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Interaction of thermal and moisture stresses in materials dried convectively

S. J. KOWALSKI and A. RYBICKI (POZNAŃ)

JOINT ACTION of the moisture concentration field and the temperature field in generation of drying stresses is considered in the paper. A question whether the thermal stresses and the moisture stresses are superimposed on each other or neutralize each other is answered. The problem is illustrated by an example of convective drying of a bar of rectangular cross-section. The numerical results are presented in diagrams.

Notation

$x_1 \equiv x,\ x_2 \equiv y,\ x_3 \equiv z$ [m]	spatial coordinates,
t [s]	time,
$\mathbf{u}(u_x, u_y, u_z)$ [m]	displacement vector of the porous material,
A [N/m^2]	bulk modulus of the porous material,
M [N/m^2]	shear modulus of the porous material,
σ_{ij} [N/m^2]	components of the stress tensor,
ε_{ij} [1]	components of the strain tensor,
T [°K]	absolute temperature,
$\vartheta = T - T_r$ [deg]	relative temperature,
ρ_0 [kg/m^3]	mass density of the porous material,
ρ_m [kg/m^3]	mass density of the moisture referred to the total volume,
$\Theta = \rho_m/\rho_0$ [1]	specific moisture content,
$\mathbf{q}$ [W/m^2]	heat flux vector,
$\boldsymbol{\eta}$ [kg/m^{2}s]	moisture flux vector,
μ [J/kg]	moisture potential density,
c_v [J/m^{3}deg]	specific heat of the medium at constant volume,
c_ϑ [J/m^{2}deg]	temperature coefficient of the moisture potential,
c_Θ [J/m^3]	moisture content coefficient,
α_ϑ [deg^{-1}]	coefficient of the linear thermal expansion,
α_Θ [1]	coefficient of the linear moisture expansion,
α_T [W/m^{2}deg]	coefficient of the convective heat exchange,
α_m [kg s/m^4]	coefficient of the convective mass exchange,
l [J/kg]	latent heat of evaporation,
Λ_T [W/m °K]	thermal conductivity,
Λ_m [kg s/m^3]	moisture conductivity.

1. Introduction

IN TRADITIONAL understanding drying of moist materials is a process of removing moisture due to evaporation. It is a thermal process conditioned by supplying heat to the dried material. During this process both the temperature and the moisture content fields appear in the material. The first one is connected with the temperature distribution and the second one — with the moisture content distribution. These fields are generally non-homogeneous and nonstationary, and as such they can induce self-stresses called „drying stresses". The drying stresses consist of thermal and moisture stresses.

The main aim of this paper is to analyse the interaction between the thermal stresses and the moisture stresses. We intend to answer the question whether these two kinds of stresses intensify or rather neutralize each other. Furthermore, we are going to show that controlling the temperature and the moisture content fields through an appropriate alteration of drying conditions (boundary conditions) can appease the drying stresses and stop their concentration leading in extreme cases to destruction of the material. We will also show that too intensive heating of the material at the beginning of the drying process is disadvantageous. Namely, it can generate a maximum of the moisture potential function (a quantity responsible for the moisture transport) close to the boundary surface. This means an impediment of the moisture flow from inside to outside of the material and too fast drying of the boundary layer. As a consequence of this, a strong shrinkage of that layer takes place and thus the self-stresses which can cause its cracking are generated.

The present considerations are based on the model proposed by KOWALSKI [3, 4], describing the thermomechanical behaviour of dried materials. A two-dimensional problem of convective drying, i.e. the drying of a bar with rectangular cross-section is analysed. The coupled system of four second-order differential equations is solved with the use of the finite element method for the derivatives with respect to the spatial coordinates and the three-point finite differences for the time derivatives, as it was shown by RYBICKI [7]. The numerical results are shown in diagrams.

2. Mathematical formulation of the problem

For the sake of clarity in the mathematical formulation of the problem in hand, we rewrite here the model presented in KOWALSKI [3, 4] and adapt it for the two-dimensional problem which we are going to consider in this paper. The model describing the thermomechanical behaviour of dried materials consists of the following system of differential equations:

$$
\begin{gathered}
M\nabla^2\mathbf{u} + \left(M + A - \frac{\gamma_\Theta^2}{C_\Theta}\right)\operatorname{grad}\operatorname{div}\mathbf{u} = \frac{\gamma_\vartheta c_\vartheta}{c_\Theta}\operatorname{grad}\vartheta + \frac{\gamma_\Theta}{c_\Theta^\rho}\operatorname{grad}\mu,\\
K_m\nabla^2\mu = \dot{\mu} + \gamma_\Theta^\rho\operatorname{div}\dot{\mathbf{u}} - c_\vartheta^\rho\dot{\vartheta},\\
K_T\nabla^2\vartheta = \dot{\vartheta} + K_E\operatorname{div}\dot{\mathbf{u}} - K_\Theta\dot{\mu}.
\end{gathered}
\tag{2.1}
$$

Here $\mathbf{u}$, μ, ϑ, denote the displacement vector of the porous solid, the moisture potential, and the temperature, in that order, and

$$
\begin{gathered}
K_m = \Lambda_m c_\Theta, \qquad \gamma_\Theta^\rho = \gamma_\Theta/\rho_0, \qquad c_\vartheta^\rho = c_\vartheta/\rho_0,\\
c_\Theta^\rho = c_\Theta/\rho_0, \qquad K_T = \Lambda_T/\overset{*}{c}_v, \quad c_\Theta^\rho = c_\Theta/\rho_0,\\
K_E = T_r(\gamma_\vartheta - c_\vartheta\gamma_\Theta/c_\Theta)\overset{*}{c}_v, \qquad K_\Theta = T_r c_\vartheta/c_\Theta^\rho\,\overset{*}{c}_v,\\
\overset{*}{c}_v = c_v + T_r c_\vartheta^2/c_\Theta, \qquad \gamma_\vartheta = (2M + 3A)\alpha_\vartheta, \qquad \gamma_\Theta = (2M + 3A)\alpha_\Theta,
\end{gathered}
\tag{2.2}
$$

where T_r is a reference temperature, for example, the initial temperature.

The equations in (2.1) describe: the deformation of the dried material (first one), the moisture potential distribution, its gradient being responsible for the moisture transport (second one), and the temperature distribution (third one).

The drying-induced stresses σ_{ij} are calculated from the relation

$$\sigma_{ij} = M(u_{i,j} + u_{j,i}) + [Au_{l,l} - \gamma_\vartheta \vartheta - \gamma_\Theta(\Theta - \Theta_r)]\delta_{ij}, \tag{2.3}$$

where Θ_r is the reference moisture content, for example the minimum value of Θ and of the drying process under the given conditions of drying.

The relation between the moisture potential and the parameters of state is

$$\mu = c_\vartheta^\rho \vartheta - \gamma_\vartheta u_{i,i} + c_\Theta^\rho(\Theta - \Theta_r). \tag{2.4}$$

We make use of the following equations for heat and mass transport,

$$\begin{aligned} \mathbf{q} &= -\Lambda_T \operatorname{grad} \vartheta, \\ \eta &= -\Lambda_m \operatorname{grad} \mu. \end{aligned} \tag{2.5}$$

For a two-dimensional problem, the displacement of the porous solid in z-direction is assumed to be zero, and all other functions are assumed to be dependent on the coordinates x, y, and time t, i.e. $u_x = u_x(x, y, t)$, $u_y = u_y(x, y, t)$, $\mu = \mu(x, y, t)$, $\vartheta = \vartheta(x, y, t)$. Thus, the system of equations (2.1) reduced to the two-dimensional case takes the form

$$\begin{aligned} &\left(2M + A - \frac{\gamma_\Theta^2}{c_\Theta}\right)\frac{\partial^2 u_x}{\partial x^2} + M\frac{\partial^2 u_x}{\partial y^2} + \left(M + A - \frac{\gamma_\Theta^2}{c_\Theta}\right)\frac{\partial^2 u_y}{\partial x \partial y} \\ &\qquad = \left(\gamma_\vartheta - \frac{\gamma_\Theta c_\vartheta}{c_\Theta}\right)\frac{\partial \vartheta}{\partial x} + \frac{\gamma_\Theta}{c_\Theta^\rho}\frac{\partial \mu}{\partial x}, \\ &\left(2M + A - \frac{\gamma_\Theta^2}{c_\Theta}\right)\frac{\partial^2 u_y}{\partial y^2} + M\frac{\partial^2 u_y}{\partial x^2} + \left(M + A - \frac{\gamma_\Theta^2}{c_\Theta}\right)\frac{\partial^2 u_x}{\partial x \partial y} \\ &\qquad = \left(\gamma_\vartheta - \frac{\gamma_\Theta c_\vartheta}{c_\Theta}\right)\frac{\partial \vartheta}{\partial y} + \frac{\gamma_\Theta}{c_\Theta^\rho}\frac{\partial \mu}{\partial y}, \\ &K_m\left(\frac{\partial^2 \mu}{\partial x^2} + \frac{\partial^2 \mu}{\partial y^2}\right) = \frac{\partial \mu}{\partial t} + \gamma_\Theta^\rho\left(\frac{\partial^2 u_x}{\partial x \partial t} + \frac{\partial^2 u_y}{\partial y \partial t}\right) - c_\vartheta^\rho \frac{\partial \vartheta}{\partial t}, \\ &K_T\left(\frac{\partial^2 \vartheta}{\partial x^2} + \frac{\partial^2 \vartheta}{\partial y^2}\right) = \frac{\partial \vartheta}{\partial t} + K_E\left(\frac{\partial^2 u_x}{\partial x \partial t} + \frac{\partial^2 u_y}{\partial y \partial t}\right) - K_\Theta \frac{\partial \mu}{\partial t}. \end{aligned} \tag{2.6}$$

We formulate the initial-boundary value problem as follows: find functions u_x, u_y, ϑ and μ which, within the rectangle $(-L, L) \times (-H, H)$ and for $t \in \mathbb{R}^+$, satisfy the system of equations (2.6) under the following boundary conditions (see Fig. 1a):

for stresses

$$\begin{aligned} \sigma_{xx}|_{x=\pm L} &= 0, & \sigma_{yy}|_{y=\pm H} &= 0, \\ \sigma_{xy}|_{x=\pm L} &= 0, & \sigma_{xy}|_{y=\pm H} &= 0, \end{aligned} \tag{2.7}$$

for the mass exchange

$$\begin{aligned} \Lambda_m \frac{\partial \mu}{\partial x}\bigg|_{x=\pm L} &= \pm\alpha_m(\mu|_{x=\pm L} - \mu_a), \\ \Lambda_m \frac{\partial \mu}{\partial y}\bigg|_{y=\pm H} &= \pm\alpha_m(\mu|_{y=\pm H} - \mu_a), \end{aligned} \tag{2.8}$$

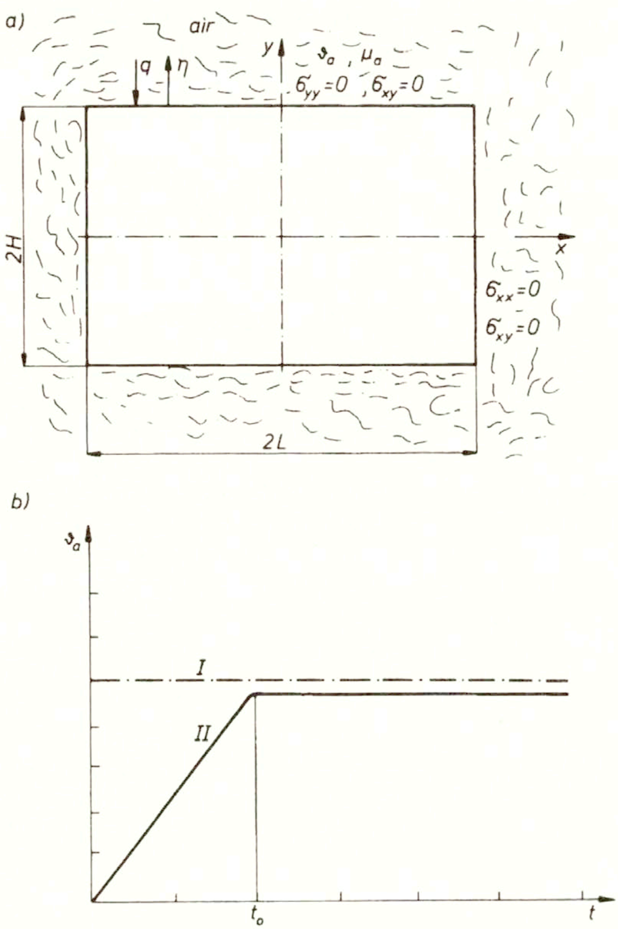


FIG. 1. Boundary conditions: a) rectangular cross-section of the drying bar, b) two different temperatures of the drying medium.

and for the heat exchange

$$
\begin{aligned}
&\Lambda_T \frac{\partial \vartheta}{\partial x}\bigg|_{x=\pm L} = \pm\alpha_T(\vartheta_a - \vartheta|_{x=\pm L}) \pm l\alpha_m(\mu|_{x=\pm L} - \mu_a),\\
&\Lambda_T \frac{\partial \vartheta}{\partial y}\bigg|_{y=\pm H} = \pm\alpha_T(\vartheta_a - \vartheta|_{y=\pm H}) \pm l\alpha_m(\mu|_{y=\pm H} - \mu_a),
\end{aligned} \tag{2.9}
$$

under the initial conditions

$$
\sigma_{ij}(x,y,0) = 0, \qquad \mu(x,y,0) = \mu_0, \qquad \vartheta(x,y,0) = \vartheta_0. \tag{2.10}
$$

In the above equations μ_a and ϑ_a denote the chemical potential and the temperature of the surrounding atmosphere (drying medium).

In order to demonstrate some advantages of a controlled drying process in comparison with a non-controlled one, we solve our problem for two different temperatures of the drying medium (see Fig. 1b). In the first case the drying medium acquires high and constant temperature ϑ_a^{I} at once, and in the second one the temperature increases slowly from zero to $\vartheta_a^{\mathrm{II}}$, where $\vartheta_a^{\mathrm{I}} = \vartheta_a^{\mathrm{II}}$ for $t \geq t_0$.

3. Numerical solution

Let us rewrite the system of differential equations (2.6) in a matrix form

$$
\begin{pmatrix} A_{xx} & A_{xy} & A_{xm} & A_{xT} \\ A_{yx} & A_{yy} & A_{ym} & A_{yT} \\ 0 & 0 & A_{mm} & 0 \\ 0 & 0 & 0 & A_{TT} \end{pmatrix} \begin{pmatrix} u_x \\ u_y \\ \mu \\ \vartheta \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ C_{mx} & C_{my} & C_{mm} & C_{mT} \\ C_{Tx} & C_{Ty} & C_{Tm} & C_{TT} \end{pmatrix} \begin{pmatrix} \dot{u}_x \\ \dot{u}_y \\ \dot{\mu} \\ \dot{\vartheta} \end{pmatrix} = \begin{pmatrix} b_x \\ b_y \\ b_m \\ b_T \end{pmatrix}, \tag{3.1}
$$

$$
\begin{aligned}
A_{xx} &= k_1 \frac{\partial^2}{\partial x^2} + k_2 \frac{\partial^2}{\partial y^2}, \\
A_{xy} &= k_2 \frac{\partial^2}{\partial x \partial y} + k_3 \frac{\partial^2}{\partial y \partial x} \\
A_{xm} &= -k_4 \frac{\partial}{\partial x}, \qquad \text{etc.,}
\end{aligned} \tag{3.2}
$$

in which $k_1, k_2, \ldots, k_l$ express the respective material constants or their combination (see Eqs. (2.6)). The vector of free terms

$$
\mathbf{b} = (b_x, b_y, b_m, b_T)^T
$$

is here equal zero.

