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Pressure Dependent Compressibility of Single Carbon Nanotubes and Graphite

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Abstract

Carbon nanotubes got a lot of attention due to their unusual mechanical and electronic properties. These nanotubes show their peculiar elastic behavior to the external force or stress. Such behavior of carbon nanotubes are very important for their applications in the engineering, industry and medical field. Well known 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 and graphene. Comparing the calculated values of Pressure obtained by using Holzapfel EOS and Vineet EOS with available experimental results, it is found that Holzaplef EOS are in close agreement with the experimental data but Vinet EOS deviates with experimental data at higher compression. The result for P, K_T and dK_T/dP at different compressions has been used to study the relationship between dK_T/dP and P/K_T.

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

1. INTRODUCTION

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 variety of 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 and Graphite

2. METHODS OF ANALYSIS

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. He has also consider the effects of uncertainties in the theoretically derived Grüneisen parameter, to derive an EOS [11,12]. Holzepfel EOS is given as:

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

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] given as

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

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

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

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

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

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

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

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

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

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 single carbon nano tube and Graphene. The input parameters are given in table-1. The expression (1) and (2) has been used for calculation of Pressure P (GPa) at different compressions. Equations (3) & (4) has been used for calculation of K_T and also equations (6) and (7) has been used for calculation of K_T' at different compressions.

The calculated values of pressure P computed at different compression along with its experimental values are displayed in table-2 & table-3 for carbon nanotube and graphene respectively. The calculate values of isothermal bulk modulus and its first order pressure derivatives are also displayed in table 2 & 3. The graph (fig.1&4) plotted for pressure P vs compression V/V_0 shown in fig.1 and fig. 4 for single wall carbon nanotubes and graphene respectively. These graphs shows that Holzepfel EOS is in close agreement with experimental values. The analysis of graph plotted between P vs K_T (fig.2&5) and P vs K_T' (fig. 3 & 6) shows that the both equations of state are in close agreement with each other.

The good agreement of compression behavior of carbon nanotubes as computed by Holzepfel EOS with the available experimental results is related to the basic assumptions made for the deduction of this equation of state. Actually these assumptions are closely associated to the surface effect of atom/molecules constituting the material. While the basis of Vinet equation of state is very much related to the bulk effect of materials. Since the compression of carbon nanotubes and graphene have much effect of surface molecules so the Holzepfel EOS is more suitable to compute the results than Vinet equation of state. Other elastic parameters such as bulk modulus and its first order derivative depicting the bulk properties of the materials. These parameters are less affected by surface atom/ molecules due to this

reason both equation of states are leading almost same result.

Table 1. Input values [14]

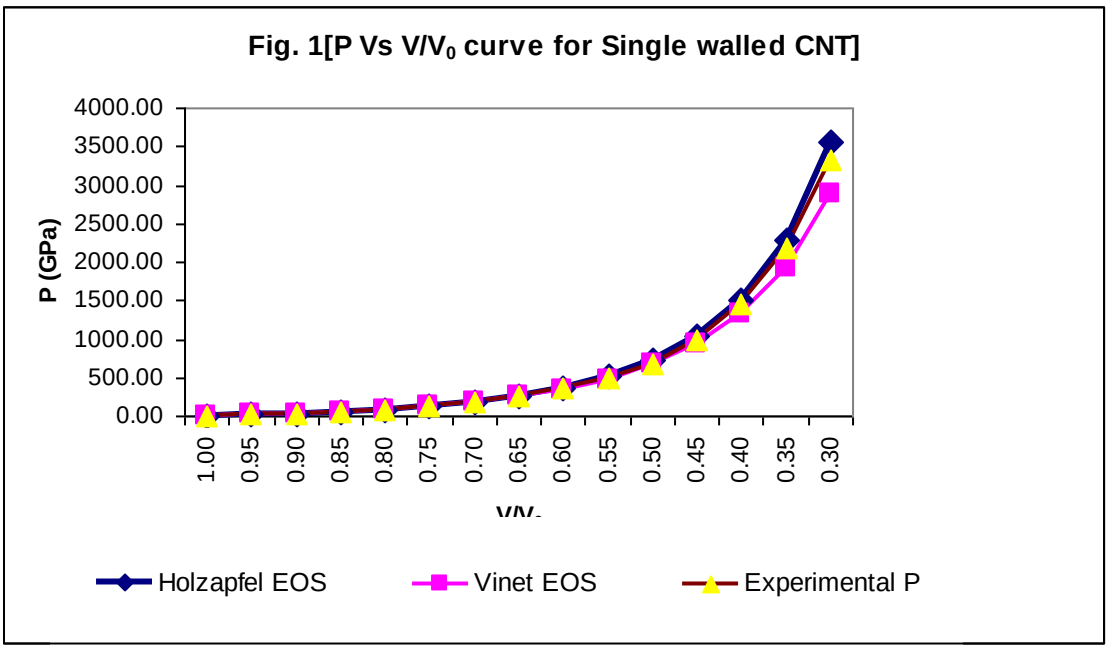
SrNo	Sample	K_0(Gpa)	K_0'
1	Inividual Carbon-nanotube	230	4.5
2	Graphene	33.8	8.9

