Stress and strain along radial and axial directions in single-walled carbon nanotubes at high temperatures

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Abstract— ***In this paper we derive expression of radial and axial stress, strain for (n,n) armchair, (n,0) zigzag and (n,m) chiral single-walled carbon nanotubes in terms of thermal expansion and calculate these parameters above room temperature (T >300 K). With the help of stress and strain we also calculate Young's modulus and Poisson's ratio. We have found that radial and axial stress both decreases with increase in temperature and axial stress is higher than the radial stress. Radial and axial stresses both are higher for (9,0) SWCNT than (5,5) SWCNT. Radial strain increases equally with increase in temperature for all type of SWCNT and does not depends upon the type of nanotube while axial strain is higher for (5,5) than (9,0) SWCNT.***

Keywords — ***Stress, Strain, Young's modulus, Poisson's ratio and interatomic potential.***

I. Introduction

Carbon nanotubes (CNTs) [1] have extraordinary material properties [2-10], which make them to a verity of application [11-14]. The CNT based nanoelectronic devices [15-20] may experience high temperature during manufacture and operation. This leads to thermal expansion and residual stress in devices, and affects the device reliability. Therefore, thermal expansion, stress, strain and Young modulus of carbon nanotubes are important properties for CNT-based nanoelectronics. In view of the wide application of CNTs for producing carbon based materials, it is necessary to have good knowledge of their properties at high temperatures.

Mechanical properties of carbon nanotubes have been studied by several workers [21-25] by using different experimental techniques and theoretical approaches. Lourie and Wagner [21] obtained the axial Young modulus for a series of temperature by micro-Raman spectroscopy from measurements of cooling-induced compressive deformation of nanotubes embedded in an epoxy matrix. They found that Young's modulus is 3 TPa at 81 K for Single-walled carbon nanotubes (SWCNTs) and 2.4 TPa for Multi-walled carbon nanotubes (MWCNTs). Wong et al. [22] found Young modulus is 1.28 ± 0.5 TPa by using atomic force microscope (AFM) and measure force displacement relation for anchored multi-walled carbon nanotubes on a substrate. Sinnott et al. [23] calculated Young's modulus for SWCNT theoretically by using MD simulation. They found that SWCNT have a modulus of approximately 1.25-1.40 TPa. Yokobson et al. [24] found axial modulus for SWCNT ranges from 1.4 to 5.5 TPa by using many body interatomic potential with a continuum shell model. Zhou et al. [25] described mechanical properties of SWCNTs by applying the strain energy directly from electronic band structure without introducing empirical potentials and continuum elastic theory. The estimated value of axial modulus was 5.0 TPa. They told that Young's modulus and wall thickness are independent of the radius and helicity.

All studies on mechanical properties of SWCNTs give very high Young's modulus but the effect of high temperatures on these properties is not clear. In this paper we study the effect of high temperature on mechanical properties of (n,n) armchair, (n,m) chiral and (n,0) zigzag SWCNT and derive expressions for radial and axial stress, strain. We calculate radial and stress, strain, Young modulus at high temperatures (T > 300) for (5,5), (7,3) and (9,0) SWCNTs by using thermal expansion data [26]. These parameters are also calculated in axial direction for only two (5,5) and (9,0) SWCNTs due to shortage of axial thermal expansion data. We also obtain Poisson's ratio for (5,5) and (9,0) SWCNTs. We compare these results with each other and find the effect of high temperatures on mechanical properties of SWCNTs.

II. Method of Analysis

In structure of SWCNT we take four atoms A, B, C and D (as shown in figure 1and 2) because other atoms show symmetry of these four atoms. In these figures r_{AB}, r_{AC} and r_{AD} are bond lengths; ∠BAC, ∠CAD and ∠DAB are bond angles; a_1, a_2 and a_3 are distance between atom B and C, atom D and C and atom B and D respectively. Angle DBC represented by ϕ_1 and angle ABC is represented by ϕ_2. $\mathbf{C_h}$ is chairl vector and θ is chairl angle.

Rise in temperature employ a stress in CNT which lead to thermal expansion. This stress can be in radial and axial direction in CNTs. Therefore, radial and axial thermal expansion takes place due to radial and axial stresses. Thermal expansion is different at different temperatures due to different stresses. When thermal expansion takes place in single walled carbon nanotubes a work is done, this will be equal to interatomic potential between carbon-carbon atoms of SWCNTs. Interatomic potential can be given by [27]

$$V(r) = -\frac{A}{r^6} + B\exp(-\alpha r) \tag{1}$$

where V(r) is the interatomic potential between C-C atoms. A, B and α are interaction parameters. The value of A is 358 kcal/mole-A^6, B is 42000 kcal/mole and α is 3.58 A^{-1}. In radial thermal expansion, a force work in radial direction which can be written in terms of interatomic potential for all type of SWCNT as

$$F_{radial} = \frac{V(r)}{(d'_t - d_t)} \tag{2}$$

where F_{radial} is force in radial direction, V(r) is interatomic potential, d_t is the diameter of tube at initial temperature (T = 300K) and d_t' is the diameter of tube at final temperature. (d_t'- d_t) gives change in diameter at a particular temperature, which is equal to the displacement at that temperature. Radial stress can be written as

