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Homogenization in thermoelasticity: application to composite materials

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ABSTRACT : One of the obstacles to the industrial use of metal matrix composite materials is the damage they rapidly undergo when they are subjected to cyclic thermal loadings; local thermal stresses of high level can develop, sometimes nearby or over the elastic limit, due to the mismatch of elastic and thermal coefficients between the fibers and the matrix. For the same reasons, early cracks can appear in composites like ceramic-ceramic. Therefore, we investigate the linear thermoelastic behaviour of heterogeneous materials, taking account of the isentropic coupling term in the heat conduction equation. In the case of periodic materials, recent results, using the homogenization theory, allowed us to describe macroscopic and microscopic behaviours of such materials.

This paper is concerned with the numerical simulation of this problem by a finite element method, using a multiscale approach.

1) INTRODUCTION

One of the obstacles to the industrial use of metal matrix composite materials is the damage they rapidly undergo when they are subjected to cyclic thermal loadings; high level local thermal stresses can develop, sometimes nearby or over the elastic limit, due to the elastic and thermal coefficients mismatch between the fibers and the matrix. In the case of brittle elastic composites, like ceramic-ceramic, damage due to cracking can occur always at a local level, and will lead to global damage.

Classically, structure made of an heterogeneous material is computed using a multiscale approach and defining an equivalent homogeneous material which is supposed to give the "averaged" behaviour at the macroscopic scale. It can be also interesting to be able to compute the microscopic fields. In the purely elastic case this homogenization technique [1] is a rather standard approach. In the coupled thermoelastic case we are dealing with, recent theoretical results allowed us to work out this localisation stage.

Therefore, we investigated the linear thermoelastic behaviour of heterogeneous materials, taking account of the isentropic coupling term in the heat conduction equation. The present study is concerned with numerical simulations using multiscale approaches.

II) PRESENTATION OF THE MECHANICAL PROBLEM

We consider a structure S , constituted by a heterogeneous material, the heterogeneities being distributed in a periodic way. The spatial period is described by an elementary volume Y^ε . More specifically, $Y^\varepsilon = \varepsilon x Y$, where ε is a small parameter characterizing the ratio between the microstructure scale and the structure scale. Therefore, Y is a reference cell which contains all the relevant information about the microstructure.

The behaviour law choosen for the different materials leads to the following equations, binding the stress tensor σ^ε , the displacement field u^ε , and θ^ε the increment of temperature field with respect to a uniform reference temperature T^0 :

$$(P^\varepsilon) \quad \begin{cases} \sigma^\varepsilon = a^\varepsilon (\varepsilon (u^\varepsilon) - \alpha^\varepsilon \theta^\varepsilon) \\ \beta^\varepsilon \dot{\theta}^\varepsilon = \lambda^\varepsilon \nabla \theta^\varepsilon - a^\varepsilon \alpha^\varepsilon \varepsilon (\dot{u}^\varepsilon) \end{cases}$$

where a^ε is the elasticity tensor, α^ε the thermal expansion tensor, $\beta^\varepsilon = \frac{\rho^\varepsilon C_p^\varepsilon}{T^0}$ with $\rho^\varepsilon C_p^\varepsilon$ the specific heat, $\lambda^\varepsilon = \frac{k^\varepsilon}{T^0}$ with k^ε the thermal conductivity.

The superscript ε in the above thermomechanical coefficients denotes the Y^ε - periodicity.

These equations are completed by the movement equations and initial conditions, the structure S being subjected to classical conditions with fixed efforts and displacements. For the sake of simplicity no body forces or thermal sources are considered.

III) HOMOGENIZATION RESULTS

III.1) MICRO -> MACRO TRANSITION

The homogenization theory allows us to show that [2], when the small parameter ε goes to 0, the fields σ^ε , u^ε and θ^ε converge to σ^0 , u^0 and θ^0 . Mechanically, these fields are usually regarded as good approximations of the macroscopic behaviour of S . In addition, they verify a set of equations (P^0) structurally identical to (P^ε) , showing that the macroscopic behaviour is thermoelastic with coupling.

