6

OTHER RESEARCH ACTIVITIES

Among other research activities, the mechanical properties of Penta-Graphene nanostructures are investigated. The Stress-Strain behaviour of Penta-Graphene nanowire has been estimated using molecular dynamics simulations. The mass density of Penta-Graphene nanotube is determined for the first time in the literature.

Inside

- Mechanical properties of Penta-Graphene nanowire using molecular dynamics simulation
- Structural properties of Penta-Graphene nanotube
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6.1 Mechanical properties of Penta-Graphene nanowire using molecular dynamics simulation

The Penta-Graphene structure (Figure 6.1) is consist of five carbon atoms connected with two different bonds. Unlike the graphene structures, which are in monoplane, the Penta-Graphene structures are found in different planes. The molecular simulation studies are used to investigate

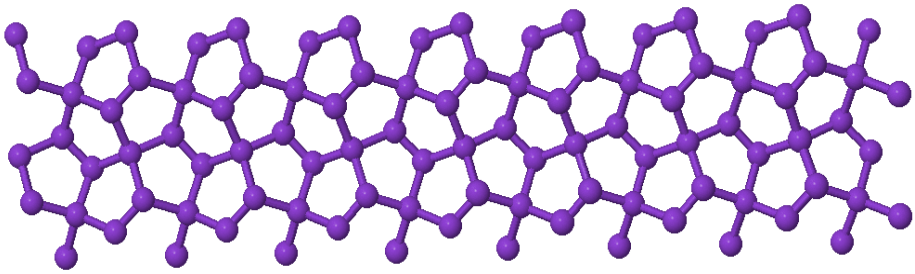

Figure 6.1 Penta-Graphene nanowire

the critical strain/strain of Penta-Graphene nanowire. The Tersoff potential has been considered in the present study. It has been observed that the stress-strain curve of Penta-Graphene nanowire (Figure 6.2) is not linear when compared with Carbon nanowire, which is linear. This might be due to the Penta-Graphene atoms are located in different planes in comparison with carbon nanowire, which are in monoplane.

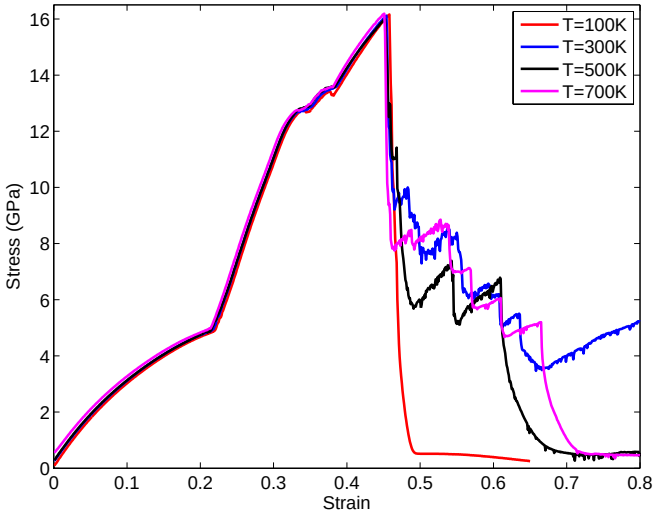

Figure 6.2 Stress-Strain Curve of Penta-Graphene nanowire

6.2 Structural properties of Penta-Graphene nanotube

The structural properties of Penta-Graphene nanotube like length of unit cell along tube axis (T), the atoms in one unit cell (N), Translational vectors and Chiral angles are found out using mathematical expression with different chirality shapes for the first time. Table 6.1 shows the structural parameters of different chirality (n, m) of Penta-Graphene nanotubes like Armchair, Zigzag and Chiral.

Table: 6.1 Structural Parameters of Penta-Graphene nanotube

Type of Penta-Graphene Nanotube	(n,m)	T (Angstrom)	N
Armchair	(3,3)	5.15	36
	(6,3)	8.14	90
Zigzag	(7,0)	3.64	42
	(8,0)	3.64	48
Chiral	(7,7)	5.15	84
	(5,10)	8.14	150
	(9,9)	5.15	108

6.3 Mass density of Penta-Graphene nanotube

For the first time, the mass density of the Penta-Graphene nanotube has been reported for various diameters (Figure 6.3). It has been observed that the Mass density of Penta-Graphene nanotube increases with the increasing diameter for short diameter tubes in the range of up to 0-5 nm. But the diameter in the range of 6-25 nm, the mass density decreases with the increasing diameter of Penta-Graphene nanotube.

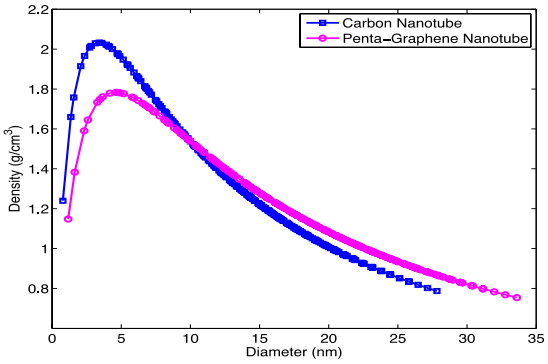

Figure 6.3 Mass density comparison of Penta-Graphene nanotube with Carbon nanotube

6.4 Wave dispersion of penta-graphene nanorod

Various types of nonlocal continuum model like Challamel, Born-Karman, Stress-Gradient, bi-Helmholtz, 2nd Order and 4th Order with stress and strain gradient approach are investigated for the wave propagation of Penta-Graphene nanorod. The Born-Karman model, which is based on the atomic approach, predicts the dispersion characteristics (Figure 6.4) correctly. Among the other models, the Challamel model predicts close agreement of dispersion behaviour in comparison with Born-Karman model. It is interesting to observe that the Challamel model works beyond the first Brillouion zone where as the other models fail.

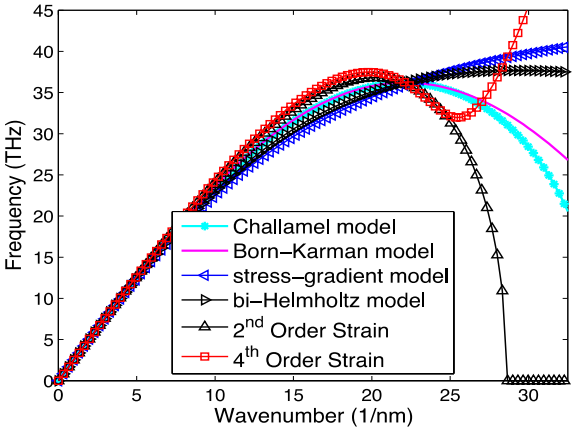

Figure: 6.4 Beyond First Brillouion