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Effects of nanobuds and heat welded nanobuds chains on mechanical behavior of carbon nanotubes

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ABSTRACT

This study reports an investigation on the effects of nanobuds and heat welded nanobuds chains (C_{60} chains attached or embedded on the surface of a SWCNT) on the mechanical properties of carbon nanotubes by molecular dynamics (MD) simulations. The bond order change and the stress concentration in the distorted connection area of nanobuds when C_{60} attaches to the surface of the SWCNT are first studied. Then the effect of multiple randomly scattered and attached C_{60} fullerenes on the ultimate tensile strength of SWCNT is discussed. It is found that both nanobuds and heat welded nanobuds chains lower the ultimate tensile strength of individual defect-free SWCNT. However, the mean post-peak strength of the CNT (after necking) is significantly enhanced by heat welded nanobuds chains. Moreover, the ultimate tensile strength of the SWCNT with vacancy defects does not decrease by heat welded nanobuds chains; interestingly, the maximum tensile strength of the SWCNTs bundles with inter-tube bridging and vacancy defects even can be enhanced by more than 20% by heat welded nanobuds chains.

1. Introduction

Fullerenes and carbon nanotubes (CNTs) have attracted a great deal of attention due to their unique physical and chemical properties [1–8]. Experimental and theoretical studies have shown that fullerenes and CNTs can be combined into nanobuds by covalently bonding fullerenes to the outer wall of carbon nanotubes, and nanobuds exhibit properties of both CNTs and fullerenes [9–14]. Nanobuds can be used as molecular anchors to prevent slipping of SWNTs in composites, thus improving the composite's mechanical properties [9]. Additionally, nanobuds possess high emission characteristics and are promising for the development of new types of vacuum electronic devices [9,12]. In recent years, the properties of nanobuds have been extensively studied, including their structures [15–18], electronic properties [19–20], chemical properties [21–24], thermal transport properties [25], magnetic properties [26] and mechanical property [14,19]. Our recent study also showed that nanobuds can promote heat welding of carbon nanotubes and SWCNTs independent of their diameters can be welded together via nanobuds even at a temperature below 1500 K [27].

It is well-known that point defects on carbon nanotubes adversely affect their mechanical properties in general, and thus nanobuds with embedding configuration should lower the stiffness and strength of carbon nanotubes. However, it should be different for nanobuds with attaching configuration where both the structure of fullerene and carbon nanotube in one nanobud are defect-free [28]. We have reported the effect of bombardment formed nanobuds with attaching configuration on the tensile strength of carbon nanotube [14], however the bombardment formed nanobuds with attaching configuration is not so typical because their distortion and stress concentration in the connection area between C_{60} and the SWCNT by collision are generally more serious than those nanobuds synthesized by chemical functionalization or formed by applying pressure [27]. More importantly, how the nanobuds with attaching configuration affect the tensile strength of carbon nanotubes is not fully understood at present, and how multiple attached C_{60} molecules or nanobuds chain with attaching configuration will affect the tensile strength of carbon nanotubes still need to be investigated.

Based on the above discussion, this paper has examined the tensile strength of SWCNTs with nanobuds or nanobuds chain with attaching configuration formed by applying pressure. A series of

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molecular dynamics (MD) simulations are conducted to test how the nanobuds or nanobuds chain with attaching configuration will affect the tensile strength of carbon nanotubes. First, nanobuds with attaching configuration formed by applying pressure are investigated for their effect on the tensile strength of SWCNTs; the bond order change and the stress concentration in the distorted connection area of nanobuds when C_{60} attaches to the surface of the SWCNT are studied, and the effect of multiple randomly scattered and attached C_{60} fullerenes on the ultimate tensile strength of SWCNT is discussed. Then, the effects of heat welded nanobuds chain on the tensile strength of CNT with or without defects are also presented and discussed in details. In the following works, the temperatures for getting the mechanical behavior of SWCNT are 300 K.

2. Effects of individual Nanobud with attaching configuration on the Mechanical Behavior of SWCNT

Different from the C_{60} bombardment formed nanobuds with attaching configuration, the configuration and the electronic structures of the nanobuds formed by applying pressure are more similar to those synthesized by chemical functionalization. The simulation method of the nanobuds formation by applying pressure has been described in details in our previous works [27] and will be employed in this work as well. In the simulations, the initial distance between C_{60} and single-walled CNT (SWCNT) is set to a certain value ranging from 0.8 to 1.6 Å which is less than the van der Waals distance of 3.4 Å, and thus the effect is similar to applying a pressure to make the C_{60} and CNT close. Since no constraints are set, any atoms are free to move during the simulations. If interlinking bonds between C_{60} and CNT form, the structures will equilibrate at 300 K in 0.2 ns with a fixed timestep 0.5 fs using the Nosé–Hoover thermostat. Four typical nanobuds A, B, C and D with respective number of interconnected bonds 1, 3, 4 and 5 as formed by applying pressure with the attaching configuration are shown in Fig. 1. The details of the configuration of the nanobuds in which the atoms of the interconnected bonds in both tubes and C_{60} are highlighted in yellow color as shown in Fig. 2.

