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A STUDY TO EVALUATE ELASTIC PROPERTIES OF 2-PHASE CNT COMPOSITES USING DIFFERENT APPROACH

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Abstract - The objective of the paper is to present a comparative study to determine elastic properties of 2-phase carbon nanotube composites using different approach i.e. Halpin-Tsai Model, Moritanaka (aligned & random distribution) and Modified Series Model. CNT is dispersed in an isotropic manner in a matrix and the improved elastic properties of matrix polymer are obtained. Effect of different volume fraction of carbon nanotube, aspect ratio with different method is studied here

Keywords - Carbon nano tube, Mathematical model.

I. Introduction

Carbon nanotubes are molecular scale tubes of graphitic carbon with outstanding properties having Young's Moduli as high as 1TPa and tensile strength up to 63 GPa. The Single-walled and Multi-walled carbon nanotubes are used in the composites to improve mechanical properties rapidly. It has been observed that the CNT ranging between 0.1% to 5% results in an improvement in tensile, shear and flexural properties [1-2]. Allaoui etal [3] shown that tensile strength and yield strength of composites containing 1% to 4 % CNT is doubled and quadrupled as compared to neat resin sample. Kim etal [4] showed that with 0.3% of SWCNT and MWCNT in the ratio 1:2 by weight results in 8.46% increase in Young's modulus of resin. Kanagaraj et al. [5] shown that with 0.44 % volume fraction of CNT in a polymer, the percentage increase in the Young's Modulus is 22.23%. In the present, the effect of % CNT reinforcement on the Mechanical properties of Multi-Scale composites is presented.

Several research works have been reported on different models.

II. Mathematical Modeling

The mathematical model is based on the assumption that: the fiber and matrix are homogenous and isotropic. There is perfect bonding between the matrix and fiber and no interface between CNT and matrix.CNT is dispersed into the matrix in an isotropic manner. The properties of CNT reinforced matrix are evaluated using micromechanics based on Halpin-Tsai model and Modified Series Model. The CNT reinforced matrix is considered as the new matrix and further to be reinforced with carbon fibers. The elastic properties of multi-scale composites (CNT-matrix/fiber) are evaluated using micromechanics approach for composites with continuous fibers.

Halpin-Tsai Model

Halpin Tsai Model is used for evaluating the properties CNT reinforced nanocomposite. The elastic Modulus of the nanocomposite, and expressed as (Kim et.al) [4]:

To evaluate the mechanical properties of carbon nanotube composite, Halpin-Tsai Model is also used. In this model both the volume fraction and aspect ratio of CNT in the nanocomposite can be varied for determining the elastic properties of carbon nanocomposite. This model is used for determining the elastic properties of nanocomposite for short as well as long CNT.

The Halpin-Tsai model determines the tensile modulus of nanocomposite, and expressed by Kim (2009):

$$E_{NC} = \left[\frac{3}{8} \times \frac{1 + 2(l_{NT}/d_{NT})\eta_L V_{NT}}{1 - \eta_L V_{NT}} + \frac{5}{8} \times \frac{1 + 2\eta_D V_{NT}}{1 - \eta_D V_{NT}} \right] E_{epoxy}$$

$$\eta_L = \frac{(E_{NT}/E_{epoxy}) - (d_{NT}/4t)}{(E_{NT}/E_{epoxy}) + (l_{NT}/2t)}$$

$$\eta_D = \frac{(E_{NT}/E_{epoxy}) - (d_{NT}/4t)}{(E_{NT}/E_{epoxy}) + (d_{NT}/2t)}$$

Where E, l_{NT}, d_{NT}, V_{NT} and t arerepresents the tensile modulus, length, diameter, and volume fraction of nanotube and thickness of graphite layer respectively. Based on isotropic assumption, the shear modulus can be calculated as follows:

$$G_{NC} = \frac{E_{NC}}{2(1+\nu)}$$

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Modified Series Model for Randomly oriented nanotube Kanagaraj [2007]:

The Modified Series Model is used to determine the properties of CNT reinforced composite in a randomly oriented manner. Then the improved Properties of matrix are obtained. The Modified Series Model is quietly used for determining the mechanical properties of the carbon nanotube composite. In this model, both the volume fraction and aspect ratio can be varied for determining the elastic properties of carbon nanotube composite. Thus the Modified Series Model is used for determining the elastic properties of carbon nanotube composite for short as well as long CNT.