$$stress_{radial} = \frac{F_{radial}}{A} = \frac{V(r)}{A(d'_t - d_t)} \tag{3}$$

where A is the cross-section area of SWCNT, given as

$$A = \pi d_t t \tag{4}$$

where d_t is the diameter of tube and t is the thickness of tube which is taken as the interatomic spacing of the graphite sheet (t = 0.34nm) [28]. In axial thermal expansion a force work in axial direction which can be given in terms of interatomic potential for (n,n) armchair SWCNT as

$$Force_{axial(n,n)} = \frac{V(r)}{a_3'(T') - a_3(T)} \tag{5}$$

where $a_3(T)$ is the length of vector $\mathbf{a_3}$ (shown in figure 1) at initial temperature (T = 300K), a_3'(T') is the length of vector a_3 at final temperature and a_3'(T') – a_3(T) gives displacement in axial direction at a particular temperature. From equation (5), axial stress can be written as

$$Stress_{axial(n,n)} = \frac{Force_{axial(n,n)}}{A} = \frac{V(r)}{\{a_3'(T') - a_3(T)\}A} \tag{6}$$

Where A is the cross-section area of (n,n) armchair SWCNT. For (n,0) zigzag SWCNT force in axial direction can be given in terms of interatomic potential as

$$Force_{axial(n,0)} = \frac{V(r)}{a'_3(T')\sin'\varphi_1(T') - a_3(T)\sin\varphi_1(T)} \tag{7}$$

where $a_3(T)\sin\phi_1(T)$ is length of axial component of vector $\mathbf{a_3}$ (shown in figure 2) at initial temperature (T = 300K), $a'_3\sin'\phi_1(T')$ is length of axial component of vector $\mathbf{a_3}$ at final temperature and $a_3(T)\sin\phi_1(T)$- $a'_3\sin'\phi_1(T')$ gives displacement in axial direction at a particular temperature. Stress in axial direction can be given as

$$Stress_{axial(n,0)} = \frac{Force_{axial(n,0)}}{A} = \frac{V(r)}{\{a'_3(T')\sin'\varphi_1(T') - a_3(T)\sin\varphi_1(T)\}A} \tag{8}$$

where A is the cross-section area of (n,0) zigzag SWCNT.

Radial and axial strain in SWCNT can be obtained by thermal expansion at different temperatures. Radial thermal expansion in SWCNT is given by [26]

$$d'_t(T) - d_t(T) = \alpha_{radial}(T' - T)\, d_t(T) \tag{9}$$

where T (300K) is initial temperature, T' is final temperature, $d_t(T)$ is the diameter at initial temperature, $d_t'(T')$ is the diameter of SWCNT at final temperature and α_{radial} is the radial thermal expansion coefficient. Radial strain for all type SWCNT can be given from equation (9) as

$$strain_{radial} = \frac{d_t'(T') - d_t(T)}{d_t(T)} = \alpha_{radial}(T' - T) \tag{10}$$

For (n,n) armchair SWCNT, axial thermal expansion can be given as [26]

$$a'_3(T') - a_3(T) = \alpha_{axial}(T' - T)\, a_3(T) \tag{11}$$

where, T is the initial temperature and T' is the final temperature, $a'_3(T')$ is length BD at temperature T', $a_3(T)$ is length BD at initial temperature T. α_{axial} is the coefficient of thermal expansion in axial direction and (T'-T) is change in temperature. Axial strain for (n,n) armchair SWCNT can be given from equation (11) as

$$strain_{axial(n,n)} = \frac{a'_3(T') - a_3(T)}{a_3(T)} = \alpha_{axial}(T' - T) \tag{12}$$

For (n,0) zigzag SWCNT, axial thermal expansion can be given as [26]

$$a'_3(T')\sin'\phi_1(T') - a_3(T)\sin\phi_1(T) = \alpha_{axial}(T' - T)a_3(T)\sin\phi_1(T) \tag{13}$$

where, T is the initial temperature and T' is the final temperature, $a'_3(T')\sin'\phi_1(T')$ is the length of the component of $\mathbf{a_3}$ in axial direction at temperature T', $a_3(T)\sin\phi_1(T)$ is the length of the component of $\mathbf{a_3}$ in axial direction at temperature T. α_{axial} is the coefficient of thermal expansion in axial direction and (T'-T) is change in temperature. Axial strain for (n,0) zigzag SWCNT can be given from equation (13) as

$$strain_{axial(n,0)} = \frac{a'_3(T')\sin'\phi_1(T') - a_3(T)\sin\phi_1(T)}{a_3(T)\sin\phi_1(T)} = \alpha_{axial}(T' - T) \tag{14}$$

III. Results and Discussions

Numerical results of stress, strain, interatomic potential and Young's modulus above room temperatures for (5,5), (7,3) and (9,0) SWCNTs in radial direction are given in table 1-3 respectively and these calculated parameters in axial direction for (5,5) and (9,0) SWCNTs are given in table 4 and 5 respectively.

Figure 3 gives the variation in radial stress for (5,5), (7,3) and (9,0) SWCNTs at high temperatures (T > 300 K). This shows that (7,3) gives higher stress than (5,5) and (9,0) SWCNTs, (9,0) gives higher stress than (5,5) SWCNT. Figure 4 gives the variation in axial stress for (5,5) and (9,0) SWCNTs at high temperatures (T > 300 K). This shows that (5,5) gives higher axial stress than (9,0) SWCNT. These figures show that radial and axial stresses are decreased with increase in temperature. If we compare figure 3 and 4, it is found that radial stress is higher than axial stress at high temperatures.