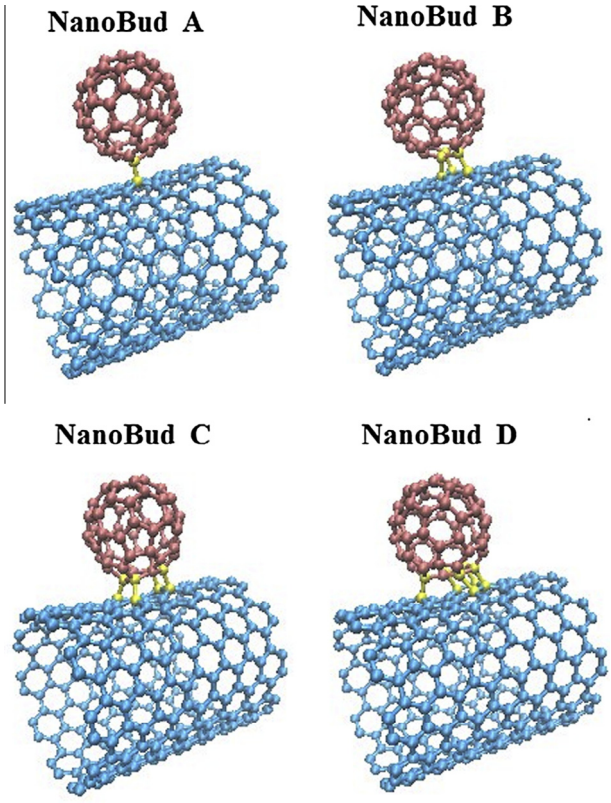

Fig. 1. Typical nanobuds with attaching configuration formed by applying pressure.

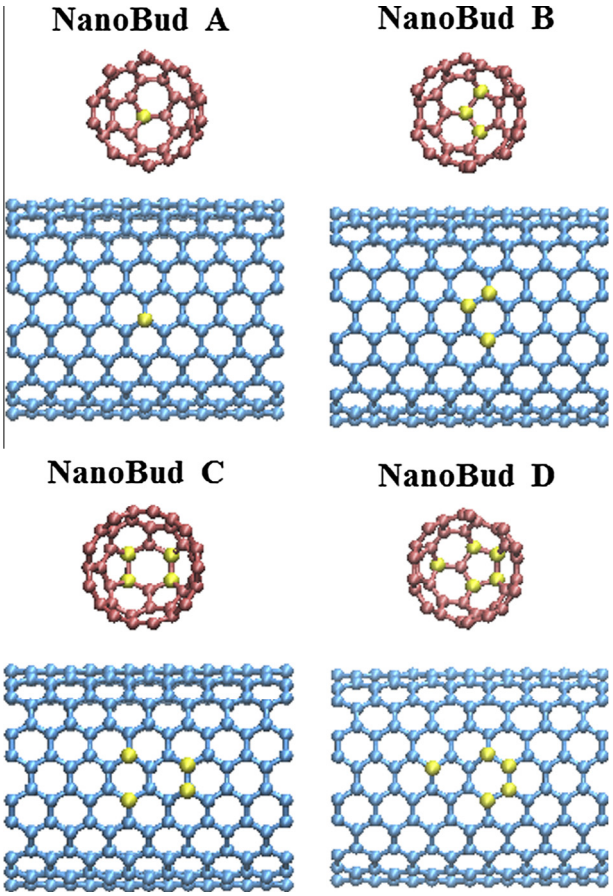

Fig. 2. Pattern of the atoms involved in the formation of the different nanobuds.

The second generation Reactive Empirical Bond Order (REBO) potential proposed by Brenner [29], which has been used widely to study the mechanical behavior of various carbon nanostructures, is employed in our MD simulations. In the MD simulations,

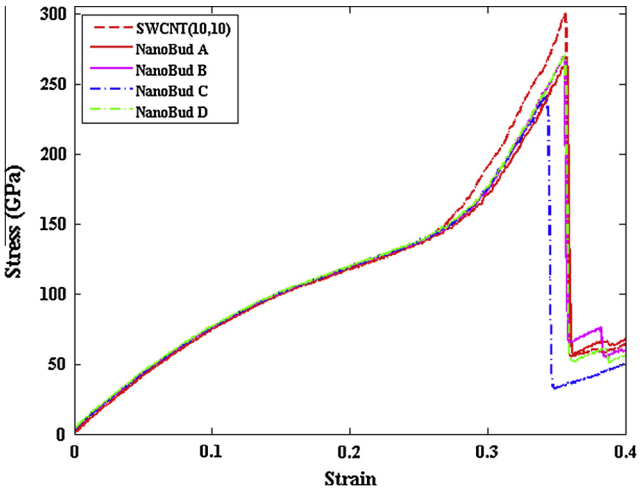

Fig. 3. Tensile stress versus strain relationships for a defect free CNT (10, 10) with or without nanobud with attaching configuration.