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Micromechanical investigation of creep-recovery behavior of carbon nanotube-reinforced polymer nanocomposites

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ABSTRACT

Creep-recovery behavior of polymer nanocomposites reinforced by carbon nanotubes (CNTs) is investigated using a 3-dimensional unit cell-based micromechanical model. The representative volume element (RVE) of the model consists of three phases including aligned CNTs, polymer matrix and CNT/polymer interphase formed due to non-bonded van der Waals interaction. The CNTs and polymer are assumed to be as transversely isotropic elastic and isotropic nonlinear viscoelastic materials, respectively. The effects of volume fraction and diameter of the CNTs, loading level and interphase including the materials behavior and size on the creep-recovery strain of the nanocomposite are examined. The predicted elastic and creep-recovery responses for pure polymer and CNT-reinforced polymer nanocomposite are found to be in good agreement with available experiment. Also, the isochronous stress–strain curves during the creep cycle for the nanocomposite under transverse and axial loadings are presented. The results clearly demonstrate that the overall transverse creep strain is dependent on the polymer nonlinear viscoelastic behavior and interphase material, as the applied loading increases. The results also reveal that the overall behavior of the nanocomposite is similar to the elastic response in the axial direction. Moreover, the isochronous stress–strain curves are extracted for biaxial and triaxial loading.

1. Introduction

Since the discovery of CNTs [1], many studies including experimental [2–4] and theoretical [5–7] ones have been performed to predict their effective properties. CNTs possess exceptional mechanical properties such as high stiffness and strength as well as excellent electronic and thermal properties [8–11]. The elastic properties of CNTs have been widely investigated, since their exact values are of great importance in many applications. According to previous studies, it is well known that the elastic properties of the CNT are transversely isotropic [12–16]. For example, Shen and Li [13,14] extracted five independent elastic parameters of the CNT. They examined the effect of CNT diameter on its elastic moduli. Liu et al. [15] employed a hybrid atom/continuum method to determine five independent elastic moduli of the CNT. Tsai et al. [16] modeled the hollow cylindrical molecular structure of CNTs as an equivalent transversely isotropic solid and used the molecular mechanics method to estimate the elastic properties of the CNTs. Hence, the CNT must be considered as a transversely isotropic material in the analytical or numerical modeling of the CNT-based composites.

The CNT is extensively used as a very good reinforcement phase in polymer composite materials due to its exceptional mechanical properties. The experimental results have confirmed that with just 0.75% (by weight) of the CNTs added in polypropylene, the elastic modulus and yield strength of the nanocomposite can increase 39% and 26.5%, respectively [17]. Also, according to the experimental results reported by So et al. [18], it has been revealed that in comparison with the pure polyimide, CNT-reinforced polyimide composites have higher tensile strength and modulus. With adding just 1% (by weight) of the CNTs in polyimide, Young's modulus and tensile strength of polyimide nanocomposite can increase 18.2% and 16%, respectively [18]. Both experimental [19–21] and theoretical [22–27] approaches have been applied in order to predict the elastic properties of the CNT-reinforced polymer composites.

Recently, it is found that CNT/polymer matrix interphase region is one of the most important factors that include a significant effect on the mechanical behavior of the nanocomposites [16,28–31]. The interphase is formed through non-bonded van der Waals interaction between the CNT and surrounding polymer. Tsai et al. [16] calculated the interphase elastic modulus and thickness between the CNT and polyimide matrix using the molecular dynamics (MD). They studied the effects of interphase on the axial and transverse Young's moduli of the CNT-reinforced

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nanocomposite. Joshi and Upadhyay [29] numerically examined the effects of interphase stiffness and thickness on the elastic modulus of the CNT-based composites. Herasati et al. [30] estimated the elastic modulus and thickness of the interphase in the CNT-reinforced polyvinylchloride composite using atomistic simulations. Their results revealed that ignoring the CNT/polymer matrix interphase region can lead to misleading outcomes. The influence of Young's modulus of the interphase on the nanocomposite tensile, bending and torsional properties was numerically explored in [31]. By the use of MD method, Xiong and Meguid [32] studied the interphase mechanical properties for the CNT-reinforced epoxy composite. According to the previous results, the interphase characteristics such as material and geometry significantly affect the mechanical behavior of the CNT-reinforced nanocomposites. Hence, the effects of interphase region must be considered on the effective properties of the CNT/polymer nanocomposites.

It should be noted that with adding CNTs into the polymer matrix, owing to the viscoelastic response of the polymer under mechanical and environmental conditions, the resulting system is a viscoelastic nanocomposite. The viscoelastic behavior is one of the most important aspects of the mechanical characteristics of the polymer nanocomposites. Several factors such as temperature, humidity, and stress level affect the viscoelastic response of the polymer nanocomposites. It is also important to be noted that at high stress levels of loading, the viscoelastic behavior of the material becomes complex and nonlinear. Although numerous studies have been done on the elastic behavior of the CNT-based composites, however, very limited attention has been paid to the viscoelastic response of these materials. Li et al. [33] theoretically predicted the creep response of the CNT-reinforced polymer composites. They studied the effects of temperature and CNT volume fraction on the linear viscoelastic behavior of the nanocomposites [33]. They did not examine the effect of interphase properties on the overall behavior of the nanocomposite. Furthermore, various creep-recovery experiments for the CNT-reinforced polymer nanocomposites have been conducted [34–39]. A literature survey shows that the effects of interphase including material and thickness on the nonlinear viscoelastic response of the CNT-reinforced polymer nanocomposites have not been investigated up to now. Moreover, the isochronous stress–strain curves for multiaxial loading have not been studied.

