Mesomechanical Modeling of Polymer/Clay Nanocomposites Using a Viscoelastic-Viscoplastic-Viscodamage Constitutive Model

In this study, damage evolution in a nanocomposite containing the polymethyl methacrylate polymer (PMMA) embedded with silicate nanoclay particles is simulated by using a nonlinear viscoelastic, viscoplastic, and viscodamage constitutive model. Mesomechanical two-dimensional representative volume elements (RVEs) of fully intercalated and fully exfoliated nanoclay polymer composites have been arbitrarily generated assuming a uniform dispersion of nanoclay particles with random length, aspect ratio, and orientation. Proper size of the RVE has been determined by studying the effect of the RVE size on the stress-strain response and toughness. Several simulations including different intercalated and exfoliated nanoclay weight fractions under different strain rates at room temperature have been conducted. It is concluded that the strength of exfoliated nanoclay composite is higher than intercalated one due to more distributed damage within many narrow localized zones for the case of exfoliated nanoclay polymer composite.

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Keywords: nanoclay particles, nanocomposite, PMMA polymer, viscoelastic-viscoplastic-viscodamage, mesomechanical

1 Introduction

Polymer and polymer composite materials offer a wide range of advantages such as high strength-to-weight ratio, impact resistance, high flexibility, recyclability, corrosion resistance, low cost, and fast processing time, which make them very attractive materials [1]. Polymer nanocomposites have been and still are the subject of many experimental studies as the next-generation materials since they offer the potential of designing materials with tailored multifunctional properties, but there has been much less emphasis on computational modeling of such nanocomposites that can be used effectively in understanding the structure-property relationship. Researchers have shown that remarkable enhancements can be achieved in mechanical properties in these nanocomposites by adding small amounts of nanoclay particles of very high aspect ratios [2,3]. The resulting enhanced properties are related to the material’s microstructure attained in processing these nanocomposite materials. In 1974, it was proposed that single clay layers are ideal reinforcing agents [2] due to their exceptionally high aspect ratio. Also, the nanometer thickness of these fillers is comparable to the scale of the chain of polymer matrix.

To date, material optimization is still an obscure goal for nanocomposite and nanostructured materials. For example, the effect of good filler dispersion has been verified to be critical for gaining of higher properties relative to those of less dispersed nanocomposites, but it is still indeﬁnite how other parameters such as the aspect ratio and the ﬁller surface functionality can control the overall properties of the nanocomposites [3]. The microstructure of polymer/clay nanocomposite can be classiﬁed as intercalated or exfoliated [4]. In an intercalated nanocomposite, the polymer penetrates the interlayer spaces of nanoclay particles. Usually an intercalated nanocomposite is interlayered by only a few molecular layers of polymer [5,6]. But, in an exfoliated (delaminated) nanoclay composite, the individual thick clay layers (each layer is about one nanometer) are broken up in a continuous polymer matrix with average expanse that depend on the amount of loading. This is a process whereby the polymer chains penetrate the interlayer spaces of clay particles, causing an increase in the layer spacing (d-spacing). Typically, the nanoclay content of exfoliated nanoclay polymer composite is much lower than that of an intercalated nanocomposite [7]. As a result, an exfoliated nanocomposite has a monolithic structure with properties related primarily to those of the polymer matrix [8]. As a matter of fact, if the clay was not well dispersed, it most likely would represent the role of just ﬁller, and a nanocomposite would not be formed [9].