In case of CNT-HDPE (High Density Poly Ethylene) composites, it is considered as randomly oriented short fiber arrangement. Based on the Modified form of rule of mixtures for series model, the composite Modulus is given byKanagaraj [2007]:

$$E_c = (\eta_l \eta_o E_{CNT} - E_{HDPE})V_{CNT} + E_{HDPE}$$

$$\eta_l = 1 - \frac{Tanh\ (a.(l/d))}{a.(l/d)}$$

$$a = \sqrt{\frac{-3E_{HDPE}}{2E_{CNT}\ \ln(V_{CNT})}}$$

$$\eta_0 = 0.2$$

Where, $\eta_l =$ Length Efficiency Factor,

$\eta_o =$ Orientation efficiency factor for randomly oriented fiber

$l/d =$ Aspect Ratio

Mori-Tanaka Method for Randomly Oriented Nanotube J. Wuite[2005]:

The mechanical properties of composite are evaluated by dispersing the CNTs in a randomly oriented (isotropic) manner in a matrix. improved properties of matrix are determined using the Mori-Tanaka Method for randomly oriented Nanotube. The effect of the percentage content of CNT on the mechanical properties of composite is investigated for randomly oriented Nanotube. This method is valid for short fibers only and the effect of aspect ratio on the mechanical properties of Nano composite cannot be studied using this method. The derived expression for the Bulk Modulus K and Shear Modulus G of a composite reinforced with randomly oriented, straight Nanotube using the Mori- Tanaka method which are given as:

$$K = K_m + \frac{C_r(C - 3K_m A)}{3(C_m + C_r A)}$$

$$G = G_m + \frac{C_r(D - 2G_m B)}{2(C_m + C_r B)}$$

Where,

$$A = \frac{3(K_m + G_m) + k_r - l_r}{3(G_m + k_r)}$$

$$B = \frac{1}{5}\left\{ \frac{4G_m + 2k_r + l_r}{3(G_m + k_r)} + \frac{4G_m}{G_m + p_r} + \frac{2[G_m(3K_m + G_m) + G_m(3K_m + 7G_m)]}{G_m(3K_m + G_m) + mr(3K_m + 7G_m)} \right\}$$

$$C = \left[n_r + 2l_r + \frac{(2k_r + l_r)(3K_m + 2G_m - l_r)}{(G_m + k_r)} \right]$$

$$D = \frac{1}{5}\left[\frac{2}{3}(n_r - l_r) + \frac{8G_m p_r}{G_m + p_r} + \frac{2(k_r - l_r)(2G_m + l_r)}{3(G_m + k_r)} + \frac{8m_r G_m(3K_m + 4G_m)}{3K_m(m_r + G_m) + G_m(7m_r + G_m)} \right]$$

Where K_m and G_m are the bulk and shear modulus of the matrix. The effective young's Modulus E and the Poisson's ratio of the material are given by the following relationship.

$$E = \frac{9KG}{3K + G}$$

$$\nu = \frac{3K = 2G}{6K + 2G}$$

Where k_r, m_r, l_r, n_r and prare the Hill's elastic Moduli for the Reinforcing phase.

D. Mori-Tanaka method for Aligned Nanotube J. Wuite [2007]:

The mechanical properties of composite are obtained by dispersing the CNTs in an aligned manner in a matrix. The improved properties of matrix are evaluated using the Mori-Tanaka Method. The effect of the percentage content of CNT on the mechanical properties of composite is investigated for aligned Nanotube using Mori-Tanaka Method. This method is valid for short fibers only and the effect of aspect ratio on the mechanical properties of Nano composite cannot be studied using this method.

Using the Mori Tanaka Method, the Hill's elastic Moduli are found to be:

$$k = \frac{E_m \begin{Bmatrix} E_m C_m + 2k_r(1+\nu_m) \\ [1 + c_r(1-2\nu_m)] \end{Bmatrix}}{2(1+\nu_m)\begin{bmatrix} E_m(1+c_r-2\nu_m) \\ +2c_m k_r(1-\nu_m-2\nu_m^2) \end{bmatrix}}$$

$$l = \frac{E_m \begin{Bmatrix} C_m \nu_m [E_m + 2k_r(1+\nu_m)] \\ +2C_r l_r(1-\nu_m^2) \end{Bmatrix}}{(1+\nu_m)\begin{bmatrix} 2C_m k_r(1-\nu_m-2\nu_m^2) \\ +E_m(1+C_r-2\nu_m) \end{bmatrix}}$$

$$n_1 = \frac{\begin{matrix} E_m^2 C_m(1+C_r-C_m\nu_m) + \\ 2C_m C_r(k_r n_r - l_r^2)(1+\nu_m)^2(1-2\nu_m) \end{matrix}}{(1+\nu_m)\begin{Bmatrix} 2C_m k_r(1-\nu_m-2\nu_m^2) \\ +E_m(1+C_r-2\nu_m) \end{Bmatrix}}$$

$$n = n_1 + n_2$$

$$p = \frac{E_m \begin{bmatrix} E_m C_m + \\ 2(1+C_r)p_r(1+\nu_m) \end{bmatrix}}{2(1+\nu_m)\begin{bmatrix} E_m(1+C_r) \\ +2C_m p_r(1+\nu_m) \end{bmatrix}}$$

Where k, l, m, n, p are the Hill's Elastic Moduli

n is the uniaxial tension modulus in the fiber direction.

k is the bulk modulus normal to fiber direction.

l is the associated cross modulus.

m is the shear modulus in plane normal to fiber direction.

p is the shear modulus parallel to the fiber direction.

k_r, m_r, p_r, n_r, l_r are the hill's Elastic Modulus for the reinforcing phase.