Figure 5 shows the variation in radial strain for (5,5), (7,3) and (9,0) SWCNTs at high temperatures (T > 300 K). This figure shows same graph for all SWCNTs. This suggests that radial strain does not depend on type of tubes and increase equally for all types of SWCNTs with increase in temperature. Figure 4 shows the variation in axial strain for (5,5) and (9,0) SWCNTs at high temperatures (T > 300 K). This shows that (5,5) SWCNT gives higher axial strain than (9,0) SWCNT. If we compare figure 5 and 6, it is found that axial strain is higher than radial strain and both are increased with increase in temperature.

Figure 7 shows the variation in radial Young's modulus for (5,5), (7,3) and (9,0) SWCNTs at high temperatures (T > 300 K). This shows that (5,5) gives higher Young's modulus than (7,3) and (9,0), (7,3) gives higher Young's modulus than (5,5). Figure 8 gives the variation in axial Young's modulus for (5,5), (9,0) SWCNTs at high temperatures (T > 300 K). This shows that axial Young's modulus for (9,0) is higher than (5,5) SWCNT. If we compare figure 7 and 8, it is found that axial Young's modulus is greater than the radial Young's modulus and both are decreased with increase in temperature.

Figure 9 shows the variation in Poisson's ratio for (5,5) and (9,0) SWCNTs at high temperatures (T > 300 K). It is found from this figure that Poisson's ratio for (5,5) SWCNT increases with increase in temperature while for (9,0) it decreases with increase in temperature and near 900 K temperature becomes almost constant. It is clear that Poisson's ratio is higher for (9,0) than (5,5) SWCNT.

IV. CONCLUSIONS

We derive expressions for radial and axial stress, strain and find that radial and axial stresses both decrease with increase in temperature. (9,0) gives higher radial stress than (5,5) SWCNT while it hold opposite in axial direction. Radial and axial strains both increase with increase in temperature. Radial strain increases equally with increase in temperature for all type of SWCNTs while axial strain for (5,5) is higher than (9,0) SWCNT. Radial and axial Young's modulus both are higher for (9,0) than (5,5) SWCNT and decrease with increase in temperature. Poisson's ratio for (9,0) increases while decreases for (5,5) with increase in temperature and higher for (9,0) than (5,5) SWCNT. Strain and Young's modulus in axial direction are higher than that in radial direction while stress in radial direction is higher than that in axial direction.

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TABLE 1

Calculated values of interatomic potential, stress, strain and Young's modulus for (5,5) SWCNT in radial direction at high temperatures

Temperature (K)	d_t' (nm) [26]	(d_t'-d_t) (nm)	α x10^{-6} (K^{-1}) [26]	Inter-atomic potential (V) x10^{-16} Jule	(5,5) Stress x10^3 N/m^2	(5,5) Strain x10^{-6}	(5,5) Young's modulus (Y) TPa
400	0.678122	0.000013	0.20	2.298632	24423.597112	20	1.221180
500	0.678170	0.000061	0.70	2.298592	5204.571052	140	0.037176
600	0.678262	0.000153	1.36	2.298516	2074.675269	408	0.005085
700	0.678384	0.000275	1.80	2.298416	1154.015890	720	0.001603
800	0.678533	0.000424	2.20	2.298293	748.273012	1100	0.000680
900	0.678700	0.000591	2.46	2.298156	536.667898	1476	0.000364
1000	0.678884	0.000775	2.70	2.298005	409.114681	1890	0.000216
1100	0.679081	0.000972	2.91	2.297843	326.079778	2328	0.000140
1200	0.679292	0.001183	3.10	2.297669	267.816704	2790	0.000096
1300	0.679511	0.001402	3.23	2.297489	225.891740	3230	0.000070
1400	0.679735	0.001626	3.30	2.297305	194.692784	3630	0.000054
1500	0.679966	0.001857	3.40	2.297115	170.402128	4080	0.000042
1600	0.680203	0.002094	3.48	2.296920	151.050458	4524	0.000033

TABLE 2

Calculated values of interatomic potential, stress, strain and Young's modulus for (7,3) SWCNT in radial direction at high temperatures

Temperature (K)	d_t (nm) [26]	$(d_t'-d_t)$ (nm)	α x10^{-6} (K^{-1}) [26]	Inter-atomic potential (V) x10^{-16} Jule	(7,3) Stress x10^{3} N/m^2	(7,3) Strain x10^{-6}	(7,3) Young's modulus (Y) TPa
400	0.695999	0.000014	0.20	13.749485	132172.532622	20	6.608627
500	0.696050	0.000065	0.73	13.749234	28465.324517	146	0.194968
600	0.696143	0.000158	1.33	13.748776	11708.464054	399	0.029345
700	0.696265	0.000280	1.76	13.748176	6605.472826	704	0.009383
800	0.696416	0.000431	2.16	13.747432	4290.096079	1080	0.003972
900	0.696585	0.000600	2.43	13.746601	3080.784955	1458	0.002113
1000	0.696771	0.000786	2.67	13.745685	2350.959902	1869	0.001258
1100	0.696971	0.000986	2.88	13.744701	1873.419844	2304	0.000813
1200	0.697186	0.001201	3.08	13.743643	1537.452286	2772	0.000555
1300	0.697409	0.001424	3.20	13.742546	1296.167427	3200	0.000405
1400	0.697638	0.001653	3.28	13.741420	1116.143550	3608	0.000309
1500	0.697873	0.001888	3.37	13.740264	976.805537	4044	0.000242
1600	0.698114	0.002129	3.45	13.739078	865.858690	4485	0.000193

