

Morphological Analysis and Variational Formulation in Heterogeneous Thermoelasticity

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1. INTRODUCTION

This paper is devoted to several applications of morphological analysis applied to the bounding of the overall behavior of composite materials. In particular we focus our attention to the generalization of the Hashin Shtrikman variational principles to thermoelasticity.

The analysis of the inhomogeneous elastic random media is based on the description of the spatial distribution of the phases. The structural morphology is described by n -points-correlation function. This description gives closer bounds depending on the increasing knowledge of their structural morphology.

This description gives rise to a systematic theory in the sense of Kröner, but in particular cases it is better to take into account some morphological characteristics which are not easy to describe by a limited number of point-correlation functions. In these cases, it is better to combine a detailed description of the material by using a decomposition in families of morphological patterns with spatial distribution of the patterns.

The Hashin-Shtrikman method is extended to take into account this new description, and then is applied to particular cases of spatial distribution of some typical representative patterns, as the composite spheres assemblage of Hashin. Some other composite materials are investigated, for which bounds of thermoelastic effective behavior are given.

2. GENERALITIES

In a thermodynamical description of the homogenization, we find that the overall behavior is determined by the definition of the free energy of a representative volume element (RVE). This volume is small enough to distinguish

the heterogeneities and sufficiently large to be considered as homogeneous at the macroscopical scale, at this scale the average quantities defined on the RVE vary slowly with the position.

For the RVE, the free energy is the value of the total free energy for a state of thermodynamical equilibrium. In our case, the equilibrium state is given as the solution of a suitable boundary value problem, defined over the RVE.

In thermoelasticity the behavior of each constituent phase is given by the definition of the local free energy, function of the strain ε and of the temperature variation τ ,

$$w(\varepsilon, \tau) = \frac{1}{2} \varepsilon : C(x) : \varepsilon + \phi(x) : \varepsilon \tau + \frac{1}{2} c_v \tau^2 .$$

The coefficients of thermoelasticity are the elastic moduli $C(x)$, the thermal expansion $\alpha = -C^{-1} : \phi$, the specific heat c_v , all these moduli depend on the spatial position of the point x inside the RVE.

The local equation of state are given by

$$\begin{aligned} \sigma &= \frac{\partial w}{\partial \varepsilon} = C(x) : \varepsilon + \phi(x) \tau , \\ s &= -\frac{\partial w}{\partial \tau} = -\phi(x) : \varepsilon - c_v \tau , \end{aligned}$$

where σ are the stresses, s is the specific entropy.

At any quantity f an unique macroscopic state is defined thanks to an averaging process defined on the RVE:

$$F = \langle f \rangle = \frac{1}{\Omega} \int_{\Omega} f d\omega ,$$

where Ω is the volume of the RVE.

Conversely to define a local field f for a given macroscopic one F , we must solve a complex boundary value problem. In thermoelasticity, this boundary value problem is well defined and gives rise to the definition of the macroscopic free energy as the potential of the system.

By definition, the free energy of the homogenized material is $W = \langle w(\varepsilon) \rangle$ determined by studying a complex boundary value problem associated to a choice of suitable boundary conditions given in terms of macroscopical quantities as the macroscopic strain $E = \langle \varepsilon \rangle$.

Here, we assume that the macroscopic strain E is given and prescribed over the boundary value of the medium. The displacement u solution of the boundary value problem verifies

