Research paper

Effects of superimposed eigenstrains on the overall thermoelastic moduli of composites

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ABSTRACT

This study investigates the effects that an initial local eigenstrain field, when superimposed on the thermal eigenstrain field, has on the overall thermal expansion coefficients and heat capacities of thermoelastic composites. The study can also be seen as an investigation into how a local residual stress field affects these overall moduli, as initial eigenstrains are generally a source of residual stresses. The approach taken is thermodynamic. Expressions that include the superimposed eigenstrain field are developed for the overall moduli within the framework of small strain thermoelasticity with temperature dependent materials. These expressions, which are written in terms of the concentration tensors and residual fields (stress and strain fields given rise to by the eigenstrains under zero overall stress and strain, respectively), contain correction terms that are absent in the expressions developed within linear thermoelasticity. Taking into account the temperature dependence of the constituent moduli is shown to be essential to capture the effects of the superimposed eigenstrain field. A Ti–6Al–4V/ZrO$_2$ composite is investigated for which the correction terms are found to be negligible for the heat capacities but significant for the thermal expansion coefficients. This suggests that, for applications with large temperature changes, using the linear-thermoelasticity-based expressions can affect the accuracy of the estimates of the overall moduli, and therefore the accuracy of thermostructural analyses of composite structures. The proposed expressions can be of use to estimate the overall thermoelastic moduli in contexts in which the strains remain small, temperature changes are large, and superimposed eigenstrains may be present.

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1. Introduction

This study investigates how the thermal expansion coefficients and heat capacities of thermoelastic composites are affected by the presence of an initial local eigenstrain field superimposed on the thermal eigenstrain field. Eigenstrains being generally a source of residual stresses, this study can also be seen as an investigation into how local residual stresses affect the overall thermoelastic moduli of composites.

A broader framework than linear thermoelasticity is needed to explore the effects of the superimposed eigenstrain field on the overall thermoelastic moduli. Linear thermoelasticity assumes that the Helmholtz potential is quadratic in strain and temperature (Lubarda, 2004). This assumptions implies, among other things, temperature independent elasticities, which turns out to be too restrictive for the purposes of this study. One such broader framework, and the one used here, is that of small strain thermoelasticity with temperature dependent materials (Kovalenko, 1970). This framework is used in many studies on components having to with-

stand large temperature changes, including ceramic components under thermal shocks (Han and Wang, 2011; Cheng et al., 2015). For applications of this kind, considering the temperature dependence of the materials is essential in the processes of materials selection (de Faoite et al., 2013), structural analysis (Ching and Chen, 2007), and structural optimization (Bobaru, 2007; Boussaa, 2009).

Being more general, the framework accounts for more phenomena than does linear thermoelasticity. Thus, within the broader framework, Nadeau and Ferrari (2004) showed theoretically that the presence of a superimposed local eigenstrain field can induce anisotropy in the overall thermal expansion response in an otherwise macroscopically isotropic composite of isotropic constituents. They also drew a parallel between their findings and a "most surprising" thermal expansion anisotropy experimentally observed in a polycrystal, one explanation for which could be the presence of residual stresses (Finlayson et al., 1981; Gibbs et al., 1981).

Several approaches have been developed in small strain thermoelasticity to estimate the overall thermoelastic moduli for composites with temperature-dependent constituents. A first approach relies on numerical homogenization. E.g., the finite-element method was used to estimate the overall elasticities and ther-

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mal expansion coefficients of silicon nitride (Wippler et al., 2011). A second approach is analytical and yields the overall moduli in terms of the strain and stress concentration tensors and residual fields. One variant of this approach consists in combining the stress-strain relation with the concentration relations (Benveniste and Dvorak, 1990; Bahei-El-Din and Dvorak, 1997; Nadeau and Ferrari, 2004; Dvorak, 2012, pp. 250–252). A second variant consists in combining thermodynamic potentials with the concentration relations (Boussaa, 2011). This second variant has the advantage of providing not only the overall elasticities and thermal expansion coefficients but also the overall heat capacities.

This paper adopts and extends this second variant to accommodate the presence of the superimposed eigenstrain field, and assesses the effects of that presence on the overall thermal expansion coefficients as well as on the overall heat capacities.

The paper is organized as follows. Section 2 provides notation and the definitions of the material moduli of interest here. Section 3 develops expressions for the Gibbs and Helmholtz potentials of a homogeneous material in which an initial eigenstrain is superimposed on the thermal eigenstrain. Section 4 recalls the concentration relations and obtains the macroscopic Gibbs and Helmholtz potentials of a heterogeneous material with an initial superimposed eigenstrain field. Section 5 derives the overall moduli from the macroscopic thermodynamic potentials. Section 6 provides Levin-type formulas for two-phase composites. Section 7 discusses a numerical example illustrating the application of the developed framework to estimate the overall moduli of a high temperature composite with a superimposed eigenstrain field. Finally, Section 8 gives some concluding remarks.