This system of second order differential equations is solved by the finite element method for the spatial derivatives and the three-point finite differences for the time derivatives (see LEES [5]). The functions of displacement u_x and u_y, the moisture potential μ, and the temperature ϑ are expressed in a form of polynomials for each instant of time t_k, $k = 0, \ldots, M$.

$$
\begin{aligned}
u_x(x, y, t_k) &= \sum_{n=1}^{N} B_n^x(t_k) \phi_n(x, y), \\
u_y(x, y, t_k) &= \sum_{n=1}^{N} B_n^y(t_k) \phi_n(x, y), \\
\mu(x, y, t_k) &= \sum_{n=1}^{N} B_n^m(t_k) \phi_n(x, y), \\
\vartheta(x, y, t_k) &= \sum_{n=1}^{N} B_n^T(t_k) \phi_n(x, y),
\end{aligned} \tag{3.3}
$$

where $\{\Phi_n(x, y)\}$ is a set of base function (shape function) and N is the number of these functions.

The coefficient vector

$$\mathbf{B}_n(t_k) = (B_n^x(t_k), B_n^y(t_k), B_n^m(t_k), B_n^T(t_k))$$

is determined for each instant t_k by the three-point method, (see LEES [5]), according to the following recurrent formula:

$$\mathbf{B}_n(t_{k+1}) = -\left(\frac{1}{3}\mathbf{A} + \frac{1}{2\Delta t}\mathbf{C}\right)^{-1} \cdot \left\{\frac{1}{3}\mathbf{A}(\mathbf{B}_n(t_k))^T + \left(\frac{1}{3}\mathbf{A} + \frac{1}{2\Delta t}\mathbf{C}\right)(\mathbf{B}_n(t_{k-1}))^T + \mathbf{b}_n\right\}, \tag{3.4}$$

where **A** and **C** are the stiffness and the time coefficient matrices, respectively, $\mathbf{b}_n$ is the vector of free terms (it is equal to zero in (3.1) but not in (3.4) where boundary conditions are taken into account), and $\Delta t = t_k - t_{k-1}$ is the time step.

Using the notation applied in (3.1) we can easily put down the Galerkin form of those equations. The respective elements of the stiffness matrix **A** are expressed as follows:

$$\begin{aligned}
(A_{xx})_{ij} &= k_1 \int\int \left(\frac{\partial \phi_j}{\partial x}\frac{\partial \phi_i}{\partial x}\right) + k_2 \int\int \left(\frac{\partial \phi_j}{\partial y}\frac{\partial \phi_i}{\partial y}\right),\\
(A_{xy})_{ij} &= k_2 \int\int \left(\frac{\partial \phi_j}{\partial y}\frac{\partial \phi_i}{\partial x}\right) + k_3 \int\int \left(\frac{\partial \phi_j}{\partial x}\frac{\partial \phi_i}{\partial y}\right),\\
(A_{xm})_{ij} &= k_4 \int\int \left(\frac{\partial \phi_j}{\partial y}\phi_i\right),\\
(A_{xT})_{ij} &= k_5 \int\int \left(\frac{\partial \phi_j}{\partial y}\phi_i\right), \quad \text{etc.}
\end{aligned} \tag{3.5}$$

To determine the elements of the time matrix **C**, the following formulas may be applied:

$$\begin{aligned}
(C_{mx})_{ij} &= k_{23} \int\int \left(\phi_j \frac{\partial \phi_i}{\partial x}\right),\\
(C_{my})_{ij} &= k_{24} \int\int \left(\phi_j \frac{\partial \phi_i}{\partial x}\right),\\
(C_{mm})_{ij} &= k_{25} \int\int (\phi_j \phi_i), \quad \text{etc.}
\end{aligned} \tag{3.6}$$

The objective of our analysis are stresses, i.e. quantities expressed by the spatial derivatives of the displacement. Then, we have to pay attention to a suitable selection and adjustment of the base function, in order to assure the continuity of these functions and their linear combinations in all boundary element points, also in boundary points of elements having different dimensions. Here we have solved this problem by making use of the bicubic Hermite interpolation on rectangular elements (see [6]). Slight modernization of this method was made to assure the above mentioned continuity.

Note that the boundary conditions for stresses (2.7) are natural conditions for the first two equations of (2.6), as they express the divergence of stresses. For example, the first one can be written as

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0. \tag{3.7}$$

The boundary conditions for heat and mass transfer, Eqs. (2.8) and (2.9), are more complicated and require additional integrals over the boundary regions to evaluate the elements of the matrix **A** and vector $\mathbf{b}_n$ (see [7]).

Because of symmetry of the problem (see boundary conditions (2.7) to (2.9)), we confine our considerations to the quarter of the whole rectangle, namely to the domain $(0, L) \times (0, H)$. The solutions in the other quarters will be the same since x and y are the symmetry axes.

4. Results and analysis

It is obvious that the thermal and moisture stresses arise as a consequence of the nonuniform temperature and moisture concentration fields, respectively.

Therefore we devote some attention to the analysis of these fields, strictly speaking to the analysis of the temperature field and the moisture potential field. The relation between the moisture potential μ and the moisture concentration Θ is given by Eq. (2.4). They are proportional to each other when the temperature and the dilatation of the porous body are constant.

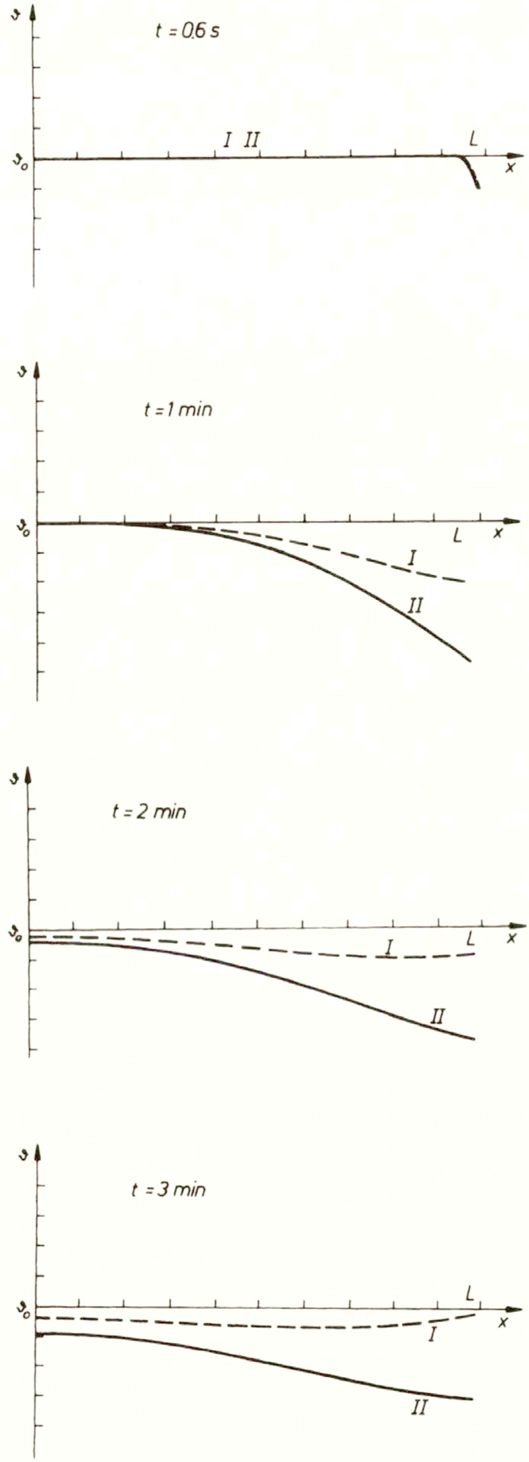
The computer calculations were carried out for the following data taken from the literature (see, for example, [1, 2]),

$$
\begin{aligned}
L &= 0.05\ [\mathrm{m}], & H &= 0.1\ [\mathrm{m}],\\
A &= 10^9\ [\mathrm{N/m^2}], & M &= 6.25\cdot 10^8\ [\mathrm{N/m^2}],\\
\Lambda_T &= 0.44\ [\mathrm{W/m^\circ K}], & \Lambda_m &= 6.04\cdot 10^{-8}\ [\mathrm{kgs^3/m}],\\
\alpha_\vartheta &= 3\cdot 10^{-8}\ [\mathrm{deg^{-1}}], & \alpha_\Theta &= 3\cdot 10^{-5}[-],\\
\alpha_T &= 40\ [\mathrm{W/m^{2\circ}K}], & \alpha_m &= 8.64\cdot 10^{-5}\ [\mathrm{kgs/m^4}],\\
\rho_0 &= 1200\ [\mathrm{kg/m^3}], & c_\Theta &= 6.66\cdot 10^5\ [\mathrm{J/m^3}],\\
l &= 2.5\cdot 10^6\ [\mathrm{J/kg}], & \Delta t &= 0.3\ [\mathrm{s}],\\
\mu_0 &= 100\ [\mathrm{J/kg}], & \mu_a &= 40\ [\mathrm{J/kg}],\\
\vartheta_0 &= 0\ [\mathrm{deg}], & \vartheta_a &= 60\ [\mathrm{deg}].
\end{aligned}
$$

Figure 2 illustrates the evolution in time of the temperature distribution for the points lying in the section $(0, L)$ of the x-axis, i.e. for $y = 0$ and $0 \le x \le L$, for two different courses of drying according to the programs I and II performed in Fig. 1b.

The temperature of the dried material can be altered due to heating and evaporation. The first alteration is clear. In order to explain the second one, let us define an equilibrium state between the drying material and the surrounding atmosphere. The equilibrium means equality of the temperature and moisture potential of the atmosphere and the dried material. For example, let us assume at the beginning $\vartheta(x, y, 0) = \vartheta_0 = \vartheta_a$ and $\mu(x, y, 0) = \mu_0 = \mu_a$. In such a case also gradients of the temperature and the moisture potential are equal zero (see boundary conditions (2.8) and (2.9)), and there is no flow of heat and moisture (see Eqs. (2.5)).

Let us now change the potential μ_a to be less than μ_0. In such a case the process of evaporation starts and the temperature of the dried material decreases tending to the wet bulb temperature.



[Fig. 2]

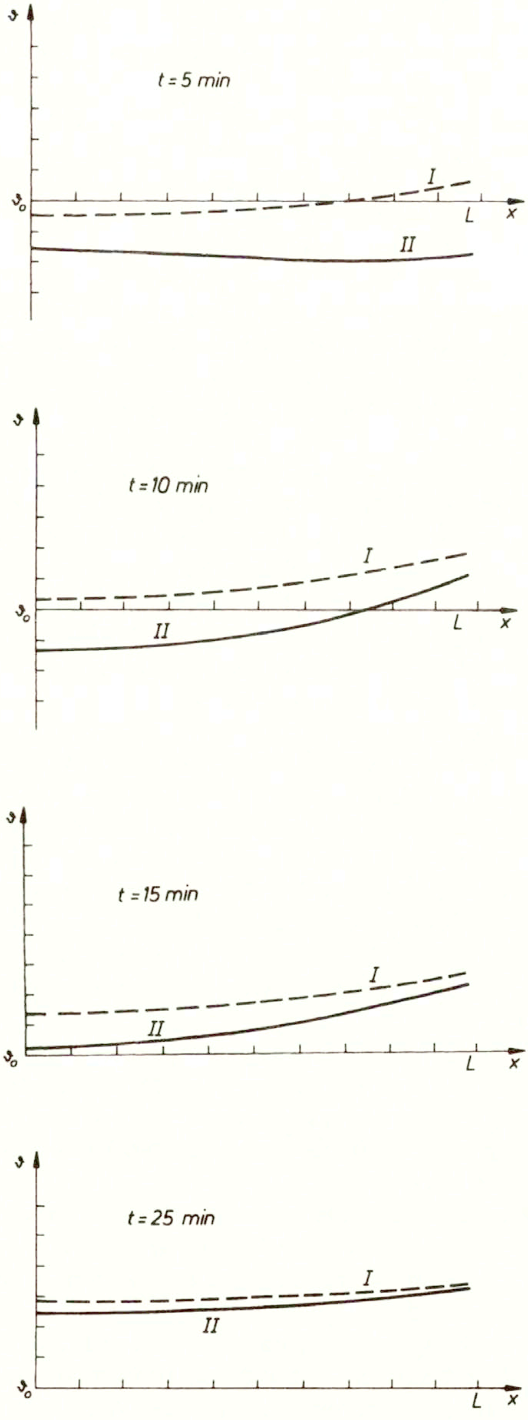


FIG. 2. Evolution of the temperature distribution along section $y = 0, 0 \leq x \leq L$: I — intensive heating, II — slow heating.

The temporary temperature decrease of the dried body takes place also when the drying conditions are such, that at the same time $\mu_a < \mu_0$ and $\vartheta_a > \vartheta_0$, i.e. when the dried body is heated convectively from the very beginning. This situation is shown in the Fig. 2.

It is interesting to analyse the gradient of the temperature. At the beginning this gradient is negative because the boundary surface is cooler than the inside of the body, and the heat flows from inside towards the boundary surface. After ca 2 min in the case of intensive heating, the temperature gradient tends to be positive near the boundary, but that in the case of slow heating does not. The latter one does not start to be positive until after 5 min. The former one is positive after this time in the whole domain, and at the boundary its value exceeds the initial value. Positive temperature gradient makes the heat flow from the boundary towards the inside of the material. After about 25 min the temperature distribution becomes almost constant in the whole domain. It is known that such a distribution of the temperature does not produce thermal stresses.

Figure 3 shows the evolution in time of the moisture potential distribution for the points lying in the section $(0, L)$ of the x-axis, for two different heating programs I and II. As it is seen, the moisture potential in the case of intensive heating is everywhere higher than that in the case of slow heating. It is important to analyse the gradient of the moisture potential, since it is responsible for the moisture transport (see Eq. $(2.5)_2$).

The negative moisture potential gradient means that the moisture flows from inside to outside. Such a situation occurs in the first two minutes, however, the gradient for the case I is higher near the boundary than in the case II.

A bad symptom appears in the 5th minute in the case of intensive heating. There is a maximum of the moisture potential which is denoted by „hump" in the figure. There is a negative moisture potential gradient on the right-hand side of the „hump", and a positive one on the left side. This means blocking of the moisture flow from inside to outside and very quick drying of the boundary layer. This layer shrinks rapidly, whereas the inside of the material does not or even swells a bit. The shrinkage stresses which appear in the boundary layer at that moment can cause its cracking.

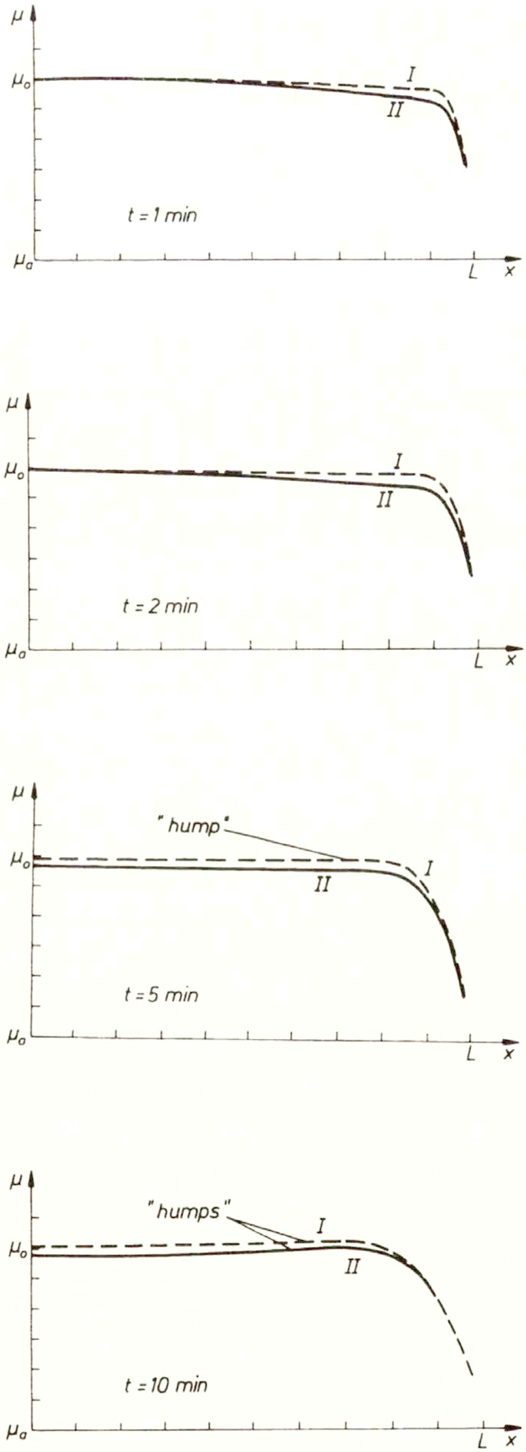
In the case of slower outside heating II, the "hump" appears later and has smaller value than during the intensive heating I. After some time (in Fig. 3 after 33.0 min) the "humps" disappear completely.

