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Dynamic properties of polyurea-milled glass composites part II: Micromechanical modeling

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ABSTRACT

In Part I, the results of experimental evaluation of the mechanical properties of pure polyurea (PU) and polyurea with milled glass composites (PU-MG) in low (1–20 Hz) and high (0.5–1.5 MHz) frequency ranges (Nantasetphong et al., 2016a) have been reported, focusing on the dependence of these properties on frequency, temperature, and the milled glass volume fraction. Here, we report the results of the corresponding micromechanical modeling. The models are developed, based on three different approximations: (1) dilute random, (2) non-dilute random, and (3) non-dilute periodic distributions of inclusions. Different orientation distributions of fibers, e.g., uniaxial parallel, in-plane random, and 3D random are considered and their results are compared with experimentally measured data presented in (Nantasetphong et al., 2016a). Moreover, the computational results are used to construct master curves of dynamic Young's storage and loss moduli and compare these with those constructed from experimental data. The 3D random and in-plane random calculation results are compared with the dynamic longitudinal and shear moduli of PU-MG composites obtained from ultrasonic wave measurements. These comparisons demonstrated that, as expected, the orientation distribution of the short fibers was affected by the thickness of the composite sample, and this effect was manifested in overall elasticity tensor of the composite.

1. Introduction

Polyurea with milled glass composites (PU-MG) are introduced and their mechanical behavior was experimentally characterized and reported in an accompanying paper (Nantasetphong et al., 2016a). In this paper, micromechanical models that describe their behavior with varying geometrical and mathematical complexity are presented.

One of the first models for short-fiber composites is the shear lag model developed by Cox (1952); Tucker III and Liang (1999). Later, Eshelby solved the elasticity problem of an ellipsoidal inclusion embedded in infinitely large matrix for the elastic stress field in and around the inclusion (Eshelby, 1957, 1961). In these celebrated works, he showed that within an ellipsoidal inclusion the strain field is uniform, and is related to a uniform transformation strain through a tensor now commonly referred to as Eshelby's tensor. The tensor depends only on the inclusion aspect ratios and the matrix elastic constants (Mura, 2013). By letting the inclusion be a prolate ellipsoid, one can use Eshelby's results to find the stiffness of a composite with cylindrical fibers at dilute concentrations (Tucker III and Liang, 1999; Chow, 1978; Nemat-Nasser and Hori, 2013). For non-dilute discontinuous fiber composite models, the interaction between fibers is taken into account either directly or indirectly. Mori and Tanaka proposed that the average strain in the fiber should be proportional to the average strain in the matrix. This idea was used to treat non-dilute composite materials (Mori and Tanaka, 1973). Taya and Mura applied Eshelby's and Mori-Tanaka's ideas to create models to predict the longitudinal modulus of a short-fiber composite containing fiber-end cracks in resin (Taya and Mura, 1981). Another approach to account for finite fiber volume fraction is the self-consistent method. In the self-consistent method, one has to numerically find the properties of a composite in which a single particle is embedded in an infinite matrix that has the, yet unknown, average properties of the composite. The solution of the self-consistent approach for some composites may require using iterative scheme (Chou et al., 1980; Laws and McLaughlin, 1979). Nemat-Nasser and Hori (2013); Nemat-Nasser et al. (1982); Iwakuma and Nemat-Nasser (1983) developed a method based on the periodic distribution of inclusions, in which

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the inclusion can be void or solid and can have various shapes. At high volume fraction, this method accounts for the interaction between particles in a more direct manner than either Mori–Tanaka or self-consistent methods. However, this method might not appropriately represent the microstructure of a composite material that has inclusions randomly distributed in the matrix. Despite this concern, the assumption of periodicity has been proved very powerful in predicting mechanical properties of composites with high inclusion-interaction effects and random distribution of inclusions (Nemat-Nasser and Hori, 2013; Nemat-Nasser et al., 1982; Iwakuma and Nemat-Nasser, 1983). Another method that accounts for the interaction between inclusion and their surrounding matrix material in a direct manner is the double inclusion model (or three-phase model) developed by Hori and Nemat-Nasser (1993). It is the generalized version of the Mori–Tanaka method. The model uses averaging scheme and produces the overall moduli of two-phase composites with greater flexibility and effectiveness than the self-consistent and the Mori–Tanaka method. The average stress and strain in a typical inclusion is estimated by embedding the typical inclusion in a finite ellipsoidal region of matrix elasticity and then this double inclusion is embedded in an infinite uniform solid with the yet-unknown overall elasticity of the composite (Nemat-Nasser and Hori, 2013; Hori and Nemat-Nasser, 1993). By replacing the yet-unknown overall elasticity with the elasticity of the matrix, the model gives the Mori–Tanaka or two-phase model, while setting it as the unknown composite value gives the self-consistent estimate in the case both inclusions are coaxial. In general, other estimates may be achieved by any choice of combination of inclusion, matrix, and composite material properties. For other interesting methods, Tucker III and Liang have provided a thorough literature review (Tucker III and Liang, 1999).