2. Thermoelastic material moduli of interest

The material moduli of interest here are the isothermal elasticity tensor, L; the isothermal compliance tensor, M; the coefficient of thermal expansion (CTE) tensor, α; the stress-temperature tensor, β; the heat capacity per unit reference volume at constant strain, C_ϵ; and the heat capacity per unit reference volume at constant stress, C_σ. These moduli are defined as follows:

$$L = \left(\frac{\partial \sigma}{\partial \epsilon}\right)_T, \quad M = \left(\frac{\partial \epsilon}{\partial \sigma}\right)_T, \tag{1}$$

$$\alpha = \left(\frac{\partial \epsilon}{\partial T}\right)_\sigma, \quad \beta = \left(\frac{\partial \sigma}{\partial T}\right)_\epsilon, \tag{2}$$

$$C_\epsilon = T\left(\frac{\partial \eta}{\partial T}\right)_\epsilon, \quad C_\sigma = T\left(\frac{\partial \eta}{\partial T}\right)_\sigma, \tag{3}$$

where σ is the stress tensor, ϵ is the small strain tensor, T is the absolute temperature, and η is the entropy.

The moduli thus defined depend a priori on the two independent variables used to describe the thermodynamic state of the material, which here are taken to be either stress and temperature or strain and temperature. When stress and temperature are used as independent variables, the dual variables, strain and entropy, are given by

$$\epsilon = -\left(\frac{\partial g}{\partial \sigma}\right)_T, \quad \eta = -\left(\frac{\partial g}{\partial T}\right)_\sigma, \tag{4}$$

where g is the Gibbs potential per unit reference volume. Similarly, when strain and temperature are used as independent variables, the dual variables, stress and entropy, are given by

$$\sigma = \left(\frac{\partial f}{\partial \epsilon}\right)_T, \quad \eta = -\left(\frac{\partial f}{\partial T}\right)_\epsilon, \tag{5}$$

where f is the Helmholtz potential per unit reference volume.

From the above definitions, it follows that the moduli enjoy the usual symmetries.

The symbols f_0, g_0 and η_0 will be used to denote the values of f, g, and η at some reference state, respectively. The reference state referred to will be specified at each use. The dot "." will denote the usual inner product between second-order tensors: For any two second-order tensors X and Y, $X \cdot Y = X_{ij}Y_{ij}$, with summation over repeated indices.

The overall or effective moduli will be denoted with superscript "eff".

3. Gibbs and Helmholtz potentials of a homogeneous thermoelastic material with a superimposed eigenstrain

In (Boussaa 2011), which deals with the case without superimposed eigenstrain, the starting point for developing expressions for the Gibbs and Helmholtz potentials is the postulation of appropriate forms for them. Here, it is more straightforward to start with the postulation of constitutive relations, and then integrate them to obtain expressions for the potentials. The constitutive relations are

$$\epsilon = M(T)\sigma + m(T), \tag{6}$$

$$m(T) = m_{\text{th}}(T) + m_*, \tag{7}$$

where m is the total eigenstrain, m_{th} is the thermal eigenstrain, and m_* is the superimposed eigenstrain, which is assumed not to depend on T and whose physical origin is irrelevant to the analysis. The linear stress-strain relationship (6), the additive decomposition (7), and the compliance tensor dependence on the temperature but not on the superimposed eigenstrain are the core assumptions of the constitutive model. These are common assumptions in the framework of small strains.

3.1. Gibbs potential

In view of the stress-strain relation (6), integrating (4-1) gives

$$g(\sigma, T) = -\frac{1}{2}\sigma \cdot M(T)\sigma - m(T) \cdot \sigma + \phi(T), \tag{8}$$

where ϕ is a function of the temperature alone. From (3-2), (4-2) and (8), one can relate ϕ to C_σ as follows:

$$C_\sigma(\sigma, T) = T\left(\frac{1}{2}\sigma \cdot \frac{d^2 M}{dT^2}\sigma + \frac{d^2 m}{dT^2} \cdot \sigma - \frac{d^2 \phi}{dT^2}\right). \tag{9}$$

Writing this equation for $\sigma = 0$, dividing both sides by T, and integrating the resulting equation twice with respect to temperature gives

$$\phi(T) = -\int_{T_0}^{T}\left(\int_{T_0}^{\xi} C_\sigma(0, \nu)\frac{d\nu}{\nu}\right)d\xi$$
$$-(T - T_0)\eta_0 + g_0, \tag{10}$$

where T_0 is an arbitrary temperature, and η_0 and g_0 are the entropy and the Gibbs potential in the state characterized by $\sigma = 0$ and $T = T_0$, respectively.

Substituting (10) back into (8) gives the desired expression for the Gibbs potential:

$$g(\sigma, T) = -\frac{1}{2}\sigma \cdot M(T)\sigma - m(T) \cdot \sigma$$
$$-\int_{T_0}^{T}\left(\int_{T_0}^{\xi} C_\sigma(0, \nu)\frac{d\nu}{\nu}\right)d\xi$$
$$-(T - T_0)\eta_0 + g_0. \tag{11}$$