The above analysis brings us to a conclusion that there are some periods during the drying process which are particularly dangerous as far as the destruction of the material is concerned. There is, however, a possibility to avoid those dangerous situations — namely by controlling the outside heating (presented here) and the outside drying medium potential (to be presented later).

The fact that the temperature at the boundary of the material decreases at the beginning of the drying process is unfavourable for the stresses. Very intensive shrinkage appears, caused by both the thermal and moisture contractions. The thermal stresses and the moisture stresses are added together.

Figure 4 shows the distribution of thermal, moisture, and total stresses along the $(0, L)$ section of the x-axis at the beginning of the drying process by intensive heating.

We have to explain that the thermal stresses were calculated under the assumption that there was no outflow of the moisture from the dried body, i.e. the moisture content of the body was kept constant all the time during heating.


μ
μo
μa
I
II
t = 1 min
L
x
μ
μo
μa
I
II
t = 2 min
L
x
μ
"hump"
μo
μo
I
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"humps"
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[Fig. 3]

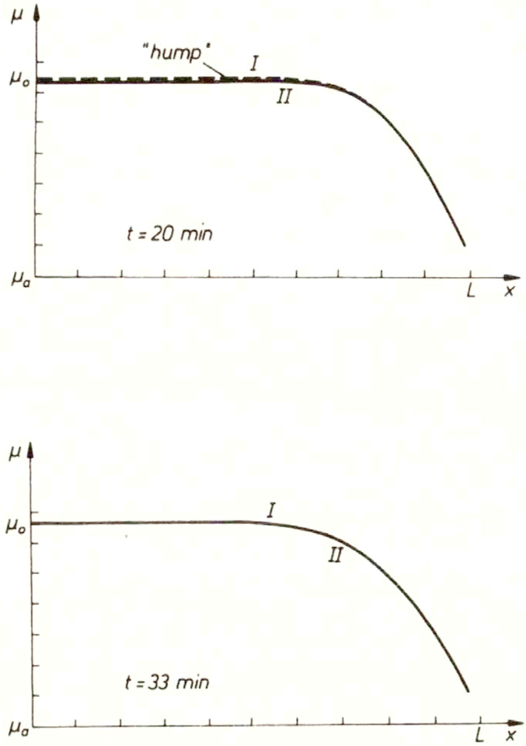

FIG. 3. Evolution of the moisture potential distribution along section $y = 0, 0 \leq x \leq L$: I — intensive heating, II — slow heating.

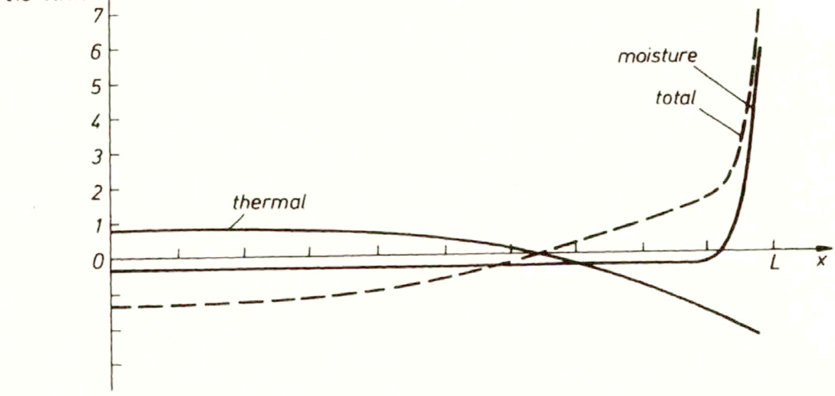

FIG. 4. Evolution of the thermal, moisture, and total stresses along section $y = 0, 0 \leq x \leq L$ at the beginning of the drying process.

The moisture stresses, on the other hand, were calculated under the assumption that the temperature of the body was kept constant all the time during the outflow of the moisture.

The total stresses were calculated without the above assumptions, i.e. by changing both the temperature and moisture content (coupled heat and mass transfer). Therefore the total stresses are not a simple superposition of the above mentioned thermal and moisture stresses.

We can state therefore that, at the beginning, the thermal and moisture stresses are summed up because the total stresses are greater than the moisture ones. After 7 minutes of drying, however, the total stresses are smaller than the moisture ones and this means that, after this time, the thermal stresses neutralize the moisture ones (see Fig. 5).

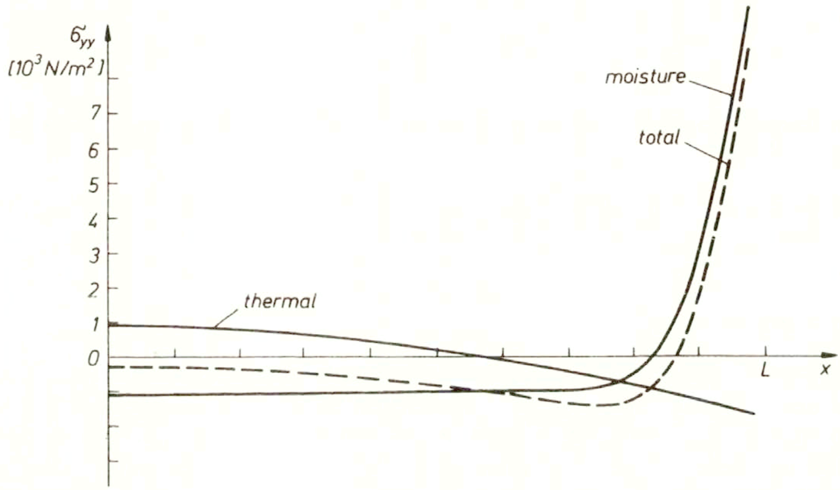

Fig. 5. Evolution of the thermal, moisture, and total stresses along section $y = 0$, $0 \leq x \leq L$ after 7 minutes of the drying process.

This becomes clear when we look at the temperature distribution in Fig. 2 after 5 minutes of drying. We state then that, after this time, the temperature of the boundary layer increases above the initial temperature. This means that the boundary layer starts to expand because of heating. However, the shrinkage due to outflow of the moisture still dominates. After 33 minutes of drying the thermal expansion and the thermal stresses disappear completely. After this time the temperature distribution becomes constant and equal to the wet bulb temperature.

Figure 6 presents the evolution of the stresses σ_{yy} at the point $y = 0$, $x = L$ (maximal σ_{yy}) for the cases of intensive (I) and slow (II) heating. At the beginning, the stresses during slow heating are greater than those due to intensive heating. This is because in the former case the boundary layer becomes cooler and contracts more than in the latter case (see Fig. 2).

After 5 minutes of drying, the "hump" appears in the moisture potential distribution close to the boundary (see Fig. 3). As we have already mentioned, the gradient of moisture potential at the boundary due to intensive heating is higher than that due to slow heating, and therefore faster drying of the boundary layer takes place due to intensive heating. That

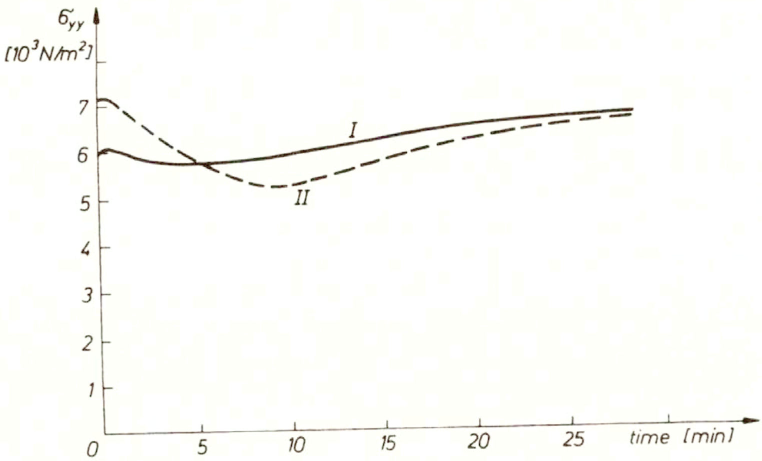

FIG. 6. Evolution of stresses σ_{yy} in point ($x = L$, $y = 0$); I — intensive heating, II — slow heating.

means more intensive shrinkage and an increase of the drying stresses in the boundary layer.

5. Final remarks

Analysing the results of our considerations we can draw some conclusions of considerable practical meaning. We can state that heating of the dried material at the very beginning of the convective drying process is a positive step. After a short time, however, heating should be reduced in order to avoid the disadvantageous "humps" in the moisture potential distributions, since they render the outflow of the moisture from the dried body difficult. The heating program should be therefore optimized. This is going to be the task for our future studies.

Optimization of the temperature program for the drying medium is not the only possibility to control the drying process. Another one is a suitable batching of the moisture (vapor) in the drying medium (air). The vapor content in the drying medium is one of the fundamental parameters governing the drying medium potential μ. Examination of the influence of this parameter on the drying process and its control will be presented in a separate paper.

In this paper we are interested in the interaction of the thermal and moisture stresses. The thermal stresses appear at the beginning of the drying process, i.e. during heating of the dried material. They disappear in the constant drying rate period, in which the temperature of the dried material is kept constant and equal to the wet bulb temperature.

They can appear again in the reduced drying rate period, when the temperature of the drying material increases again and tends to the temperature of the external environment.

For materials like clay and ceramics the most important period, taking into account shrinkage, is the first period of drying.

Therefore, we have confined our considerations only to the period of heating of the dried material, i.e. to the beginning of the drying process.

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Thermodiffusion in heterogeneous elastic solids and homogenization

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OVERALL BEHAVIOUR of microheterogeneous elastic solids in which thermodiffusion occurs is studied by using homogenization methods. Heterogeneities are characterized by a small positive parameter ε. The material coefficients of the coupled system of linear equations describing thermodiffusion depend on ε. In the periodic case, when heterogeneities are distributed periodically, the homogenization is performed by applying the method of two-scale asymptotic expansions. The convergence and corrector theorems are formulated for a nonperiodic microstructure. It is shown, that the initial conditions for the temperature and chemical potential of the homogenized system are changed in comparison with the primal one provided that the initial conditions for the latter system are nonhomogenous. For a layered composite with periodically distributed layers, analytical formulae are derived for all the effective material coefficients. Particular cases are studied by exploiting some available experimental data.

Introduction

OVERALL BEHAVIOUR of micro-heterogeneous materials and composites is justified either mathematically, yet still referring to physical notions [1–12], or rather based on physical concepts [13–24]. Obviously those two points of view overlap [3, 7, 8, 10, 11, 12, 25, 26, 27].

Composites are often designed for structures working at elevated temperatures, cf. [13, 24, 28, 29]. Effects of moisture and mass diffusion may also be important [30–32]. Section 1 of [155] provides an overview of papers dealing with heat, mass and moisture transfer in heterogeneous media and composite materials. The main aim of the present paper is a study of the equations of thermodiffusion [33–36] in anisotropic and micro-heterogeneous solids from the point of view of homogenization. In our previous paper [37], similar problem was investigated under a simplifying assumption that the coupling term in the flow equations may be neglected. Neither convergence nor corrector theorems were formulated and only periodic microstructure was studied. However, inhomogeneous initial conditions were imposed and the change in the initial temperature and chemical potential was observed. In the note [38] the coupling term was taken into account.

The plan of the present paper, consisting of two parts, is as follows. Part 1 presents theoretical results concerning homogenization of three-dimensional elastic solids in which thermodiffusion occurs. Particularly, in Sec. 2 the basic equations of thermodiffusion in an anisotropic and nonhomogenous body are formulated. Next, in Sec. 3, for such a body the initial-boundary value problem is formulated and existence and uniqueness theorem is given. Section 4 deals with the homogenization provided that the microstructure of the body is periodic or quasi-periodic. The method of two-scale asymptotic expansions is used. The local problems, posed on the basic cell Y, and the effective or homogenized material coefficients are examined in Sec. 5. As in our previous paper [37], the change in the initial conditions for the temperature and chemical potential occurs. This problem is investigated in Sec. 6. A general convergence theorem, without the assumption of periodicity, is formulated in Sec. 7.

Two topics are investigated in the second part of the paper. In Sec. 8 the corrector theorems formulated in [39, 40] are extended so as to include the diffusion. Analytical formulae for the effective material coefficients are derived in Sec. 9, provided that the body consists of periodically distributed layers (one-dimensional homogenization). By using these formulae some specific cases are discussed in Sec. 10.

Part 1. Theoretical developments

1. Thermal effects in heterogeneous bodies and composites: very brief overview

In our report [155] an elaborate review has been performed. Here we shall only summarize the main points. In [155] the contributions dealing with thermal and thermomechanical response of heterogeneous bodies and composites are discussed under the following subheadings:

1.1. General treatments [4, 13, 17, 24, 28, 29, 41–44].
1.2. Thermal conduction and thermal expansion [13, 17, 27, 45–52].
1.3. Thermoelasticity, thermoviscoelasticity and thermodiffusion [5, 8, 10, 37, 39, 40, 53–74].
1.4. Thermopiezoelectric composites [75–83].
1.5. Thermoelastic contact problem and homogenization [84, 85].
1.6. Influence of moisture on the overall behaviour of composites [8, 18, 28, 30–32, 37, 41, 86, 87].
1.7. Porous materials [19, 88–94, 154].
1.8, Damage, cracked laminates [95–99].
1.9. Fibrous composites [28, 100–110].
1.10. Plates and shells [111–123].
1.11. Random media and composites [124–130].
1.12. Micro-heat exchangers and micro-heat pipes [131, 132].

2. Thermodiffusion in an elastic body

2.1. Nonequilibrium thermodynamics of diffusion

The phenomenon of diffusion belongs to irreversible processes, and, if it is developing under the conditions in which the deviation from the equilibrium of the system is not too large, it obeys the laws of linear nonequilibrium thermodynamics (**LNT**), cf. DE GROOT and MAZUR [133].

Essential role in **LNT** is played by the balance equation of entropy. It expresses the obvious fact that the variation of entropy (as every other quantity) is composed of two parts

$$dS = d_e S + d_i S, \tag{2.1}$$

where $d_e S$ is due to the entropy flow and its exchange with the surrounding, and $d_i S$ is due to the entropy source (because of irreversibility of phenomena occurring in the system).

If all quantities describing the system are continuous as functions of space variables, the exchange term variation per unit time has a divergence form

$$\frac{\partial_e S}{\partial t} = -\operatorname{div} \mathbf{j}_e\,, \tag{2.2}$$

where $\mathbf{j}_e$ is the entropy flow per unit area and unit time.

If the variation of entropy in the system is due to flows of heat (i.e. energy) and mass, we have the following balance equation

$$T\dot{s} = -q_{i,i} + Mj_{i,i}\,, \tag{2.3}$$

where s is the entropy of unit volume, $\mathbf{q}$ and $\mathbf{j}$ are heat and diffusion fluxes, respectively; T is the absolute temeperature and M denotes the chemical potential.

