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Investigation of Agglomeration and Dispersion of Reinforcement on the Viscoelastic Properties of CNT Reinforced Polymeric Composites

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ABSTRACT

In this research, effect of agglomeration and dispersion of Carbon nanotubes (CNTs) on viscoelastic properties of CNT-reinforced polymeric nanocomposites is investigated. The effective properties of the nanocomposite are obtained by the Mori-Tanaka micromechanical approach, assuming completely random oriented CNTs. Considering spherical shaped inclusions for CNTs agglomerated region, two parameters are presented and applied to the Mori-Tanaka micromechanical method to model the agglomeration and dispersion of the CNTs. The polymeric matrix is assumed to be viscoelastic. The viscoelastic properties of polymer matrix are simulated by standard linear solid model with three structural parameters. Due to time-dependency of constitutive equation of the matrix, direct using of the micromechanical method is not possible. Hence, the constitutive equations of the matrix are transferred to the Laplace domain and algebraic form of the mentioned equations are inserted to the Mori-Tanaka relations. To verify the model, predicted results of that are compared with available experimental data for CNT reinforced polymeric nanocomposites. Investigation of agglomeration parameters shows that the overall properties of the composite can be improved by decreasing agglomeration of the CNTs.

KEYWORDS:

Polymeric Nanocomposite, Carbon Nanotube, Viscoelasticity, Agglomeration and Dispersion.

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1- Brief Introduction

Carbon nanotubes (CNTs) have been widely used in many applications due to their superior properties. Regarding CNT-reinforced composites as an important application of nano-scale structures, prediction of mechanical and physical properties is necessary due to restriction of experiments on them. Many polymeric nanocomposites have viscoelastic properties, so that micromechanical approaches have been implemented to simulate their structural behavior. According to time-dependent structural equations of viscoelastic materials, micromechanical formulations are presented in time, frequency and Laplace domains [1-6]. Effects of agglomeration and dispersion of CNTs on the elastic properties were firstly investigated by Shi et al. [7] using the Mori-Tanaka method. The effect of CNT agglomeration on the viscoelastic properties has not been considered yet in the literature.

In this study, two parameters are introduced to model CNT agglomeration. The standard linear solid model with three structural parameters are used to simulate the viscoelastic properties of the matrix. By applying Laplace transform on the time-dependent constitutive equations, the algebraic form of them can be obtained and inserted in the micromechanical formulations. A parametric study is performed on the model and the effect of CNT agglomeration is investigated. The results of the model are compared with available experimental data.

2- Micromechanics

The viscoelastic properties of the polymer are modeled by standard linear solid shown in Figure 1, schematically.

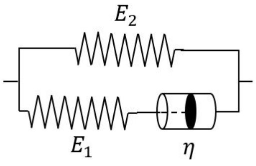

Figure 1. Standard linear solid for viscoelastic materials

The constitutive equation of this model is expressed as:

$$\sigma + p_1\dot{\sigma} = q_0\varepsilon + q_1\dot{\varepsilon} \tag{1}$$

where

$$p_1 = \frac{\eta}{E_1}, \qquad q_0 = E_2, \qquad q_1 = \frac{E_1 + E_2}{E_1}\eta \tag{2}$$

Considering Polypropylene (PP) as polymeric matrix, the model parameters are obtained as:

$$\begin{aligned} p_1 &= 273.60 \text{ sec} \\ q_0 &= 3.0300 \text{ GPa} \\ q_1 &= -756.50 \text{ GPa.sec} \end{aligned} \tag{3}$$

Applying Laplace transform on Eq. (1), the algebraic form of the constitutive equation is found

$$\bar{\sigma}(s) = \frac{q_0 + q_1 s}{1 + p_1 s}\bar{\varepsilon}(s) \tag{4}$$

The Mori-Tanaka formulations for overall properties of the composite are given by:

$$\bar{\mathbf{C}}(s) = (c_m\bar{\mathbf{C}}_m(s) + c_r\mathbf{C}_r{:}\,\mathbf{A}){:}\,(c_m\mathbf{I} + c_r\mathbf{A})^{-1} \tag{5}$$

where A is strain concentration tensor, given by:

$$\mathbf{A} = \left[\mathbf{I} + \mathbf{S}{:}\,(\bar{\mathbf{C}}_m(s))^{-1}{:}\,(\mathbf{C}_r - \bar{\mathbf{C}}_m(s))\right]^{-1} \tag{6}$$