To date, material-by-design is still an obscure goal especially for nanocomposite and nanostructured materials. For example, the effect of good nanofiller dispersion has been veriﬁed to be critical for gaining of higher properties relative to those of less dispersed nanocomposites, but it is still indeﬁnite how other parameters such as the ﬁller’s aspect ratio and the interfacial properties can control the overall properties of the nanocomposites [3]. Although the micromechanical behavior of nanocomposite polymers can be obtained through experimental testing, it is not easy to characterize the micromechanical response of nanoclay polymer composites in a laboratory because controlling the microstructural features including, for example, nanoclay particle shape, size, orientation, distribution, volume fraction, and interfacial properties is expensive and time consuming. Therefore, it is highly desirable to develop accurate constitutive models and multiscale computational techniques that enable researchers to simulate effectively the micromechanical behavior of nanocomposite polymers, which provide an understanding of the inﬂuence of micromechanical characteristics on the overall macroscopic response. Therefore, the main advantage of the mesoscale modeling approach is to be able to establish the property-structure relationship based on
simulating explicitly the material’s microstructure and to explore the key microstructural features that control the overall macroscopic thermomechanical responses of nanocomposites. Based on this approach, one can design the material for a specific desirable property (e.g., fracture toughness) by directly tailoring the thermomechanical properties of its constituents and their distributions.

Numerous experimental studies have shown that the material response of nanocomposite polymers is very complex and is time-, rate-, and temperature-dependent and exhibits both recoverable (viscoelastic) and irreversible (viscoplastic) deformations. However, there are very few studies that have developed mechanistic constitutive models that couple the thermoviscoelastic, thermoviscoplastic, and thermoviscodamage (i.e., rate- and time-dependent damage) of composite polymers. Therefore, the main objective of this study is to employ a coupled nonlinear viscoelastic, viscoplastic, and viscodamage constitutive model for simulating the mesomechanical response of nanoclay polymer composites. Two-dimensional representative volume element (RVE)-based meso-scale finite element computational modeling of fully intercalated and fully exfoliated nanoclay polyethylene methacrylate (PMMA) polymer composites are conducted in order to obtain their overall macroscopic mechanical response in terms of key microstructural features. The simulations are conducted under uniaxial tension at different strain rates.

2 Constitutive Models

In this section, the recently-developed coupled nonlinear viscoelastic, viscoplastic, and viscodamage constitutive model based on the laws of thermodynamic are recalled here [10,11].

2.1 Nonlinear Viscoelastic Model. Generally, the total deformation of polymeric materials and composites subjected to an applied stress can be decomposed into recoverable (viscoelastic) and irreversible (viscoplastic) components, where the extent of each is mainly affected by the loading time, temperature, and loading rate. Thus, the total Eulerian strain tensor, \( \varepsilon \), can be additively decomposed into a viscoelastic component, \( \varepsilon^{ve} \), and a viscoplastic component, \( \varepsilon^{vp} \), as follows:

\[
\varepsilon_{ij} = \varepsilon_{ij}^{ve} + \varepsilon_{ij}^{vp} \tag{1}
\]

The Eulerian strain tensor \( \varepsilon \) is related to the deformation gradient \( F \) as following:

\[
\varepsilon_{ij} = \frac{1}{2} \left( \delta_{ij} - F_{ki}^{-1} F_{kj}^{-1} \right) \tag{2}
\]

where \( \delta_{ij} \) is the Kronecker delta and \( A^{-1} \) is the inverse of \( A \). Also, based on continuum damage mechanics definition of the effective (undamaged) stress, the relation between Cauchy stress in the undamaged and the damaged material is written as [12]

\[
\sigma_{ij} = \sigma_{ij}^D \frac{1 - \phi}{1 - \phi^D} \tag{3}
\]

where \( \sigma \) is the effective stress tensor in the undamaged configuration, \( \sigma^D \) is the nominal Cauchy stress tensor in the damaged configuration, and \( \phi \) is the so-called damage density or damage variable that starts from \( \phi = 0 \) for undamaged material and ending with 1 at complete rupture. Since \( \sigma \) is the true stress driving the nonlinear behaviors (e.g., viscoelastic, viscoplastic, and viscodamage), the constitutive equations in the subsequent equations are presented in terms of the effective (undamaged) stress \( \sigma^D \).