The last equation can be written as follows

$$\dot{s} = -\left(\frac{q_i - Mj_i}{T}\right)_{,i} + \sigma\,. \tag{2.4}$$

The first term at the r.h.s. is equal to $\partial_e S/\partial t$ and describes the entropy exchange with the surrounding, while the second term, i.e.

$$\sigma = (q_i - Mj_i)\left(\frac{1}{T}\right)_{,i} - j_i\frac{M_{,i}}{T}\,, \tag{2.5$_1$}$$

or

$$\sigma = q_i\left(\frac{1}{T}\right)_{,i} - j_i\left(\frac{M}{T}\right)_{,i}\,, \tag{2.5$_2$}$$

represents the entropy production and corresponds to $\partial_i S/\partial_t$.

Equations (2.5) is a specific example of the *LNT* law: *the entropy production is a bilinear form in the fluxes $\dot{x}^\alpha$ and thermodynamic forces X^α appearing in the phenomenological equations for which the Onsager relation is satisfied*, cf. [133, 134],

$$\dot{x}^\alpha = \sum_\beta L^{(\alpha\beta)}X^{(\beta)}\,, \tag{2.6}$$

$$L^{(\alpha\beta)} = L^{(\beta\alpha)}\,, \tag{2.7}$$

$$\sigma = -\sum_\alpha X^{(\alpha)}\dot{x}^\alpha\,. \tag{2.8}$$

Since $\sigma \geq 0$, the quadratic form

$$\sum_{\alpha,\beta} L^{(\alpha\beta)}X^{(\alpha)}X^{(\beta)}$$

must be *positive definite* or at least *positive.*

Comparison of (2.8) with (2.5) indicates a certain flexibility in the choice of fluxes and conjugate forces. For instance, in [133, 134] the following fluxes are considered

$$\dot{\mathbf{x}}^{(1)} = \mathbf{q}' \equiv \mathbf{q} - M\mathbf{j}, \qquad \dot{\mathbf{x}}^{(2)} = \mathbf{j}\,, \tag{2.9}$$

conjugate to the forces

$$\mathbf{X}^{(1)} = \frac{1}{T^2}\nabla T, \qquad \mathbf{X}^{(2)} = \frac{1}{T}\nabla M\,. \tag{2.10}$$

NOWACKI ([34], Ch. 4) assumes the fluxes

$$\dot{\mathbf{x}}^{(1)} = \mathbf{q}, \qquad \dot{\mathbf{x}}^{(2)} = \mathbf{j}\,, \tag{2.11}$$

as conjugate to the forces

$$\mathbf{X}^{(1)} = \frac{1}{T^2}\nabla T, \qquad \mathbf{X}^{(2)} = \nabla \frac{M}{T}, \tag{2.12}$$

respectively.

The difference between $\mathbf{q}$ and $\mathbf{q}'$ represents heat transferred by the diffusion and provides an example that *in diffusing mixtures the concept of heat flow can be defined in different ways* [133].

Therefore the first [133, 134] *alternative* has more clear physical meaning. In the linear case both approaches coincide.

The appropriate phenomenological relations of the type (2.6), corresponding to the choice (2.9) and (2.10) are given by

$$\begin{aligned} q_i - Mj_i &= -\widehat{L}^{(11)}_{ij} X^{(1)}_j - \widehat{L}^{(12)}_{ij} X^{(2)}_j ,\\ j_i &= -\widehat{L}^{(21)}_{ij} X^{(1)}_j - \widehat{L}^{(22)}_{ij} X^{(2)}_j , \end{aligned}$$

or explicitly

$$\begin{aligned} q_i - Mj_i &= -\widehat{L}^{(11)}_{ij} \frac{1}{T^2} T_{,j} - \widehat{L}^{(12)}_{ij} \frac{1}{T} M_{,j},\\ j_i &= -\widehat{L}^{(21)}_{ij} \frac{1}{T^2} T_{,j} - \widehat{L}^{(22)}_{ij} \frac{1}{T} M_{,j} , \end{aligned} \tag{2.13}$$

where

$$\widehat{L}^{(12)}_{ij} = \widehat{L}^{(21)}_{ij} = \widehat{L}^{(21)}_{ji} . \tag{2.14}$$

If we put

$$\begin{aligned} L^{(11)}_{ij} &= \frac{1}{T^2} \widehat{L}^{(11)}_{ij} ,\\ L^{(12)}_{ij} &= L^{(21)}_{ij} = \frac{1}{T^2} \widehat{L}^{(12)}_{ij} ,\\ L^{(22)}_{ij} &= \frac{1}{T} \widehat{L}^{(22)}_{ij} , \end{aligned}$$

the phenomenological relations take the form

$$\begin{aligned} \mathbf{q} - M\mathbf{j} &= -\mathbf{L}^{(11)}\nabla T - \mathbf{L}^{(12)} T \nabla M ,\\ \mathbf{j} &= -\mathbf{L}^{(21)}\nabla T - \mathbf{L}^{(22)}\nabla M . \end{aligned} \tag{2.15}$$

Here $\mathbf{L}^{(11)}$ is the heat conductivity matrix, below denoted also by $\mathbf{K}$. The matrix $\boldsymbol{\lambda} = \mathbf{K}/T_0$ will also be used.

Below, the matrix $\mathbf{L}^{(22)}$ will be denoted by $\mathbf{D}$. It is related to the generally accepted definition of the diffusion matrix $\underline{\mathcal{D}}$ according to the formula

$$\mathcal{D}_{ij} = \left(\frac{\partial M}{\partial c}\right)_{T,\boldsymbol{\sigma}} D_{ij} = \left(\frac{\partial M}{\partial c}\right)_{T,\boldsymbol{\sigma}} L^{(22)}_{ij} , \tag{2.16}$$

where $\boldsymbol{\sigma}$ is the stress tensor.

To corroborate this statement we calculate, after LANDAU and LIFSHITZ [134], the *gradient* of the chemical potential M considered as a function of σ, T and c. We have

$$\nabla M = \left(\frac{\partial M}{\partial c}\right)_{T,\sigma} \nabla c + \left(\frac{\partial M}{\partial T}\right)_{c,\sigma} \nabla T + \left(\frac{\partial M}{\partial \sigma}\right)_{T,c} \nabla \sigma . \tag{2.17}$$

We note that the derivative $(\partial M/\partial\sigma)_{T,c}$ in the last term can be replaced by $(\partial \varepsilon/\partial c)_{T,\sigma}$, since

$$d\mathcal{G} = -SdT - \mathbf{e}d\sigma + Mdc , \tag{2.18}$$

where $\mathcal{G} = \mathcal{G}(T, \sigma, c)$ is the termodynamic potential (Gibbs' function or free enthalpy) of the unit volume, cf. [34, 134]. Hence

$$\left(\frac{\partial M}{\partial \sigma}\right)_{T,c} = \frac{\partial^2 \mathcal{G}}{\partial\sigma\partial c} = -\left(\frac{\partial \mathbf{e}}{\partial c}\right)_{T,\sigma} . \tag{2.19}$$

Substituting (2.17) into (2.15) we get (2.16) and the matrix of thermodiffusion $[\mathfrak{k}_{Tik}\mathcal{D}_{kj}]$ such that

$$\mathfrak{k}_{Tik}\mathcal{D}_{kj} = T\left(L_{ij}^{(12)} + \left(\frac{\partial M}{\partial T}\right)_{c,\sigma} L_{ij}^{(22)}\right) . \tag{2.20}$$

The matrix $\underline{\mathfrak{k}}_T$ with dimensionless components in the scalar case reduces to the thermodiffusive ratio. Similarly, we get the components of barodiffusion $\mathfrak{k}_P$

$$\mathfrak{k}_{Pij} = -\left(\frac{\partial \varepsilon_{ij}}{\partial c}\right)_{T,\sigma} \Big/ \left(\frac{\partial M}{\partial c}\right)_{T,\sigma} .$$

The matrix $\mathbf{L}^{(12)}$ describes the phenomenon of thermal diffusion, i.e. flow of matter as a result of temperature gradient (*Soret-type effect*) and the reciprocal phenomenon, i.e. flow of heat as a result of the concentration gradient (*Dufour effect*).

The linearization of Eqs. (2.15) consists in rejection of the nonlinear term, namely $M\mathbf{j}$ and assuming small changes of temperature

$$\Theta = T - T_0, \qquad \Theta \ll T_0 . \tag{2.21}$$

In such a case $\mathbf{L}^{(\alpha\beta)}$ do not depend on temperature. Thus we arrive at the following relations

$$\begin{aligned} q_i &= -L_{ij}^{(11)}\Theta_{,j} - L_{ij}^{(12)}T_0 M_{,j} , \\ j_i &= -L_{ij}^{(21)}\Theta_{,j} - L_{ij}^{(22)} M_{,j} . \end{aligned} \tag{2.22}$$

For NOWACKI's [34] choice of fluxes (2.11) and forces (2.12), we obtain

$$\begin{aligned} q_i &= -\mathcal{L}_{ij}^{(11)} X_j^{(1)} - \mathcal{L}_{ij}^{(12)} X_j^{(2)} , \\ j_i &= -\mathcal{L}_{ij}^{(21)} X_j^{(1)} - \mathcal{L}_{ij}^{(22)} X_j^{(2)} , \end{aligned}$$

or

$$\begin{aligned} q_i &= -\mathcal{L}_{ij}^{(11)}\frac{1}{T^2}T_{,j} - \mathcal{L}_{ij}^{(12)}\frac{1}{T}\left(M_{,j} - \frac{M}{T}T_{,j}\right) , \\ j_i &= -\mathcal{L}_{ij}^{(21)}\frac{1}{T^2}T_{,j} - \mathcal{L}_{ij}^{(22)}\frac{1}{T}\left(M_{,j} - \frac{M}{T}T_{,j}\right) , \end{aligned} \tag{2.23}$$

where $\mathcal{L}_{ij}^{(\alpha\beta)}$ are new transport coefficients; their form readily follows from (2.22): after the linearization and appropriate definition of the material coefficients we recover the relations (2.22).

Now let us focus our considerations on *linear thermoelastic solids*.

2.2 Basic equations of diffusion in a thermoelastic solid

Let $\Omega \subset R^3$ be a bounded domain and $\Gamma = \partial\Omega$ its boundary. A thermo-elastic solid in which diffusion takes place will be denoted, for the sake of simplicity, by **TED**. Only physically and geometrically linear problems are investigated.

$\overline{\Omega}$ is the domain occupied by **TED** body in its natural state. Physical fields depend on $\mathbf{x} = (x_i) \in \Omega$ $(i = 1, 2, 3)$ and on time t. The following notations are used: $\mathbf{u} = (u_i)$ — the displacement vector, $\mathbf{e} = (e_{ij})$ — the strain tensor, $\boldsymbol{\sigma} = (\sigma_{ij})$ — the stress tensor, T — the absolute temperature, T_0 — the absolute temperature of a natural state, $\Theta = T - T_0$ — the relative temperature, $\mathbf{q} = (q_i)$ — the heat flux vector, s — the entropy, M — the chemical potential, $\mathbf{j} = (j_i)$ — the mass flux of a diffusing substance, $\mathbf{B} = (B_i)$ — the prescribed body forces.

The equations describing **TED** body are specified by

(i) Field equations

$$e_{ij}(\mathbf{u}) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{2.24}$$

$$\rho \ddot{u}_i = \frac{\partial \sigma_{ij}}{\partial x_j} + B_i, \tag{2.25}$$

$$T_0 \dot{s} = -\frac{\partial q_i}{\partial x_i}, \tag{2.26}$$

$$\dot{c} = -\frac{\partial j_i}{\partial x_i}, \tag{2.27}$$

where $\dot{u}_i = \partial u_i/\partial t$, etc.

(ii) Constitutive equations

$$\sigma_{ij} = c_{ijkl}e_{kl} - \gamma_{ij}\Theta - \xi_{ij}c, \tag{2.28}$$

$$s = \gamma_{ij}e_{ij} + b\Theta + dc, \tag{2.29}$$

$$M = -\xi_{ij}e_{ij} - d\Theta + ac. \tag{2.30}$$

iii) Flow laws

$$q_i = -K_{ij}\frac{\partial \Theta}{\partial x_j} - L_{ij}T_0\frac{\partial M}{\partial x_j}, \tag{2.31}$$

$$j_i = -L_{ij}\frac{\partial \Theta}{\partial x_j} - D_{ij}\frac{\partial M}{\partial x_j}. \tag{2.32}$$

Here ρ denotes the density, (c_{ijkl}) is the tensor of elastic moduli satisfying the usual symmetry conditions: $c_{ijkl} = c_{klij} = c_{jikl}$; (γ_{ij}) and (ξ_{ij}) are the stress-temperature tensor and the stress-diffusion tensor, respectively; moreover

$$\gamma_{ij} = c_{ijkl}\alpha_{kl}^T, \quad \xi_{ij} = c_{ijkl}\alpha_{kl}^D,$$

where (α^T_{kl}) and (α^D_{kl}) are the thermal expansion tensor and the diffusion expansion tensor, respectively; the last one describes the influence of diffusion on the change of dimensions of the body (swelling); $b = c_{e,c}/T_0$ and $c_{e,c}$ is the specific heat for fixed $\mathbf{e}$ and c; (K_{ij}) and (D_{ij}) denote the thermal conductivity and diffusion tensor, respectively, while (L_{ij}) stands for the thermodiffusion tensor. Obviously, the tensors $\boldsymbol{\alpha}$, $\boldsymbol{\gamma}$, $\mathbf{D}$, $\mathbf{K}$ and $\mathbf{L}$ are symmetric.

On account of the symmetric role played by γ_{ij} and ξ_{ij} in the linear **TED** equations, the following notation will also be used

$$\gamma_{ij} = \gamma^{(1)}_{ij}, \qquad \xi_{ij} = \gamma^{(2)}_{ij}.$$

The material coefficients are not necessarily constant. Nevertheless, we make the following assumption :

$$(2.33) \qquad \rho, b, d, a \in L^\infty(\Omega), \qquad 0 < \rho_0 \le \rho(\mathbf{x}) \quad \text{a.e.} \quad \mathbf{x} \in \Omega,$$

$$(2.34) \qquad \lambda_1(e_1^2 + e_2^2) \le [e_1, e_2] \begin{bmatrix} b(\mathbf{x}) & d(\mathbf{x}) \\ d(\mathbf{x}) & a(\mathbf{x}) \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} \le \lambda_2(e_1^2 + e_2^2) \quad \text{a.e.} \quad \mathbf{x} \in \Omega,\ \forall e_1, e_2 \in \mathbb{R},$$

$$(2.35) \qquad \lambda_1|\mathbf{e}|^2 \le c_{ijkl}e_{ij}e_{kl} \le \lambda_2|\mathbf{e}|^2 \quad \text{a.e.} \quad \mathbf{x} \in \Omega,\ \forall \mathbf{e} \in \mathbb{E}^3_s$$

$$(2.36) \qquad \lambda_1(|\mathbf{e}_1|^2 + |\mathbf{e}_2|^2) \le [\mathbf{e}_1, \mathbf{e}_2] \begin{bmatrix} \boldsymbol{\lambda}(\mathbf{x}) & \mathbf{L}(\mathbf{x}) \\ (\mathbf{L})^T(\mathbf{x}) & \mathbf{D}(\mathbf{x}) \end{bmatrix} \begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \end{bmatrix} \le \lambda_2(|\mathbf{e}_1|^2 + |\mathbf{e}_2|^2), \quad \text{a.e. } \mathbf{x} \in \Omega,\ \forall \mathbf{e}_1, \mathbf{e}_2 \in \mathbb{E}^3_s,$$

where $\mathbb{E}^3_s$ is the space of symmetric 3×3 matrices and $0 < \lambda_1 < \lambda_2$ are constants.