TABLE 3

Calculated values of interatomic potential, stress, strain and Young's modulus for (9,0) SWCNT in radial direction at high temperatures

Temperature (K)	d_t (nm) [26]	$(d_t'-d_t)$ (nm)	α x10^{-6} (K^{-1}) [26]	Inter-atomic potential (V) x10^{-16} Jule	(9,0) Stress x10^{3} N/m^2	(9,0) Strain x10^{-6}	(9,0) Young's modulus (Y) TPa
400	0.704992	0.000009	0.13	6.751374	99668.265463	13	7.666790
500	0.705036	0.000053	0.63	6.751268	16923.476970	126	0.134313
600	0.705124	0.000141	1.25	6.751055	6360.312672	375	0.016961
700	0.705246	0.000263	1.72	6.750760	3409.162693	688	0.004955
800	0.705395	0.000412	2.11	6.750400	2175.661608	1055	0.002062
900	0.705565	0.000582	2.41	6.749989	1539.694280	1446	0.001065
1000	0.705750	0.000767	2.63	6.749542	1167.937213	1841	0.000634
1100	0.705950	0.000967	2.83	6.749059	926.049571	2264	0.000409
1200	0.706164	0.001181	3.04	6.748542	757.959339	2736	0.000277
1300	0.706388	0.001405	3.16	6.748001	636.864315	3160	0.000202
1400	0.706618	0.001635	3.26	6.747445	547.051659	3586	0.000153
1500	0.706854	0.001871	3.34	6.746875	477.848902	4008	0.000119
1600	0.707096	0.002113	3.43	6.746291	422.939840	4459	0.000095

TABLE 4
Calculated values of interatomic potential, stress, strain Young's modulus and Poisson's ratio for (5,5) SWCNT in axial direction at high temperatures

Temperature (K)	**a_3' (nm) [26]**	**(a_3'-a_3) x10^{-6} (nm)**	**αx10^{-6} (K^{-1}) [26]**	**Inter-atomic potential (V) x10^{-16} Jule**	**(5,5)Stress x10^3 N/m^2**	**Strain x10^{-6} (5,5)**	**Young's modulus (Y) (5,5) TPa**	**Poission's ratio (σ)**
400	0.246007	9	0.37	7.956751	122.117206	37	3.300465	–
500	0.246030	32	0.93	7.956686	34.342751	186	0.184638	0.752688
600	0.246069	71	1.56	7.956575	15.476108	468	0.033069	0.871795
700	0.246119	121	2.03	7.956433	9.079227	812	0.011181	0.886700
800	0.246178	180	2.41	7.956265	6.101789	1205	0.005064	0.912863
900	0.246243	245	2.66	7.956081	4.481740	1596	0.002808	0.924812
1000	0.246315	317	2.91	7.955876	3.462778	2037	0.001700	0.927835
1100	0.246391	393	3.09	7.955660	2.792245	2472	0.001130	0.941748
1200	0.246471	473	3.25	7.955433	2.319197	2925	0.000793	0.953846
1300	0.246555	557	3.40	7.955195	1.968750	3400	0.000579	0.950000
1400	0.246642	644	3.53	7.954947	1.702171	3883	0.000438	0.934844
1500	0.246731	733	3.61	7.954695	1.494940	4332	0.000345	0.941828
1600	0.246823	825	3.71	7.954433	1.327725	4823	0.000275	0.938005

Table 5
Calculated values of interatomic potential, stress, strain Young's modulus and Poisson's ratio for (9,0) SWCNT in axial direction at high temperatures

Temperature (K)	**a_3'sinϕ_1' (nm) [26]**	**(a_3'sinϕ_1' –$a_3$sinϕ_1) x10^{-6} (nm)**	**α x10^{-6} (K^{-1}) [26]**	**Inter-atomic potential (V) x10^{-16} Jule**	**(9,0)Stress x10^3 N/m^2**	**Strain x10^{-6} (9,0)**	**Young's modulus (Y) (9,0) TPa**	**Poission's ratio (σ)**
500	0.214026	10	0.47	8.047940	110.363210	94	1.174077	1.340426
600	0.214048	32	1.04	8.047877	34.483589	312	0.110524	1.201923
700	0.214082	66	1.59	8.047780	16.716104	636	0.026283	1.081761
800	0.214125	109	2.00	8.047657	10.119316	1000	0.010119	1.055000
900	0.214173	157	2.26	8.047520	7.023666	1356	0.005180	1.066372
1000	0.214228	212	2.54	8.047363	5.199759	1778	0.002924	1.035433
1100	0.214286	270	2.73	8.047197	4.081687	2184	0.001869	1.036630
1200	0.214349	333	2.93	8.047017	3.308371	2637	0.001255	1.037543
1300	0.214414	398	3.06	8.046831	2.767102	3060	0.000904	1.032680
1400	0.214482	466	3.16	8.046636	2.362485	3476	0.000680	1.031646
1500	0.214552	536	3.23	8.046436	2.053202	3876	0.000530	1.034056
1600	0.214622	606	3.30	8.046236	1.815357	4290	0.000423	1.039394

