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A variable-order fractional differential equation model of shape memory polymers

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ABSTRACT

A shape-memory polymer (SMP) is capable of memorizing its original shape, and can acquire a temporary shape upon deformation and returns to its permanent shape in response to an external stimulus such as a temperature change. SMPs have been widely used industrial and medical applications. Previously, differential equation models were developed to describe SMPs and their applications. However, these models are often of very complicated form, which require accurate numerical simulations.

In this paper we argue that a variable-order fractional differential equation model of the shape-memory behavior is more suitable than constant-order fractional differential equation models in terms of modeling the memory behavior of SMPs. We develop a numerical method to simulate the variable-order model and, in particular, to identify the unknown variable order of the model. Numerical experiments are presented to show the utility of the method.

1. Introduction

A shape-memory polymer (SMP) is a polymeric material that is capable of memorizing its original shape, and can acquire a temporary shape upon deformation and returns to its permanent shape in response to an external stimulus such as a temperature change [22]. In recent years SMPs have found increasingly more applications in a variety of areas, ranging from industrial to medical applications and even everyday life. Examples in industrial applications of SMPs include shape-memory foams used in the building industry which can expand with temperature to seal window frame, heat-shrinkable tubes used for electronics, and self-deployable sun sails used in a spacecraft. Examples in medical applications of SMPs include intelligent medical devices and implants for minimally invasive surgery [2,7,25].

The transition between the temporary and permanent shape changes in an SMP is often triggered by a temperature change. An SMP has both a visible, current (temporary) shape and an invisible, stored (permanent) shape. Once the SMP is manufactured in its permanent shape, it is reformed into a different, temporary shape by processes of heating, deformation, and cooling. Then the SMP will maintain this temporary shape. The SMP will return to its original (permanent) state only after it is activated by a predetermined external temperature change. In short, the properties of SMPs are temperature dependent and in fact often very sensitive to an external temperature change by the nature of SMPs. Differential equation models have been developed to describe the time-dependent evolution processes in the study and design of SMPs.

In many important applications of SMPs, the response of SMPs to the external stimulus temperature must be very accurate. Moreover, both the temporary and the permanent shapes of SMPs must be placed exactly in the desired locations. Since the properties of SMPs are very sensitive to their external environment, the corresponding numerical models must have very high accuracy and fidelity in their prediction of the thermo-mechanical behavior of the SMPs under various conditions and circumstances. What further complicates the scenario is that the physical mechanism and, correspondingly, the properties of thermally-induced SMPs depend heavily on polymer types, and may vary significantly in response to the same external environment. For example, the melting transition is responsible for the semicrystalline polymers [8]. The nematic-isotropic transition can induce the shape-memory effect (SME) in liquid crystalline elastomers [2]. The thermally-induced SME in amorphous polymers originates from the glass transition [15], the modeling and numerical simulation of which is the main objective of this paper although the modeling technique developed in the paper can be applied to other types of SMPs.

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Two main approaches, namely the phase transition modeling approach and the thermo-viscoelastic modeling approach, have been used to model the SME [14]. The thermo-viscoelastic modeling approach is physically relevant and is based upon the one-dimensional rheological models. This is the reason why it has attracted wide attentions. To model the SME, the modulus or the viscosity the model are assumed to be temperature dependent [14,21,22]. However, the resulting (integer-order) differential equation models for accurately describing the SME are of a very complicated form and typically contain a large number of parameters to be determined [15,24]. This introduces mathematical and numerical difficulties as well as uncertainty that are difficult and costly in numerical simulations.

In recent years fractional-order differential equation (FDE) models are emerging as powerful tools for modeling challenging phenomena involving long-time memory or long-range spatial interactions in many disciplines and applications [12,16]. In particular, it was shown that FDE models can accurately describe complex viscoelastic behaviors with only a few parameters used [6,16,18,23]. This is not an coincidence but has deep physical reasons behind. Recall that classical integer-order differential equation models were derived under the assumption that there exist (i) a mean free path and (ii) a mean waiting time in the underlying particle movements at the microscopic scale [11,12]. These assumptions virtually hold for evolution processes in homogeneous media. The fundamental reason why SMPs work lies in their molecular network structure which consists of at least two separate phases, as well as their change in response to an external stimulus temperature change. As the material structure is heterogeneous in general, an integer-order differential equation model often fails to provide an appropriate description of the evolution process. In contrast, an FDE model has been shown to provide a more accurate description of the evolution process. Moreover, as SMPs have long-time memory effect, a fractional-order-in-time differential equation model is well suited for modeling the behavior of SMPs [3,11,12,16]. Finally, because SMPs can have significant changes of their shapes depending on whether an external stimulus temperature change exceeds their prescribed temperature, which in turn will significantly affect their microscopic network structure. Hence, a variable-order FDE model seems to be a more appropriate model to describe the shape-memory behaviors of amorphous polymers, which we will study in this paper.