- the momentum equation

$$\operatorname{div} \sigma = 0,$$

- the kinematical relation

$$2\varepsilon(u) = \nabla u + \nabla^t u,$$

- the local constitutive law

$$\sigma = C : \varepsilon + \tau \phi,$$

- the boundary conditions

$$u = E \cdot x, x \in \partial\Omega.$$

The global free energy is then a function of the global strain E , and of the variation of the temperature τ . The displacement u is the solution of a linear problem, then the local strain field takes the form

$$\varepsilon(x; E, \tau) = B(x) : (E - \langle \varepsilon_{res}(\tau) \rangle) + \varepsilon_{res}(\tau)$$

the strain concentration tensor B is the local strain for an isothermal evolution of the RVE. The local strain ε_{res} is the strain due to the temperature τ , this field is kinematically admissible with a free expansion of the body Ω . These strains are associated with a self-equilibrated stress field r , which verifies

$$r = C : \varepsilon_{res}(\tau) + \phi \tau,$$

$$0 = \operatorname{div} r,$$

$$0 = \langle r \rangle.$$

Under these conditions, the global free energy of the system is a quadratic function of the macroscopic strain E , and of the temperature variation τ :

$$W(E, \tau) = \langle w(\varepsilon(E, \tau), \tau) \rangle = \frac{1}{2} E : C_{eff} : E + \Phi : E \tau + \frac{1}{2} C_v \tau^2$$

the coefficients of the overall thermoelastic behavior are given by

$$C_{eff} = \langle B^t : C : B \rangle,$$

$$\Phi = \langle B^t : \phi \rangle,$$

$$C_v \tau = \langle c_v \rangle \tau - \langle \phi : B \rangle : \tau + \langle \phi : \varepsilon_{res} \rangle.$$

In these expressions, the influence of the residual stresses due to the incompatibility of the field of the thermal expansion is emphasized. The value of the global free energy is determined for the given state (E, τ) by using all the properties of the local fields, the kinematical admissibility of the strains $(\varepsilon, \varepsilon_{res}, B)$, and the statical admissibility of the stresses (σ, r) . In particular the relations $\langle r : \varepsilon_{res} \rangle = 0$, and $\langle r : B \rangle = 0$ are verified.

The overall behavior takes then the form

$$\begin{aligned}\Sigma &= \langle \sigma \rangle = C_{eff} : E + \tau \langle \phi : B \rangle = \frac{\partial W}{\partial E}, \\ S &= \langle s \rangle = -\frac{\partial W}{\partial \tau}.\end{aligned}$$

These relations gives rise to the overall thermal expansion:

$$E_{th} = -C_{eff}^{-1} : \Phi \tau = \langle \varepsilon_{res} \rangle .$$

Dually, we can use the complementary energy:

$$w^*(\sigma, \tau) = \min -\sigma : \varepsilon + w(\varepsilon, \tau)$$

to obtain the overall complementary energy of the RVE.

3. BOUNDING METHOD

Let us rewrite the boundary value problem on a reference homogeneous medium with macroscopic elastic moduli C_o . Denoting by δC the perturbation $C(x) - C_o$ and by $p(x)$ the stress polarization field defined by

$$p = \delta C : \varepsilon, H = \delta C^{-1} .$$

A state of equilibrium verifies the conservation of the momentum, the kinematical admissibility of the strain and the local constitutive law, then it is the solution of the new boundary value problem:

- the momentum equation

$$\operatorname{div} \sigma = 0,$$

- the kinematical relation

$$2\varepsilon = \nabla u + \nabla^t u,$$

- the local constitutive law

$$\sigma = C_o : \varepsilon + \tau \phi + p ,$$

- the boundary conditions

$$u = E \cdot x , x \in \partial\Omega ,$$

- the internal constraint

$$\varepsilon = H : p .$$

Let $\eta = \varepsilon - E$, a kinematically admissible strain field, $\langle \eta \rangle = 0$, the value of the total potential energy for the displacement solution of the boundary value problem is then a stationary point of the functional F :

$$\begin{aligned} F = & \frac{1}{2} E : C_o : E + \langle p + \phi \tau \rangle : E + \frac{1}{2} \langle c_v \rangle \tau^2 \\ & + \frac{1}{2} \langle \eta : C_o : \eta \rangle + \langle (p + \phi \tau) : \eta \rangle - \frac{1}{2} \langle p : H : p \rangle . \end{aligned}$$