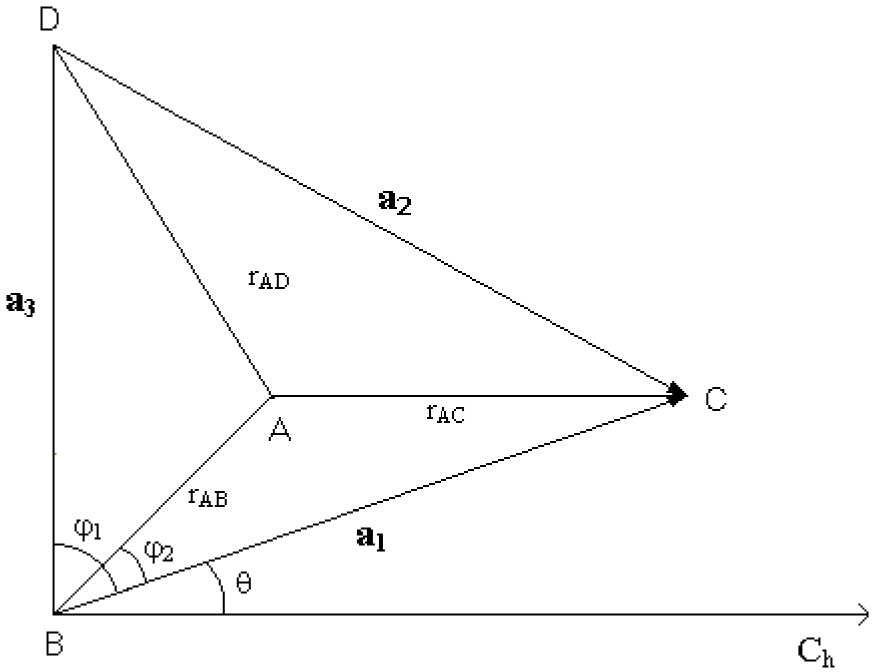

Fig. 1 A represented atom A and its three nearest neighbor atoms B, C and D in armchair (n,n) SWCNT (θ = 30°).

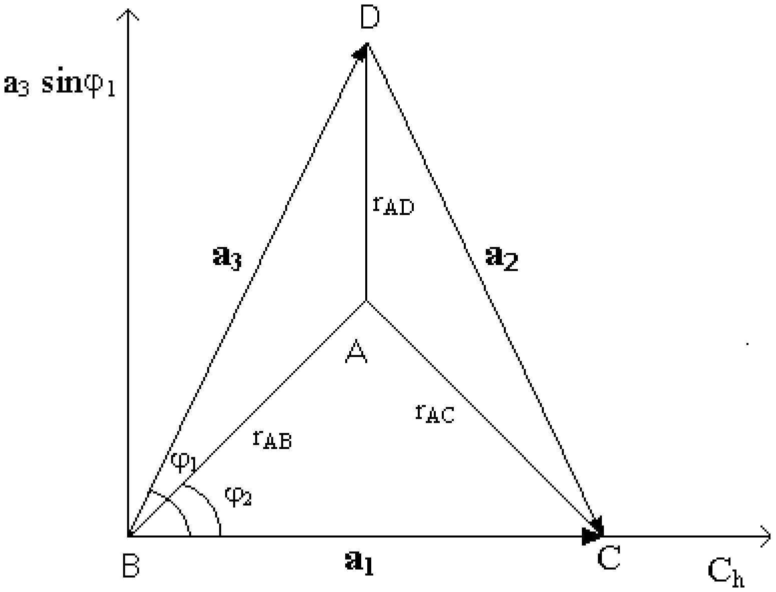

Fig. 2 A represented atom A and its three nearest neighbor atoms B, C and D in Zigzag (n,0) SWCNT (θ = 0).