The Schapery’s nonlinear viscoelastic model [13] is employed here to model the viscoelastic response of the polymer. In one-dimension, the Schapery’s single integral model can be expressed in terms of the effective stress \( \sigma^D \) as follows:

\[
\varepsilon^{ve} = g_0(\sigma^D) D_0 \sigma^D + g_1(\sigma^D) \int_0^\tau \Delta D(\psi^D - \psi^D) d(\sigma^D^t \sigma^D^t) d\tau \tag{4}
\]

where \( D_0 \) is the instantaneous compliance, \( \Delta D \) is the transient compliance, \( g_i \) (i = 0, 1, 2) are nonlinear parameters related to the effective stress and temperature at specific time \( \tau \). The parameter \( g_0 \) measures the increase or decrease in the instantaneous compliance. The parameter \( g_1 \) assesses the nonlinear effect in the transient compliance and \( g_2 \) relates the loading rate effect on the creep response. In Eq. (4), \( \psi^D = \frac{1}{2} \int_0^\tau d\xi^D / (a_0 a_1 a_2) \) is the reduced time and \( \psi^D = a_0 \) is the temperature, strain or stress, and environment (e.g. moisture and aging) time-shift factors, respectively. For numerical convenience, the Prony series is used to represent the transient compliance as:

\[
\Delta D^D = \sum_{i=1}^N D_i \left[ 1 - \exp \left( -\lambda a_i \psi^D \right) \right], \tag{5}
\]

where \( \psi^D \) and \( \psi^D_0 \) are the deviatoric and volumetric strain tensors, respectively, and \( G \) and \( K \) are the undamaged shear and the bulk moduli, respectively. \( J_0, B_0, \) and \( S_0 \) are the undamaged shear and the bulk compliances, and the deviatoric components of the effective stress tensor, respectively. By using the Schapery’s integral constitutive model in Eq. (4), the deviatoric and the volumetric viscoelastic strain components can be expressed at time \( \tau \) as follow, respectively:

\[
\varepsilon_{ij}^{ve} = \frac{1}{2} g_0 J_0 S_{ij}^D + \frac{1}{2} g_1 \int_0^\tau \Delta D(\psi - \psi^D) d(\sigma^D_{ij} S_{ij}^D) d\tau \tag{6}
\]

\[
\varepsilon_{ik}^{vp} = \frac{1}{3} \sigma_{ik} B_0 \varepsilon_{ik}^D + \frac{1}{3} g_1 \int_0^\tau \Delta \varepsilon_{ik} (\psi - \psi^D) d(\sigma^D_{ij} \varepsilon_{ij}^D) d\tau \tag{7}
\]

where \( J_0 \) and \( B_0 \) are the instantaneous effective elastic shear and bulk compliances, respectively.

In the above equations, the superimposed \( \tau \) and \( \tau \) designate a value at current and previous time increments, respectively.

2.2 Viscoplastic Model. In order to calculate the viscoplastic deformations in polymers, a Perzyna-type [15] viscoplasticity constitutive model can be utilized. Therefore, since a large deformation theory is used here, the viscoplastic rate of deformation \( \dot{d}^p \)(i.e., the symmetric part of the spatial velocity gradient) can be expressed using the following flow rule:

\[
\dot{d}_{ij}^p = \Gamma^p(T) (\Phi(f))^N \frac{\partial g}{\partial \sigma_{ij}}, \quad (\Phi(f)) = \begin{cases} 0 & \Phi(f) \leq 0 \\ f / f_0 & \Phi(f) > 0 \end{cases} \tag{8}
\]