For given value (p', τ) , denoting by $\eta'(p', \tau)$ the solution of the variational equation $\frac{\partial F}{\partial \eta} \bullet \delta \eta = 0$, this field depends linearly on the prescribed quantities (p', τ) , and realizes a local minimum for F . The value of this minimum is the Hashin-Shtrikman functional $HS(E, p', \tau)$:

$$\begin{aligned} HS = & \frac{1}{2} E : C_o : E + \langle p' + \phi \tau \rangle : E + \frac{1}{2} \langle c_v \rangle \tau^2 \\ & + \frac{1}{2} \langle (p' + \phi \tau) : \eta'(p', \tau) \rangle - \frac{1}{2} \langle p' : H : p' \rangle . \end{aligned}$$

A statically admissible stress field σ' is obtained for each η'

$$\sigma' = C_o : (E + \eta') + p' + \phi \tau .$$

For the given prescribed boundary conditions the free energy of the system is the value of the potential energy for the solution of the problem of equilibrium then the free energy of the system can be bounded by the application of the energy principles:

$$- \langle w^*(\sigma', \tau) \rangle + \langle \sigma' \rangle : E \leq W(E, \tau) \leq \langle w(\varepsilon', \tau) \rangle .$$

By using the properties of η' , $\langle \eta' \rangle = 0$, $\langle \sigma' : \eta' \rangle = 0$, and for a suitable choice of the reference medium C_o , the Hill's classical results are recovered:

- if H is negative definite:

$$W(E, \tau) \leq HS^+(E, p, \tau),$$

- if H is positive definite:

$$HS^-(E, p, \tau) \leq W(E, \tau).$$

This functional is different of the proposed one in J. Willis (1981). Here the formulation is based on a purely elastic reference medium, and τ is considered as an external given loading. After a suitable choice of the reference medium, we must determined an optimal value for the polarization field p by the variational equation

$$\frac{\partial HS}{\partial p} \bullet \delta p = 0.$$

The optimal value of HS is then a quadratic function of the prescribed quantities (E, τ) :

$$\begin{aligned} Q^o(E, \tau) = HS(E, p(E, \tau), \tau) &= \frac{1}{2} E : C_o : E + \frac{1}{2} \langle p + \phi\tau \rangle : E \\ &+ \frac{1}{2} \langle \tau\phi : \varepsilon(p, \tau) \rangle + \frac{1}{2} \langle c_v \rangle \tau^2. \end{aligned}$$

In this expression the local strain $\varepsilon(p, \tau)$ is the solution of the problem of thermoelasticity. This strain is kinematically admissible with E for any given τ and p .

To explain the value of the Q^o it is necessary to determine the strain field ε defined on the reference medium for any choice of the polarization p and any choice of τ .

This solution ε is given by the integral equation

$$\varepsilon + \int_{\Omega} \Gamma^o(x, y)(p(y) + \phi(y)\tau) d\omega = E_o$$

where Γ^o is the modified Green operator ($\Gamma = G_{ij, pq(ip)(jq)}^o$) deduced from the Green tensor $G^o(x, y)$, and E_o is chosen such $E = \langle \varepsilon \rangle$. The Green tensor is the elementary solution of the problem of elasticity:

- the momentum equation

$$\frac{\partial}{\partial x_i} C_{ijkl}^o \frac{\partial}{\partial x_l} G_{kp}^o(x, x') + \delta_{ip} \delta(x - x') = 0, \quad x \in \Omega, \quad x' \in \Omega$$

in which we have taken the local constitutive law into account:

