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Modeling nonlinear thermo-elastic response for glassy polycarbonate using ultrasonic results under compression in a confined cell

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A B S T R A C T

We develop a nonlinear thermo-elastic model for polycarbonate (PC) using ultrasonic longitudinal and shear waves applied on a sample under confined compression. The model is a thermodynamically consistent model developed based on data obtained from a modified pressure–volume–temperature measurement system that also provides the longitudinal and shear wave moduli (Masubuchi et al., 1998. Materials Science Research International 4(3), 223–226). The heat capacity data was obtained by using a differential scanning calorimeter. The resulting model reproduces the ultrasonic behavior of the PC over the temperature range of 35 °C to 150 °C and under pressures from 0 to 70 MPa. Since the response at constant pressure is close to linear below the glass transition temperature of 147 °C, one may extend the use of the model to temperatures below 35 °C, possibly covering most of the range of use for most applications.

1. Introduction

Most of the models that are used to characterize the thermo-elastic behavior of glassy polymers such as polycarbonate (PC) at large deformations are based on visco-elastic models that have components resembling finite deformation plasticity (Argon, 1975; Argon and Bessonov, 1977a,b; Boyce et al., 1988, 1989, 1994, 1995; Boyce and Arruda, 1990; Arruda and Boyce, 1993a,b; Arruda et al., 1993, 1995; Hasan et al., 1995; Krempl and Ho, 1995; Krempl and Bordonaro, 2000). For the stress response, these models describe the stress as a function of the elastic deformation gradient and temperature. Even though the models are nonlinear, they are normally fit to the initial bulk and shear moduli measured from tension or compression tests at infinitesimal strains. As a result, in the nonlinear range the models may or may not predict response consistent with the material's nonlinear response. To improve the modeling, we propose to build a nonlinear thermo-elastic response model for PC based on ultrasonic wave speed measurements done in a pressure–volume–temperature (PVT) device by Masubuchi et al. (1998).

We model the response by building a thermo-elastic model of the free energy based on the measured response. The method to construct free energy functions for models that depend on the invariants of the deformation has been used by many authors and recently reviewed by Marckmann and Verron (2006). These hyperelastic models are also used to create large deformation thermo-elastic models based on separating the deformation into elastic and thermal parts and assuming the stress to depend only on the elastic deformation and temperature. Such models use the total deformation as a multiplicative deformation of elastic and thermal parts as introduced by Stojanović (Stojanovic et al., 1964, 1970) and being used by many authors including, for example, (Miehe, 1995; Holzapfel and Simo, 1996; Imam and Johnson, 1998; Vujosevic and Lubarda, 2002). We will also use a similar construct to make the nonlinear thermo-elastic model.

Our model is based on the experiments of Masubuchi et al. (1998) on a pressurized samples of PC confined laterally in a pressure chamber and subjected to longitudinal

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and shear ultrasonic waves. They report the volume change, pressure, temperature, and the longitudinal and shear wave speeds at different temperatures. A description of the results and model follow.

2. Experimental measurements

The experimental measurements discussed here were performed by Masubuchi et al. (1998). The authors combined a pressure–volume–temperature (PVT) test system with an ultrasonic velocity measurement system to calculate the longitudinal and shear wave speeds of PC under high pressure using a closed and sealed system. The samples were processed into a cylindrical shape and were set into a PVT system (since the temperature and pressure need to be controlled during the test) and, in addition to the PVT measurements, they also measured the longitudinal and shear wave velocities for this PC. The description of the experimental procedure is provided in Masubuchi et al. (1998), Kuttruff (1991), Shutilov (1988), Nishiwaki et al. (1994). The compression and shear wave moduli were calculated using the standard wave equations

$$E = \rho v_l^2, \tag{1}$$

$$G = \rho v_s^2, \tag{2}$$

where E is the longitudinal (compression/tension) wave modulus, G is the shear wave modulus, ρ is the density, v_l is the longitudinal wave speed, and v_s is the shear wave speed. Fig. 1 shows the specific volume they measured as a function of temperature at various pressures. The density can be calculated as the reciprocal of the specific volume using the PVT curves shown in Fig. 1, and Figs. 2 and 3 show the wave moduli calculated at different temperature and pressures.