The macroscopic coefficients a^0 , α^0 and λ^0 involved in these equations are obtained by the resolution on the reference cell of 3 kinds of problems with periodic boundary conditions. The two first are usual when homogenizing purely elastic (problem P^E) or purely thermal (problem P^G) behaviour laws. They are defined by respectively assigning given homogeneous strain E and thermal gradient G , the solutions being respectively noted u^E and θ^G . The third one, P^C , takes account of the isentropic coupling and is defined by assigning a stress equal to $a \cdot \alpha \cdot 1$, the solution being this time noted u^C . The coefficient β^0 is simply the average on the reference cell of the differents β . Besides, the initial conditions for (P^0) are not exactly those of the initial problem (P^ε) , but are derived from (P^ε) by modifying some results obtained in the three previous cell problems.

III.1) MACRO -> MICRO TRANSITION

In order to obtain the local fluctuations of σ , u and θ , it is necessary to be able to derive the microscopic behaviour, in a point of S , during its evolution under the loading.

The problem can be expressed in the following way :

In a given (macroscopic) point and at a given time, the resolution of (P^0) gives the macroscopic values of the strain $\bar{\mathbf{E}}$, the temperature $\bar{\Theta}$ and the thermal gradient $\bar{\mathbf{G}}$. We then search for the fields \mathbf{u} and θ , in this point but at a microscopic scale. Recent results in homogenization theory [3] allow us to write these fields under the following form :

$$\begin{cases} \mathbf{u} &= \mathbf{u}^{\bar{\mathbf{E}}} + \bar{\Theta} \mathbf{u}^{\mathbf{C}} + \tilde{\mathbf{u}} \\ \theta &= \theta^{\bar{\mathbf{G}}} + \tilde{\theta} \end{cases}$$

The terms $\mathbf{u}^{\bar{\mathbf{E}}}$, $\theta^{\bar{\mathbf{G}}}$ and $\mathbf{u}^{\mathbf{C}}$ are derived from the cell problems $(P^{\bar{\mathbf{E}}})$, $(P^{\bar{\mathbf{G}}})$ and $(P^{\mathbf{C}})$. The terms $\tilde{\mathbf{u}}$ and $\tilde{\theta}$, resulting from the aforementioned modification of initial conditions, are the solutions of a transient thermoelastic problem (\tilde{P}) , defined on the reference cell and with periodic boundary conditions.

IV) THE NUMERICAL METHOD

The numerical method relies upon a finite element spatial discretisation using piecewise affine functions. Two types of problems are to be solved :

* Stationary thermoelasticity with periodic conditions. The main difficulty is to take account of the periodic conditions, and this is done by using a method of nodal unknowns elimination [4].

* Transient thermoelasticity. We used a time discretisation by an implicit scheme. This leads to resolving, at each step, a same linear system, corresponding to a stationary coupled thermoelastic problem. This coupling generates a non symmetric system. Again, a method of nodal unknowns elimination is used for the periodic conditions in (\tilde{P}) . This "detail" required a systematic use of a skyline storage.

V) A FEW APPLICATIONS

Several examples have been worked out, rather dedicated to a best comprehension of the mechanisms of the thermoelastic behaviour of materials. :

- Parametric analysis of macroscopic thermoelastic coefficients : influence of various geometric and material parameters and comparison with other approaches (Self-consistent scheme, Mori-Tanaka method and homogenization by Fourier series [5]).

- Under mechanical loadings, the coupling term induces non-negligible temperature changes. They have been successfully compared to experimental results [6].

- Numerical simulations of theoretically predicted phenomena [2] : Persistence of fast oscillations of the temperature field around the macroscopic value.

- Prediction of the evolution of the microscopic stresses when the material is subjected to thermal cycling, and analysis of the rôle of the interface.

VI) PERSPECTIVES

This study tends to show the importance of the coupling term. We now aim to focus on two particular points :

* Extension of the modelling of the behaviour to dissipative materials such as linear viscoelastic materials, taking account of dissipation in the heat equation.

* Numerical simulations of applications of industrial nature :

- Design and optimization of heterogeneous materials (choice of the interface).
- Structure analysis in thermoviscoelasticity.
- Multiscale numerical computations in thermoelasticity.

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