



Thermomechanical material modelling based on a hybrid free energy density depending on pressure, isochoric deformation and temperature



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ABSTRACT

In order to represent temperature-dependent mechanical material properties in a thermomechanical consistent manner it is common practice to start with the definition of a model for the specific Helmholtz free energy. Its canonical independent variables are the Green strain tensor and the temperature. But to represent calorimetric material properties under isobaric conditions, for example the exothermal behaviour of a curing process or the dependence of the specific heat on the temperature history, the temperature and the pressure should be taken as independent variables. Thus, in the field of calorimetry the Gibbs free energy is usually used as thermodynamic potential whereas in continuum mechanics the Helmholtz free energy is normally applied. In order to simplify the representation of calorimetric phenomena in continuum mechanics a hybrid free energy density is introduced. Its canonical independent variables are the isochoric Green strain tensor, the pressure and the temperature. It is related to the Helmholtz free energy density by a Legendre transformation. In combination with the additive split of the stress power into the sum of isochoric and volumetric terms this approach leads to thermomechanical consistent constitutive models for large deformations. The article closes with applications of this approach to finite thermoelasticity, curing adhesives and the glass transition.

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1. Introduction

In engineering, constitutive theories are usually formulated to represent mechanical material properties under isothermal conditions. In this context, the reader is referred to the articles of Lion (1997), Boyce et al. (2000), Laiarinandrasana et al. (2009), Miehe et al. (2009) or Jöhrlitz et al. (2010) in which the temperature-dependent stress–strain behaviour of elastomers and other polymers under finite deformations is addressed. Since stress- or temperature-induced changes in volume are relatively small under typical loading states and magnitudes, the stress–strain behaviour of a large number of polymers can be assumed as nearly isochoric. Accordingly, under such loadings the effect of the volumetric part of the constitutive model to the stress–strain response is relatively small, for example in the case of tensional loadings of tall specimens. In order to identify the material parameters of constitutive models or to implement them into finite element programs, formulations in which the stress tensor is the dependent mechanical state variable are required. For this reason, the specific Helmholtz free energy is usually taken as fundamental thermodynamic potential in continuum mechanics. It should be mentioned that the isochoric specific heat which is needed for the evaluation of the

related differential equation of heat conduction can easily be calculated from the Helmholtz free energy because it is its thermodynamically associated caloric quantity. But caused by their high bulk modulus, the isochoric specific heat cannot be measured for solids. If, for example, the isobaric specific heat has been measured in a standard calorimetric experiment but the isochoric specific heat is needed as input parameter for a finite element program, the difference between them is frequently ignored because in many situations it has minor influence to the simulation results. Following Haupt (2002), in linear thermoelasticity the isochoric and isobaric specific heats c_v and c_p are constant material parameters and are connected as follows:

$$c_p - c_v = \frac{9\theta_0 K \alpha^2}{\rho} \quad (1)$$

The application of (1) is only possible in sufficient small temperature intervals in which c_v and c_p are nearly constant. In the case of polymers, the mass density is about $\rho \approx 10^3 \text{ kg m}^{-3}$, a typical value for the bulk modulus is about $K \approx 3000 \text{ MPa}$, the linear thermal expansion coefficient is of the order of $\alpha \approx 10^{-4} \text{ K}^{-1}$ and $\theta_0 \approx 300 \text{ K}$ is a rough estimate for the reference temperature. Based on these values, $9\theta_0 K \alpha^2 / \rho \approx 81 \text{ J kg}^{-1} \text{ K}^{-1}$ is calculated. Since $c_p - c_v$ depends in a quadratic manner on the expansion coefficient, a larger value of $\alpha \approx 2 \times 10^{-4} \text{ K}^{-1}$ leads to $9\theta_0 K \alpha^2 / \rho \approx 324 \text{ J kg}^{-1} \text{ K}^{-1}$. Assuming $c_p \approx 1500 \text{ J kg}^{-1} \text{ K}^{-1}$ as a typical value

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for the isobaric specific heat of polymers, the relative difference $(c_p - c_v)/c_p$ is between 5% and more than 20%. In the case of mechanically incompressible but thermally expandable materials like rubber, the term “isochoric specific heat” makes no sense.

In thermochemistry, on the other hand, the caloric material properties as well as the thermal expansion behaviour are often in the centre of interest (cf. Kamal et al., 1973; Bauer et al., 2000; Gutzow et al., 2007; Garden, 2007a,b; Bailey et al., 2008; Richert, 2011 and the citations therein). In order to represent this type of material behaviour, the specific Gibbs free energy is typically taken as fundamental thermodynamic potential (cf. Gutzow et al., 2007; Lion et al., 2011). The main reason for this choice is the fact that calorimetric and thermal expansion experiments are commonly carried out under prescribed pressure and temperature histories. In many commercial differential scanning calorimetry apparatuses, the pressure is constant and the temperature is a user-definable function of time. It would be quite strange in this situation to take the specific Helmholtz free energy as thermodynamic potential because its associated caloric quantity is the isochoric specific heat. In the case of isotropic materials under free boundary conditions, only changes in volume occur when the pressure and the temperature are varying. Therefore, the isochoric part of a three-dimensional constitutive model (cf. Lion et al., 2010; Lion et al., 2011) has no influence to the caloric response and the thermal expansion behaviour. Consequently, Gutzow et al. (2007) formulated their model only for the volumetric material behaviour, i.e. the Gibbs free energy depends on temperature, pressure and an internal variable which they denoted as order parameter. The application of the Gibbs free energy approach in the field of three-dimensional solid mechanics is promising in the case of linear thermoviscoelasticity (cf. Lion et al., 2010) when the mechanical model is solvable for the stress tensor. But in the case of large deformations or pronounced physical nonlinearities such a formulation would lead to implicit constitutive equations which are no more solvable for the stress tensor.