C_r is the reinforcing phase volume fraction.

C_m is the matrix phase volume fraction.

Em is the Young's Modulus.

ν_m is the Poisson's ratio of matrix.

The expression for the Moduli of the CNRP as function of the stiffness constants is determined for a unidirectional composite as follows:

$$E_l = n - \frac{l^2}{k}$$

$$E_t = \frac{4m(kn - l^2)}{kn - l^2 + mn}$$

$$G_{lt} = 2p$$

$$\nu_{lt} = \frac{l}{2k}$$

III. Results and Discussions

The elastic properties of Multi-Scale composite are evaluated by using Halpin-Tsai Model, Modified Series Model and Continuous fiber reinforced micromechanics. Table I shows the effect of aspect ratio on Young's modulus and Shear modulus.

TABLE I. Effect of aspect ratio (L/D) on elastic properties of CNT composite for Vcnt=2%

S.N	Aspect Ratio	E	G
1	10	4.766334	1.833206
2	20	5.263471	2.024412
3	30	5.698885	2.191879
4	40	6.083399	2.339769
5	50	6.425445	2.471325
6	60	6.731691	2.589112
7	70	7.007477	2.695184
8	80	7.257133	2.791205
9	90	7.484205	2.87854
10	100	7.691624	2.958317

The elastic properties of Multi-Scale composite are evaluated by using Halpin-Tsai Model, Modified Series Model and Continuous fiber reinforced micromechanics and submmerized in Table II.

Figure 1 shows the effect of CNT % on the Young's Modulus of HDPE (High Density polyethylene) polymer reinforced with CNT. It is observed that with 2% CNT, the percentage increase in the Young's Modulus is 112.72% and 158.97% using the Halpin-Tsai Model and Modified Series Model, respectively.

Figure 2 shows the effect of percentage of CNT on the Shear Modulus of the Multi-scale composite. It is observed that there is variation in the Shear Modulus as the percentage content of CNT is increased in the multi-scale composite. For 2% CNT, the increase in the Shear

Modulus is 86.52% and 116.10% for the Halpin-Tsai Model and Modified Series Model, respectively.

Effect of Aspect ratio (L/D) on elastic properties of CNT composite for Vcnt=1%

	Halpin-Tsai Model		Modified Series Model		Mori Tanaka (aligned nanotubes)		Mori Tanaka (random nanotubes)	
Aspect ratio	Young's modulus	Shear Modulus	Young's modulus	Shear modulus	Young's modulus	Shear Modulus	Young's Modulus	Shear Modulus
10	4.409831	1.696089	4.047231	1.566589	4.3299	1.5552	4.1096	1.5324
20	4.656411	1.790927	4.293811	1.661427	4.576481	1.650039	4.356181	1.627239
30	4.872628	1.874088	4.519638	1.747665	4.802308	1.736276	4.582008	1.713476
40	5.063765	1.947602	4.745465	1.833902	5.028134	1.822513	4.807834	1.799713
50	5.233946	2.013056	4.922446	1.901856	5.205115	1.890467	4.984815	1.867667
60	5.386438	2.071707	5.059638	1.955007	5.342307	1.943618	5.122007	1.920818
70	5.523863	2.124563	5.150543	1.991074	5.433213	1.979686	5.212913	1.956886
80	5.648349	2.172442	5.241449	2.027142	5.524118	2.015753	5.303818	1.992953
90	5.761641	2.216016	5.292816	2.048491	5.575486	2.037102	5.355186	2.014302
100	5.865184	2.25584	5.344184	2.06984	5.626853	2.058451	5.406553	2.035651

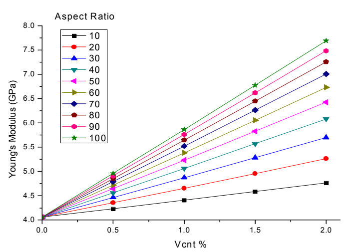

Figure 1: Effect of Vcnt on young's modulus of CNT composite along different aspect ratio.

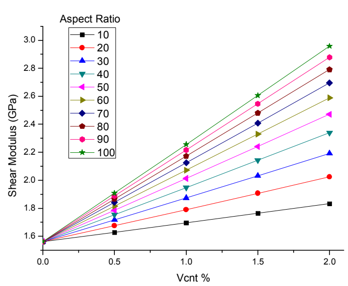

Figure 2: Effect of Vcnt on shear modulus of CNT composite along different aspect ratio.

Conclusions

- There is significant improvement in the elastic properties of matrix, even with a small percentage of CNT
- The Modified Series Model values are on higher side as compared to Halpin-Tsai Model.
- Also there has been a significant improvement in transverse and shear modulus value as we increase the percentage of CNT. The reason being that there is matrix dominance in transverse and in plane shear direction.

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