Effective thermoelastic moduli of FGMs with temperature-dependent constituents and initial eigenstrains

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Abstract. We outline a procedure for incorporating the effects on the effective thermoelastic moduli of composites of (i) the temperature dependence of the constituents and (ii) the presence of initial eigenstrains. The procedure uses a unified thermodynamic treatment, which assumes small strains, finite changes in temperature, and initial eigenstrains. The procedure is illustrated by deriving the effective values of the isothermal compliance tensor, the thermal expansion tensor, and the heat capacity per unit reference volume at constant stress. The procedure is of particular interest in the modeling of thermoelastic FGMs operating under thermal conditions where the material properties are liable to depend on temperature.

1. Introduction
Many FGM applications are intended to operate under severe thermomechanical conditions that involve considering both the temperature dependence of the constituents [1, 2] and the residual stresses [3, 4]. The micromechanical models usually used to estimate the effective thermoelastic moduli of FGMs, on the other hand, are based on linear thermoelasticity, where (i) the changes in temperature are assumed to be small, (ii) the material moduli are assumed to be independent of temperature, and (iii) the effects of initial eigenstrains associated with the residual stresses are neglected. A method to take into account the temperature dependence of the constituents on the effective thermoelastic moduli has recently been proposed by the present author [5]. The present study outlines a procedure to extend this method to include the effects of initial eigenstrains.

More specifically, the purpose of the paper is to illustrate the procedure by developing the effective values of three moduli—the isothermal compliance tensor, the thermal expansion tensor, and the heat capacity per unit reference volume at constant stress—the definitions of which are recalled in Section 2. The thermodynamic potential most convenient to use for that purpose is the Gibbs potential. Its expression in the case of the homogeneous material is developed in Section 3. Its analogue in the case of the heterogeneous material, the macroscopic Gibbs potential, is obtained in Section 4, along with the corresponding localization relations. The effective moduli are obtained from the macroscopic potential in Section 5.

2. The moduli of the material
The moduli of the material whose effective values are developed below are the isothermal compliance tensor $M$, the thermal expansion tensor $\alpha$, and the heat capacity per unit reference
volume at constant stress \( C_\sigma \). These moduli are defined as follows:

\[
M = \left( \frac{\partial \varepsilon}{\partial \sigma} \right)_T, \quad \alpha = \left( \frac{\partial \varepsilon}{\partial T} \right)_\sigma, \quad C_\sigma = T \left( \frac{\partial s}{\partial T} \right)_\sigma, \tag{1}
\]

where \( \varepsilon \) is the strain tensor, \( \sigma \) is the stress tensor, \( T \) is the temperature, and \( s \) is the entropy.

The Gibbs potential, denoted by \( g \), is most convenient to implement the thermodynamic approach to obtain the effective values of these moduli. The stress and the temperature are the natural variables for this potential, to which the stress and the entropy are related by

\[
\varepsilon = - \left( \frac{\partial g}{\partial \sigma} \right)_T, \quad s = - \left( \frac{\partial g}{\partial T} \right)_\sigma. \tag{2}
\]

3. The Gibbs potential of a homogeneous material

To obtain the Gibbs potential for a homogeneous material, we start from the following state equation:

\[
\varepsilon = M(T)\sigma + m_\theta(T) + m_0 \tag{3}
\]

where \( M \) is assumed to depend on the temperature, \( m_\theta \) is the thermal strain, and \( m_0 \) is the constant initial eigenstrain, the physical origin of which is irrelevant for the present analysis.

From this equation, it is clear that the thermal expansion tensor is independent of \( m_0 \), as

\[
\alpha(\sigma, T) = \frac{dM}{dT}\sigma + \frac{dm_\theta}{dT}. \tag{4}
\]

In view of (3), integrating (2-1) gives

\[
g(\sigma, T) = -\frac{1}{2} \sigma \cdot M(T)\sigma - m(T) \cdot \sigma + \phi(T), \tag{5}
\]

where \( m \) denotes the total eigenstrain, \( m = m_\theta + m_0 \), and \( \phi \) is a function only of the temperature.

