MACROSCOPIC RELATIONS FOR THERMODIFFUSION IN HETEROGENEOUS ELASTIC MEDIUM

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Summary We consider heterogeneous thermoelastic body with periodic microstructure in which diffusion takes place. Using homogenisation methods we derive macroscopic coefficients describing thermodiffusion in a nonlinear elastic composite. In the case of layered composites, exact analytical formulae for the overall coefficients have been obtained.

INTRODUCTION

Temperature gradients lead to thermal stresses and influence diffusion in solids. The effect of large thermal gradients on the mass transport in gold and nonlinearity of hydrogen diffusion in nickel is is well known, [1-3]. Overall properties of elastic composites with coefficients independent of temperature in which thermodiffusion takes place were investigated by homogenisation method in several papers where the temperature-displacement and entropy-displacement formulations of thermoelastic solid were used, cf. [4]. Also in [4] the procedure of homogenisation of quasi-linear heat equation was performed. Here we extend this procedure to thermodiffusive processes in solids.

ASYMPTOTIC METHOD

We consider an elastic body occupying a volume $\Omega \subset \mathbb{R}^3$ and exhibiting a microperiodic structure characterized by the cell ϵY. The physical properties of the body change in microperiodic manner. The relation of the characteristic dimension of the cell ℓ to the characteristic dimension of the body L is taken as a small parameter $\epsilon = \ell/L$. The following balance laws are to be satisfied:
(*i*) *The equation of motion*

$$\rho \ddot{u}_i = \frac{\partial}{\partial x_j}\sigma_{ij} \tag{1}$$

with σ_{ij} given by

$$\sigma_{ij} = c_{ijmn}\varepsilon_{mn} - g_{ij}^T(T - T_0) - g_{ij}^c c \tag{2}$$

where the deformation ε_{ij} and displacement u_i are related by the linear expression $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$, T and T_0 denote the absolute and reference temperatures, while c_{ijmn}, g_{ij}^T and g_{ij}^c are the elasticity, stress-temperature and stress-diffusion coefficients, respectively. The coefficients may depend on the position $\mathbf{x}$, temperature T and concentration c in a given manner.
(*ii*) *The conservation of mass and heat*

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x_i}j_i + r^c \quad \text{and} \quad c_p\frac{\partial T}{\partial t} = -\frac{\partial}{\partial x_i}q_i + r^T \tag{3}$$

with c_p - the specific heat at constant pressure, r^c and r^T - the mass and heat sources depending on ε_{ij} and T. The mass and heat currents j_i and q_i are given by

$$j_i = -D\frac{\partial}{\partial x_i}c + M\frac{\partial}{\partial x_i}T \quad \text{and} \quad q_i = -N\frac{\partial}{\partial x_i}c + \lambda_T\frac{\partial}{\partial x_i}T \tag{4}$$

where D, M, N and λ_T are the coefficients of diffusion, thermodiffusion (direct and reciprocal) and heat conduction, which can depend also on $\mathbf{x}$, T and c.
In composite with a periodic microstructure all material coefficients are ϵY-periodic functions, where Y is the basic cell. For instance,

$$c_{ijmn}^\epsilon = c_{ijmn}^\epsilon(\mathbf{x}, T) = c_{ijmn}(\frac{\mathbf{x}}{\epsilon}, T), \quad g_{ij}^{T\epsilon} = g_{ij}^{T\epsilon}(\mathbf{x}, T) = g_{ij}^T(\frac{\mathbf{x}}{\epsilon}, T) \qquad x \in \Omega$$

and so on. For any fixed $\epsilon > 0$ both the displacement, concentration and the temperature fields are denoted by $\mathbf{u}^\epsilon, c^\epsilon$ and T^ϵ and have the ϵ - expansions. For instance,

$$u_i^\epsilon(\mathbf{x}) = \overset{0}{u}_i(\mathbf{x}) + \epsilon\ \overset{1}{u}_i(\mathbf{x}, \mathbf{y}) + \epsilon^2\ \overset{2}{u}_i(\mathbf{x}, \mathbf{y}) + \cdots$$

$$T^\epsilon(\mathbf{x}) = \overset{0}{T}(\mathbf{x}) + \epsilon\ \overset{1}{T}(\mathbf{x}, \mathbf{y}) + \epsilon^2\ \overset{2}{T}(\mathbf{x}, \mathbf{y}) + \cdots$$

where $\mathbf{y} = \mathbf{x}/a$. Also, the material coefficients are to be expanded, e.g.

