International Journal of Materials Science ISSN 0973-4589 Volume 12, Number 1 (2017)

Theoretical Prediction of Equation of State for Carbon Nanotube Bundle

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Abstract- The elastic properties of Carbon nanotubes have been matter of great interest among scientific community due to their potential uses in the devices exploiting their unusual mechanical and electronic properties. Experimentally it has also been observed that the elastic behavior of carbon nanotubes to the stress are very important due to their excellent applications in the engineering, industry and medical field. But the appropriate theoretical model for the prediction of mechanical behavior of carbon nanotube bundles is still lacking. Equation of state for solids developed by Holzaplef and Vinet have been used here to determine the pressure-volume relationships, bulk modulus and its pressure derivatives for single carbon nano tube bundle. The obtained results using Holzaplef EOS and Vinet EOS are in close agreement with the experimental data. The result for P, K_T and dK_T/dP at different compressions has been used to study the relationship between K_T and K'_T with P.

Keywords: Equation of state, Pressure-volume relationship, Pressure derivatives, CNT, Bulk modulus and derivatives of bulk modulus.

Introduction: The elastic properties of Carbon nanotubes were widely studied both for promising application, e.g. in composite nanotube materials, and to gain a better understanding of this one dimensional carbon based materials. Carbon nanotubes [1] got a lot of attention due to their potential uses in the devices exploiting their unusual mechanical and electronic properties. The elastic behavior of carbon nanotubes to the external force or stress are very important due to their excellent applications in the engineering, industry and medical field[2,3]. When one sheet or multiple sheets of graphene rolled into a cylinder gives a one-dimensional structure of carbon nanotubes. Single-walled carbon nanotube bundles typically consist of several nested tubes, each like a graphene sheet bent into the cylindrical form with an overall diameter of a few nanometers. Single-walled carbon nanotubes can be classified according to different chiral angles, for example zigzag (θ =0°), armchair (θ = 30°), and chiral tubes (0° < θ < 30°) [4]. The elastic properties such as Young's modulus and Poisson's ratio of nanotube have been studied by the previous workers [5–9]. The hardness and its

important relation with mechanical properties of single-walled carbon nanotubes have been intensively studied during the last decade [6, 10].

Grain-size and grain-shape parameters have a great influence on the physical properties of materials and on geophysical processes. With the decrease of grain size, the deformation mechanism passes from dislocation-controlled creep to diffusion-controlled creep.

In present work Equation of state for solids developed by Holzaplef and Vinet have been used here to determine the pressure-volume relationships, bulk modulus and its pressure derivatives for single carbon nano tube bunle.

2. THEORY:

Shock wave reduced isotherms (SWRI) are commonly considered as most reliable EOS data for the realization of a practical pressure scale. Holzaplef considered a comparison of SWRI for different metals and also the calibration of the ruby luminescence line shift stresses as secondary pressure scale and discussed corrections for the deviatory stresses, effects from uncertainties in the theoretically derived Grüneisen parameter, to derive an EOS [11,12] called Holzepfel EOS given as:

$$P = 3K_0 x^{-5}(1-x)\exp\left[f(1-x)\right] \qquad (1)$$

where $x = \left(\frac{V}{V_0}\right)^{\frac{1}{3}}$ and $f = \frac{3}{2}\left(K_0^{'} - 3\right)$

The Vinet equation of state (EOS) based on the Rydberg potential function derived by using the thermodynamic formulation for the Grüneisen parameter [13, 14] given as

$$P = 3K_0 x^{-2}(1-x)\exp\left[\eta(1-x)\right] \qquad (2)$$

Where $\eta = \frac{3}{2}\left(K_0^{'} - 1\right)$

Expression for isothermal bulk modulus corresponding to equation (1) and (2) obtained by using relationship $K_T = -V\left(\frac{dP}{dV}\right)_T$ given as

$$K_T = \frac{1}{3} fPx - K_0 x^{-5}(4x-5)\exp\left[f(1-x)\right] \qquad (3)$$

$$K_T = K_0 x^{-2}\left[1+(\eta x+1)(1-x)\right]\exp\left\{\eta(1-x)\right\} \qquad (4)$$

The expression for first pressure derivative of isothermal bulk modulus be given as

$$K_T^{'} = \frac{\partial K_T}{\partial P} = \frac{\partial K_T}{\partial V}\frac{\partial V}{\partial P} \qquad (5)$$

Using equation (5) in equation (3) and (4) the first derivative of isothermal bulk modulus $K_T^{'}$ becomes

$$K_T^{'} = \frac{fx}{3}\left[\left(1-\frac{P}{3K_T}\right)-\frac{1}{K_T}\left(\frac{fPx}{3}-K_T\right)\right]-\frac{K_0 x^{-5}}{3K_T}(16x-25)\exp\left[f(1-x)\right] \qquad (6)$$

$$K_T^{'} = \frac{1}{3}\left[\frac{x(1-\eta)+2\eta x^2}{1+(\eta x+1)(1-x)}+\eta x+2\right] \qquad (7)$$

3. Results and Discussion

In present work Holzaplef equation of state and Vinet equation of state have been used to determine the pressure-volume relationships, bulk modulus and its pressure derivatives for carbon nano tube bundle. The input parameters are taken from [15] as given in table-1. The equation 1 & 2, used to calculate P at different compressions. Equations 3 & 4 are used to calculate K_T while equation 6 & 7 are used to calculate K_T'. The calculated values of pressure P along with its experimental values at different compressions are displayed in table-2 for carbon

nanotube bundle. The computed values of isothermal bulk modulus and its first order pressure derivative are also given in table- 2. The graph plotted between pressure P vs compression V/V_0 is depicted in Fig.1 which shows that Holzaplef EOS and Vinet EOS are in close agreement with experimental values. The analysis of graph plotted between P vs K_T (Fig.2) and P vs K_T' (Fig. 3) shows that the both equations of state are in close agreement with each other and can be used for the prediction of the variation of isothermal bulk modulus (K_T) and its first order pressure derivative (K'_T) for corbon nanotube bundles at varying pressure.

