its nanostructures. The accuracy and efficiency of these models are also evaluated.

From the aspect of material properties, the variations of thermodynamic and mechanical properties of silicon are investigated with different temperature, strain, and surface conditions. As a promising two-dimensional material, graphene shows its excellent electrical, optical and mechanical properties in nano-technology. In this work, systematical investigations are carried out to study the strength and stiffness variations of graphene with different chiralities, sizes, temperatures, loading conditions, and defects. A theoretical expression for fracture strength of graphene as a function of temperature, strain rate, and defect size is developed. The accuracy is validated by MD simulation results.

Host: Chong Long Fu (574-5161, fucl@ornl.gov)