Equivalent form of the constitutive equations is the following one

$$(2.37) \qquad \sigma_{ij} = \bar{c}_{ijkl}e_{kl} - \bar{\gamma}_{ij}\Theta - \bar{\xi}_{ij}M,$$

$$(2.38) \qquad s = \bar{\gamma}_{ij}e_{ij} + \bar{b}\Theta + \bar{d}M,$$

$$(2.39) \qquad c = \bar{\xi}_{ij}e_{ij} + \bar{d}\Theta + \bar{a}M,$$

or

$$(2.40) \qquad \sigma_{ij} = \tilde{c}_{ijkl}e_{kl} - \tilde{\gamma}_{ij}s - \tilde{\xi}_{ij}c,$$

$$(2.41) \qquad \Theta = -\tilde{\gamma}_{ij}e_{ij} + \tilde{b}s - \tilde{d}c,$$

$$(2.42) \qquad M = -\tilde{\xi}_{ij}e_{ij} - \tilde{d}s + \tilde{a}c,$$

where

$$(2.43) \qquad \begin{aligned} \bar{c}_{ijkl} &= c_{ijkl} - \frac{1}{a}\xi_{ij}\xi_{kl}, \\ \bar{\gamma}_{ij} &= \gamma_{ij} + \frac{d}{a}\xi_{ij} := \bar{\gamma}^{(1)}_{ij}, \\ \bar{\xi}_{ij} &= \frac{1}{a}\xi_{ij} := \bar{\gamma}^{(2)}_{ij}, \\ \bar{b} = b + \frac{d^2}{a}, &\quad \bar{d} = \frac{d}{a}, \quad \bar{a} = \frac{1}{a}, \end{aligned}$$

are isothermal-isopotential material coefficients, while

$$
\begin{aligned}
\widetilde{c}_{ijkl} &= c_{ijkl} - \frac{1}{b}\gamma_{ij}\gamma_{kl} := c_{ijkl} - \widetilde{\gamma}_{ij}\gamma_{kl}\,,\\
\widetilde{\gamma}_{ij} &= \frac{1}{b}\gamma_{ij} := \widetilde{\gamma}^{(1)}_{ij}\,,\\
\widetilde{\xi}_{ij} &= \xi_{ij} - \frac{d}{b}\gamma_{ij} := \widetilde{\gamma}^{(2)}_{ij}\,,\\
\widetilde{b} &= \frac{1}{b}, \qquad \widetilde{d} = \frac{d}{b}, \qquad \widetilde{a} = a + \frac{d^2}{b}
\end{aligned}
\tag{2.44}
$$

are adiabatic-isopotential ones. Here the "potential" means the chemical potential.

The following relations are also readily obtained:

$$
\begin{gathered}
\widetilde{c}_{ijkl} = \overline{c}_{ijkl} + \frac{\overline{a}}{\overline{\Delta}}\overline{\gamma}_{ij}\overline{\gamma}_{kl} + \frac{\overline{b}}{\overline{\Delta}}\overline{\xi}_{ij}\overline{\xi}_{kl} - \frac{\overline{d}}{\overline{\Delta}}(\overline{\gamma}_{ij}\overline{\xi}_{kl} + \overline{\xi}_{ij}\overline{\gamma}_{kl})\,,\\
\widetilde{d} = \overline{d}/\overline{\Delta}, \qquad \widetilde{a} = \overline{b}/\overline{\Delta}, \qquad \widetilde{b} = \overline{a}/\overline{\Delta}, \qquad \overline{\Delta} = \overline{a}\overline{b} - \overline{d}^2\,.
\end{gathered}
\tag{2.45}
$$

From Eqs. (2.24)–(2.32) we readily obtain the basic system of equations for the determination of three unknown fields: $\mathbf{u}$, s and c:

$$
\begin{aligned}
\rho\ddot{u}_i &= \frac{\partial}{\partial x_j}[\widetilde{c}_{ijkl}e_{kl}(\mathbf{u}) - \widetilde{\gamma}_{ij}s - \widetilde{\xi}_{ij}c] + B_i\,,\\
\dot{s} &= \frac{\partial}{\partial x_i}\left\{\lambda_{ij}\frac{\partial}{\partial x_j}[-\widetilde{\gamma}_{kl}e_{kl}(\mathbf{u}) + \widetilde{b}s - \widetilde{d}c] + L_{ij}\frac{\partial}{\partial x_j}[-\widetilde{\xi}_{kl}e_{kl}(\mathbf{u}) - \widetilde{d}s + \widetilde{a}c]\right\},\\
\dot{c} &= \frac{\partial}{\partial x_i}\left\{L_{ij}\frac{\partial}{\partial x_j}[-\widetilde{\gamma}_{kl}e_{kl}(\mathbf{u}) + \widetilde{b}s - \widetilde{d}c] + D_{ij}\frac{\partial}{\partial x_j}[-\widetilde{\xi}_{kl}e_{kl}(\mathbf{u}) - \widetilde{d}s + \widetilde{a}c]\right\},
\end{aligned}
\tag{2.46}
$$

where

$$
\lambda_{ij} = K_{ij}/T_0\,. \tag{2.47}
$$

It is worth noting that Eq. $(2.46)_2$ for the evolution of entropy is formally the same as Eq. $(2.46)_3$ for the evolution of concentration. Thus, the system (2.46) may be written in the following abbreviated form:

$$
\begin{aligned}
\rho\ddot{u}_i &= \frac{\partial}{\partial x_j}[\widetilde{c}_{ijkl}e_{kl}(\mathbf{u}) - \widetilde{\gamma}^{\alpha}_{ij}s^{\alpha}] + B_i\,,\\
\dot{s}^{\alpha} &= \frac{\partial}{\partial x_i}\left[L^{\alpha\beta}_{ij}\frac{\partial}{\partial x_j}(-\widetilde{\gamma}^{\beta}_{kl}e_{kl}(\mathbf{u}) + \widetilde{a}^{\beta\gamma}s^{\gamma})\right],
\end{aligned}
\tag{2.48}
$$

provided that the following notation is introduced

$$
(s^{\alpha}) = (s^1, s^2) = (s, c) \tag{2.49}
$$

$$
[\widetilde{a}^{\alpha\beta}] = \begin{bmatrix} \widetilde{a}^{11} & \widetilde{a}^{12} \\ \widetilde{a}^{21} & \widetilde{a}^{22} \end{bmatrix} = \begin{bmatrix} \widetilde{b} & -\widetilde{d} \\ -\widetilde{d} & \widetilde{a} \end{bmatrix}, \tag{2.50}
$$

$$
[\widetilde{\gamma}^{\alpha}_{ij}] = [\widetilde{\gamma}^{(1)}_{ij}, \widetilde{\gamma}^{(2)}_{ij}] = [\widetilde{\gamma}_{ij}, \widetilde{\xi}_{ij}]\,, \tag{2.51}
$$

$$
[\mathbf{L}^{\alpha\beta}] = \begin{bmatrix} \mathbf{L}^{11} & \mathbf{L}^{12} \\ \mathbf{L}^{21} & \mathbf{L}^{22} \end{bmatrix} = \begin{bmatrix} \boldsymbol{\lambda} & \mathbf{L} \\ \mathbf{L}^{T} & \mathbf{D} \end{bmatrix}. \tag{2.52}
$$

The Greek superscripts take values 1 and 2, and indicate the relation between the matrix element and the relevant fluxes of heat and diffusion, respectively. The summation convention applies also to these indices. The following symmetries are evident:

$$\tilde{a}^{\alpha\beta} = \tilde{a}^{\beta\alpha}, \qquad L^{\alpha\beta}_{ij} = L^{\beta\alpha}_{ij} = L^{\alpha\beta}_{ji}. \tag{2.53}$$

In order to facilitate the formulation of the initial-boundary value problems, we introduce the following notations:

$$(\Theta^{\alpha}) = (\Theta^1, \Theta^2) = (\Theta, M). \tag{2.54}$$

For further convenience we set

$$[\overline{\gamma}^{\alpha}] = [\overline{\gamma}^{(1)}, \overline{\gamma}^{(2)}] = [\overline{\gamma}_{ij}, \overline{\xi}_{ij}], \tag{2.55}$$

$$[\gamma^{\alpha}] = [\gamma^{(1)}, \gamma^{(2)}] = [\gamma_{ij}, -\xi_{ij}], \tag{2.56}$$

$$[\overline{a}^{\alpha\beta}] = \begin{bmatrix} \overline{b} & \overline{d} \\ \overline{d} & \overline{a} \end{bmatrix}, \tag{2.57}$$

and

$$[a^{\alpha\beta}] = \begin{bmatrix} b & d \\ -d & a \end{bmatrix}. \tag{2.58}$$

The matrix $[\overline{a}^{\alpha\beta}]$ is symmetric while $[a^{\alpha\beta}]$ skew-symmetric. As it is seen from the definitions (2.45), the matrices $[\overline{a}^{\alpha\beta}]$ and $[\tilde{a}^{\alpha\beta}]$ are mutually inverse

$$\tilde{a}^{\alpha\gamma}\overline{a}^{\gamma\beta} = \delta^{\alpha\beta}. \tag{2.59}$$

Also from (2.39) we find

$$\tilde{a}^{\alpha\beta}\overline{\gamma}^{\beta}_{ij} = \tilde{\gamma}^{\alpha}_{ij}. \tag{2.60}$$

By using (2.54) and (2.55), the constitutive equations (2.38) and (2.39) assume the following concise form

$$s^{\alpha} = \overline{\gamma}^{\alpha}_{ij}e_{ij} + \overline{a}^{\alpha\beta}\Theta^{\beta}. \tag{2.61}$$

REMARK 2.1. KUBIK [135] derived general equations of thermodiffusion on the basis of the mixture theory. The field equations are obtained by using the balance equations, cf. also KUBIK [136], KUBIK and WYRWAŁ [137].

Various physical aspects of the diffusion in solids are presented in the book by MROWEC [138], cf. also WERES [139].

3. Existence and uniqueness theorem

The initial-boundary value problem of the thermodiffusion in a nonhomogeneous anisotropic elastic body is formulated in the following form

$$\rho\frac{\partial^2 u_i}{\partial t^2} - \frac{\partial}{\partial x_j}(\overline{c}_{ijkl}e_{kl}(\mathbf{u}) - \overline{\gamma}_{ij}\Theta - \overline{\xi}_{ij}M) = B_i, \qquad \text{in } \Omega \times (0, t_0), \tag{3.1}$$

$$\overline{b}\frac{\partial\Theta}{\partial t} + \overline{d}\frac{\partial M}{\partial t} - \frac{\partial}{\partial x_i}\left(\lambda_{ij}\frac{\partial\Theta}{\partial x_j} + L_{ij}\frac{\partial M}{\partial x_j}\right) + \overline{\gamma}_{ij}\frac{\partial \dot{u}_i}{\partial x_j} = g_1, \qquad \text{in } \Omega \times (0, t_0), \tag{3.2}$$

$$\overline{d}\frac{\partial\Theta}{\partial t} + \overline{a}\frac{\partial M}{\partial t} - \frac{\partial}{\partial x_i}\left(L_{ij}\frac{\partial\Theta}{\partial x_j} + D_{ij}\frac{\partial M}{\partial x_j}\right) + \overline{\xi}_{ij}\frac{\partial \dot{u}_i}{\partial x_j} = g_2, \qquad \text{in } \Omega \times (0, t_0), \tag{3.3}$$

(3.4) $$\mathbf{u}(\mathbf{x},t)=0,\quad \Theta(\mathbf{x},t)=0,\quad M(\mathbf{x},t)=0,\quad \text{on } \partial\Omega\times(0,t_0),$$

(3.5) $$\mathbf{u}(\mathbf{x},0)=\mathbf{U}(\mathbf{x}),\quad \Theta(\mathbf{x},0)=\Theta_0(\mathbf{x}),\quad M(\mathbf{x},0)=M_0(\mathbf{x}),\quad \dot{u}(\mathbf{x},0)=\mathbf{V}(\mathbf{x}$$

where $\dot{u}_i=\partial u_i/\partial t$; B_i, g_1 and g_2 are given functions of $\mathbf{x}$ and t.

We make the following, rather weak assumptions, cf. (2.33)–(2.36):

(H_1)
$$\rho,\overline{b},\overline{d},\overline{a}\in L^{\infty}(\Omega),\qquad 0<\rho_0\le\rho(\mathbf{x}),$$
$$\lambda_1(e_1^2+e_2^2)\le[e_1,e_2]\begin{bmatrix}\overline{b}(\mathbf{x}) & \overline{d}(\mathbf{x})\\ \overline{d}(\mathbf{x}) & \overline{a}(\mathbf{x})\end{bmatrix}\begin{bmatrix}e_1\\ e_2\end{bmatrix}\le\lambda_2(e_1^2+e_2^2),$$
$$\text{a.e. } \mathbf{x}\in\Omega\ \forall e_1,e_2\in\mathbb{R},$$

where $\lambda_2>\lambda_1>0$; λ_2, λ_1 — constants;

(H_2)
$$\overline{c}_{ijkl}\in L^{\infty}(\Omega),\ \lambda_1|\mathbf{e}|^2\le\overline{c}_{ijkl}(x)e_{ij}e_{kl}\le\lambda_2|\mathbf{e}|^2,\qquad \text{a.e. } \mathbf{x}\in\Omega\forall\mathbf{e}\in\mathbb{E}^3_s,$$
$$\lambda_1(|\mathbf{e}_1|^2+|\mathbf{e}_2|^2)\le[\mathbf{e}_1,\mathbf{e}_2]\begin{bmatrix}\boldsymbol{\lambda}(\mathbf{x}) & \mathbf{L}(\mathbf{x})\\ (\mathbf{L})^T(\mathbf{x}) & \mathbf{D}(\mathbf{x})\end{bmatrix}\begin{bmatrix}\mathbf{e}_1\\ \mathbf{e}_2\end{bmatrix}\le\lambda_2(|\mathbf{e}_1|^2+|\mathbf{e}_2|^2),$$
$$\text{a.e. } \mathbf{x}\in\Omega\ \forall\mathbf{e}_1,\mathbf{e}_2\in\mathbb{E}^3_s.$$

Here $\mathbb{E}^3_s$ denotes the space of symmetric 3×3 matrices.

(H_3) $$\overline{\gamma}_{ij},\overline{\xi}_{ij}\in L^{\infty}(\Omega),\quad |\overline{\gamma}_{ij}(\mathbf{x})|\le\lambda_2,\quad |\overline{\xi}_{ij}(\mathbf{x})|\le\lambda_2,\quad \text{a.e. } \mathbf{x}\in\Omega.$$

(H_4) $$B_i\in L^2(0,t_0;L^2(\Omega)),\quad g_\alpha\in L^{\infty}(0,t_0;H^{-1}(\Omega))\quad (\alpha=1,2).$$

(H_5) $$u_i\in H^1_0(\Omega);\quad V_i,\Theta_0,M_0\in L^2(\Omega).$$

We set $H^1(\Omega)^3=[H^1(\Omega)]^3$, etc.

We can now formulate

Theorem 3.1. *Under the assumptions* (H_1)–(H_5) *there exists a unique solution* $(\mathbf{u},\Theta,M)$ *of* (3.1)–(3.5) *and*

$$\mathbf{u}\in L^{\infty}(0,t_0;H^1_0(\Omega)^3),\qquad \frac{\partial u_i}{\partial t}\in L^{\infty}(0,t_0;L^2(\Omega)),$$
$$\Theta;M\in L^{\infty}(0,t_0;L^2(\Omega))\cap L^2(0,t_0;H^1_0(\Omega)).$$

Remark 3.1

(i) The proof of this theorem can be performed either by using the semigroup theory [140] or by the Galerkin's method [141]. In fact, under (H_1)–(H_5) existence of a solution $(\mathbf{u},\Theta,M)$ holds in the smaler class, cf. [39, 40],

$$\mathbf{u}\in C^0(0,t_0;H^1_0(\Omega)^3),\qquad \frac{\partial\mathbf{u}}{\partial t}\in C^0(0,t_0;L^2(\Omega)^3),$$
$$\Theta;M\in C^0(0,t_0;L^2(\Omega))\cap L^2(0,t_0;H^1_0(\Omega)).$$

(ii) For the definitions and properties of the function spaces used throughout this paper, the reader may refer to [142, 143].