For randomly oriented CNT, the overall properties can be considered isotropic. The relaxation modulus of the composite in Laplace domain is expressed as

$$\begin{aligned} E(s) = {}& \frac{3}{8}[c_r E_{\text{CNT}} + (1 - c_r)\bar{E}_m(s)] \\ & + \frac{5}{8}\left[\frac{E_{\text{CNT}}\bar{E}_m(s)}{(1 - c_r)E_{\text{CNT}} + c_r\bar{E}_m(s)}\right] \end{aligned} \tag{7}$$

To model CNT agglomeration, it is assumed that the CNTs are agglomerated in spherical inclusions and dispersed in other places. Therefore, two parameters can be defined, accordingly:

$$\xi = \frac{V_{\text{Inc}}}{V} \qquad \zeta = \frac{V_{\text{CNT}}^{\text{Inc}}}{V_{\text{CNT}}} \tag{8}$$

where ξ and ζ are the ratio of inclusion volume to composite volume and the ratio of CNT volume inside the inclusion to CNT volume of the composite, respectively.

By inserting agglomeration parameters in Eq. (7), the relaxation moduli of inner and outer of the inclusions are obtained:

$$\begin{aligned} E_{\text{in}}(s) = {}& \frac{3}{8\xi}[c_r\zeta E_{\text{CNT}} + (\xi - c_r\zeta)\bar{E}_m(s)] \\ & + \frac{5}{8}\frac{\xi\bar{E}_m(s)E_{\text{CNT}}}{(\xi - c_r\zeta)E_{\text{CNT}} + c_r\zeta\bar{E}_m(s)} \\ E_{\text{out}}(s) & \\ = {}& \frac{3}{8}\left\{\frac{c_r(1-\zeta)}{1-\xi}E_{\text{CNT}} + \left[1 + \frac{c_r(1-\zeta)}{1-\xi}\right]\bar{E}_m(s)\right\} \\ & + \frac{5}{8}\frac{(1-\xi)E_{\text{CNT}}\bar{E}_m(s)}{[(1-\xi) - c_r(1-\zeta)]E_{\text{CNT}} + c_r(1-\zeta)\bar{E}_m(s)} \end{aligned} \tag{9}$$

Finally, the overall properties can be expressed as

$$\bar{E}(s) = \xi E_{\text{in}}(s) + (1 - \xi)E_{\text{out}}(s) \tag{10}$$

By applying inverse Laplace transform, the time-dependent properties can be found.

3- Numerical Results

In this section, effects of agglomeration parameters are studied. The volume fraction of the CNT is considered 0.5% and the CNTs are assumed to be isotropic with elastic modulus 1.2 TPa.

At first, assuming ζ=0.5, the relaxation modulus of the composite for different magnitudes of ξ are shown in Figure 2. It is observed that, increasing ξ parameter, leads to improve overall properties of the composite. It is also seen that the effect of ξ is significant at higher values.

Figure 3 indicates the variations of relaxation modulus for different magnitudes of ζ. In this figure, the magnitude of ξ are taken as 0.5. It can be found that the relaxation modulus is decreased with increasing ζ and for higher values of ζ, considerable effects on the relaxation modulus is observed.

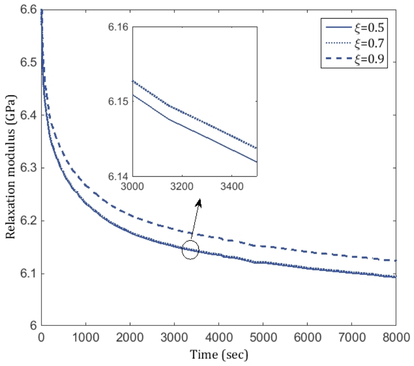

Figure 2. Relaxation modulus of the composite for ζ=0.5 and different magnitudes of ξ

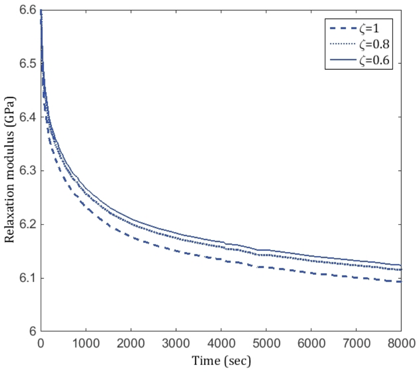

Figure 3. Relaxation modulus of the composite for ξ=0.5 and different magnitudes of ζ

4- Conclusions

According to importance of CNT agglomeration in the composites, in this research, a micromechanical model is developed to investigate viscoelastic behavior of the composite with agglomerated reinforcement.

From numeral results, it can be concluded that the effect of ζ and ξ are different. In the case of constant ζ, the relaxation modulus is increased with increasing ξ. For constant ξ, increasing ζ leads to decreasing the relaxation modulus.

By applying appropriate agglomeration parameters, the overall properties of the composite can be obtained realistically compared to experimental results.

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