3. Modeling considerations

We propose to make an isotropic thermo-elastic model for PC based on deformation, ultrasonic, and calorimetric measurements. To do this, we start from a general framework assuming the specific free energy ψ, the Cauchy stress tensor $\mathbf{T}$, the specific entropy η, and the heat flux vector $\mathbf{q}$ each is given by a function of the elastic deformation gradient $\mathbf{F}^e$, the thermal deformation gradient $\mathbf{F}^\theta$, temperature gradient $\mathbf{G}$, and temperature θ. We write this as

$$\begin{aligned} \psi &= \psi^+\ (\mathbf{F}^e, \mathbf{F}^\theta, \mathbf{G}, \theta),\\ \mathbf{T} &= \mathbf{T}^+\ (\mathbf{F}^e, \mathbf{F}^\theta, \mathbf{G}, \theta),\\ \eta &= \eta^+\ (\mathbf{F}^e, \mathbf{F}^\theta, \mathbf{G}, \theta),\\ \mathbf{q} &= \mathbf{q}^+\ (\mathbf{F}^e, \mathbf{F}^\theta, \mathbf{G}, \theta), \end{aligned} \tag{3}$$

where the superscript "+" indicates the constitutive function used to model the variable, and we assume that the deformation gradient $\mathbf{F}$ is decomposed through the multiplicative decomposition $\mathbf{F} = \mathbf{F}^e\mathbf{F}^\theta$ introduced by Stojanovic' (Stojanovic et al., 1964, 1970) and others. Standard arguments (see Negahban, 1995) based on imposing the entropy production inequality remove the dependence of the free energy on $\mathbf{G}$ and provide the relations

$$\begin{aligned} &\psi = \psi^+(\mathbf{F}^e, \mathbf{F}^\theta, \theta),\\ &\mathbf{T}^T = \rho\partial_{\mathbf{F}^e}(\psi^+)\mathbf{F}^{eT},\\ &\eta = -\partial_\theta(\psi^+) - \left[\partial_{\mathbf{F}^\theta}(\psi^+)\mathbf{F}^{\theta T} - \tfrac{1}{\rho}\mathbf{F}^{eT}\mathbf{T}^T\mathbf{F}^{e-T}\right] : \boldsymbol{\alpha},\\ &\tfrac{1}{\theta}\mathbf{q}\circ\mathbf{g} \le 0, \end{aligned} \tag{4}$$

where ρ is the current density, $\boldsymbol{\alpha}$ is the multidimensional coefficient of thermal expansion and $\mathbf{g} = \mathbf{G}\mathbf{F}^{-1}$ is the temperature gradient relative to the current configuration while $\mathbf{G}$ was the temperature gradient relative to the reference configuration. It follows from the dependence on the free energy that the stress and entropy do not depend on the temperature gradient.

We further assume that the response is appropriately invariant to rigid body motions, and that the free energy, and hence the stress and entropy, do not directly depend on the thermal deformation gradient. Standard arguments allow us to write the free energy as a new function of the right Cauchy stretch tensor $\mathbf{C}^e = \mathbf{F}^{eT}\mathbf{F}^e = \mathbf{U}^{e2}$ and of temperature.

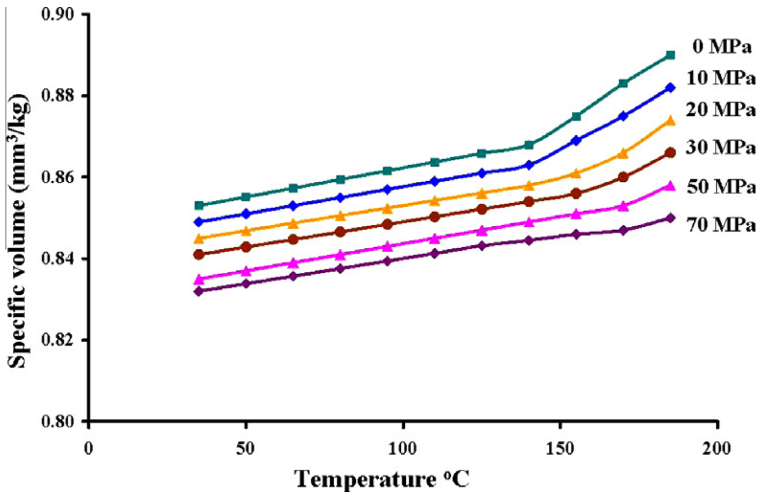

Fig. 1. Specific volume for PC as a function of temperature and pressure (data extracted from Masubuchi et al. (1998)).