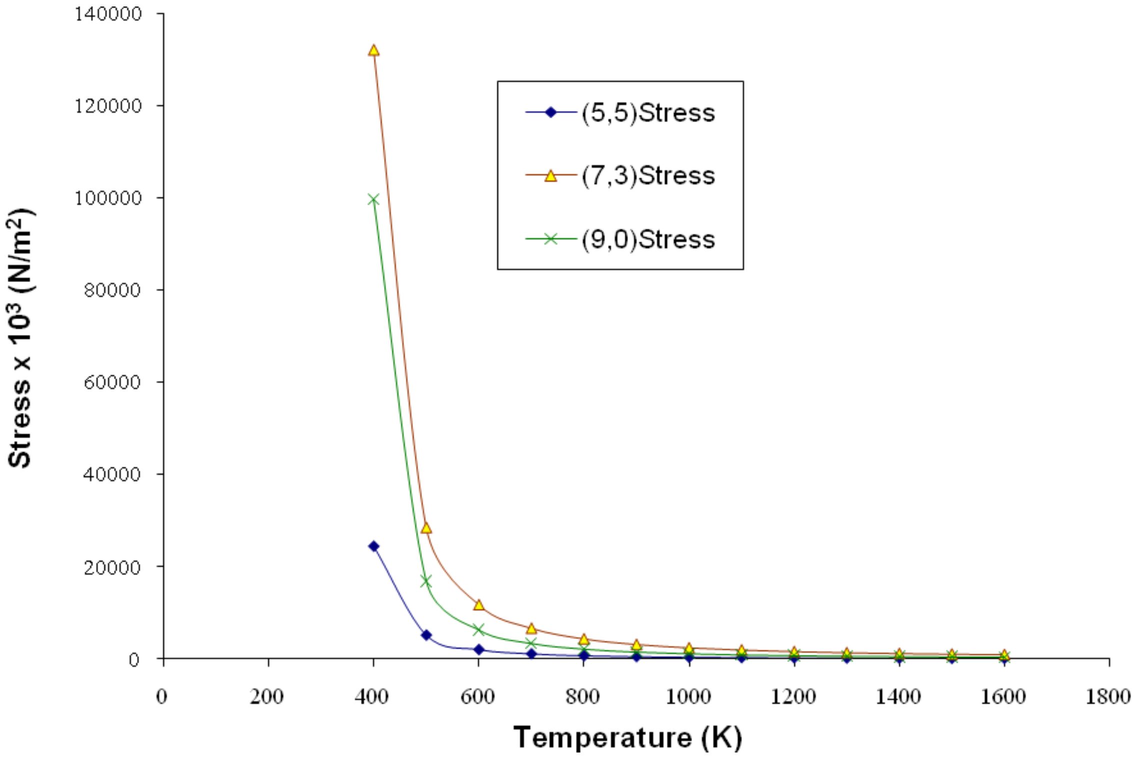

Fig. 3 Variation in radial stress for (5,5), (7,3) and (9,0) SWCNT at high temperatures.

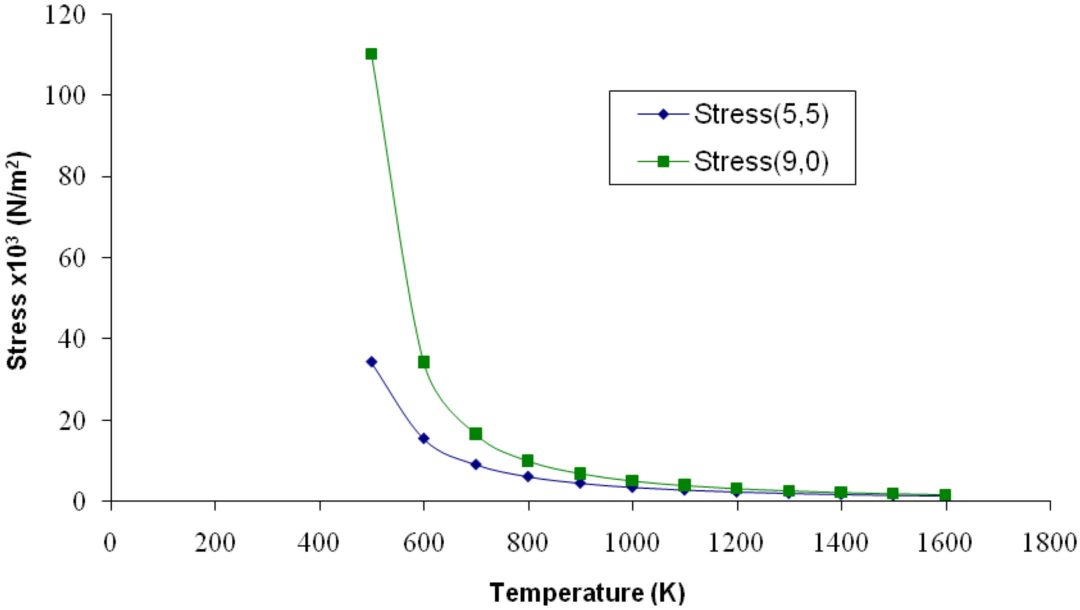

Fig. 4 Variation in axial stress for (5,5) and (9,0) SWCNT at high temperatures.

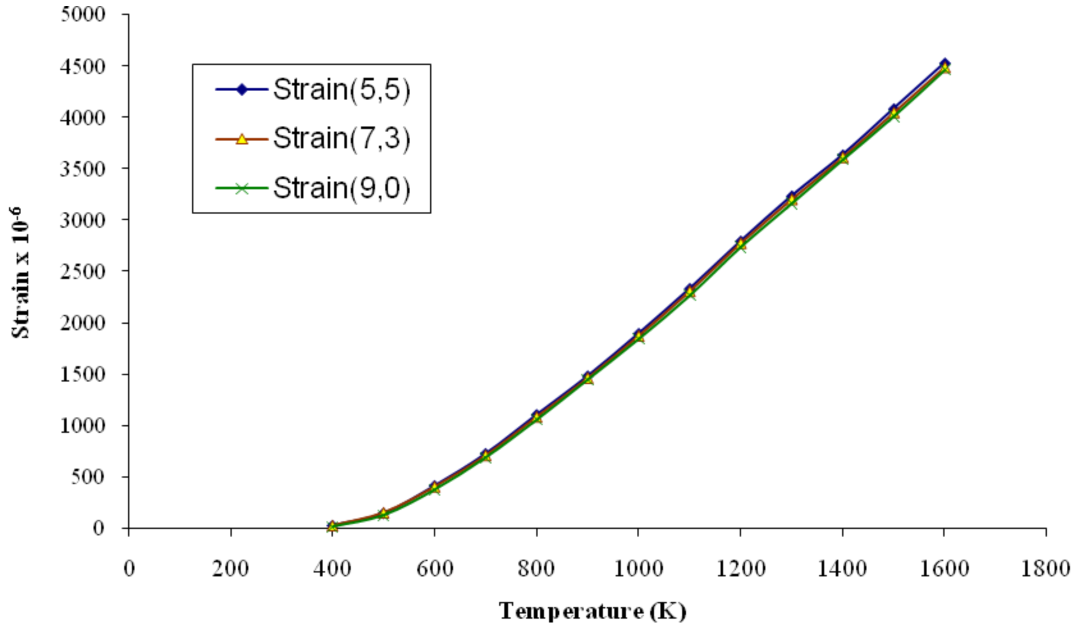

Fig. 5 Variation in radial strain for (5,5), (7,3) and (9,0) SWCNT at high temperatures.