Table 2. Calculated values of P, K_T(GPa) and K_T' for Individual Carbonnanotube

V/V_0	**P(Hol)**	**P(VEOS)**	**P(Exp)**	**K_T(Hol)**	**K_T(VEOS)**	**K_T'(Hol)**	**K'_T(VEOS)**
1.00	0.00	0.00	0.00	230.00	230.00	4.50	4.50
0.95	13.24	13.23	13.23	287.68	287.33	4.23	4.19
0.90	30.68	30.62	30.65	359.40	357.69	4.01	3.92
0.85	53.71	53.48	53.65	449.32	444.56	3.81	3.69
0.80	84.30	83.62	84.15	563.09	552.56	3.64	3.49
0.75	125.19	123.53	124.70	708.59	687.89	3.49	3.31
0.70	180.36	176.72	179.80	896.92	859.01	3.35	3.14
0.65	255.68	248.25	253.53	1144.17	1077.70	3.22	2.99
0.60	359.99	345.49	354.30	1474.13	1360.64	3.11	2.84
0.55	507.03	479.52	498.48	1923.04	1732.03	3.00	2.71
0.50	718.87	667.43	687.67	2547.96	2227.94	2.90	2.58
0.45	1032.34	936.50	998.83	3442.29	2903.86	2.81	2.45
0.40	1511.96	1332.02	1457.76	4766.36	3848.53	2.72	2.33
0.35	2277.62	1933.09	2185.74	6811.90	5210.69	2.63	2.21
0.30	3569.37	2886.71	3333.38	10150.48	7254.90	2.55	2.09

Table 3. Calculated values of P, K_T(GPa) and K_T' for Graphene

V/V_0	P(Hol)	P(VEOS)	P(Exp)	K_T(Hol)	K_T(VEOS)	K_T'(Hol)	K'_T(VEOS)
1	0	0	0	230	230	4.5	4.5
0.95	2.18	2.17	2.18	51.99	51.93	7.95	7.91
0.90	5.66	5.65	5.66	78.35	78.01	7.26	7.19
0.85	11.18	11.13	11.16	116.81	115.72	6.74	6.64
0.80	19.88	19.72	19.85	173.42	170.61	6.32	6.19
0.75	33.64	33.19	33.58	257.65	251.19	5.97	5.81
0.70	55.54	54.42	55.51	384.72	370.85	5.67	5.49
0.65	90.84	88.20	89.62	579.64	551.00	5.40	5.20
0.60	148.68	142.69	147.53	884.72	826.73	5.17	4.94
0.55	245.54	232.21	241.80	1373.82	1257.31	4.95	4.70
0.50	412.26	382.75	406.73	2181.05	1946.01	4.75	4.47
0.45	709.33	643.48	685.74	3561.08	3080.10	4.56	4.25
0.40	1262.22	1112.00	1217.76	6025.07	5015.35	4.37	4.03
0.35	2349.72	1994.28	2265.37	10670.55	8467.59	4.19	3.82
0.30	4648.35	3759.33	4369.76	20064.73	14984.54	4.01	3.59



