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MD Simulation of Structural and Mechanical Transformation of Single-Walled Carbon Nanotubes Under Pressure

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Abstract. We investigate the structural and mechanical properties of single-walled carbon nanotubes (SWNTs) under hydrostatic pressure, using constant-pressure molecular dynamics (MD) simulations. We observed that all the SWNTs, independent of their size and chirality, behave like a classical elastic ring exhibiting a buckling transition transforming their cross-sectional shape from a circle to an ellipse. The simulated critical transition pressure agrees well with the prediction from continuum mechanics theory, even for the smallest SWNT with a radius of 0.4nm. Accompanying the buckling shape transition, there is a mechanical hardness transition, upon which the radial moduli of the SWNTs decrease by two orders of magnitude. Further increase of pressure will eventually lead to a second transition from an elliptical to a peanut shape. The ratio of the second shape transition pressure over the first one is found to be very close to a constant of $\sim$1.2, independent of the tube size and chirality.

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Key words: Carbon nanotube, high-pressure solid-state phase transformation, MD simulation.

1 Introduction

The discovery of carbon nanotubes [1] has opened up a new area for experimental and theoretical research. Carbon nanotubes have exhibited many fascinating properties as well as intriguing structure-property relationships. For example, the mechanical properties of carbon nanotubes have been extensively studied, with a wide range of potential

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applications, such as to be used as the strengthening elements in composites. Single-walled carbon nanotubes (SWNT) can be either metallic or semi-conducting depending on their size and chirality [2], and the correlations between their electrical property and mechanical deformation have been studied both experimentally [3–7] and theoretically [8–15] for potential applications as nano-elements in electromechanical devices [13, 16]. First-principles calculations have shown that armchair metallic SWNTs may become semiconductor under a large flattening distortion [15]; while band gap of zigzag semiconductor SWNTs display a high sensitivity to external strain [9].

One way to study the structural and mechanical properties of carbon nanotubes is by applying hydrostatic pressure. A number of high-pressure experiments have been carried out on bundles of SWNTs [17–21], showing pressure induced structural transitions in the range of 1-2 *GPa* [17–19]. Recent experiments also showed that pressure may induce transitions in electrical and magneto transport properties in SWNT bundles [22], which correlate closely with the pressure induced structural shape transitions [22]. In parallel, extensive theoretical studies, ranging from first-principles calculations [23–25], molecular dynamics (MD) simulations [25–27], to continuum mechanics modeling [25, 27] have been performed by several groups to study properties of both isolated single SWNTs and bundles of SWNTs under pressure.

For isolated single tubes, so far theoretical studies have mostly focused on armchair and zigzag tubes [25, 27] under pressure, which have a high symmetrical radial atomic structure and a short axial period. It has been shown that pressure induces a series of shape transitions in both armchair and zigzag SWNTs, transforming their cross sections from a circle to an elliptical and then from an elliptical to a peanut shape [27]. And a universal geometric constant was discovered to define these two shape transitions [27]. Furthermore, a mechanical (hardness) transition was found at the first shape transition, at which the radial moduli of SWNTs decrease by as much as two orders of magnitude [25]. Here, we report constant-pressure MD simulations of isolated SWNTs to investigate their shape and mechanical transitions under hydrostatic pressure. In particular, we extend previous works to chiral tubes to complete a systematic study of all three types of tubes (armchair, zigzag and chiral). We will present some details of the method for atomic volume partition in all three types of tubes, to facilitate the constant-pressure MD simulations of a finite system. Our simulations show that all three types of tubes behave, essentially, in the same manner under pressure. They follow closely the prediction of isotropic continuum mechanics analysis, down to the smallest tubes we simulated with a radius of 0.4nm.

2 Calculation details

The molecular dynamics (MD) method is a powerful simulation tool, widely used in chemistry, physics and materials science [28], but the traditional constant-pressure MD method is designed for an infinite system with periodic boundary conditions and cannot