In this study, micromechanical models were developed based on 3 different methods: (1) dilute random, (2) non-dilute random, and (3) non-dilute periodic distributions of inclusions. The first method implements Eshelby's works (Eshelby, 1961, 1957; Mura, 2013; Nemat-Nasser and Hori, 2013). The second method uses Mori–Tanaka averaging method (Tucker III and Liang, 1999; Nemat-Nasser and Hori, 2013; Mori and Tanaka, 1973; Taya and Mura, 1981). The third method follows Nemat-Nasser and coworkers' works (Nemat-Nasser and Hori, 2013; Nemat-Nasser et al., 1982; Iwakuma and Nemat-Nasser, 1983). In contrast with method 1, methods 2 and 3 take into account the effect of particles interaction in two different unit cell structures. Each method has its own advantage. The dilute random distribution is the least complex approach and takes less computational time, but it is less accurate for high volume fractions of inclusions. The non-dilute random distribution of inclusions improves the accuracy of method 1, while it takes the same computational time. The non-dilute periodic distribution of inclusions requires more computational time due to the calculation of Fourier series representation of field variables (Nemat-Nasser and Hori, 2013; Nemat-Nasser et al., 1982; Iwakuma and Nemat-Nasser, 1983), but it provides the most accurate results among the three-presented methods. In each method, three models with different fiber orientations; uniaxial, in-plane random, and 3D random orientations were addressed using proper averaging techniques. Originally, these models were created for estimating mechanical properties of elastic composites; however Hashin showed that by replacement of the real elastic moduli by their complex counterparts (including storage and loss components), they can be directly utilized for viscoelastic composites (Hashin, 1970).

2. Theory

Consider the applied uniform strain ϵ^o (linear displacement) or uniform stress σ^o on boundary of a composite. The average strain $\bar{\epsilon}$ or stress $\bar{\sigma}$ over total volume of the composite will be:

$$\bar{\boldsymbol{\epsilon}} = \boldsymbol{\epsilon}^{\boldsymbol{o}}, \tag{1}$$

$$\bar{\boldsymbol{\sigma}} = \boldsymbol{\sigma}^{\boldsymbol{o}}, \tag{2}$$

respectively (Nemat-Nasser and Hori, 2013). The overall constitutive tensors for the composite can be written as:

$$\bar{\boldsymbol{C}} : \boldsymbol{\epsilon}^{\boldsymbol{o}} = \boldsymbol{C}^{\boldsymbol{m}} : \boldsymbol{\epsilon}^{\boldsymbol{o}} + f_{\Omega}\left(\boldsymbol{C}^{\boldsymbol{\Omega}} - \boldsymbol{C}^{\boldsymbol{m}}\right) : \bar{\boldsymbol{\epsilon}}^{\boldsymbol{\Omega}}, \tag{3}$$

$$\bar{\boldsymbol{D}} : \boldsymbol{\sigma}^{\boldsymbol{o}} = \boldsymbol{D}^{\boldsymbol{m}} : \boldsymbol{\sigma}^{\boldsymbol{o}} + f_{\Omega}\left(\boldsymbol{D}^{\boldsymbol{\Omega}} - \boldsymbol{D}^{\boldsymbol{m}}\right) : \bar{\boldsymbol{\sigma}}^{\boldsymbol{\Omega}}, \tag{4}$$

