

Modeling and homogenization of shape memory polymer nanocomposites



M. Taherzadeh^a, M. Baghani^{a,*}, M. Baniassadi^a, K. Abrinia^a, M. Safdari^b

^a School of Mechanical Engineering, College of Engineering, University of Tehran, Tehran, Iran

^b Aerospace Engineering Department, University of Illinois, 104 S Wright St., Urbana, IL 61801, USA

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ABSTRACT

Increasing applications of shape memory polymer nanocomposites calls for reliable and effective modeling techniques. Finite element analysis (FEA) is one of the popular modeling techniques mostly used for this purpose. To perform FEA, an effective constitutive law is needed to extract the behavior of material in each integration point. In this study, we have employed 3D finite element modeling to study shape memory polymers (SMPs) loaded with perfectly dispersed Graphene Nanoplatelets (GNPs). In the current work, a novel scheme is used to create representative volume elements for the purpose of modeling, and a 3D constitutive equation is derived to describe the characteristic *thermomechanical behavior of SMPs*. Several realizations of SMP nanocomposites with different volume fractions and aspect ratios of GNP inclusions are generated and modeled, and effective mechanical properties of generated microstructures are estimated using volume-averaged values. It is observed that SMPs loaded with 3% by volume GNP inclusions recover their permanent shape when they are subjected to a small strain thermomechanical cycle. Furthermore, a considerable improvement on the elastic modulus of the composites is observed upon increasing volume fraction or aspect ratio of GNP inclusions.

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1. Introduction

Shape memory materials are a class of smart materials that recover their original (permanent) shape from a deformed state (temporary shape) which is known as shape memory recovery. In most cases, external stimulus such as heat, magnetism, or electricity is applied to stimulate shape memory recovery [1–3]. Since first discovery of shape memory effect in polymers, many research efforts in this field have been carried [4,5]. Compared to other types of smart materials such as shape memory alloys, shape memory polymers (SMPs) have low density, low cost, low energy consumption, excellent manufacturing capability and the ability to withstand large elastic deformation [6–8]. Shape memory polymers are utilized in wide range of applications such as medical, micro-electromechanical systems and advanced technologies in the aerospace [9,10].

Despite all impressive characteristics of SMPs, the most noticeable drawback for SMPs is their poor elastic properties [11] which impedes the applications of SMPs when large recovery

stress is required, e.g. in actuators. In order to overcome such limitations, a variety of reinforcements are used in SMP composites [12,13]. Needless to say, recent developments in the fabrication of nanoscale materials such as Graphene [14], graphite, carbon nanotubes [15,16], and clay also increased academic and industrial interests on using these nanomaterials as reinforcement in other materials including SMPs.

Due to difficulties in experimental characterizations, other methods such as analytical and numerical simulations may be employed as an alternative to experimental methods [17,18]. Mori-Tanaka (MT) [19], and the Halpin-Tsai [20] are two of the most popular analytical mechanic-based composite stiffness models that are widely used for modeling composite structures [21]. These methods are not able to precisely account for the interaction between adjacent particles. Additionally, the micro-stress that is involved with each individual inclusion cannot be evaluated by these methods [22]. In last decades, numerical methods, e.g., finite element method (FEM), has attracted a great deal of interest to be utilized in simulation as well as design of composite structures [23,24]. Statistical continuum mechanics techniques also offer useful tools for characterization and reconstruction of heterogeneous materials based on statistical correlation function [23,25].

* Corresponding author.

E-mail address: baghani@ut.ac.ir (M. Baghani).

In this study, 3D representative volume elements (RVEs) are generated to simulate the stress–strain–temperature relationship of randomly distributed Graphene nanoplatelets-reinforced shape memory polymer composite. In order to evaluate thermo-mechanical response of the composite, the model has been assumed as a mixture of elastic Graphene Nanoplateletes (GNPs) inclusions and SMP matrix. SMP matrix itself is divided into two phases, rubbery and glassy, and the fraction of each phase is directly related to the temperature [26]. To capture the thermo-mechanical response of SMP, a thermodynamically-consistent constitutive model has been developed [3,26]. The stiffness tensor of the elastic GNP is identified by ultrasonic and static tests [27]. In all cases, 7% axial strain is applied and the effects of aspect ratio of the inclusions and volume fraction on the effective elastic properties are presented. Two different thermomechanical cycles are applied on the model, stress–free strain recovery cycle and fixed-strain stress recovery cycle. In the stress–free strain recovery cycle, the model returns from deformed state (temporary shape) to their original (permanent) shape due to rising the temperature. However, in the second cycle, the model is prevented to return to its original shape during the heating the materials. This study also investigates the important effect of imperfect GNP/SMP interfaces on shape memory polymer nanocomposites. Cohesive surface energy between GNP nanoparticles and a polymer reported elsewhere [28] is introduced into finite element models to capture GNP/polymer debonding and its subsequent effect on the mechanical properties of the nanocomposite system under investigation. Finally, key observations of the study are summarized followed by a series of concluding remarks.

2. Constitutive equations for SMP

In this section, the shape memory effect in a stress–strain–temperature diagram is described. As it is shown in Fig. 1, point [a] is the start state in this diagram where SMP holds its permanent shape. At this state a specified strain is applied on the SMP and it demonstrates a rubbery behavior up to point [b] . Then the strain is fixed and the temperature is decreased until the rubbery phase is converted into Glassy phase T_l (temporary shape at point [c]). Then the material is unloaded. Because of the high stiffness of the glassy phase polymer, the strain slightly recovers (point [d]). Finally the temperature rises and SMP recovers its permanent shape at point [a] . This cycle is called stress–free strain recovery in SMP applications. On the other hand, SMP could have gone from point [d] to point [e] , if the strain at point [d] was kept fixed and the temperature was increased. In this way, the cycle is called fixed-strain stress recovery (shown in Fig. 1 with dotted line).