where \( \Gamma^p = \Gamma^0 \theta^p(T) \) with \( \theta^p = \exp \left[ \theta (T - T_0) / T_0 \right] \) is the viscoplastic viscosity parameter as a function of temperature \( T \) (1/\( \Gamma^0 \) is the relaxation time of viscoplastic deformation according to the notion of Perzyna) in which \( \Gamma^0 \) is the viscosity parameter at a reference temperature \( T_0 \) and \( \theta \) is a material parameter. \( f \) is the overstress function that is expressed in terms of the yield function \( f \). In Eq. (8), \( \sigma_0^D \) is a yield stress quantity used to normalize the overstress function. Also, the exponent \( N \) is the viscoplastic rate sensitivity parameter. A modified Drucker–Prager yield function that can distinguish between the polymer’s behavior in compression and tension and the sensitivity for confining pressures is employed, as follows:
in Eq.(8) can be presumed as a Drucker–Prager-type form which is nonassociated such that the viscoplastic potential characteristics of the material is complex in general; thus, we assume that the visco-hardening rate. Also, the viscoplastic deformation of polymeric materials. In general, the damage evolution, \( \phi \), can be a function of effective stress, \( \bar{\sigma} \), hydrostatic stress, \( \bar{\sigma}_{\text{tot}} \), total strain, \( \varepsilon \), strain rate, \( k \), temperature, \( T \), and damage history, \( \phi \). Because the time of rupture in a creep test and the peak point in the stress-strain diagram for the constant strain rate test (displacement control) are highly stress dependent, and also, the damage density evolution is highly temperature-dependent; therefore, coupling the damage law with temperature is imperative. Recently, Darabi et al. [11] have proposed a viscodamage evolution law which has also been used for studying damage growth and evolution in polymers by Abu Al-Rub and Tahani [10], as follows:

\[
\phi = \Gamma_0^\text{d} \left[ \left( \frac{Y - Y_0}{Y_0} \right)^2 \right] q \exp \left( k \varepsilon_{\text{eff}}^a \right) \exp \left[ - \delta \left( 1 - \frac{T}{T_0} \right) \right]
\]  

(14)

where \( \Gamma_0^\text{d} \) is the damage viscosity parameter evaluated at a reference temperature \( T_0 \) and \( \delta, k, \) and \( q \) are material constants. \( \varepsilon_{\text{eff}}^a = \varepsilon_{\text{eff}} / C_0 \) is the effective or equivalent total strain, \( Y_0 \) is the damage threshold that specifies at which stress level damage initiates, and \( Y = (\tau - \bar{\mu}_1) \) is the damage driving force where \( \tau \) is given in Eq. (10) and \( \bar{\mu}_1 \) is the Macaulay bracket. The dependency of the damage density evolution equation, Eq. (14), on the total strain couples it to viscoelasticity and viscoplasticity, and also

\[
f = \tau - \bar{\mu}_1 - \kappa (\varepsilon_{\text{eff}}^a) \leq 0
\]  

(9)

\[
\bar{\tau} = \frac{1}{2} \left[ (1 + 1/d) \sqrt{J_2} + (1 - 1/d)J_1 / J_2 \right]
\]  

(10)

\[
\kappa = \left[ \kappa_0 + \kappa_1 \left( 1 - \exp \left( -\kappa_2 (\varepsilon_{\text{eff}}^a) \right) \right) \right] \theta^p(T)
\]  

(11)

where \( \kappa \) relates to the material’s internal friction, \( \bar{\mu}_1 \) is the first invariant of the effective stress tensor, \( J_2 \) and \( J_1 \) are the second and third invariants of the deviatoric part of the effective stress tensor, respectively. The material parameter \( d \) is the ratio of the yield stress in uniaxial tension to that in compression. \( \kappa_0 (\varepsilon_{\text{eff}}^a) \) is an isotropic hardening function associated with the cohesive characteristics of the polymer and is a function of the equivalent viscoplastic strain \( \varepsilon_{\text{eff}}^a \), in which \( \kappa_0 \) defines the initial yield stress, \( \kappa_0 + \kappa_1 \) determines the saturated yield stress, and \( \kappa_2 \) is the strain hardening rate. Also, the viscoplastic deformation of polymeric materials is complex in general; thus, we assume that the viscoplastic effect is nonassociated such that the viscoplastic potential in Eq. (8) can be presumed as a Drucker–Prager-type form

\[
g = \bar{\tau} - \beta \bar{\mu}_1
\]  

(12)

where the material parameter \( \beta \) describes the dilatation or contraction behavior of the material. The effective viscoplastic strain in Eq. (11) can be expressed as follows:

\[
\varepsilon_{\text{eff}}^a = A^{-1} \sqrt{d_\beta^p d_\beta^p}, \quad A = \sqrt{1 + 2 \left( \frac{0.5 + \beta / 3}{1 - \beta / 3} \right)^2}
\]  