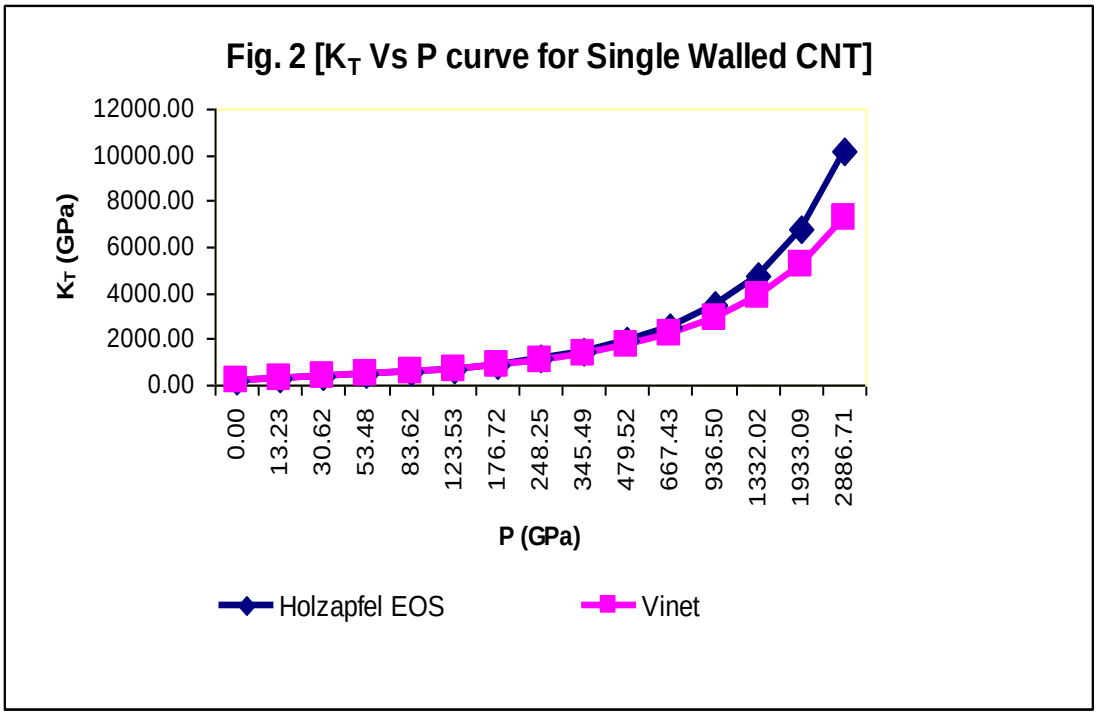


Fig. 2 [K_T Vs P curve for Single Walled CNT]
12000.00
10000.00
8000.00
6000.00
4000.00
2000.00
0.00
K_T (GPa)
0.00
13.23
30.62
53.48
83.62
123.53
176.72
248.25
345.49
479.52
667.43
936.50
1332.02
1933.09
2886.71
P (GPa)
Holzapfel EOS
Vinet

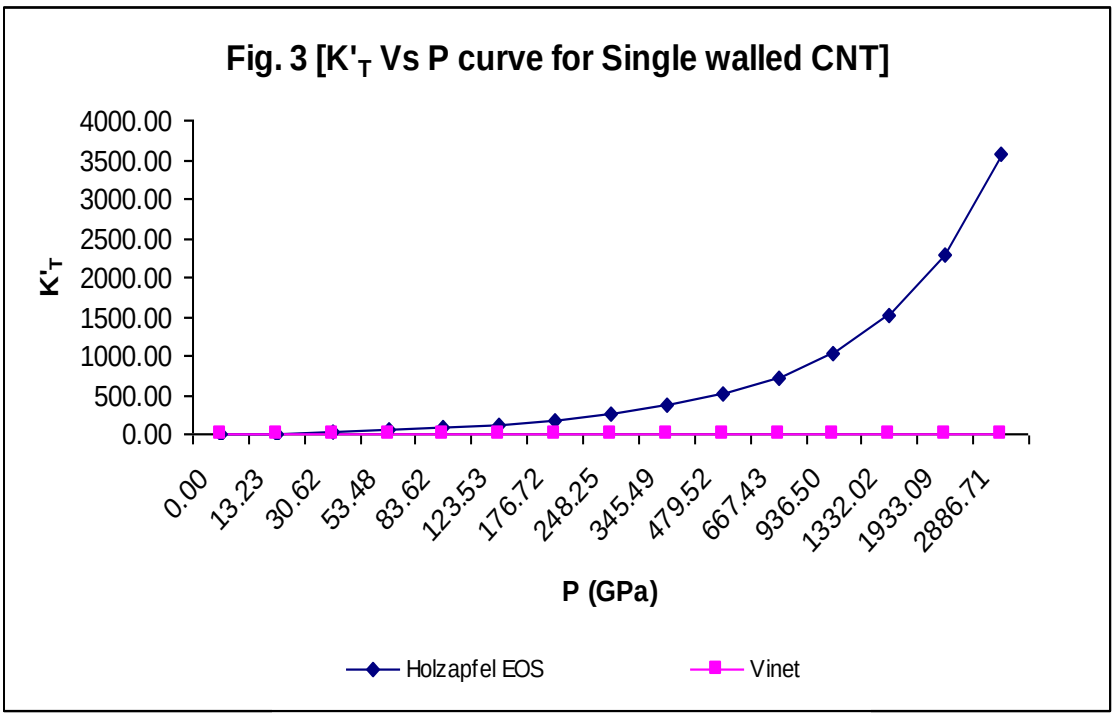


Fig. 3 [K'_T Vs P curve for Single walled CNT]
4000.00
3500.00
3000.00
2500.00
2000.00
1500.00
1000.00
500.00
0.00
K'_T
0.00
13.23
30.62
53.48
83.62
123.53
176.72
248.25
345.49
479.52
667.43
936.50
1332.02
1933.09
2886.71
P (GPa)
Holzapfel EOS
Vinet