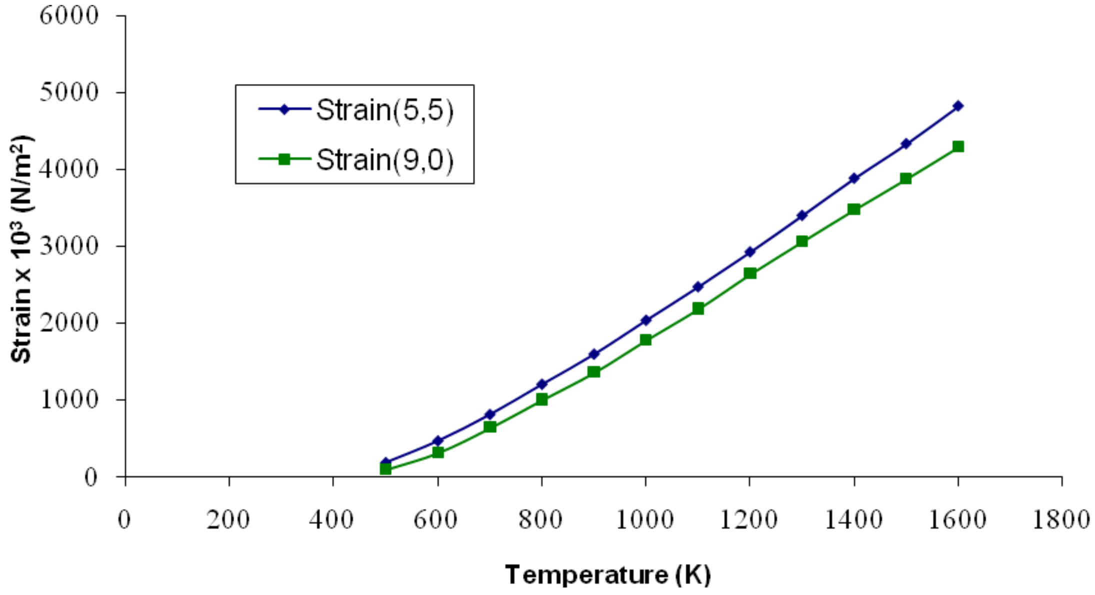

Fig. 6 Variation in axial strain for (5,5) and (9,0) SWCNT at high temperatures.

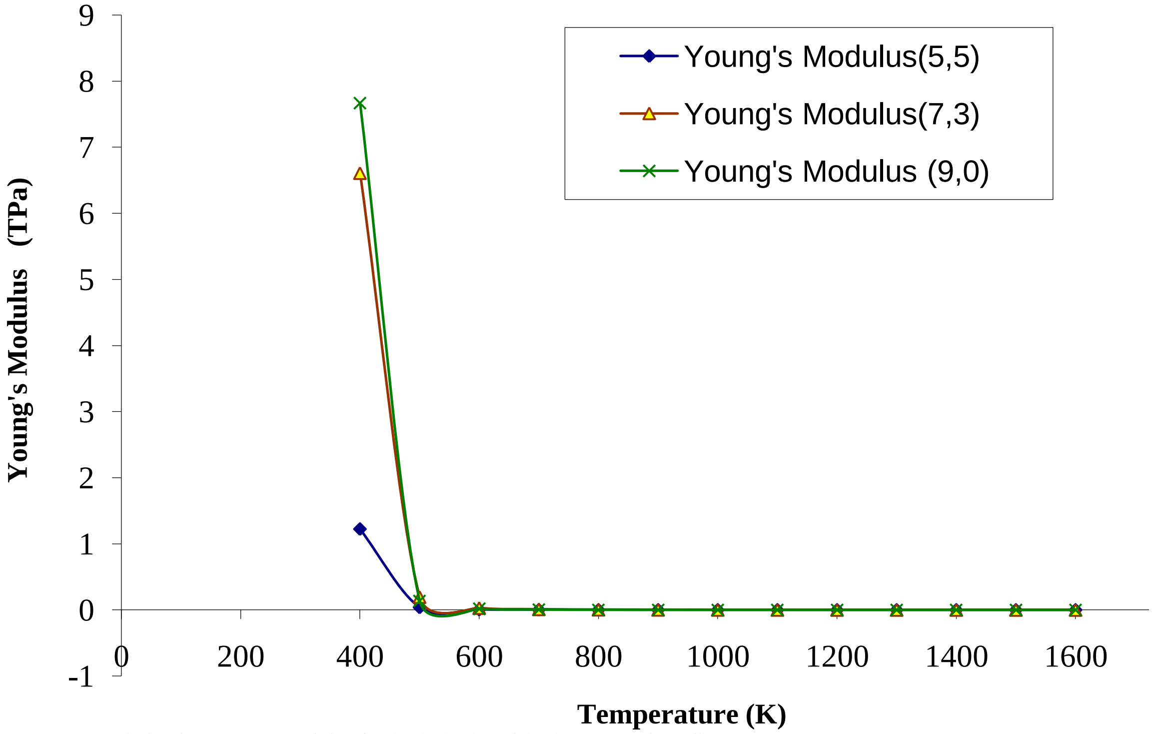

Fig. 7 Variation in Young's modulus for (5,5), (7,3) and (9,0) SWCNT in radial direction at high temperatures.