(13)

2.3 Viscodamage Model. Time-, rate-, and temperature-independent evolution equations for the damage variable, \( \phi \), are not proper to predict the damage nucleation and the growth in polymeric materials. In general, the damage evolution, \( \phi \), can be a

<table>
<thead>
<tr>
<th>n</th>
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<th>4</th>
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<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
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<td>( \lambda_0 ) (s(^{-1}))</td>
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<td>0.1</td>
<td>0.01</td>
<td>10(^{-5})</td>
<td>10(^{-4})</td>
<td>10(^{-5})</td>
<td>10(^{-6})</td>
<td>10(^{-7})</td>
<td>10(^{-8})</td>
</tr>
<tr>
<td>( D_0 ) (MPa(^{-1})) \times 10^{-6}</td>
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<td>5.66</td>
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<td>18.88</td>
<td>28.58</td>
<td>40.06</td>
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<table>
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<th>( \alpha )</th>
<th>( \beta )</th>
<th>( \Gamma_0^\text{eff} ) (s(^{-1}))</th>
<th>( N )</th>
<th>( d )</th>
<th>( \kappa_0 ) (MPa)</th>
<th>( \kappa_1 ) (MPa)</th>
<th>( \kappa_2 )</th>
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<td>0.3</td>
<td>0.15</td>
<td>2 \times 10^{-4}</td>
<td>1.3</td>
<td>0.85</td>
<td>48</td>
<td>75</td>
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<table>
<thead>
<tr>
<th>( \Gamma_0^\text{d} ) (s(^{-1}))</th>
<th>( Y_0 ) (MPa)</th>
<th>( q )</th>
<th>( k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>8 \times 10^{-5}</td>
<td>60</td>
<td>16</td>
<td>0.8</td>
</tr>
</tbody>
</table>

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\]  

(13)

Fig. 1 RVEs with 3 wt. % of nanoclay particles: (a) fully intercalated and (b) fully exfoliated

Table 1 List of material parameters at 20 °C for the PMMA polymer [10]

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Value (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Modulus ( C_0 )</td>
<td>3500</td>
</tr>
<tr>
<td>Shear modulus ( C_1 )</td>
<td>2200</td>
</tr>
<tr>
<td>Young’s modulus ( C_2 )</td>
<td>1100</td>
</tr>
<tr>
<td>Poisson’s ratio ( C_3 )</td>
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</tr>
<tr>
<td>Thickness ( C_4 )</td>
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</tr>
<tr>
<td>Length ( C_5 )</td>
<td>1</td>
</tr>
<tr>
<td>Thickness ( C_6 )</td>
<td>10</td>
</tr>
<tr>
<td>Length ( C_7 )</td>
<td>4</td>
</tr>
<tr>
<td>Thickness ( C_8 )</td>
<td>100</td>
</tr>
<tr>
<td>Length ( C_9 )</td>
<td>1000</td>
</tr>
<tr>
<td>Thickness ( C_{10} )</td>
<td>10000</td>
</tr>
</tbody>
</table>

Table 2 Mechanical and geometrical properties of nanoclay particles

<table>
<thead>
<tr>
<th>Nanoclay particles</th>
<th>Young’s Modulus (GPa)</th>
<th>Poisson’s ratio</th>
<th>Length (nm)</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Interlamellar</td>
<td>136 GPa</td>
<td>0.28</td>
<td>150–180</td>
<td>7.0–9.0</td>
</tr>
<tr>
<td>Exfoliated</td>
<td>400 GPa</td>
<td>0.20</td>
<td>150–180</td>
<td>1.0–1.5</td>
</tr>
</tbody>
</table>

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Fig. 2 RVE size convergence study: (a) toughness; (b) maximum stress

Fig. 3 Stress-strain behavior of nanoclay PMMA composite at three different strain rates and for three different weight fractions: (a), (c), and (e) are for fully intercalated composite; (b), (d), and (f) are for fully exfoliated composite
implicitly incorporates the dependency on the effects of time, rate, and temperature.

