A Comparative Study of Armchair Carbon Nanotubes under Shear Deformation using Molecular Dynamics Simulation

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***Abstract*— The properties found so far for CNTs make them suitable for almost any application that requires high thermal conductivity, high electrical conductivity, high strength, durability and lightweight properties. A comparative study for the shear deformation of CNTs with different chirality, change in temperature, strain rates and a double walled CNT was performed. It resulted that CNTs can fracture only after experiencing great stress rates with a reduction in strain rate, but with constant strain rate a double walled nanotube is mechanically stronger. There is not much effect with change in temperature on the deformation curves of CNTs. AIREBO (Adaptive Intermolecular Reactive Empirical Bond Order) is the potential used in the paper for all cases of carbon nanotube as it indicates a carbon environment. The potential of AIREBO depends on three terms, as it accounts for interactions between covalent bonds and Van der Waals at large atom distances.**

Keywords—Carbon Nanotubes, Molecular Dynamics Simulation, Uniaxial deformation, Mechanical strength

I. Introduction

Carbon nanotubes have extraordinary interesting characteristics that have attracted the scientific world, yet scientists still know a little about them. But the properties discovered till now make them well-suited for nearly any application requiring high thermal conductivity, high electrical conductivity, high strength, durability, and lightweight properties. Therefore, all researchers are now striving to discover the mechanism of growth of the CNTs because of their huge potential in various areas. A carbon nanotube can be considered as a graphene sheet rolled into a cylinder, where the graphene is a single layer of carbon atoms bonded together by the carbon – carbon bonds (covalent bonds). It is regarded as one of the thinnest materials discovered, and also the strongest [1].

II. Numerical Modeling

The potential used in the paper is AIREBO [2] for all carbon nanotube cases as it demonstrates a carbon environment. The AIREBO potential depend on three terms as denoted by the equation below as it accounts for covalent bonds and van der Waals interactions at large distances between atoms.

$$\mathrm{E} = \frac{1}{2}\sum_{i}\sum_{j\neq i}[E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k\neq i,j}\sum_{l\neq i,j,k} E_{kijl}^{TORSION}]$$

E^{REBO} has the same functional form as the possible REBO hydrocarbons formed in Brenner [3]. For AIREBO the coefficients for are the same as the potential of Brenner, but some designed spline values are slightly dissimilar. The AREBO would mostly create forces, energies and statistical average similar to its derived REBO potential. Using a form like the typical Lennard Jones potential, the E^{LJ} term encounters long raged interactions (2<r<cutoff). The parameter E^{LJ} in AIREBO contains several switching functions to prevent the short-range LJ repulsion, and $E^{TORSION}$ is an explicit four-body potential that defines the different dihedral angle preferences in carbon atom configurations.

For equilibration, energy minimization and a constant temperature and pressure (NPT) ensemble was used for 100 ps, and the uniaxial deformation was performed with the use of the same ensemble.

III. Molecular Dynamics Cases

The carbon nanotubes for all cases will be for an Armchair pattern with bond length and height of 0.1418 and 8 nanometers. The cases were modelled using Visual Molecular Dynamics modeler [4] and simulation was performed using LAMMPS [5]. The following tables below contains information of the variable parameters in the cases:

TABLE I. CNTs with Different Chirality

	CNT 1	CNT 2	CNT 3
Chirality (n,m)	4,4	6,6	8,8
Temperature (K)	300	Stain Rate (s^{-1})	10^{10}

TABLE II. CNTs Placed in Different Temperature Systems

	CNT 4	CNT 5	CNT 6
Temperature (K)	200	300	400
Chirality (n,m)	6,6	Stain Rate (s^{-1})	10^{10}

TABLE III. CNTs under Different Strain Rates

	CNT 7	CNT 8	CNT 9
Stain Rate (s^{-1})	10^{9}	10^{10}	10^{11}
Temperature (K)	300	Chirality (n,m)	6,6

TABLE IV. Comparison of Single and Double Walled CNT

	CNT 1	CNT 2	CNT 3
Chirality (n,m)	6,6	Wall1: 4,4 Wall 2: 6,6	Wall 1: 4,4 Wall 2: 8,8
Temperature (K)	300	Stain Rate (s^{-1})	10^{10}

IV. Results and Discussion

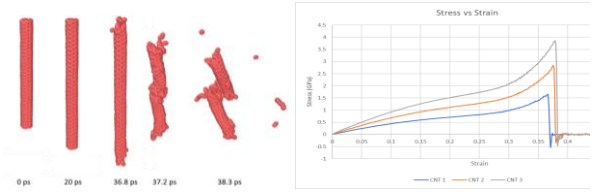

Figure 1: CNT of Chirality (4,4) under Uniaxial Deformation
Figure 2: Stress vs Strain Curves for Different Chirality

From Figure 2, the simulation results showed that the carbon nanotube with the highest chiral value showed greater strength than the ones with smaller chiral values and higher value of young's modulus.