- the boundary conditions

$$G_{kp}^o(x, x') = 0, x \in \partial\Omega, x' \in \Omega.$$

Finally we obtain the bounds of the overall behavior as

$$\begin{aligned} Q^-(E, \tau) &= \frac{1}{2}E : C^- : E + \Phi^- : E\tau + \frac{1}{2}C_v^- \tau^2 \\ &\leq W(E, \tau) = \frac{1}{2}E : C_{eff} : E + \Phi : E\tau + \frac{1}{2}C_v \tau^2 \\ &\leq Q^+(E, \tau) = \frac{1}{2}E : C^+ : E + \Phi^+ : E\tau + \frac{1}{2}C_v^+ \tau^2. \end{aligned}$$

Then as the two quadratic functions $W - Q^-$ and $Q^+ - W$ are positive definite, we have immediately:

$$\begin{aligned} E : C^- : E &\leq E : C_{eff} : E \leq E : C^+ : E, \\ C_v^- &\leq C_v \leq C_v^+, \end{aligned}$$

and for the non diagonal terms, the two reduced quadratic functions must be positive definite

$$\begin{aligned} (C^+ - C_{eff})(C_v^+ - C_v) - (\Phi^+ - \Phi)^T \otimes (\Phi^+ - \Phi) &\geq 0, \\ (C^- - C_{eff})(C_v^- - C_v) - (\Phi^- - \Phi)^T \otimes (\Phi^- - \Phi) &\geq 0. \end{aligned}$$

4. APPLICATIONS

4.1. CASE OF AN n -PHASE COMPOSITE. For an isotropic reference medium, the solution ε of the problem of polarization is

$$\varepsilon + \int_{\Omega} \Gamma^o(x, y)(p(y) + \phi(y)\tau) d\omega = \varepsilon_o$$

where the Γ^o is known exactly for the infinite medium. Γ^o has a singular part E_o , value of which is related to the Eshelby problem of spherical inclusion or heterogeneity, and a regular contribution F_o .

Following Hashin-Shtrikman and Walpole, we can choose for $p(x)$ piecewise uniform function

$$p(x) = \sum_{r=1}^n p_r \chi_r(x)$$

where χ_r is the characteristic function of the phase r .

In the Hashin Shtrikman functional, only appear the average quantities $\bar{\varepsilon}_r$ of the local strain on each phase r . As pointed out by Walpole, the solution at the optimum for an isotropic spatial distribution of the phases, extended here for thermoelastic case, is given by the resolution of n problems of spherical inclusions, the solution of each being given by

$$\begin{aligned}\bar{\varepsilon}_r &= B_r : (E + \langle \varepsilon_{res} \rangle) + \varepsilon_{res}^r, \\ A_r &= I + E_o \delta c_r, B_r = A_r^{-1} \langle A_r^{-1} \rangle_n^{-1}, \\ \varepsilon_{res}^r &= -A_r^{-1} E_o \phi \tau, \langle f \rangle_n = \sum_1^n f_r \chi_r.\end{aligned}$$

The functional HS takes the final form

$$\begin{aligned}HS &= \frac{1}{2} E : C^{HS} : E + \langle \phi : B \rangle_n E \tau \\ &+ \frac{1}{2} [\langle \phi : \varepsilon_{res} \rangle_n \tau - \tau \langle \phi : B \rangle_n \langle \varepsilon_{res} \rangle_n] + \langle \frac{1}{2} c_v \tau^2 \rangle_n\end{aligned}$$

for the value $\tau = 0$, the classical bounds for the elastic moduli are recovered

$$C^{HS} = \langle c A_r^{-1} \rangle_n \langle A^{-1} \rangle_n^{-1}$$

and the other coefficients take naturally the value

$$\begin{aligned}\Phi^{HS} &= \langle \phi B \rangle_n = \langle \phi A^{-1} \rangle_n \langle A^{-1} \rangle_n^{-1}, \\ C_v^{HS} &= \langle c_v \rangle_n - \langle (\phi - \Phi^{HS}) : A^{-1} : E_o : \phi \rangle_n.\end{aligned}$$