The above viscoelastic, viscoplastic, and viscodamage constitutive models have been implemented in the well-known commercial finite element code ABAQUS via the user material subroutine User Material (UMAT). The reader is referred to Darabi et al. [11] for details about the numerical algorithms for implementing these models. Moreover, the detailed procedure for determining the viscoelastic, viscoplastic, and viscodamage models’ parameters in a systematic way is thoroughly discussed in Ref. [11]. These parameters have been identified for the PMMA polymer by Abu Al-Rub and Tehrani [10]. PMMA is the matrix phase of the nano-clay polymer composite that is micromechanically simulated in the Sec. 3. All the models parameters are listed in Table 1.

3 Mesomechanical Numerical Simulations

3.1 RVE Size and Microstructure. In this section, we focus on a two-dimensional dispersion of perfectly bonded nanoclay particles in a PMMA polymer matrix, and predict the effects of the particles’ distribution in both fully intercalated and fully exfoliated nanoclay particles through simulating the mesomechanical response of RVEs subjected to uniaxial compressive loading.
under isothermal conditions. In Fig.1, two generated RVEs are shown representing the random distribution of nanoclay particles in fully intercalated (Fig. 1(a)) and fully exfoliated (Fig. 1(b)) polymer composites.

For creating the geometry of such RVEs that contain nanoclay particles in different random distributions, length, aspect ratio, and orientation, a c++ program has been written to generate and disperse nanoclay particles in the RVE and then export it to Abaqus [16] by using a Python script code. Elliptical shape of the nanoclay particles is assumed. The elastic mechanical properties and geometry of the nanoclay particles, which are presented in Ref. [17], are listed in Table 2 and employed in the current meso-scale finite element simulations. The RVEs are constrained from the bottom in the vertical direction and from the left in the horizontal direction, whereas periodic boundary conditions are applied to the right edge. Plane strain finite element simulations under displacement control compression up to 1 \( \text{m} \) are conducted. A 4-node bilinear quadrilateral element is used in the simulations. The focus of future studies will be on constructing three-dimensional representation of the nanoclay polymer composites. However, in spite of its limitations, a two-dimensional analysis is still a viable approach to gain qualitative insight, rather than to evaluate the quantitative response, of the material response at the microstructural level.

The size of the RVE should be large enough as compared with the characteristic size of the nanoclay particles so that the size

Fig. 6 Damage distribution in nanoclay composites at 1.0 / s strain rate for 1 wt. %: (a) intercalated, (b) exfoliated; 3 wt. %: (c) intercalated, (d) exfoliated, and 8 wt. %: (e) intercalated, (f) exfoliated
effect of the RVE is negligible. Therefore, in order to determine the proper size of the RVE, several RVE sizes with many random distributions of nanoclay particles are simulated. From these various simulated random distributions of nanoclay particles, the maximum and the minimum peak stresses from a stress-strain response and the toughness modulus as the area under the stress-strain diagram are predicted for each RVE size in order to finding a precise statistical representation of the RVE and distribution of the nanoclay particles. For example, from the results in Fig. 2 with a 3 wt. % of fully intercalated nanoclay particles, a 3 × 3 μm² size for the RVE is selected with the corresponding distributions of nanoclay particles that are shown in Fig. 1. Any RVE that is larger than 3 × 3 μm² with any random distribution of nanoclay particles results in a negligible effect of the RVE’s size on the ultimate strength and toughness of the nanocomposite response. It is worthy to mention that other mechanical properties (e.g., initial modulus), which are not reported here, are also RVE’s size-independent when simulating the response of an RVE that is larger than 3 × 3 μm².

