Compressive Buckling of Boron Nitride Nanotubes with Hydrogen Storage

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Abstract Energy and environment are two of the most significant issues for the world in the next 50 years [1]. Energy consumption is intimately linked with CO_2 emission, a major human contributor to undesirable climate change. The simplest solution to both problems lies in the use of alternative green energy sources, such as hydrogen. Hydrogen is the most abundant element on the earth and an ideal alternative energy source; it has the highest energy content per weight, it is versatile and renewable, and it is easily produced anywhere without the current geopolitical dependencies [1, 2].
However, under ambient conditions, hydrogen is a very low density gas: 10 times lower than air, demanding efficient storage systems to enable exploiting the available energy. The US Department of Energy (DOE) recently set the 2015 automotive hydrogen storage target of system gravimetric and volumetric densities of 5.5 %wt and 40 g of H_2/L [3]. Despite significant efforts, the solution has not yet been found.
Cryogenic liquid hydrogen, compressed gaseous hydrogen and metal hydrides have been investigated as possible hydrogen storage forms [4], which, however, have drawbacks such as low capacity, safety problems, or impractical release temperatures. Since the discovery of carbon nanotubes (CNTs) in 1997 [5], they were considered as a promising candidate for gas adsorption and many theoretical and experimental studies investigated the hydrogen storage capacity of these carbon nanostructures. However, detailed investigations conclude that high hydrogen storage capacity at ambient conditions, which meets the DOE targets for vehicular fuel cells, cannot occur in bare carbon nanotubes [1, 2].
The structure of Boron nitride nanotubes (BNNTs) [6, 7], which are made from group-III and -V elements neighboring C in the Periodic Table, is very similar to that of CNTs and they can be imagined as rolled up hexagonal BN layers or as CNTs in which alternating B and N atoms entirely substitute for C atoms [8]. BNNTs have outstanding physical and mechanical properties [9] and, compared to CNTs, have an enhanced chemical and high-temperature stability and exhibit superior mechanical properties at high temperatures and enhanced resistance to oxidization. Their diameters can also reach hundreds of nanometers, much greater than that of CNTs, suitable for hydrogen storage applications.
Therefore, BNNTs have been tested as a new material for hydrogen storage and studies have revealed that they have better hydrogen storage characteristics and are a better hydrogen storage medium than CNTs, which is partly explained by the increased tube-hydrogen interactions due to the polar nature of their bonds. Furthermore, Tang et al. [10], revealed an implicit relation between the structure of BNNTs and their hydrogen storage behavior, and showed that BNNTs with a collapsed structure could store up to 4.2 %wt hydrogen at room temperature.
This work investigates the effect of hydrogen storage on the mechanical properties of BNNTs (Figure 1). Molecular dynamics simulations have been performed to study the buckling behavior of BNNTs under uniaxial compressive loading with different percentages of hydrogen storage (Figure 2). The structural stability and compressive resistance properties of these nanotubes were investigated in a hydrogen environment and the critical buckling loads and critical buckling strains of the nanotubes and their susceptibility were determined.

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Figures

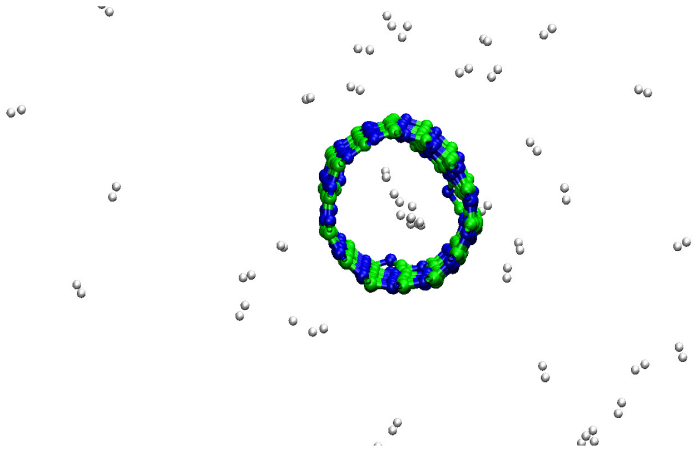

Figure 1

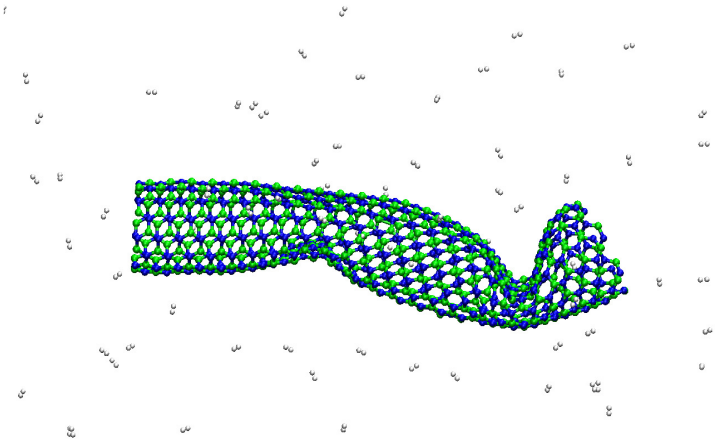

Figure 2