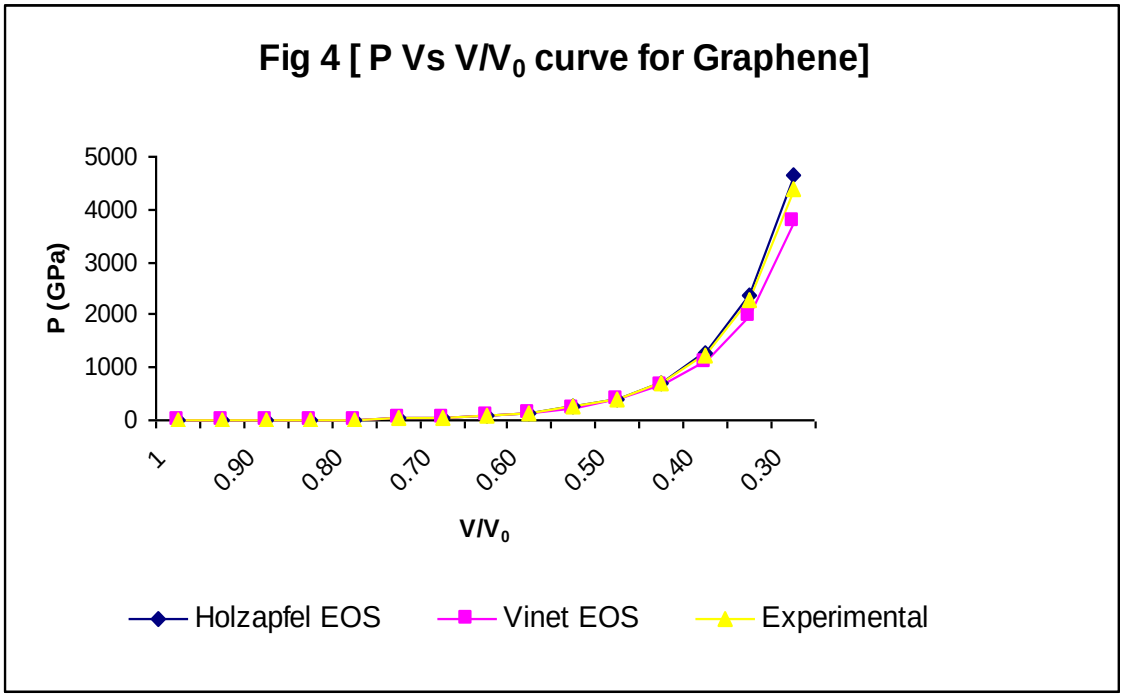


Fig 4 [P Vs V/V0 curve for Graphene]
P (GPa)
5000
4000
3000
2000
1000
0
1
0.90
0.80
0.70
0.60
0.50
0.40
0.30
V/V0
Holzapfel EOS
Vinet EOS
Experimental