3.2 Computational Results. In this section, the results of the simulations are presented. In Fig. 3, the stress-strain responses of the nanoclay composites at three strain rates (0.001, 0.1, and 1.0/s) and three different weight fractions (1, 3, and 8 wt. %.) are shown and compared with that of the pure polymer matrix response. It can be seen that the stress-strain response of the polymer matrix is improved with dispersing nanoclay particles. It is also obvious from Fig. 3 that the exfoliated nanocomposite outperforms the intercalated nanocomposite as the initial modulus, strength, and strain hardening rates are higher for the exfoliated nanocomposite. Moreover, one can notice that the initial modulus, strength, and strain hardening rates increase as the weight fraction of the nanoclay particles increases for both nanocomposites, where this increase is more pronounced for the exfoliated nanocomposite. These mechanical properties are higher as the strain rate increases. Comparing the stress-strain responses at 1 and 3 wt. %, more pronounced effect of nanoclay particles is seen for the exfoliated nanocomposite. These results are in qualitative agreements with experimental results in Refs. [8,18]. In Fig. 4, the presented bar diagrams show the difference between the toughness (i.e., area under the stress-strain diagram) in each of the simulated RVEs. One can notice that although the toughness has increased in the intercalated clay composite (8wt. %/PMMA = 1.52) (Fig. 4(a)) in comparison to pure polymer, this ratio is almost doubled, when the clay nanoparticles have been fully exfoliated in polymer matrix (8wt. %/PMMA = 2.14) (Fig. 4(b)).

Figure 5 shows the initiation and evolution of damage in the RVE with 3 wt. % of intercalated clay particles in Fig. 1(a) subjected to a compressive strain rate of 1/s. As can be seen, damage has initiated close to the tip of nanoclay clusters and then propagated and merged to other damaged regions. Several localized damaged bands are seen that govern the overall response of the composite. Figures 6(a)–6(f) show the contour of damage distribution for different weight fractions in the intercalated and exfoliated nanocomposites at 1/s strain rate. By comparing the intercalated and exfoliated composite responses with the same nanoclay weight fraction, it can be recognized that when the nanoclay particles are completely exfoliated in the polymer matrix the damage is well-distributed with many narrow localized damage bands unlike that for the fully intercalated nanocomposite where few narrow localized damage bands are evolved. As the weight fraction of the exfoliated nanoparticles increases the amount of damage diminishes so that the stress-strain responses (Fig. 3) show more capacity for carrying the applied load. In fact, the nanoparticles delay the damage evolution and cause smooth damage distributions. This clearly explains why the exfoliated nanocomposite outperforms the intercalated nanocomposite.

4 Conclusion
In this study, a coupled nonlinear viscoelastic, viscoplastic, and viscosdamage constitutive model is used to simulate the mesomechanical response of nanoclay PMMA polymer composite under uniaxial compressive loading. It is shown that the model described in this paper has considerable promise as a mesoscale computational framework for predicting the overall thermomechanical response of polymer composites based on the nature of their microstructure. In this paper, two main types of nanoclay polymer composites are simulated; fully intercalated and fully exfoliated nanoclay PMMA polymer composites. The effect of the weight fraction of nanoclay particles on the overall mechanical response and damage evolution is investigated under different uniaxial compressive strain rates. It is shown that the mechanical response of the pure polymer is significantly enhanced by dispersing small fractions of nanoclay particles. However, the fully exfoliated nanoclay PMMA composite had a higher modulus/strain to failure in comparison to the response of the fully intercalated nanocomposite. This is attributed to ability of the exfoliated nanoparticles for delaying damage initiation and evolution and distributing the damage into many localized narrow bands. Therefore, the maximum benefit of nanoclay particles in a polymer matrix is achieved when the platelets of clay have been well dispersed or exfoliated. In fact, a more pronounced enhancement in the stress-strain response of fully exfoliated nanocomposite is observed when small fractions of nanoclay particles are dispersed within the polymer matrix. Future work will focus on conducting three-dimensional mesosimulationations under different loading conditions. Furthermore, emphasis will be placed on the effect of nanoclay particle-matrix interfacial properties on the overall thermomechanical response, which is a much less understood issue.

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References