For isotropic phases, these terms are isotropic, and the bounding problem is reduced to solve two scalar inequalities

$$\begin{aligned}3(K^+ - K_{eff})(C_v^+ - C_v) - (\Phi^+ - \Phi)^2 &\geq 0, \\ 3(K^- - K_{eff})(C_v^- - C_v) - (\Phi^+ - \Phi)^2 &\geq 0.\end{aligned}$$

As proposed by Rosen (1970), if K_{eff} is assumed to be known as

$$K_{eff} = K^* = \gamma K^+ + (1 - \gamma) K^-, \quad 0 \leq \gamma \leq 1,$$

the two inequalities determine the intersection of two domains defined by two parabola in the (Φ, C_v) plane, the intersection of the parabola are two points (Φ^*, C_v^*) coordinates of which are defined by

$$\begin{aligned}3(K^+ - K^*)(C_v^+ - C_v^*) - (\Phi^+ - \Phi^*)^2 &= 0, \\ 3(K^- - K^*)(C_v^- - C_v^*) - (\Phi^- - \Phi^*)^2 &= 0.\end{aligned}$$

the solution is given by

$$\begin{aligned} \Phi_{\pm}^* &= \gamma\Phi^+ + (1 - \gamma)\Phi^- \pm \sqrt{\Psi}, \\ \Psi &= 3\gamma(\gamma - 1)[3\Delta C_v \Delta K - (\Delta\Phi)^2] \geq 0, \\ \Delta K &= K^+ - K^-, \Delta C_v = C_v^+ - C_v^-, \Delta\Phi = \Phi^+ - \Phi^-. \end{aligned}$$

Then for all $K_{eff} : K^- \leq K_{eff} \leq K^+$, $\Phi_-^* \leq -3K_{eff}\alpha_{eff} \leq \Phi_+^*$.

These equations determine bounds of the expansion coefficient in a easier manner than by using the translational method as proposed by Gibiansky and Torquato (1997). A particular case is the case of a two phase materials, then the bounds of the expansion coefficient are given by the Levin formula:

$$\alpha_{HS} = \langle \alpha \rangle + \frac{\frac{1}{K_{HS}} - \langle \frac{1}{K} \rangle}{\frac{1}{K_2} - \frac{1}{K_1}} (\alpha_2 - \alpha_1).$$

It is noticed that the upper bound is not related to the upper Hashin Shtrikman bounds it depends on the sign of $(\alpha_2 - \alpha_1)(K_2 - K_1)$.

4.2. THE COMPOSITE SPHERE ASSEMBLAGE. For the Hashin Sphere Assemblage, the kernel is made from material 2 inside a core of material 1. The modulus of compressibility is perfectly determined:

$$K_{eff} = K_2 + \frac{\chi_1(K_1 - K_2)(3K_2 + 4\mu_2)}{3K_2 + 4\mu_2 + 3(1 - \chi_1)(K_1 - K_2)}$$

and then by application of the Levin formula we have

$$\alpha_{eff} = \langle \alpha \rangle + \frac{\frac{1}{K_{eff}} - \langle \frac{1}{K} \rangle}{\frac{1}{K_2} - \frac{1}{K_1}} (\alpha_2 - \alpha_1),$$

then also the specific heat is determined

$$C_v = \langle c_v \rangle - \frac{3\chi_1(1 - \chi_1)(\phi_2 - \phi_1)^2}{3K_2 + 4\mu_2 + 3(1 - \chi_1)(K_1 - K_2)}.$$

4.3. OTHER MORPHOLOGICAL ASSEMBLAGE. Let us consider a composite defined by N morphological patterns λ . The pattern λ has the geometry D_λ . Inside Ω , each domain belong of the family λ has a center X_k^λ , the number of such domains is N_λ .