The unit cell-based micromechanical approaches such as the method of cell (MOC) [40–42] and generalized method of cell (GMC) [43–45] can be successfully applied to investigate the overall behavior of the nanocomposites. The MOC [46] and GMC [47] are mathematically rigorous. Among unit cell-based methods which describe the overall behavior of heterogeneous materials, the simplified unit cell (SUC) micromechanical model is a simple method to investigate the effects of various material properties and different conditions between constituents of composite systems. The SUC model was applied in [48] to predict the elastic and thermoelastic properties of the unidirectional SiC/Ti Metal Matrix Composites (MMCs). Later, the SUC model was used to investigate the effects of initiation and propagation of interface damage on the elastoplastic behavior of unidirectional SiC/Ti MMCs under off-axis loading [49]. Hassanzadeh-Aghdam et al. [50] extended the governing equations of the SUC model to three dimensions mainly to study the effects of aspect ratio of reinforcement phase on the axial and transverse elastic and thermoelastic properties of composites.

In this work, SUC micromechanical model is developed to predict the creep-recovery response of the CNT-reinforced polymer composites. The main advantage of the present model is its ability to give closed-form formulations for the nonlinear viscoelastic response of the CNT-reinforced polymer composites. The nanocomposite system consists of three phases including aligned CNTs, polymer matrix and interphase. In the micromechanical modeling of the nanocomposites, the interphase region is considered as a third phase between the CNT and the polymer matrix. The CNTs are assumed to behave elastically and transversely isotropic as well, while polymer matrix is considered as a nonlinear viscoelastic material. Schapery's nonlinear viscoelastic model is used for modeling the polymer matrix. The rest of paper is organized as follows. Section 2 presents Schapery's model for the nonlinear viscoelastic behavior of the polymer matrix. Section 3 introduces the individual RVE of nanocomposite system for micromechanical modeling. Section 4 presents the SUC micromechanical equations in detail. In Section 5, the material properties of the constituents of the nanocomposites are proposed. Verification of the model in predicting viscoelastic and elastic responses of nanocomposites is given in Section 6. Also, the effects of interphase material and thickness on the creep and recovery strains are discussed. Furthermore, the effects of CNT volume fraction and diameter and applied loading level on the nonlinear viscoelastic behavior of the CNT-reinforced polymer composite are studied. The isochronous stress–strain curves during the creep cycle at different times for the CNT/polymer nanocomposite are presented in Section 6. Moreover, the isochronous stress–strain curves are obtained for biaxial and triaxial loading. Conclusions are introduced in Section 7.

2. Schapery's nonlinear viscoelastic model

In this study, the viscoelastic material is modeled based on Schapery's nonlinear viscoelastic model. For isothermal and uniaxial loading conditions, the current total strain can be written as [51,52]

$$\varepsilon(t)=\left(g_0^tD_0+g_1^tg_2^t\sum_{n=1}^{N}D_n\left[1-\frac{1-\exp(-\lambda_n\Delta\psi^t)}{\lambda_n\,\Delta\psi^t}\right]\right)\sigma(t)-g_1^t\sum_{n=1}^{N}D_n\left(\exp(-\lambda_n\,\Delta\psi^t)q_n^{t-\Delta t}-\frac{1-\exp(-\lambda_n\,\Delta\psi^t)}{\lambda_n\,\Delta\psi^t}g_2^{t-\Delta t}\sigma(t-\Delta t)\right) \quad (1)$$

where D_0 is the instantaneous compliance value at $t=0$ (t stands for the time), N is the number of terms, D_n is nth coefficient of the Prony series and λ_n is the nth reciprocal of the retardation time. g_0, g_1 and g_2 are the time-independent but stress-dependent nonlinear viscoelastic material parameters. These parameters describe the nonlinear effects on the compliance of the material. Moreover, the reduced time increment $\Delta\psi^t$ and the hereditary integral q_n^t for every term of the Prony series at the end of the current time t are defined by the following equations

$$\Delta\psi^t=\psi^t-\psi^{t-\Delta t}=\int_{t-\Delta t}^{t}\frac{ds}{a_\sigma^{\sigma(s)}} \quad (2)$$

$$q_n^t=\exp(-\lambda_n\,\Delta\psi^t)q_n^{t-\Delta t}-\frac{1-\exp(-\lambda_n\Delta\psi^t)}{\lambda_n\,\Delta\psi^t}\left(g_2^t\sigma(t)-g_2^{t-\Delta t}\sigma(t-\Delta t)\right) \quad (3)$$

where a_σ similar to g_0, g_1 and g_2, is a time-independent but stress-dependent nonlinear viscoelastic material parameter. With assuming strain components as linear functions of the stresses, the stress–strain relationship for multiaxial loading state is derived [53]. Therefore, for the multiaxial constitutive equation of nonlinear viscoelastic isotropic material, the 3-D stress–strain relationship is given by