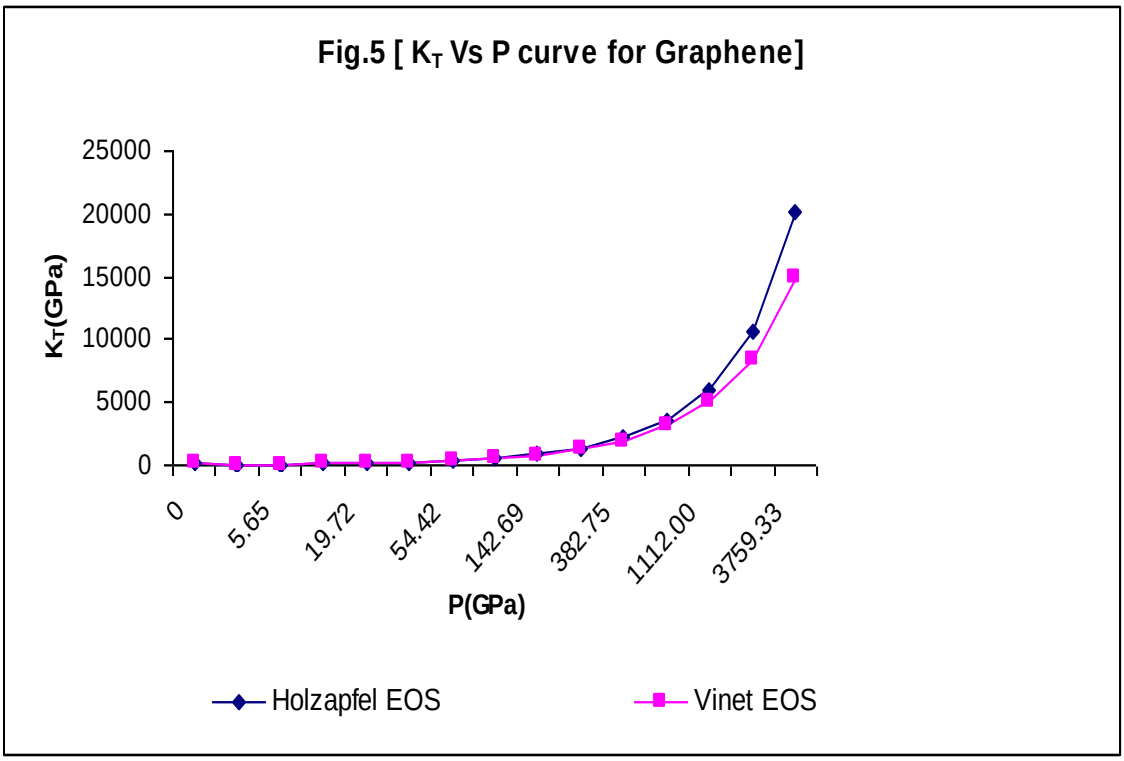
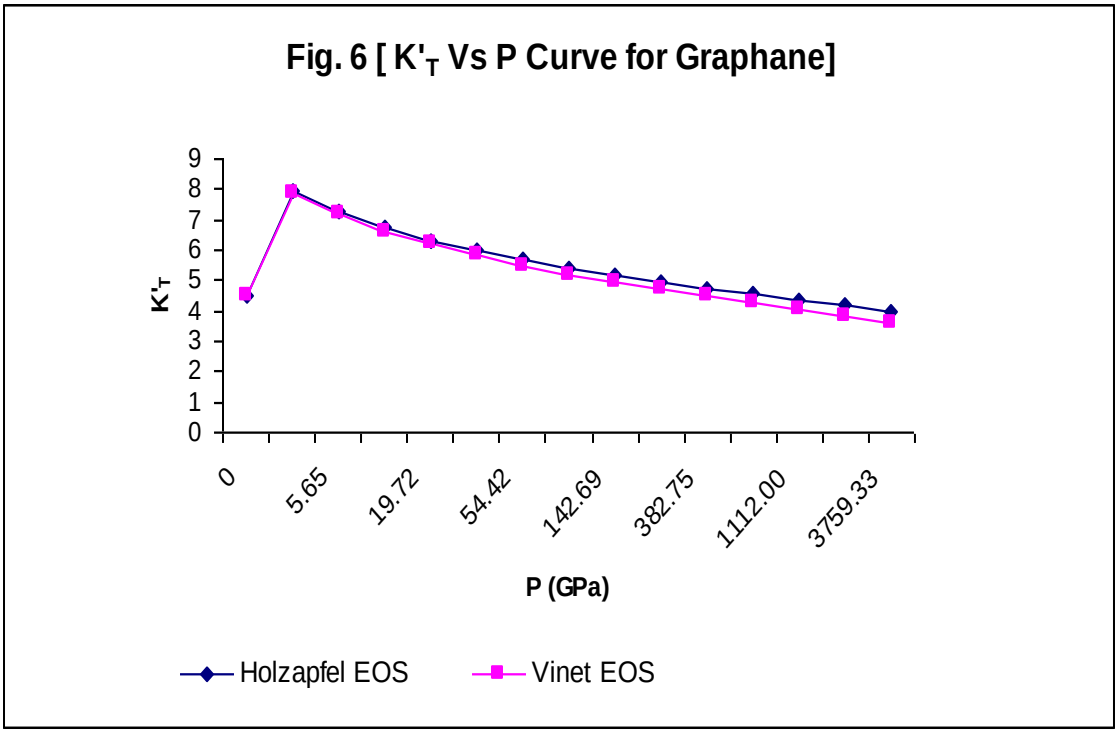


Fig.5 [KT Vs P curve for Graphene]
KT(GPa)
25000
20000
15000
10000
5000
0
0
5.65
19.72
54.42
142.69
382.75
1112.00
3759.33
P(GPa)
Holzapfel EOS
Vinet EOS



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