(iii) The related existence and uniqueness problems are discussed in [144, 145, 146].

4. Microperiodic structure of TED body and two-scale asymptotic expansions

A subclass of nonhomogeneous bodies are those with microperiodic structure. Periodicity is certainly an idealization, except man-made regular composites, yet in such a case homogenization methods yield explicit formulae for the determination of overall (effective or homogenized) moduli.

In the sequel we shall apply the method of two-scale asymptotic expansion, which can likewise be used in the case of quasi-periodic (nonuniform) structures, cf. [5, 76, 147].

Let a microperiodic structure of the **TED** body considered be εY-periodic, where $\varepsilon > 0$ is a small parameter and $Y = \overset{3}{\underset{i=1}{\pi}}(0, y_i^0)$ is the so-called basic cell. The functions:

$$c_{ijkl}(\mathbf{y}), \gamma_{ij}(\mathbf{y}), \xi_{ij}(\mathbf{y}), D_{ij}(\mathbf{y}), K_{ij}(\mathbf{y}), \lambda_{ij}(\mathbf{y}), B_i(\mathbf{y}), b(\mathbf{y}), d(\mathbf{y}), a(\mathbf{y}), \rho(\mathbf{y})$$

are Y-periodic and sufficiently regular. Later a weaker assumption will be discussed. For a fixed $\varepsilon > 0$ the material functions

$$\begin{aligned} &{}^{\varepsilon}c_{ijkl}(\mathbf{x}) = c_{ijkl}\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad {}^{\varepsilon}\gamma_{ij}(\mathbf{x}) = \gamma_{ij}\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad {}^{\varepsilon}\xi_{ij}(\mathbf{x}) = \xi_{ij}\left(\frac{\mathbf{x}}{\varepsilon}\right), \\ &{}^{\varepsilon}K_{ij}(\mathbf{x}) = K_{ij}\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad {}^{\varepsilon}L_{ij}(\mathbf{x}) = L_{ij}\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad {}^{\varepsilon}D_{ij}(\mathbf{x}) = D_{ij}\left(\frac{\mathbf{x}}{\varepsilon}\right), \\ &{}^{\varepsilon}b(\mathbf{x}) = b\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad {}^{\varepsilon}d(\mathbf{x}) = d\left(\frac{\mathbf{x}}{\varepsilon}\right), \\ &{}^{\varepsilon}a(\mathbf{x}) = a\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad {}^{\varepsilon}\rho(\mathbf{x}) = \rho\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad \mathbf{x} \in \Omega, \end{aligned} \tag{4.1}$$

are εY-periodic. We note that in sections concerned with asymptotic expansions the notation ${}^{\varepsilon}c_{ijkl}$, etc. is used, whereas the conventional notation c^{ε}_{ijkl} is employed in Secs. 7 and 8.

According to the definitions (2.48)–(2.52), the functions $a^{\alpha\beta}_{ij}$, γ^{α}_{ij} and $L^{\alpha\beta}_{ij}$ are also εY-periodic; thus we set

$$\begin{aligned} &{}^{\varepsilon}c_{ijkl}(\mathbf{x}) = c_{ijkl}\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad {}^{\varepsilon}\gamma^{\alpha}_{ij}(\mathbf{x}) = \gamma^{\alpha}_{ij}\left(\frac{\mathbf{x}}{\varepsilon}\right), \\ &{}^{\varepsilon}L^{\alpha\beta}_{ij}(\mathbf{x}) = L^{\alpha\beta}_{ij}\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad {}^{\varepsilon}a^{\alpha\beta}(\mathbf{x}) = a^{\alpha\beta}\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad {}^{\varepsilon}\rho(\mathbf{x}) = \rho\left(\frac{\mathbf{x}}{\varepsilon}\right), \quad \mathbf{x} \in \Omega. \end{aligned} \tag{4.2}$$

We observe that for a quasi-periodic structure we would have $c_{ijkl}(\mathbf{x}, \mathbf{y})$, $\gamma^{\alpha}_{ij}(\mathbf{x}, \mathbf{y})$, etc., where the functions $c_{ijkl}(\mathbf{x}, .)$, $\gamma^{\alpha}_{ij}(\mathbf{x}, .)$, etc. are Y-periodic and $\mathbf{x} \in \Omega$ is the macroscopic variable.

From a mathematical point of view the homogenization means a passage with ε to zero in an appropriate sense [2, 5, 10]. Strictly speaking, the method of asymptotic expansions is a formal homogenization method, nevertheless it is a powerful one.

In the periodic case, the basic system of Eqs. (2.48) takes on the following form ($\varepsilon > 0$ and fixed):

$$\begin{aligned} &{}^{\varepsilon}\rho\, {}^{\varepsilon}\ddot{u}_i = \frac{\partial}{\partial x_j}[{}^{\varepsilon}\tilde{c}_{ijkl}e_{kl}({}^{\varepsilon}\mathbf{u}) - {}^{\varepsilon}\tilde{\gamma}^{\alpha}_{ij}\ {}^{\varepsilon}s^{\alpha}] + {}^{\varepsilon}B_i, \\ &{}^{\varepsilon}\dot{s}^{\alpha} = \frac{\partial}{\partial x_i}\left[{}^{\varepsilon}L^{\alpha\beta}_{ij}\frac{\partial}{\partial x_j}(-{}^{\varepsilon}\tilde{\gamma}^{\beta}_{kl}e_{kl}({}^{\varepsilon}\mathbf{u}) + {}^{\varepsilon}\tilde{a}^{\beta\gamma}\ {}^{\varepsilon}s^{\gamma})\right], \quad \text{in } \Omega \times (0, t_0). \end{aligned} \tag{4.3}$$

Obviously, the functions ${}^{\varepsilon}\mathbf{u}$ and ${}^{\varepsilon}s^{\alpha}$ depend on $\mathbf{x} \in \Omega$ and the time $t \in (0, t_0)$, ($t_0 > 0$ or $t_0 = +\infty$). This system of equations has to be completed by the boundary and initial conditions. The following conditions are assumed:

(i) boundary conditions

$$ {}^{\varepsilon}\mathbf{u}(\mathbf{x},t) = 0, \qquad {}^{\varepsilon}\Theta^{\alpha}(\mathbf{x},t) = 0 \quad \text{on } \Gamma \times (0,t_0) \tag{4.4}$$

and

(ii) initial conditions

$$ \begin{gathered} {}^{\varepsilon}\mathbf{u}(\mathbf{x},0) = \mathbf{U}(\mathbf{x}), \qquad {}^{\varepsilon}\dot{\mathbf{u}}(\mathbf{x},0) = \mathbf{V}(\mathbf{x})\,, \\ ({}^{\varepsilon}\Theta^{\alpha}(\mathbf{x},0)) = (\Theta_0^{\alpha}(\mathbf{x})) = (\Theta_0^1(\mathbf{x}), \Theta_0^2(\mathbf{x})) = (\Theta_0(\mathbf{x}), M_0(\mathbf{x})), \qquad \mathbf{x} \in \Omega\,, \end{gathered} \tag{4.5}$$

where the functions $\mathbf{U}$, $\mathbf{V}$ and Θ_0^{α} are prescribed and sufficiently regular. It is worth noting here that various combinations of initial conditions are possible. As we shall see in Sec. 6, some of the non-mechanical initial conditions for the homogenized body may be different from those for the microperiodic solid.

According to the method of two-scale asymptotic expansions we make the following assumption (*ansatz*):

$$ \begin{aligned} {}^{\varepsilon}u_i(\mathbf{x},t) &= u_i^{(0)}(\mathbf{x},\mathbf{y},t) + \varepsilon u_i^{(1)}(\mathbf{x},\mathbf{y},t) + \varepsilon^2 u_i^{(2)}(\mathbf{x},\mathbf{y},t) + \ldots\,, \\ {}^{\varepsilon}s^{\alpha}(\mathbf{x},t) &= s^{(0)\alpha}(\mathbf{x},\mathbf{y},t) + \varepsilon s^{(1)\alpha}(\mathbf{x},\mathbf{y},t) + \varepsilon^2 s^{(2)\alpha}(\mathbf{x},\mathbf{y},t) + \ldots\,, \end{aligned} \tag{4.6}$$

where $\mathbf{y} = \mathbf{x}/\varepsilon$ and the functions $u^{(0)}(\mathbf{x},\cdot,t)$, $s^{(0)\alpha}(\mathbf{x},\cdot,t)$, $u^{(1)}(\mathbf{x},\cdot,t)$, etc. are Y-periodic.

Before proceeding further we recall that for a function $f(\mathbf{x},\mathbf{y})$, where $\mathbf{y} = \mathbf{x}/\varepsilon$, the space differentiation operator $\partial/\partial x_i$ should be replaced by $\partial/\partial x_i + (1/\varepsilon)/(\partial/\partial y_i)$. Substituting (4.5) into (4.2) we obtain

$$ \begin{aligned} \rho\left(\frac{\mathbf{x}}{\varepsilon}\right)&(\ddot{u}_i^{(0)} + \varepsilon\ddot{u}_i^{(1)} + \varepsilon^2\ddot{u}_i^{(2)} + \ldots) = \\ &= \left(\frac{\partial}{\partial x_j} + \frac{1}{\varepsilon}\frac{\partial}{\partial y_j}\right)\left[\tilde{c}_{ijkl}\left(\frac{\mathbf{x}}{\varepsilon}\right)\left(\frac{\partial}{\partial x_l} + \frac{1}{\varepsilon}\frac{\partial}{\partial y_l}\right)(u_k^{(0)} + \varepsilon u_k^{(1)} + \varepsilon^2 u_k^{(2)} + \ldots)\right. \\ &\left. -\tilde{\gamma}_{ij}^{\alpha}\left(\frac{\mathbf{x}}{\varepsilon}\right)(s^{(0)\alpha} + \varepsilon s^{(1)\alpha} + \varepsilon^2 s^{(2)\alpha} + \ldots)\right] + B_i\left(\frac{\mathbf{x}}{\varepsilon}\right), \end{aligned} \tag{4.7}$$

$$ \begin{aligned} \dot{s}^{(0)\alpha} + \varepsilon\dot{s}^{(1)\alpha} + \varepsilon^2\dot{s}^{(2)\alpha} + \ldots &= \left(\frac{\partial}{\partial x_i} + \frac{1}{\varepsilon}\frac{\partial}{\partial y_i}\right)\left\{L_{ij}^{\alpha\beta}\left(\frac{\mathbf{x}}{\varepsilon}\right)\left(\frac{\partial}{\partial x_j} + \frac{1}{\varepsilon}\frac{\partial}{\partial y_j}\right)\right. \\ &\cdot\left[-\tilde{\gamma}_{kl}^{\beta}\left(\frac{\mathbf{x}}{\varepsilon}\right)\left(\frac{\partial}{\partial x_l} + \frac{1}{\varepsilon}\frac{\partial}{\partial y_l}\right)(u_k^{(0)} + \varepsilon u_k^{(1)} + \varepsilon^2 u_k^{(2)} + \ldots)\right. \\ &\left.\left. +\tilde{a}^{\beta\gamma}\left(\frac{\mathbf{x}}{\varepsilon}\right)(s^{(0)\gamma} + \varepsilon s^{(1)\gamma} + \varepsilon^2 s^{(2)\gamma} + \ldots)\right]\right\}. \end{aligned} \tag{4.8}$$

According to the procedure of the method of asymptotic expansions we compare terms associated with the same power of ε. Consequently we obtain:

$\underline{\varepsilon^{-3}}$

$$ 0 = \frac{\partial}{\partial y_i}\left(L_{ij}^{\alpha\beta}(\mathbf{y})\frac{\partial}{\partial y_j}(-\tilde{\gamma}_{kl}^{\beta}(\mathbf{y})e_{ykl}(\mathbf{u}^{(0)})\right), \tag{4.9}$$

where

$$ e_{yij}(\mathbf{v}) = \left(\frac{\partial v_i}{\partial y_j} + \frac{\partial v_j}{\partial y_i}\right)/2. \tag{4.10}$$

$\underline{\varepsilon^{-2}}$

$$(4.11)\qquad 0 = \frac{\partial}{\partial y_i}(\widetilde{c}_{ijkl}(\mathbf{y})e_{ykl}(\mathbf{u}^{(0)})),$$

$$(4.12)\qquad 0 = \frac{\partial}{\partial x_i}\left(L_{ij}^{\alpha\beta}(\mathbf{y})\frac{\partial}{\partial y_j}(-\widetilde{\gamma}_{kl}^{\beta}(\mathbf{y})e_{ykl}(\mathbf{u}^{(0)}))\right) + \frac{\partial}{\partial y_i}\left(L_{ij}^{\alpha\beta}(\mathbf{y})\frac{\partial}{\partial x_j}(-\widetilde{\gamma}_{kl}^{\beta}(\mathbf{y})e_{ykl}(\mathbf{u}^{(0)}))\right)$$
$$+ \frac{\partial}{\partial y_i}\left(L_{ij}^{\alpha\beta}(\mathbf{y})\frac{\partial}{\partial y_j}(-\widetilde{\gamma}_{kl}^{\beta}(\mathbf{y})e_{kl}(\mathbf{u}^{(0)})) + L_{ij}^{\alpha\beta}(\mathbf{y})\frac{\partial}{\partial y_j}(-\widetilde{\gamma}_{kl}^{\beta}(\mathbf{y})e_{ykl}(\mathbf{u}^{(1)}))\right)$$
$$+ \frac{\partial}{\partial y_i}\left(L_{ij}^{\alpha\beta}(\mathbf{y})\frac{\partial}{\partial y_j}(\widetilde{a}^{\alpha\beta}(\mathbf{y})s^{(0)\gamma})\right).$$

Hence it can be shown (cf. Appendix) that $\mathbf{u}^{(0)}$ does not depend on the local variable $\mathbf{y}$, i.e.

$$(4.13)\qquad \mathbf{u}^{(0)} = \mathbf{u}^{(0)}(\mathbf{x}, t).$$

Further, one obtains, (cf. Appendix)

$$(4.14)\qquad s^{(0)\alpha} = \overline{\gamma}_{ij}^{\alpha}(\mathbf{y})\left(\frac{\partial u_i^{(1)}}{\partial y_j} + \frac{\partial u_i^{(0)}}{\partial x_j}\right) + \overline{a}^{\alpha\beta}(\mathbf{y})C^{\beta}(\mathbf{x}, t),$$

where *a priori* unknown functions C^{β} do not depend on y.