The rest of the paper is as follows. In Section 2 we present a fractional-order differential equation model of the shape-memory behavior of SMPs. In Section 3 we describe and discuss why a variable-order fractional differential equation model seems to be more appropriate the shape-memory behavior of SMPs.

2. A fractional-order differential equation model of shape-memory behavior of SMPs

In this section we present a fractional-order Zener differential equation model of the shape-memory behavior of SMPs. The one-dimensional rheological representative of a fractional-order Zener model is shown below in Fig. 1, which consists of an equilibrium elastic spring and a fractional damping Maxwell element.

The total strain in the non-equilibrium branch equals to that of the equilibrium branch, leading to

$$\epsilon = \epsilon^e + \epsilon^v. \tag{1}$$

The stress response is given by

$$\sigma = E^{eq}\epsilon + E^{neq}\epsilon^e, \tag{2}$$

where E^{eq} is the modulus of the equilibrium elastic spring and E^{neq} is the modulus of the spring in the non-equilibrium fractional damping Maxwell element. The evolution of ϵ^v in the fractional damping element can be determined by [5,23]

$${}_0^C D_t^\alpha \epsilon^v = \frac{\epsilon - \epsilon^v}{\tau^\alpha}, \qquad \epsilon^v|_{t=0} = 0. \tag{3}$$

Here τ is the temperature-dependent relaxation time of the Maxwell element and is given by

$$\tau = \begin{cases} \tau^{ref} 10^{-\frac{C_1(T-T_g)}{C_2+T-T_g}}, & T \geq T_g, \\ \tau^{ref} 10^{A(\frac{1}{T}-\frac{1}{T_g})}, & T < T_g \end{cases} \tag{4}$$

where the temperature profile T is a function of time t. ${}_0^C D_t^\alpha$ with $0 < \alpha < 1$ is the Caputo fractional derivative operator of order α [16] which is defined by

$${}_0^C D_t^\alpha \epsilon^v(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{d\epsilon^v(s)}{ds} (t-s)^{-\alpha} ds. \tag{5}$$

The combination of Eqs. (1), (2) and (3) yields the following fractional shape-memory behavior model

$$\begin{cases} {}_0^C D_t^\alpha \epsilon^v = \dfrac{\sigma(t) - E^{eq}\epsilon^v}{(E^{neq}+E^{eq})\tau^\alpha}, \\ \epsilon = \dfrac{\sigma(t) + E^{neq}\epsilon^v}{E^{neq}+E^{eq}}, \\ \epsilon^v|_{t=0} = 0. \end{cases} \tag{6}$$

To close the sytem (6), a constitutive relation of $\sigma(t)$ is provided in the numerical simulation. For their numerical investigation, we refer readers to, e.g., the work in [5,23].

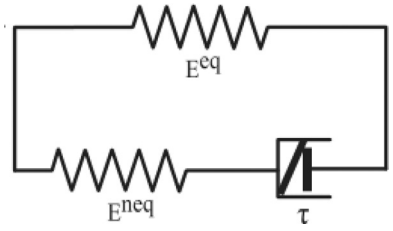

Fig. 1. Illustration of a fractional-order Zener model.

3. A variable-order FDE model of the shape-memory behavior and its numerical method

It is known that the fractional order α in an FDE model is related to the Hurst index or the fractal dimension of the material matrix [11]. Recall that the fundamental reason why SMPs can return to its original (permanent) shape from their current (temporary) shape lies in the fact that their molecular network structures, which consists of at least two separate phases, change in response to an external stimulus temperature change. As their network structures change, their fractal dimensions are anticipated to change. Hence, a variable-order FDE model is expected to be more suitable than a constant-order FDE model. Motivated by these observations, we consider the following variable-order FDE model of the shape-memory behavior [3,4,19,20]

$$\begin{cases} {}_0^C D_t^{\alpha(t)} \epsilon^v = \dfrac{\sigma(t) - E^{eq}\epsilon^v}{(E^{neq}+E^{eq})\tau^{\alpha(t)}}, & t \in [0, t_{final}] \\ \epsilon = \dfrac{\sigma(t) + E^{neq}\epsilon^v}{E^{neq}+E^{eq}}, & t \in [0, t_{final}], \\ \epsilon^v|_{t=0} = 0, \end{cases} \tag{7}$$

with $0 < \alpha(t) < 1$. The variable-order fractional derivative ${}_0^C D_t^{\alpha(t)}$ is defined by [1,4,17,19]

$${}_0^C D_t^{\alpha(t)} \epsilon^v(t) = \frac{1}{\Gamma(1-\alpha(t))} \int_0^t \frac{d\epsilon^v(s)}{ds} (t-s)^{-\alpha(t)} ds. \tag{8}$$