Abstract for an Invited Paper
for the MAR09 Meeting of
The American Physical Society

New Routes Toward Nanotube Synthesis: Computation and Experiment[1]

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The nanotechnology of the future demands controlled and consistent fabrication of different classes of nanostructures. Computational nanoscience can play an important role in the development of novel nanofabrication techniques. By revealing the fundamental differences in the mechanical bending behavior of nanofilms from that of micro- and macro-films, we have carried out atomistic simulations making significant contributions to advance a novel nanofabrication approach, the so-called "nanomechanical architecture" of thin films. This approach allows fabrication of different types of nanostructures, with a high level of control over their size and shape based on a priori theoretical/computational designs. The simulations have revealed a self-bending mechanism of Si (Ge) nanofilms leading to formation of pure Si (Ge) nanotubes, which greatly broadens the repertoire of nanotubes that can be made from multilayer films. Furthermore, applying the principle of nanomechanical architecture to the extreme case of the thinnest film possible, a single atomic layer of patterned graphene sheet, a new method for synthesizing carbon nanotubes with an unprecedented control over their size and chirality was proposed.

[1]The work is supported by DOE