The function \( \phi \) can be related to \( C_\sigma \) as follows. From (1-3), (2-2) and (4),

\[
C_\sigma(\sigma, T) = T \left( \frac{1}{2} \sigma \cdot \frac{d^2 M}{dT^2}(T)\sigma + \frac{d^2 m}{dT^2}(T) \cdot \sigma - \frac{d^2 \phi}{dT^2} \right). \tag{6}
\]

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

\[
\phi(T) = -s_0(T - T_0) - \int_{T_0}^T \left( \int_{T_0}^\xi \frac{C_\sigma(0, \nu)}{\nu} d\nu \right) d\xi + g_0, \tag{7}
\]

where \( s_0 \) and \( g_0 \) are the entropy and the Gibbs energy in the state characterized by \( \sigma = 0 \) and \( T = T_0 \), respectively.

Substituting (5) into (4) yields

\[
g(\sigma, T) = -\frac{1}{2} \sigma \cdot M(T)\sigma - m(T) \cdot \sigma - s_0(T - T_0) - \int_{T_0}^T \left( \int_{T_0}^\xi \frac{C_\sigma(0, \nu)}{\nu} d\nu \right) d\xi + g_0. \tag{8}
\]

A second state equation is readily obtained from this equation and (2-2) as

\[
s = \frac{1}{2} \sigma \cdot \frac{dM}{dT}\sigma + \frac{dm}{dT} \cdot \sigma + \int_{T_0}^T \frac{C_\sigma(0, \nu)}{\nu} d\nu + s_0, \tag{9}
\]

and the corresponding expression for the heat capacity at constant stress is

\[
C_\sigma(\sigma, T) = C_\sigma(0, T) + T \left( \frac{1}{2} \sigma \cdot \frac{d^2 M}{dT^2}\sigma + \frac{d^2 m}{dT^2} \right). \tag{10}
\]

To sum up, according to the thermoelasticity model developed here, the initial eigenstrain affects neither the compliance (by assumption), the thermal expansion tensor, nor the heat capacity at constant stress.
4. The Gibbs potential of a heterogeneous material

4.1. Localization relations

We consider a representative volume (RVE) of a heterogeneous material whose constituents show (i) a thermoelastic behavior governed by the Gibbs potential (6) and the associated constitutive equations, and (ii) perfect bonding and thermal contact at their interfaces. Within the RVE, (i) the distribution of initial eigenstrains is assumed to be given, (ii) the temperature is assumed to be uniform, and (iii) the strain is assumed to be small. In view of the potential and moduli of interest here, the RVE is considered under only controlled macroscopic (average) stress \( \sigma \) and temperature \( T \), the macroscopic stress being controlled by applying uniform boundary tractions and the temperature by applying a uniform boundary temperature.

The stress \( \sigma(x) \) within the RVE can be written as

\[
\sigma(x; \sigma, T) = B(x; T) \sigma + b(x; T),
\]

In this equation, the first term on the right-hand side is the stress that develops in the RVE under \( \sigma \) only, and the fourth-order tensor \( B \), which is independent of the eigenstrains, is the stress concentration tensor at temperature \( T \). The second term corresponds to the stress that develops in the RVE under the eigenstrains and traction free boundary conditions. This latter term can be decomposed into two terms, viz.

\[
b(x; T) = b_\theta(x; T) + b_0(x; T),
\]

which correspond to the stress developed under \( m_\theta(x; T) \) and \( m_0(x) \), respectively. Although the stress \( b_0(x; T) \) arises from the constant (and nonuniform) eigenstrain \( m_0 \), it also depends on the temperature because of the dependence on temperature of the compliance tensor.

4.2. Macroscopic Gibbs potential

The macroscopic Gibbs potential density \( G \) is defined as

\[
G(\sigma, T) = \langle g \rangle = \frac{1}{|V|} \int_V g(x; \sigma, T) \, dV.
\]

Here, \( g(x; \sigma, T) \) is of the form (6) where \( M, m, C_\sigma, s_0 \), and \( g_0 \) are made to depend also on position, and \( \sigma \) is the stress that develops in the RVE under the combined effects of \( \sigma \) and \( m \).

Substituting the expression for \( g \) given in (6) and the stress localization relation (8) into the foregoing equation yields

\[
G(\sigma, T) = -\frac{1}{2} \sigma \cdot \langle B^T MB \rangle \sigma - \langle B^T m \rangle \cdot \sigma - \frac{1}{2} \langle m \cdot b \rangle
- \int_{T_0}^{T} \left( \int_{T_0}^{\xi} \frac{C_\sigma(\sigma = 0, \nu)}{\nu} \, d\nu \right) \, d\xi - \langle s_0 \rangle (T - T_0) + \langle g_0 \rangle.
\]

The derivation of this equation uses classical properties of the stress localization tensor \( B \) as can be found in [5].

