Mechanical Properties of Nanoscale Materials Studied by Lattice Green's Function and Molecular Dynamics Methods

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The mechanical properties of nanoscale sp-bonded materials like nanographene, nanographite, and related nanoscale materials have been studied using the lattice Green's function method (LGF). Firstly, the properties of cracks and dislocations in the two-dimensional 2D graphene sheets are investigated by using the LGF. The LGF's have been determined by solving the "Dyson" equation and taking into account three-body atomic forces among the constituent atoms. After the lattice Green's functions of the absolute zero temperature have been determined, the lattice parameters and interatomic force constants are adjusted to fit to the nanomaterials at finite temperature T for simulating the mechanical properties at temperature T. We calculate the crack stability diagrams for crack extention (lattice trapping) and dislocation emissions at the cohesive region of the cracks. The fracture and strength properties are also investigated for the nanocrystalline materials like quasi one-dimensional (1D) quantum wire and nanotubes. The O(N) tight-binding molecular dynamics (TBMD) method is used to analyze the reconstruction of atomic bonding near the crack tip as well as the cleaved surface. We compare the fracture behavior of nanoscale materials with those of corresponding bulk-size materials.