$\underline{\varepsilon^{-1}}$

By taking account of (4.13) an (4.14) we arrive at the following relations, (cf. Appendix)

$$(4.15)\qquad \frac{\partial}{\partial y_j}\left(\overline{c}_{ijkl}(\mathbf{y})\left(\frac{\partial u_k^{(1)}}{\partial y_l} + \frac{\partial u_k^{(0)}}{\partial x_l}\right)\right) = \frac{\partial \overline{\gamma}_{ij}^{\alpha}(\mathbf{y})}{\partial y_j}C^{\alpha}(\mathbf{x}, t),$$

$$(4.16)\qquad \frac{\partial}{\partial y_j}\left[L_{ij}^{\alpha\beta}(\mathbf{y})\frac{\partial}{\partial y_j}\left(- \widetilde{\gamma}_{kl}^{\beta}(\mathbf{y})\left(\frac{\partial u_k^{(1)}}{\partial x_l} + \frac{\partial u_k^{(2)}}{\partial y_l}\right) + \widetilde{a}^{\beta\gamma}(\mathbf{y})s^{(1)\gamma}\right)\right] = \frac{\partial L_{ij}^{\alpha\beta}(\mathbf{y})}{\partial y_j}\frac{\partial C^{\beta}(\mathbf{x}, t)}{\partial x_j}.$$

$\underline{\varepsilon^{0}}$

$$(4.17)\qquad \rho(\mathbf{y})\ddot{u}_i^{(0)} = \frac{\partial}{\partial x_i}[\widetilde{c}_{ijkl}(\mathbf{y})e_{kl}(\mathbf{u}^{(0)}) - \widetilde{\gamma}_{ij}^{\alpha}(\mathbf{y})s^{(0)\alpha} + \widetilde{c}_{ijkl}(\mathbf{y})e_{ykl}(\mathbf{u}^{(1)})] + \frac{\partial}{\partial y_j}\{\ldots\} + B_i,$$

$$(4.18)\qquad \dot{s}^{(0)\alpha} = \frac{\partial}{\partial x_i}\left(L_{ij}^{\alpha\beta}(\mathbf{y})\frac{\partial}{\partial x_j}[-\widetilde{\gamma}_{kl}^{\beta}(\mathbf{y})e_{kl}(\mathbf{u}^{(0)}) - \widetilde{\gamma}_{kl}^{\beta}(\mathbf{y})e_{ykl}(\mathbf{u}^{(1)}) + \widetilde{a}^{\gamma\beta}(\mathbf{y})s^{(0)\gamma}]\right.$$
$$\left.+ L_{ij}^{\alpha\beta}(\mathbf{y})\frac{\partial}{\partial y_j}[-\widetilde{\gamma}_{kl}^{\beta}(\mathbf{y})e_{kl}(\mathbf{u}^{(1)}) - \widetilde{\gamma}_{kl}^{\beta}(\mathbf{y})e_{ykl}(\mathbf{u}^{(2)}) + \widetilde{a}^{\gamma\beta}(\mathbf{y})s^{(1)\gamma}]\right) + \frac{\partial}{\partial y_j}\{\ldots\}.$$

The terms in brackets $\{\ldots\}$ are unimportant for our further considerations.

5. Effective material coefficients and local problems

For a function f depending on $y \in Y$ we set

$$\langle f \rangle = \frac{1}{|Y|} \int_Y f(\mathbf{y})\, dy \,. \tag{5.1}$$

By using our previous results, after some calculations, the following field equations describing the homogenized **TED** body are obtained

$$\begin{aligned} \langle \rho \rangle \ddot{u}_i^{(0)} &= \overline{c}^h_{ijkl} \frac{\partial^2 u_k^{(0)}}{\partial x_j \partial x_l} - \overline{\gamma}^{h\alpha}_{ij} \frac{\partial C^\alpha}{\partial x_j} + \langle B_i \rangle \,, \\ \langle \dot{s}^{(0)\alpha} \rangle &= L^{h\alpha\beta}_{ij} \frac{\partial^2 C^\beta}{\partial x_i \partial x_j} \,. \end{aligned} \tag{5.2}$$

Here and in the sequel the superscript h denotes a homogenized quantity.

In the component form we have

$$\begin{aligned} \langle \rho \rangle \ddot{u}_i^{(0)} &= \overline{c}^h_{ijkl} \frac{\partial^2 u_k^{(0)}}{\partial x_j \partial x_l} - \overline{\gamma}^h_{ij} \frac{\partial C_t}{\partial x_j} - \overline{\xi}^h_{ij} \frac{\partial C_c}{\partial x_j} + \langle B_i \rangle \,, \\ \langle \dot{s}^{(0)} \rangle &= \lambda^h_{ij} \frac{\partial^2 C_t}{\partial x_i \partial x_j} + L^h_{ij} \frac{\partial^2 C_c}{\partial x_i \partial x_j} \,, \\ \langle \dot{c}^{(0)} \rangle &= L^h_{ij} \frac{\partial^2 C_t}{\partial x_i \partial x_j} + D^h_{ij} \frac{\partial^2 C_c}{\partial x_i \partial x_j} \,. \end{aligned} \tag{5.2$_1$}$$

Moreover we have

$$\langle s^{(0)\alpha} \rangle = \overline{\gamma}^{h\alpha}_{ij} e_{ij}(\mathbf{u}^{(0)}) + \overline{a}^{h\alpha\beta} C^\beta \,. \tag{5.3}$$

Hence, by comparing with (2.38) and (2.39) we infer that the functions C^α, $\alpha = 1, 2$, (i.e. C_t and C_c) stand for the temperature and chemical potential of the homogenized solid, respectively. Consequently, it is more instructive to use the following notations, cf. (2.54)

$$\Theta^{h1} = \Theta^h = C^1 = C, \qquad \Theta^{h2} = M^h = C^2 = C_c \,. \tag{5.4}$$

Then, instead of (5.3) we have

$$\langle s^{(0)\alpha} \rangle = \overline{\gamma}^{h\alpha}_{ij} e_{ij}(\mathbf{u}^{(0)}) + \overline{a}^{h\alpha\beta} \Theta^{h\beta} \,. \tag{5.4$_1$}$$

The homogenized material constants are given by

$$\begin{aligned} \overline{c}^h_{ijkl} &= \left\langle \overline{c}_{ijkl} + \overline{c}_{ijpq} \frac{\partial \chi_p^{(kl)}}{\partial y_q} \right\rangle , \\ \overline{\gamma}^{h\alpha}_{ij} &= \left\langle \overline{\gamma}^\alpha_{ij} - \overline{c}_{ijpq} \frac{\partial \Gamma^\alpha_p}{\partial y_q} \right\rangle , \\ \overline{a}^{h\alpha\beta} &= \left\langle \overline{a}^{\alpha\beta} + \overline{\gamma}^\alpha_{ij} \frac{\partial \Gamma^\beta_i}{\partial y_j} \right\rangle , \\ L^{h\alpha\beta}_{ij} &= \left\langle L^{\alpha\beta}_{ij} - L^{\alpha\gamma}_{ik} \frac{\partial \Theta^{\gamma\beta}_j}{\partial y_k} \right\rangle , \end{aligned} \tag{5.5}$$

where

$$\begin{aligned} \bar{c}_{ijkl} &= c_{ijkl} - \frac{1}{a}\xi_{ij}\xi_{kl}\,, \\ \bar{\gamma}^{(1)}_{ij} &= \bar{\gamma}_{ij} = \gamma_{ij} + \frac{d}{a}\xi_{ij}, \qquad \bar{\gamma}^{(2)}_{ij} = \bar{\xi}_{ij} = \frac{1}{a}\xi_{ij}\,, \\ \bar{a}^{\alpha\beta} &= \begin{bmatrix} \bar{b} & \bar{d} \\ \bar{d} & \bar{a} \end{bmatrix}, \qquad \bar{b} = b + \frac{d^2}{a}, \qquad \bar{d} = \frac{d}{a}, \qquad \bar{a} = \frac{1}{a}\,. \end{aligned}$$

We emphasize that the superscript h always denotes a homogenized (effective) quantity. For instance, $\bar{c}^h_{ijkl}$ are homogenized (effective) elastic moduli of $\bar{c}_{ijkl}(x/\varepsilon)$.

We observe that, cf. Eq. $(5.7)_3$ below,

$$L^{h\alpha\beta}_{ij} = L^{h\alpha\beta}_{ji}\,. \tag{5.6}$$

The functions $\boldsymbol{\chi}^{(kl)}$, $\boldsymbol{\Gamma}$, $\boldsymbol{\Theta}^{\alpha\beta}$, etc. are Y-periodic. These local functions are solutions to the local problems, which are posed on Y:

$$\begin{aligned} \frac{\partial}{\partial y_j}\left(\bar{c}_{ijkm}(\mathbf{y})\frac{\partial \chi^{(pq)}_k}{\partial y_m}\right) &= -\frac{\partial}{\partial y_j}\bar{c}_{ijpq}(\mathbf{y})\,, \\ \frac{\partial}{\partial y_j}\left(\bar{c}_{ijkm}(\mathbf{y})\frac{\partial \Gamma^{\alpha}_k}{\partial y_m}\right) &= \frac{\partial \bar{\gamma}^{\alpha}_{ij}(\mathbf{y})}{\partial y_j}\,, \\ \frac{\partial}{\partial y_i}\left(L^{\alpha\gamma}_{ij}(\mathbf{y})\frac{\partial \Theta^{\gamma\beta}_k}{\partial y_i}\right) &= \frac{\partial L^{\alpha\beta}_{ik}(\mathbf{y})}{\partial y_i}\,. \end{aligned} \tag{5.7}$$

Solutions of Eqs. $(5.7)_{1,2}$ exist up to constant vectors, while those of Eq. $(5.7)_3$ — up to constants.

Equations (5.7) are strong formulation of the local problems. In such a case the periodic functions $\bar{c}_{ijkl}(\mathbf{y})$, $\bar{\gamma}^{\alpha}_{ij}(\mathbf{y})$ and $L^{\alpha\beta}_{ik}(\mathbf{y})$ have to be of class $C^1(Y)$. This assumption may be significantly weakened provided that one passes to weak or variational formulations.

Let us define the space of Y-periodic functions

$$\begin{aligned} H_{\text{per}}(Y) &= \{v \in H^1(Y) \mid v \text{ takes equal values at opposite sides of } Y\}, \\ H_{\text{per}}(Y, \mathbb{R}^3) &= [H_{\text{per}}(Y)]^3, \end{aligned}$$

where $H^1(Y)$ is the standard Sobolev space, cf. Refs [5], [10]. Now we assume that periodic functions $c_{ijkl}(\mathbf{y})$, $\gamma^{\alpha}_{ij}(\mathbf{y})$, $L^{\alpha\beta}_{ij}(\mathbf{y})$, $B_i(\mathbf{y})$ and $\rho(\mathbf{y})$ are elements of the space $L^{\infty}(Y)$.

Such an assumption comprises, for instance, layered solids with discontinuous material constants.

From (5.7) one readily obtains the *variational* (weak) form of the local problems:

Find $\boldsymbol{\chi}^{(pq)} = (\chi^{(pq)}_k)$, $\boldsymbol{\Gamma}^{\alpha} = (\Gamma^{\alpha}_k) \in H_{\text{per}}(Y, \mathbb{R}^3)$ and $\boldsymbol{\Theta}^{\alpha\beta} = (\Theta^{\alpha\beta}_k) \in H_{\text{per}}(Y, \mathbb{R}^3)$;

$$\int_Y \bar{c}_{ijkl}(\mathbf{y})e_{ykl}(\chi^{(pq)})e_{yij}(\mathbf{v})\,dy = -\int_Y \bar{c}_{ijpq}(\mathbf{y})e_{yij}(\mathbf{v})\,dy \quad \forall\mathbf{v}\in H_{\text{per}}(Y,\mathbb{R}^3)$$

(5.8)
$$\int_Y \bar{c}_{\text{ijkl}}(\mathbf{y})e_{\text{ykl}}(\mathbf{\Gamma}^{\alpha})e_{yij}(\mathbf{v})\,dy = \int_Y \overline{\gamma}^{\alpha}_{ij}(\mathbf{y})e_{yij}(\mathbf{v})\,dy, \quad \forall\mathbf{v}\in H_{\text{per}}(Y,\mathbb{R}^3),$$

$$\int_Y L^{\alpha\gamma}_{ij}(\mathbf{y})\frac{\partial\Theta^{\gamma\beta}_k}{\partial y_j}\frac{\partial w}{\partial y_i}\,dy = \int_Y L^{\alpha\beta}_{ik}(\mathbf{y})\frac{\partial w}{\partial y_i}\,dy \quad \forall w\in H_{\text{per}}(Y).$$

Existence of solutions to the problems (5.8) results from the Lax–Milgram lemma, cf. [10].

6. Initial conditions for the temperature and chemical potential of the homogenized body

Now we shall derive the initial conditions which should be satisfied for $t=0$ by the pairs of the functions resolving the *homogenized* equations

$$(w^{h\alpha}) = (s^h, M^h), \qquad (s^{h\alpha}) = (s^h, c^h) \qquad \text{and} \qquad (\Theta^{h\alpha}) = (\Theta^h, M^h),$$

corresponding to the pairs defined by Eqs. (2.49) and (2.54), respectively, where $s^h = s^h(\mathbf{x},t)$, $M^h = M^h(\mathbf{x},t)$, $c^h = c^h(\mathbf{x},t)$ and $\Theta^h = \Theta^h(\mathbf{x},t)$. To this end the following result will be applied, cf. [5, 148, 149].

LEMMA 6.1. If f is a Y-periodic $L^\infty(Y)$ function, then $f\left(\frac{\mathbf{x}}{\varepsilon}\right)$ converges in $L^\infty(\Omega)$-weak-* to $\langle f\rangle$ as $\varepsilon\to 0$, provided that Ω is bounded. Consequently, if $g(\mathbf{x})$ is any $L^2(\Omega)$ function, then $f\left(\frac{\mathbf{x}}{\varepsilon}\right)g(\mathbf{x})$ converges weakly in $L^2(\Omega)$ to $\langle f\rangle g(\mathbf{x})$. ■

We recall that weak-* (weak-star) topology on L^∞ denotes the natural weak topology in the sense of duality $\langle\cdot,\cdot\rangle_{L^1\times L^\infty}$, cf. [10].

For $\varepsilon>0$ and $t=0$, after (2.61) and (4.5), the entropy-concentration pair $(s^\alpha) = (s,c)$ in terms of the temperature-chemical potential pair $(\Theta^\alpha) = (\Theta, M)$ is expressesd as follows

(6.1)
$$^{\varepsilon}s^{\alpha}(\mathbf{x},0) = \overline{\gamma}^{\alpha}_{ij}\left(\frac{\mathbf{x}}{\varepsilon}\right)e_{ij}(\mathbf{U}) + \overline{a}^{\alpha\beta}\left(\frac{\mathbf{x}}{\varepsilon}\right)\Theta^{\beta}_0(\mathbf{x}),$$

where

$$\Theta^{\beta}_0(\mathbf{x}) = \Theta^{\beta}(\mathbf{x},0).$$

By employing Lemma (6.1) we get

(6.2)
$$\lim_{\varepsilon\to 0}{}^{\varepsilon}s^{\alpha}(\mathbf{x},0) = \langle\overline{\gamma}^{\alpha}_{ij}\rangle e_{ij}(\mathbf{U}) + \langle\overline{a}^{\alpha\beta}\rangle\Theta^{\beta}_0(\mathbf{x}).$$

On the other hand, Eq. $(5.3)_1$ yields the following relation for $t=0$:

(6.3)
$$\langle s^{0\alpha}(\mathbf{x},\mathbf{y},0)\rangle = \overline{\gamma}^{h\alpha}_{ij}e_{ij}(\mathbf{U}(\mathbf{x})) + \overline{a}^{h\alpha\beta}\Theta^{h\beta}(\mathbf{x},0).$$

Obviously

(6.4)
$$\lim_{\varepsilon\to 0}{}^{\varepsilon}s^{\alpha}(\mathbf{x},0) = \langle s^{0\alpha}(\mathbf{x},\mathbf{y},0)\rangle.$$

Hence we finally obtain the initial condition for the pair $(\Theta^{h\alpha}) = (\Theta^h, M^h)$,

$$(6.5)\quad \begin{aligned} \Theta^h(\mathbf{x},0) &= \{(\overline{a}^h\langle\overline{b}\rangle + \overline{d}^h\langle\overline{d}\rangle)\Theta_0(\mathbf{x}) + (\overline{a}^h\langle\overline{d}\rangle + \overline{d}^h\langle\overline{a}\rangle)M_0(\mathbf{x}) \\ &\quad + [\overline{a}^h(\langle\overline{\gamma}_{ij}\rangle - \overline{\gamma}^h_{ij}) + \overline{d}^h(\langle\overline{\xi}_{ij}\rangle - \overline{\xi}^h_{ij})]e_{ij}(\mathbf{U}(\mathbf{x}))\}/\overline{\Delta}^h, \\ M^h(\mathbf{x},0) &= \{(\overline{d}^h\langle\overline{b}\rangle + \overline{b}^h\langle\overline{d}\rangle)\Theta_0(\mathbf{x}) + (\overline{d}^h\langle\overline{d}\rangle + \overline{b}^h\langle\overline{a}\rangle)M_0(\mathbf{x}) \\ &\quad + [\overline{d}^h(\langle\overline{\gamma}_{ij}\rangle - \overline{\gamma}^h_{ij}) + \overline{b}^h(\langle\overline{\xi}_{ij}\rangle - \overline{\xi}^h_{ij})]e_{ij}(\mathbf{U}(\mathbf{x}))\}/\overline{\Delta}^h, \end{aligned}$$

where Θ_0, M_0 and $\mathbf{U}$ are prescribed, cf. Eq. (3.5). Moreover, we have set

$$\overline{\gamma}^h_{ij} = \overline{\gamma}^{h1}_{ij}, \qquad \overline{\xi}^h_{ij} = \overline{\gamma}^{h2}_{ij}, \qquad \overline{d}^h = d^h = \overline{a}^{h12}, \qquad \overline{b}^h = \overline{a}^{h11}, \qquad \overline{a}^h = \overline{a}^{h22},$$

cf. Eq. (5.5) and (2.55), (2.57), and

$$\overline{\Delta}^h = \overline{a}^h\overline{b}^h - (\overline{d}^h)^2 .$$

We note that $\overline{d}^h \neq \langle\overline{d}\rangle$, in general.