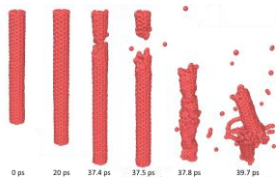

Figure 3: CNT of Chirality (6,6) at 400K

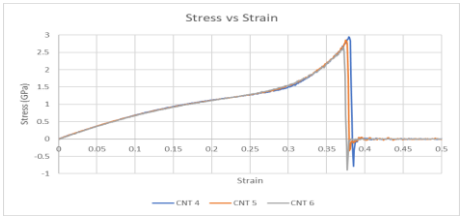

Figure 4: Stress vs Strain Curves for Change in Temperature

Based on Figure 4, the temperature was changed by 100 K in each case, and with lower the temperature, the carbon nanotube demonstrates a slightly stronger mechanical behavior, but the all three curves follow the same path initially. This could be accounted mainly due to the NPT ensemble as with higher temperature, the nanotube shows greater thermal vibrations due to greater energies in its atoms; thus, it fractures by a split percentage of strain before the ones with lower temperature.

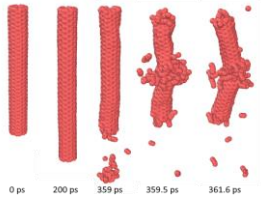

Figure 5: CNT of Chirality (6,6) at $10^9 s^{-1}$ strain rate

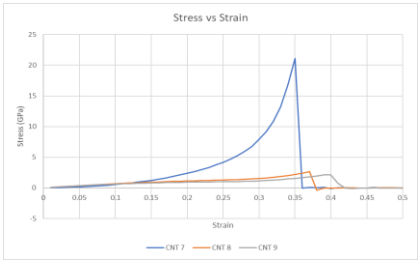

Figure 6: Stress vs Strain Curves for Change in Strain Rate

From figure 6, change in the strain rate affects drastically on the fracture point especially with respect to stress. At lower strain rates the CNTs can withstand more stress before it fractures, but the CNT will fracture faster than the cases with higher strain rates. Further, it can also be implied that the young's modulus is greater for lower strain rates.

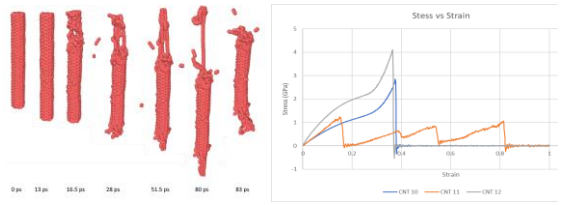

Figure 7: Double walled Carbon Nanotube with Chirality (4,4) and (6,6)
Figure 8: Stress vs Strain Curves for Change in Number of Walls for CNT

The curves in Figure 8 demonstrates a single walled CNT and two double walled CNTs; however, the double walled CNTs displayed curves with variable characteristics. One of the double walled nanotubes was created with chirality (4,4) and (6,6) and the other was with chirality (4,4) and (8,8). CNT 11 fractures under less stress because the walls were very close to each other and there were collisions with the walls under the influence of the thermodynamically ensemble. However, the nanotube completely fractures only after a Strain of 0.82 as strains of carbon atoms would tend to hold the fragments of the CNT even after the first major fracture. On the other hand, CNT 12 showed considerable strength, and is the strongest nanotube from all the previous cases for the given strain rate.

V. Conclusion

Based on the above cases obtained from the simulation by using AIREBO potential, it is noted that with the reduction in strain rate, the CNT will fracture only after experiencing great levels of stress. Moreover, this case will also result in a greater young's modulus. However, if the strain rate is kept constant that a double walled nanotube will be mechanically strongly if the walls are regularly placed. The curve obtained by closely placed CNT walls contains the most about of irregularities and will completely fracture only after a high strain value. Temperature has very little effect on the mechanical strength on CNTs.

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