Table-1-Input values [15]

Sample	K_0(Gpa)	K_0'
Carbon-nanotube bundle	37	11

Table-2; Calculated values of P, K_T (GPa) and K_T' for Carbon nanotube Bundle

V/V_0	P (Hol)	P (VEOS)	P (Exp)	K_T (Hol)	K_T (VEOS)	K_T' (Hol)	K_T' (VOS)
1	0.00	0.00	0.00	37.00	37.00	11.00	11.00
0.9769	0.98	0.98	1.0	47.44	47.42	10.29	10.30
0.9638	1.67	1.67	1.5	54.38	54.35	9.95	9.96
0.9513	2.43	2.43	2.0	61.80	61.74	9.66	9.67
0.9425	3.03	3.03	2.5	67.54	67.45	9.47	9.48
0.94	3.21	3.21	3.0	69.26	69.15	9.42	9.43
0.935	3.59	3.59	3.5	72.81	72.67	9.32	9.33
0.9238	4.52	4.51	4.0	81.35	81.15	9.10	9.11
0.9213	4.74	4.73	4.5	83.38	83.16	9.06	9.07
0.9188	4.97	4.96	5.0	85.45	85.21	9.02	9.02
0.9088	5.95	5.94	5.5	94.22	93.90	8.84	8.85
0.9063	6.21	6.20	6.0	96.54	96.19	8.80	8.81
0.8981	7.13	7.11	6.5	104.52	104.07	8.67	8.68
0.8963	7.34	7.32	7.0	106.36	105.88	8.65	8.65
0.89	8.11	8.09	7.5	113.01	112.45	8.55	8.55
0.8875	8.43	8.41	8.0	115.75	115.15	8.52	8.51

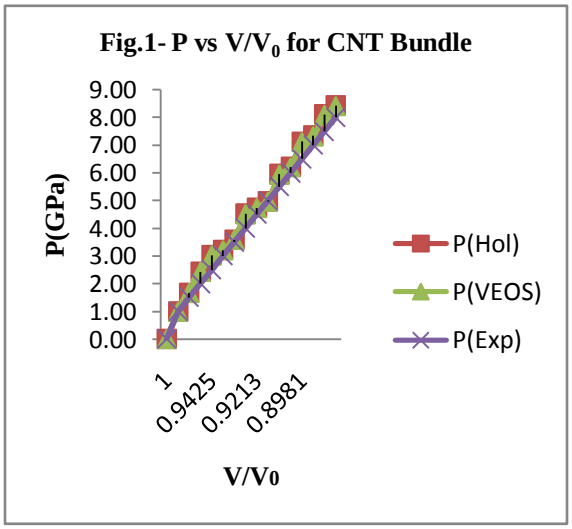

Fig. 1- Variation of Pressure with the compression ratio for the CNT Bundle

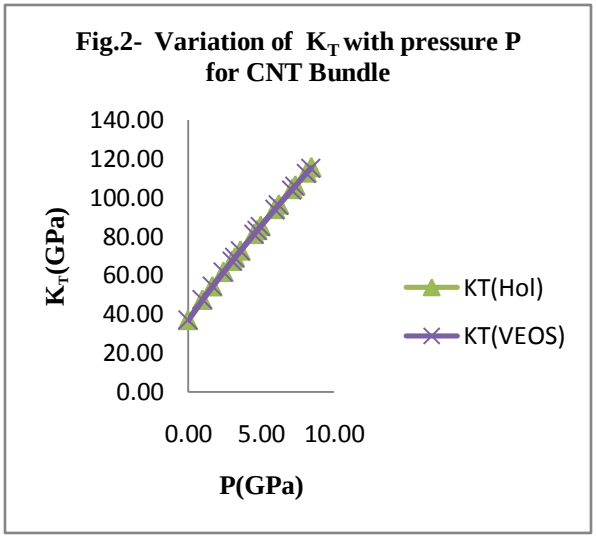

Fig. 2- Variation of K_T with Pressure for the CNT Bundle

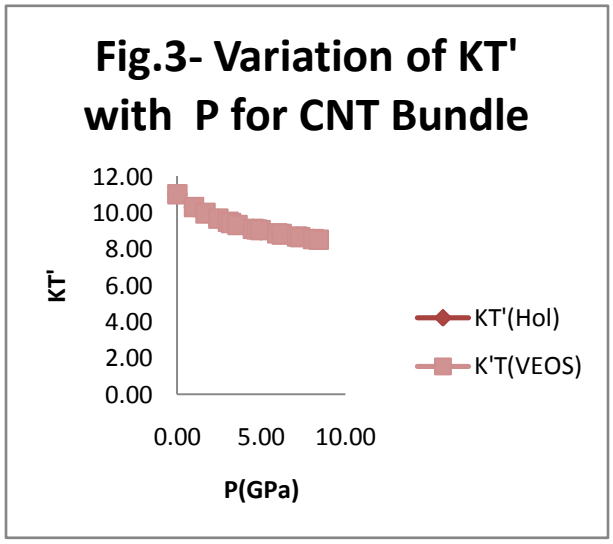

Fig. 3- Variation of K'_T with Pressure P for the CNT Bundle

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