5. Effective moduli

The macroscopic Gibbs potential (9) is that of a thermoelastic material. The macroscopic strain \( \varepsilon = \nabla G/\nabla \sigma \) takes the form

\[
\varepsilon = M^{\text{eff}} \sigma + m^{\text{eff}},
\]

where, in view of (9), the effective compliance tensor \( M^{\text{eff}} \) and thermal strain \( m^{\text{eff}} \) are given by

\[
M^{\text{eff}} = \langle B^T MB \rangle,

m^{\text{eff}} = \langle B^T m \rangle = \langle B^T m_\theta \rangle + \langle B^T m_0 \rangle.
\]
From (10), the thermal expansion tensor \( \alpha^{\text{eff}}(\sigma, T) = (\partial \sigma / \partial T)_{\sigma} \) is found to be given by

\[
\alpha^{\text{eff}}(\sigma, T) = \frac{dM^{\text{eff}}}{dT} \sigma + \alpha^{\text{eff}}(0, T),
\]

where \( \alpha^{\text{eff}}(0, T) \) is the free thermal expansion tensor,

\[
\alpha^{\text{eff}}(0, T) = \frac{d}{dT} \langle B^T m \rangle = \frac{d}{dT} \left[ \frac{1}{2} \sigma \cdot \frac{d^2 M^{\text{eff}}}{dT^2} \sigma + \frac{d^2 m^{\text{eff}}}{dT^2} \cdot \sigma \right].
\]

The macroscopic entropy \( s(\sigma, T) = - (\partial G / \partial T)_{\sigma} \) can be written as

\[
s = \frac{1}{2} \sigma \cdot \frac{dM^{\text{eff}}}{dT} \sigma + \frac{d m^{\text{eff}}}{dT} \cdot \sigma + \frac{1}{2} \frac{d}{dT} \langle b \cdot m \rangle + \int_{T_0}^{T} \frac{\langle C_{\sigma}(0, \nu) \rangle}{\nu} \, d\nu + \langle s_0 \rangle,
\]

so that the effective heat capacity at constant stress \( C_{\sigma}^{\text{eff}}(\sigma, T) = T (\partial s / \partial T)_{\sigma} \) is given by

\[
C_{\sigma}^{\text{eff}}(\sigma, T) = C_{\sigma}^{\text{eff}}(0, T) + T \left[ \frac{1}{2} \sigma \cdot \frac{d^2 M^{\text{eff}}}{dT^2} \sigma + \frac{d^2 m^{\text{eff}}}{dT^2} \cdot \sigma \right],
\]

where

\[
C_{\sigma}^{\text{eff}}(0, T) = \langle C_{\sigma}(0, T) \rangle + \frac{1}{2} \frac{d^2}{dT^2} \langle b \cdot m \rangle
\]

\[
= \langle C_{\sigma}(0, T) \rangle + \frac{1}{2} \frac{d^2}{dT^2} \langle b_\theta \cdot m_\theta \rangle + \frac{1}{2} \frac{d^2}{dT^2} \langle b_\theta \cdot m_\theta \rangle + \frac{1}{2} \frac{d^2}{dT^2} \langle b_\theta \cdot m_\theta \rangle + \frac{1}{2} \frac{d^2}{dT^2} \langle b_\theta \cdot m_\theta \rangle
\]

The following conclusions can be drawn:

- The initial eigenstrains have no influence on the effective compliance tensor.
- The initial eigenstrains affect the effective total eigenstrain.
- The initial eigenstrains affect the effective thermal expansion tensor. Their influence is made possible by the temperature dependence of the constituents’ compliance tensors. If the constituents’ compliance tensors are temperature independent, then the initial eigenstrains have no effect on the effective thermal expansion even if the constituents’ thermal expansion tensors are temperature dependent. If the constituents’ compliance tensors depend on temperature, then the initial eigenstrains affect the effective thermal expansion tensor even if the constituents’ thermal expansion tensors are temperature independent.
- The initial eigenstrains affect the effective heat capacity at constant stress. Again, their influence is made possible by the temperature dependence of the constituents’ compliance tensors. If the constituents’ compliance tensors depend on temperature, then the initial eigenstrains affect the effective heat capacity even if the constituents’ heat capacities are temperature independent.

References

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