based on the calculated average stress and strain tensors, respectively. f_{Ω} is the volume fraction of the fiber, $\bar{\boldsymbol{C}}$, $\boldsymbol{C}^{\boldsymbol{\Omega}}$, and $\boldsymbol{C}^{\boldsymbol{m}}$ are the (to be determined) overall elasticity tensor of the composite, the elasticity tensor of the fiber, and the elasticity tensor of the matrix, respectively, $\bar{\boldsymbol{D}}$, $\boldsymbol{D}^{\boldsymbol{\Omega}}$, and $\boldsymbol{D}^{\boldsymbol{m}}$ are the (to be determined) overall compliance tensor of the composite, the compliance tensor of the fiber and the compliance tensor of the matrix, respectively, $\bar{\boldsymbol{\epsilon}}^{\boldsymbol{\Omega}}$ and $\bar{\boldsymbol{\sigma}}^{\boldsymbol{\Omega}}$ are the average strain and stress over the fiber volume. $\boldsymbol{\epsilon}^{\boldsymbol{o}}$ and $\boldsymbol{\sigma}^{\boldsymbol{o}}$ are arbitrary. For a fundamental proof, (see Nemat-Nasser and Hori (2013)). If the relation between $\bar{\boldsymbol{\epsilon}}^{\boldsymbol{\Omega}}$ ($\bar{\boldsymbol{\sigma}}^{\boldsymbol{\Omega}}$) and $\boldsymbol{\epsilon}^{\boldsymbol{o}}$ ($\boldsymbol{\sigma}^{\boldsymbol{o}}$) is known, one could solve for $\bar{\boldsymbol{C}}$ ($\bar{\boldsymbol{D}}$). $\bar{\boldsymbol{\epsilon}}^{\boldsymbol{\Omega}}$ and $\bar{\boldsymbol{\sigma}}^{\boldsymbol{\Omega}}$ may be related to $\boldsymbol{\epsilon}^{\boldsymbol{o}}$ and $\boldsymbol{\sigma}^{\boldsymbol{o}}$ as:

$$\bar{\boldsymbol{\epsilon}}^{\boldsymbol{\Omega}} = \boldsymbol{P}^{\boldsymbol{\Omega}} : \boldsymbol{\epsilon}^{\boldsymbol{o}}, \tag{5}$$

$$\bar{\boldsymbol{\sigma}}^{\boldsymbol{\Omega}} = \boldsymbol{Q}^{\boldsymbol{\Omega}} : \boldsymbol{\sigma}^{\boldsymbol{o}}, \tag{6}$$

where $\boldsymbol{P}^{\boldsymbol{\Omega}}$ and $\boldsymbol{Q}^{\boldsymbol{\Omega}}$ are introduced as tensors to transform $\boldsymbol{\epsilon}^{\boldsymbol{o}}$ and $\boldsymbol{\sigma}^{\boldsymbol{o}}$ to $\bar{\boldsymbol{\epsilon}}^{\boldsymbol{\Omega}}$ and $\bar{\boldsymbol{\sigma}}^{\boldsymbol{\Omega}}$, respectively. Note that in (Tucker III and Liang, 1999; Hill, 1963), these tensors are denoted by letters A and B. Substitute Eqs. (5) and (6) into (3) and (4), to write $\bar{\boldsymbol{C}}$ and $\bar{\boldsymbol{D}}$ as:

$$\bar{\boldsymbol{C}} = \boldsymbol{C}^{\boldsymbol{m}} + f_{\Omega}\left(\boldsymbol{C}^{\boldsymbol{\Omega}} - \boldsymbol{C}^{\boldsymbol{m}}\right) : \boldsymbol{P}^{\boldsymbol{\Omega}}, \tag{7}$$

$$\bar{\boldsymbol{D}} = \boldsymbol{D}^{\boldsymbol{m}} + f_{\Omega}\left(\boldsymbol{D}^{\boldsymbol{\Omega}} - \boldsymbol{D}^{\boldsymbol{m}}\right) : \boldsymbol{Q}^{\boldsymbol{\Omega}}. \tag{8}$$

The three methods listed earlier provide different approximations to tensors $\boldsymbol{P}^{\boldsymbol{\Omega}}$ and $\boldsymbol{Q}^{\boldsymbol{\Omega}}$. Since micromechanical models for composites with short fibers based on dilute random, non-dilute random, and non-dilute periodic distributions of inclusions are well established in literatures (Eshelby, 1961, 1957; Mura, 2013; Nemat-Nasser and Hori, 2013; Nemat-Nasser et al., 1982; Iwakuma and Nemat-Nasser, 1983; Tucker III and Liang, 1999), only the important theoretical aspects and the necessary modifications of the models will be discussed here.

2.1. Dilute random distributions of inclusions (DD model)

This model considers an infinitely extended matrix with uniform-sized prolate spheroid inclusions in the matrix. Due to the low volume fraction (dilute model) the inclusions do not interact with the adjacent particles. Therefore the far-field strain (stress) experienced by any inclusion equals to the globally applied strain (stress). The average strain (stress) in the inclusion is proportional to the applied strain (stress) (Nemat-Nasser and Hori, 2013). The shape of the prolate spheroid differs from the actual shape of the milled glass fiber. However, the prolate spheroid has a relatively long semi-major axis compared to the two equal semi-minor axes ($l/r \gg 1$) and could be considered a reasonable representation of the milled glass fibers.

Fig. 1(a) represents the structure of a composite with uniaxial prolate spheriods. Geometry and dimensions of the prolate spheroid are shown in Fig. 2(a) and Table 1. The superscripted DD will be used to indicate all models developed from the method