In a recent essay by Hartmann et al. (2013), the field-assisted sintering of copper and ceramic powder in graphite tools was modelled, simulated and validated. During these processes, the transient temperature variations can reach several hundred degrees. In order to develop a realistic constitutive model for such a process, not only the knowledge about the temperature-dependent mechanical material behaviour is important but also the consideration of the caloric material behaviour. In the relevant temperature range, the experimental data of the isobaric specific heat of graphite exhibits an increase of more than 120%. As it is common practice, the authors developed a constitutive model that is based on the specific Helmholtz free energy such that the empirical function which they fitted to the experimental curve of the specific heat has to be interpreted as isochoric specific heat. This statement becomes clearly when the time derivative of the volume strain in their differential equation of heat conduction is set to zero and can be justified as follows: Since graphite possesses a relative small linear thermal expansion coefficient of $\alpha \approx 4.6 \times 10^{-6} \text{ K}^{-1}$, a density of $\rho \approx 1850 \text{ kg m}^{-3}$ and a bulk modulus of about $K \approx 6000 \text{ MPa}$, the value of $9\theta_0 K \alpha^2 / \rho \approx 0.2 \text{ J kg}^{-1} \text{ K}^{-1}$ is obtained for the difference $c_p - c_v$ when $\theta_0 \approx 300 \text{ K}$ is assumed. For this reason, it is not required to distinguish between the isochoric and the isobaric specific heat in the case of graphite at least under small temperature changes. Since the terms isochoric and isobaric are precisely defined, caution is necessary.

These considerations have shown that a temperature- and pressure-dependent free energy of the Gibbs type is advantageous when isobaric caloric or volumetric thermal expansion data have to be constitutively modelled. If mechanical stress–strain data has to be modelled or a finite element implementation has to be realised, it is more convenient to develop a model which is based

on the temperature- and deformation-dependent Helmholtz free energy. In order to separate volumetric effects from changes in shape it is useful to split the deformation gradient into the corresponding contributions. For these reasons, a hybrid free energy density is proposed which combines all these aspects. In Section 2 of this paper, the fundamentals and the general thermomechanical framework are provided. In Section 3, it is shown how caloric quantities like the enthalpy rate or the isobaric specific heat can be taken into account in a stringent manner. Section 4 discusses different applications of the theory and Section 5 closes with a discussion.

2. Thermomechanical approach

In order to represent thermomechanical material properties in nonlinear continuum mechanics the space- and time-dependent deformation gradient \mathbf{F} is a fundamental geometrical quantity (cf. Haupt, 2002). Its determinant $J = \det(\mathbf{F})$ describes the ratio of the volume elements between the reference and the current configuration. As proposed by Flory (1961), the tensor \mathbf{F} can be multiplicatively decomposed into pure volumetric and isochoric contributions:

$$\mathbf{F} = \bar{\mathbf{F}} \hat{\mathbf{F}} \quad (2)$$

$$\bar{\mathbf{F}} = J^{1/3} \mathbf{1} \quad (3)$$

$$\hat{\mathbf{F}} = J^{-1/3} \mathbf{F} \quad (4)$$

The isochoric part $\hat{\mathbf{F}}$ is not influenced by changes in volume and the volumetric part $\bar{\mathbf{F}}$ does not depend on changes in shape. Based on the tensors \mathbf{F} and $\hat{\mathbf{F}}$, two different Cauchy–Green tensors $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ and $\hat{\mathbf{C}} = \hat{\mathbf{F}}^T \hat{\mathbf{F}}$ which are calculated with the total deformation gradient and its isochoric part are introduced. This motivates the following definitions of two Green strain tensors and of the volume strain:

$$\mathbf{E} = \frac{1}{2} (\mathbf{C} - \mathbf{1}) \quad (5)$$

$$\hat{\mathbf{E}} = \frac{1}{2} (\hat{\mathbf{C}} - \mathbf{1}) \quad (6)$$

$$\varepsilon_{\text{vol}} = J - 1 \quad (7)$$

Considering these expressions, the total Green strain tensor \mathbf{E} can be expressed as follows:

$$\mathbf{E} = \frac{1}{2} (J^{2/3} \hat{\mathbf{C}} - \mathbf{1}) = J^{2/3} \hat{\mathbf{E}} + \frac{1}{2} (J^{2/3} - 1) \mathbf{1} \quad (8)$$

Since the isochoric Cauchy Green tensor $\hat{\mathbf{C}}$ is unimodular, the constraint $\det(\hat{\mathbf{C}}) = 1$ holds for arbitrary deformation histories. Differentiating this relation with respect to time, the following orthogonality relation can be derived:

$$\frac{d}{dt} \det(\hat{\mathbf{C}}(t)) = 0 \Rightarrow \hat{\mathbf{C}}^{-1} \cdot \dot{\hat{\mathbf{C}}} = 0 \quad (9)$$

The dot between two second order tensors is the scalar product, $\mathbf{A} \cdot \mathbf{B} = \text{tr}(\mathbf{A} \mathbf{B}^T) = \sum_{i,k=1}^3 A_{ik} B_{ik}$, and $\text{tr}(\mathbf{A}) = A_{11} + A_{22} + A_{33}$ is the trace of the second order tensor \mathbf{A} . In order to separate volumetric and isochoric effects also with regard to the stress, the Cauchy stress tensor \mathbf{T} is represented as the sum of a spherical and a deviatoric part:

$$\mathbf{T} = -p \mathbf{1} + \mathbf{T}^D \quad (10)$$

$$p = -\frac{1}{3} \text{tr}(\mathbf{T}) \quad (11)$$

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