On the geometry D_λ , we define a polarization field $P_\lambda(y)$. Then if the geometrical point $x \in \Omega$ is inside the k-th domain of the family λ , there

exists an unique point y of D_λ , such as $x = y + X_k^\lambda$. At the point y the thermomechanical characteristics are $C_\lambda(y), \phi_\lambda(y), c_{v\lambda}(y)$. Let us defined a set of averaging process (Bornert at al (1996)):

$$q_\lambda^M(y) = \frac{1}{N_\lambda} \sum_k q(y + X_k^\lambda),$$

$$\langle q \rangle_\lambda = \frac{1}{D_\lambda} \int_{D_\lambda} q d\omega.$$

The functional HS takes now the form

$$HS = \frac{1}{2} E : C_o : E + \frac{1}{2} \sum_\lambda f_\lambda \langle P_\lambda + \phi_\lambda \tau \rangle_\lambda : E$$

$$+ \frac{1}{2} \sum_\lambda f_\lambda \langle \phi_\lambda \tau : \varepsilon_\lambda^M(p, \tau) \rangle + \frac{1}{2} \sum_\lambda f_\lambda \langle c_{v\lambda}^M \rangle_\lambda \tau^2$$

where f_λ is the concentration of domains D_λ : $f_\lambda = \frac{N_\lambda D_\lambda}{\Omega}$.

In the particular case of spherical patterns, with isotropic constituents, which are in an isotropic spatial of their centers. The solution of the boundary value problem in thermoelasticity is given by

$$\varepsilon + \int_\Omega \Gamma^o(x, y)(p(y) + \phi(y)\tau) d\omega = \varepsilon_o$$

by application of the averaging process and by taking into account the spatial distribution of the center we have

$$\varepsilon_o = \varepsilon_\lambda^M + \int_{S_\lambda} \Gamma^o(x, y)(P_\lambda(y) + \phi_\lambda(y)\tau) d\omega,$$

$$\varepsilon_\lambda^M(x) = H_\lambda^M(x) : P_\lambda(x).$$

As in isothermal elasticity, the optimum is obtained by solving N problems of spherical composite inclusion embedded in the reference medium C_o . The value of ε_o applied at the infinity is chosen to have the average condition

$$E = \sum_\lambda f_\lambda \langle \varepsilon_\lambda^M(y) \rangle_\lambda.$$

We consider now an assemblage of N spherical patterns λ , each composed by n_λ concentric layers of an isotropic homogeneous medium. Under radial loading, the solution of the problem of thermoelastic equilibrium shows that each composite sphere is equivalent to an homogeneous one with thermoelastic

characteristics $(K_\lambda, \Phi_\lambda, c_v^\lambda)$. For this particular case the bounds are given as in the preceding section 4.1 but the reference medium is defined relatively to the local value $C_\lambda(y)$ of the mechanical phases.

For example, for two families of spherical patterns with two layers, we obtain the bounds

$$\alpha_{HSM} = f\alpha_\lambda + (1-f)\alpha_\mu + \frac{\frac{1}{K_{HSM}} - (\frac{f}{K_\lambda} + \frac{1-f}{K_\mu})}{\frac{1}{K_\lambda} - \frac{1}{K_\mu}}(\alpha_\lambda - \alpha_\mu)$$

where K_{HSM} is one of the bounds of Hashin-Shtrikman for the assemblage of two composite spheres

$$K_{HSM} = \frac{3K_\lambda K_\mu + 4\mu_o(fK_\lambda + (1-f)K_\mu)}{3K_\lambda K_\mu(\frac{f}{K_\lambda} + \frac{1-f}{K_\mu}) + 4\mu_o}.$$

5. COMMENTS

The applications of the proposed method are presented on different situations ; the extension to morphological patterns has been proposed and applied to particular cases of local morphology.

The spatial distribution of the different phases have a great influence. For example in a two phases composite, the thermal expansion coefficient is only bounded by using the Levin formula and the bounding of the modulus of compressibility, for the same phases arranged as a the composite sphere assemblage of Hashin these two moduli are closely determined.

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