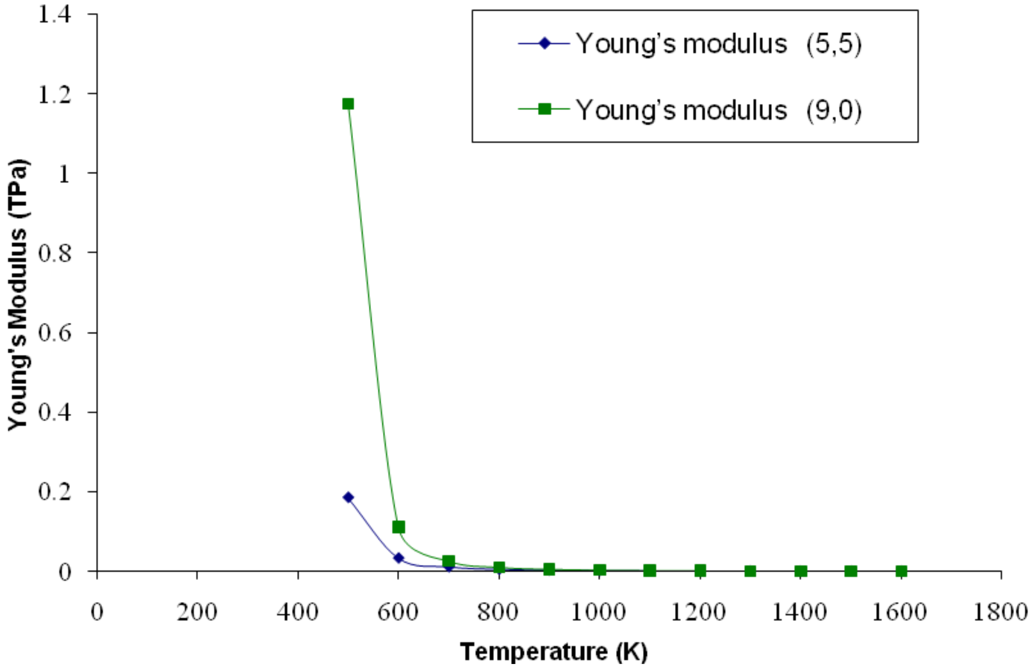

Fig. 8 Variation in Young's modulus for (5,5) and (9,0) SWCNT in axial direction at high temperatures.

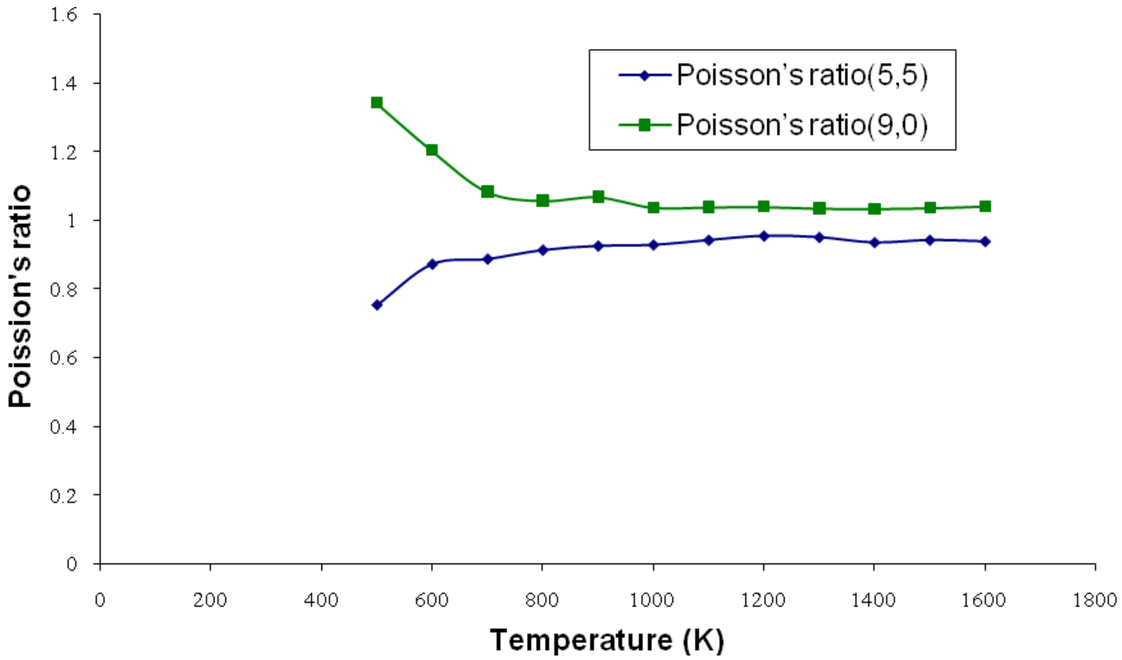

Fig. 9 Variation in Poisson's ratio for (5,5) and (9,0) SWCNT at high temperatures.

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