$$c^{\epsilon}_{ijmn} = \overset{0}{c}_{ijmn} + \epsilon^1 \overset{1}{c}_{ijmn} + \epsilon^2 \overset{2}{c}_{ijmn} + \cdots$$

After lengthy calculations the field equations are obtained. For instance,

$$\rho^{\epsilon}\ddot{u}^{\epsilon}_i = \left(\frac{\partial}{\partial x_j} + \frac{1}{\epsilon}\frac{\partial}{\partial y_j}\right)\left[c^{\epsilon}_{ijmn}\left(\frac{\partial}{\partial x_n} + \frac{1}{\epsilon}\frac{\partial}{\partial y_n}\right)u^{\epsilon}_m - g^{T\epsilon}_{ij}(T^{\epsilon} - T_0) - g^{c\epsilon}_{ij}(T^{\epsilon} - T_0)\right].$$

Homogenization means passing with ϵ to zero and yields the macroscopic field equations involving homogenized (overall) coefficients. For instance,

$$\begin{aligned} c^h_{ijpq} &= <\overset{0}{c}_{ijpq}(\mathbf{y}) + \overset{0}{c}_{ijmn}\frac{\partial \chi_{mpq}(\mathbf{y})}{\partial y_n}>, \\ g^{Th}_{ij} &= <\overset{0}{g}{}^{T}_{ij}(\mathbf{y}) - \overset{0}{c}_{ijmn}\frac{\partial \Gamma_m(\mathbf{y})}{\partial y_n}>, \\ \lambda^T_{ik} &= <\overset{0}{\lambda}_T(\mathbf{y})\delta_{ik} + \overset{0}{\lambda}_T(\mathbf{y})\delta_{ij}\frac{\partial \theta_k(\mathbf{y})}{\partial y_j}>. \end{aligned} \qquad (5)$$

Here χ_{mpq}, Γ_m and θ_k denote Y-periodic local functions. The superscript h stands for the homogenized quantities; $\chi_{mpq}, \Gamma_m, \theta_k$ are the functions obtained from solution of local problems, and $< \cdots >$ denotes the averaging over Y.

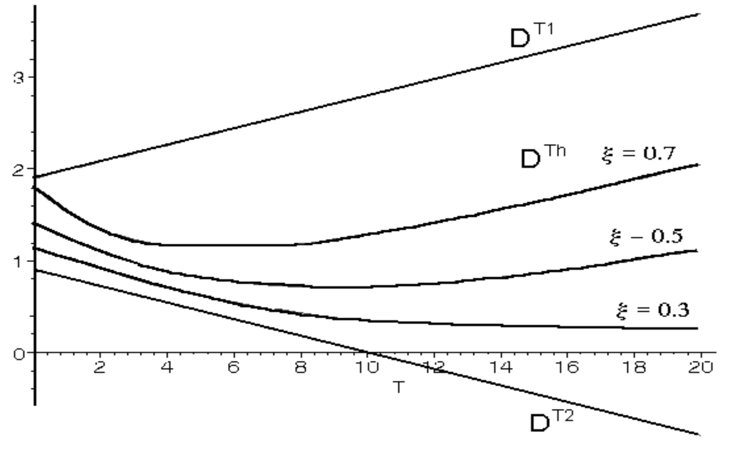

Figure: Effective direct thermodiffusion coefficient versus temperature for different volume fraction of components for: $D_1 = 1 + 0.1T$, $D^T_1 = 0.9 - 0.09T$, $\lambda^D_1 = 0.5 + 0.05T$, $\lambda_1 = 0.4 + 0.04T$, $D_2 = 5 + 0.1T$, $D^T_2 = 1.9 - 0.09T$, $\lambda^D_2 = 1.5 + 0.05T$, $\lambda_2 = 1.4 + 0.04T$.

CONCLUSIONS

The equations of nonlinear thermodiffusion in elastic solids with periodic microstructure have been analysed. By using homogenisation methods the macroscopic equations have been derived. To illustrate these general results, the microperiodic layered composite has been studied in which the coefficients depend on T and c. As an example, see Figure.

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