Now, a brief explanation of the small strain constitutive model proposed by Baghani et al. [3] is provided. In this model an

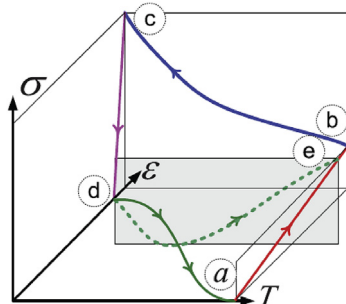


Fig. 1. Stress–strain–temperature diagram showing the thermomechanical behavior of SMP under strain or stress recovery processes.

equivalent RVE of SMP consisting of a frozen and an active phase has been used. According to the mixture rule, the total strain is given in the following relation:

$$\boldsymbol{\varepsilon} = \varphi_a \boldsymbol{\varepsilon}^a + \varphi_f \boldsymbol{\varepsilon}^F + \boldsymbol{\varepsilon}^T, \tag{1}$$

where $\boldsymbol{\varepsilon}^a$ and $\boldsymbol{\varepsilon}^F$ denote elastic strain in the active and frozen phase, respectively and $\boldsymbol{\varepsilon}^T$ denotes the thermal strain which is evaluated by $\alpha^T dT$ and α^T is the effective thermal expansion coefficient. In this relation, φ_a and φ_f denote the volume fraction of the active and frozen phase, respectively. Both φ_a and φ_f are function of temperature. The strain in the frozen phase $\boldsymbol{\varepsilon}^F$ is decomposed into two parts such that

$$\varphi_f \boldsymbol{\varepsilon}^F = \varphi_f \boldsymbol{\varepsilon}^f + \boldsymbol{\varepsilon}^{is}, \tag{2}$$

where $\boldsymbol{\varepsilon}^f$ is the elastic strain in the frozen phase and $\boldsymbol{\varepsilon}^{is}$ is the in-elastic stored strain. As a result, the total strain is the weighted summation of the strains in each phase.

Assuming temperature decreasing, the strain in the newly generated glassy phase, already been in the rubbery phase, had experienced the $\boldsymbol{\varepsilon}^a$ previously. Then $\varphi_f \boldsymbol{\varepsilon}^F$ is defined as:

$$\varphi_f \boldsymbol{\varepsilon}^F = \varphi_f (\boldsymbol{\varepsilon}^f + \bar{\boldsymbol{\varepsilon}}^f) = \varphi_f \left(\boldsymbol{\varepsilon}^f + \frac{1}{V_f} \int_{V_f} \boldsymbol{\varepsilon}^a dv \right) = \varphi_f \boldsymbol{\varepsilon}^f + \frac{1}{V} \int_{V_f} \boldsymbol{\varepsilon}^a dv, \tag{3}$$

where V_f and V are volume of the frozen phase and the total volume of the RVE, respectively. In equation (3), strain in the frozen phase is divided into two parts: strain in the old frozen phase, $\boldsymbol{\varepsilon}^f$, and strain in the newly generated frozen phase, $\bar{\boldsymbol{\varepsilon}}^f$. The term “ $\varphi_f \bar{\boldsymbol{\varepsilon}}^f$ ” is called as the stored strain and it is denoted by $\boldsymbol{\varepsilon}^{is}$. We recast equation (3) to

$$\varphi_f \boldsymbol{\varepsilon}^F = \varphi_f \boldsymbol{\varepsilon}^f + \boldsymbol{\varepsilon}^{is}. \tag{4}$$

In the cooling process, $\boldsymbol{\varepsilon}^{is}$ is defined by

$$\boldsymbol{\varepsilon}^{is} = \int \boldsymbol{\varepsilon}^a d\varphi_f. \tag{5}$$

In the heating process, the strain stored in the frozen phase should be relaxed. This is mathematically expressed by

$$\varphi_f \boldsymbol{\varepsilon}^F = \varphi_f (\boldsymbol{\varepsilon}^f + \bar{\boldsymbol{\varepsilon}}^f) = \varphi_f \left(\boldsymbol{\varepsilon}^f + \frac{1}{V_f} \int_{V_f} \frac{\boldsymbol{\varepsilon}^{is}}{\varphi_f} dv \right) = \varphi_f \boldsymbol{\varepsilon}^f + \frac{1}{V} \int_{V_f} \frac{\boldsymbol{\varepsilon}^{is}}{\varphi_f} dv, \tag{6}$$

which in a more compact form is

$$\varphi_f \boldsymbol{\varepsilon}^F = \varphi_f \boldsymbol{\varepsilon}^f + \boldsymbol{\varepsilon}^{is}. \tag{7}$$

Thus, the total strain could be recast to

$$\boldsymbol{\varepsilon} = \varphi_a \boldsymbol{\varepsilon}^a + \varphi_f \boldsymbol{\varepsilon}^F + \boldsymbol{\varepsilon}^T + \boldsymbol{\varepsilon}^{is}. \tag{8}$$

In addition, the stored strain obeys the following evolution law

$$\dot{\boldsymbol{\varepsilon}}^{is} = \dot{\varphi}_f \left[k_1 \boldsymbol{\varepsilon}^a + k_2 \frac{\boldsymbol{\varepsilon}^{is}}{\varphi_f} \right]; \begin{cases} k_1 = 1, k_2 = 0, \dot{T} < 0 \\ k_1 = 0, k_2 = 1, \dot{T} > 0 \\ k_1 = 0, k_2 = 0, \dot{T} = 0 \end{cases} \tag{9}$$

Now, based on a first order rule of mixture, the convex free-energy density function Ψ is defined by

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