Written in a concise form Eqs. (6.5) are given by

$$(6.5')\qquad (\Theta^{h\alpha}(\mathbf{x},0)) = \tilde{a}^{h\alpha\beta}[\langle\overline{a}^{\beta\gamma}\rangle\Theta^\gamma_0(\mathbf{x}) + (\langle\overline{\gamma}^\beta_{ij}\rangle - \overline{\gamma}^{h\beta}_{ij})e_{ij}(\mathbf{U}(\mathbf{x}))],$$

where $\tilde{\mathbf{a}}^h$ is the inverse of $\overline{\mathbf{a}}^h$

$$\tilde{\mathbf{a}}^h = (\overline{\mathbf{a}}^h)^{-1} \qquad \text{i.e.} \qquad \tilde{a}^{h\alpha\gamma}\overline{a}^{h\gamma\beta} = \delta^{\alpha\beta} .$$

We have

$$(6.6)\qquad \tilde{a}^{h11} = \tilde{b}^h = \overline{a}^h/\overline{\Delta}^h, \qquad \tilde{a}^{h12} = \tilde{d}^h = \overline{d}^h/\overline{\Delta}^h, \qquad \tilde{a}^{h22} = \tilde{a}^h = \overline{b}^h/\overline{\Delta}^h .$$

Let us consider another pair of the initial data, for instance the pair

$$(6.7)\qquad \begin{aligned} {}^\varepsilon\mathbf{u}(\mathbf{x},0) &= \mathbf{U}(\mathbf{x}), \qquad {}^\varepsilon\dot{\mathbf{u}}(\mathbf{x},0) = \mathbf{V}(\mathbf{x}), \\ ({}^\varepsilon Z^\alpha(\mathbf{x},0)) &= (Z^\alpha_0(\mathbf{x})) = (\Theta_0(\mathbf{x}), G(\mathbf{x})), \end{aligned}$$

where $(Z^\alpha_0) = (\Theta_0, G)$ is prescribed, and

$$(6.8)\qquad {}^\varepsilon\Theta_0(\mathbf{x},0) = \Theta_0(\mathbf{x}), \qquad {}^\varepsilon c(\mathbf{x},0) = G(\mathbf{x}) .$$

For $\varepsilon > 0$, by using (2.29) and (6.7)–(6.8), the initial entropy is expressed as follows,

$$(6.9)\qquad {}^\varepsilon s(\mathbf{x},0) = \overline{\gamma}_{ij}\left(\frac{\mathbf{x}}{\varepsilon}\right)e_{ij}(\mathbf{U}) + \overline{b}\left(\frac{\mathbf{x}}{\varepsilon}\right)\Theta_0(\mathbf{x}) + d\left(\frac{\mathbf{x}}{\varepsilon}\right)G(\mathbf{x}) .$$

By employing Lemma 6.1 once again we get

$$(6.10)\qquad \lim_{\varepsilon\to 0} {}^\varepsilon s(\mathbf{x},0) = \langle\overline{\gamma}_{ij}\rangle e_{ij}(\mathbf{U}) + \langle\overline{b}\rangle\Theta_0(\mathbf{x}) + \langle d\rangle G(\mathbf{x}) .$$

On the other hand, Eqs. (5.3) and (5.4) can be written as

$$(6.11)\qquad \begin{aligned} \langle s^{(0)}\rangle &= \overline{\gamma}^h_{ij}e_{ij}(\mathbf{u}^{(0)}) + \overline{b}^h\Theta^h + \overline{d}^h M^h, \\ \langle c^{(0)}\rangle &= \overline{\xi}^h_{ij}e_{ij}(\mathbf{u}^{(0)}) + \overline{d}^h\Theta^h + \overline{a}^h M^h . \end{aligned}$$

After elimination of M^h and taking account of (6.8), we arrive at the following relation

$$(6.12)\qquad \langle s^{(0)}(\mathbf{x},\mathbf{y},0)\rangle = \gamma^h_{ij}e_{ij}(\mathbf{U}(\mathbf{x})) + b^h\Theta^h(\mathbf{x},0) + d^h G(\mathbf{x}),$$

where

$$\gamma^h_{ij} = \overline{\gamma}^h_{ij} - \frac{\overline{d}^h}{\overline{a}^h}\overline{\xi}^h_{ij}, \qquad b^h = \overline{b}^h - \frac{(\overline{d}^h)^2}{\overline{a}^h}, \qquad d^h = \frac{\overline{d}^h}{\overline{a}^h},$$

because, cf. (6.8),

$$\lim_{\varepsilon\to 0} {}^{\varepsilon}c(\mathbf{x},0) = \langle c^{(0)}(\mathbf{x},\mathbf{y},0)\rangle = G(\mathbf{x})\,.$$

As previously

$$\lim_{\varepsilon\to 0} {}^{\varepsilon}s(\mathbf{x},0) = \langle s^{(0)}(\mathbf{x},\mathbf{y},0)\rangle\,.$$

Finally, we obtain

$$\Theta^h(\mathbf{x},0) = [\langle b\rangle\Theta(\mathbf{x}) + (\langle\gamma_{ij}\rangle - \gamma^h_{ij})e_{ij}(\mathbf{U}(\mathbf{x})) + (\langle d\rangle - d^h)G(\mathbf{x})]/b^h\,. \tag{6.13}$$

The formulae (6.5) and (6.13) generalize the corresponding result reported by FRANCFORT [61, 62] in the case of homogenization of the equations of coupled thermoelasticity. From Eq. $(6.5)_1$ we conclude that the change in the initial temperature for the homogenized **TED** body is also influenced by the diffusion. This change is implied by the fact that $\langle b\rangle \neq b^h$, $\langle\gamma\rangle \neq \gamma^h$ and $\langle d\rangle \neq d^h$, in general. The initial condition for the chemical potential also changes and is given by $(6.5)_2$.

7. Convergence theorem in the general, non-periodic case

Suppose that a microstructure of an elastic solid in which thermodiffusion occurs is characterized by a small parameter $\varepsilon > 0$. *No assumption of periodicity* is imposed.

We recall that formula (5.5) applies to a microperiodic structure only. The same symbols for the effective coefficients are used in a nonperiodic case. The reader sholud be aware that in the nonperiodic case formula like (5.5) is not available and one has to find bounds on effective coefficients. The results presented in this section are also valid in the particular case of a periodic microstructure. Consequently, the formal homogenization procedure used in Sec. 4 is justified by Theorem 7.2 below.

For a fixed $\varepsilon > 0$ the system of coupled equations of the linear thermodiffusion is assumed in the following form:

$$\rho^\varepsilon\frac{\partial^2 u_i^\varepsilon}{\partial t^2} - \frac{\partial}{\partial x_j}(\overline{c}^\varepsilon_{ijkm}e_{km}(\mathbf{u}^\varepsilon) - \overline{\gamma}^\varepsilon_{ij}\Theta^\varepsilon - \overline{\xi}^\varepsilon_{ij}M^\varepsilon = B_i, \qquad \text{in } \Omega\times(0,t_0), \tag{7.1}$$

$$\overline{b}^\varepsilon\frac{\partial\Theta^\varepsilon}{\partial t} + \overline{d}^\varepsilon\frac{\partial M^\varepsilon}{\partial t} - \frac{\partial}{\partial x_i}\left(\lambda^\varepsilon_{ij}\frac{\partial\Theta^\varepsilon}{\partial x_j} + L^\varepsilon_{ij}\frac{\partial M^\varepsilon}{\partial x_j}\right) + \overline{\gamma}^\varepsilon_{ij}\frac{\partial\dot{u}_i^\varepsilon}{\partial x_j} = g_1, \qquad \text{in } \Omega\times(0,t_0), \tag{7.2}$$

$$\overline{d}^\varepsilon\frac{\partial\Theta^\varepsilon}{\partial t} + \overline{a}^\varepsilon\frac{\partial M^\varepsilon}{\partial t} - \frac{\partial}{\partial x_i}\left(L^\varepsilon_{ij}\frac{\partial\Theta^\varepsilon}{\partial x_j} + D^\varepsilon_{ij}\frac{\partial M^\varepsilon}{\partial x_j}\right) + \overline{\xi}^\varepsilon_{ij}\frac{\partial\dot{u}_i^\varepsilon}{\partial x_j} = g_2, \qquad \text{in } \Omega\times(0,t_0), \tag{7.3}$$

$$\mathbf{u}^\varepsilon(\mathbf{x}.t) = 0, \qquad \Theta^\varepsilon(\mathbf{x},t) = 0, \qquad M^\varepsilon(\mathbf{x},t) = 0, \qquad \text{on } \partial\Omega\times(0,t_0), \tag{7.4}$$

$$\mathbf{u}^\varepsilon(\mathbf{x}.0) = \mathbf{U}(\mathbf{x}), \qquad \Theta^\varepsilon(\mathbf{x},0) = \Theta_0(\mathbf{x}), \qquad M^\varepsilon(\mathbf{x},0) = M_0(\mathbf{x}), \qquad \dot{\mathbf{u}}^\varepsilon(\mathbf{x}.0) = \mathbf{V}(\mathbf{x})\,, \tag{7.5}$$

where $\dot{u}_i = \partial u_i/\partial t$, etc.

We make the following assumptions:

$$(A_1)\quad \left|\;\begin{aligned} &\rho^\varepsilon, \overline{b}^\varepsilon, \overline{d}^\varepsilon, \overline{a}^\varepsilon \in L^\infty(\Omega), \qquad \lambda_1 \leq \rho^\varepsilon(\mathbf{x}) \leq \lambda_2, \qquad \text{a.e. } \mathbf{x}\in\Omega \\ &\lambda_1(e_1^2+e_2^2) \leq [e_1,e_2]\begin{bmatrix}\overline{b}^\varepsilon(\mathbf{x}) & \overline{d}^\varepsilon(\mathbf{x})\\ \overline{d}^\varepsilon(\mathbf{x}) & \overline{a}^\varepsilon(\mathbf{x})\end{bmatrix}\begin{bmatrix}e_1\\ e_2\end{bmatrix} \leq \lambda_2(e_1^2+e_2^2)\,, \\ &\qquad\qquad\qquad\qquad\qquad\qquad \text{a.e. } \mathbf{x}\in\Omega\ \forall e_1,e_2\in\mathbb{R}\,, \end{aligned}\right.$$

where $\lambda_2 > \lambda_1 > 0$; λ_2, λ_1 — constants;.

$$(A_2)\quad \left|\begin{array}{l} \overline{c}^\varepsilon_{ijkm} \in L^\infty \Omega), \lambda_1|\mathbf{e}|^2 \le \overline{c}^\varepsilon_{jkm}(x)e_{ij}e_{km} \le \lambda_2|\mathbf{e}|^2, \quad \text{a.e. } \mathbf{x} \in \Omega\ \forall \mathbf{e} \in \mathbb{E}^3_s, \\ \lambda_1(|\mathbf{e}_1|^2 + |\mathbf{e}_2|^2) \le [\mathbf{e}_1, \mathbf{e}_2] \begin{bmatrix} \boldsymbol{\lambda}^\varepsilon(\mathbf{x}) & \mathbf{L}^\varepsilon(\mathbf{x}) \\ (\mathbf{L}^\varepsilon)^T(\mathbf{x}) & \mathbf{D}^\varepsilon(\mathbf{x}) \end{bmatrix} \begin{bmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \end{bmatrix} \le \lambda_2(|\mathbf{e}_1^2 + |\mathbf{e}_2^2), \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{a.e. } \mathbf{x} \in \Omega\ \forall \mathbf{e}_1, \mathbf{e}_2 \in \mathbb{E}^3_s. \end{array}\right.$$

We recall that $\mathbb{E}^3_s$ is the space of symmetric 3×3 matrices.

$$(A_3)\quad \left|\ \overline{\gamma}^\varepsilon_{ij}, \overline{\xi}^\varepsilon_{ij} \in L^\infty(\Omega), \quad |\overline{\gamma}^\varepsilon_{ij}(\mathbf{x})| \le \lambda_2, \quad |\overline{\xi}^\varepsilon_{ij}(\mathbf{x})| \le \lambda_2, \quad \text{a.e. } \mathbf{x} \in \Omega. \right.$$

To obtain *a priori* estimates we multiply Eqs. (7.1)–(7.3) by $\dfrac{\partial \mathbf{u}^\varepsilon}{\partial t}$, Θ^ε and M^ε, respectively. Next, performing integration over Ω and integration by parts one gets

$$(7.6)\quad \int_\Omega \rho^\varepsilon \frac{\partial^2 u^\varepsilon_i}{\partial t^2}\frac{\partial u^\varepsilon_i}{\partial t}\,dx - \int_\Omega \frac{\partial u^\varepsilon_i}{\partial t}\frac{\partial}{\partial x_j}(\overline{c}^\varepsilon_{ijkm}e_{km}(\mathbf{u}^\varepsilon))\,dx + \int_\Omega \frac{\partial u^\varepsilon_i}{\partial t}\frac{\partial}{\partial x_j}(\overline{\gamma}^\varepsilon_{ij}\Theta^\varepsilon + \overline{\xi}^\varepsilon_{ij}M^\varepsilon) = \int_\Omega B_i \frac{\partial u^\varepsilon_i}{\partial t}\,dx,$$

$$(7.7)\quad \frac{1}{2}\frac{d}{dt}\int_\Omega \overline{b}^\varepsilon|\Theta^\varepsilon|^2\,dx + \int_\Omega \overline{d}^\varepsilon\Theta^\varepsilon\frac{\partial M^\varepsilon}{\partial t}\,dx + \int_\Omega (\lambda^\varepsilon_{ij}\Theta^\varepsilon_{,j} + L^\varepsilon_{ij}M^\varepsilon_{,j})\Theta^\varepsilon_{,i}\,dx + \int_\Omega \overline{\gamma}^\varepsilon_{ij}\Theta^\varepsilon e_{ij}\left(\frac{\partial \mathbf{u}^\varepsilon}{\partial t}\right)dx = \int_\Omega g_1\Theta^\varepsilon\,dx,$$

$$(7.8)\quad \int_\Omega \overline{d}^\varepsilon M^\varepsilon\frac{\partial \Theta^\varepsilon}{\partial t}\,dx + \frac{1}{2}\frac{d}{dt}\int_\Omega \overline{a}^\varepsilon|M^\varepsilon|^2\,dx + \int_\Omega (L^\varepsilon_{ij}\Theta^\varepsilon_{,j} + D^\varepsilon_{ij}M^\varepsilon_{,j})M^\varepsilon_{,i}\,dx + \int_\Omega \overline{\xi}^\varepsilon_{ij}M^\varepsilon e_{ij}\left(\frac{\partial \mathbf{u}^\varepsilon}{\partial t}\right)dx = \int_\Omega g_2M^\varepsilon\,dx,$$

since the boundary conditions (7.4) are homogeneous; here $\Theta^\varepsilon_{,j} = \dfrac{\partial \Theta^\varepsilon}{\partial x_j}$, etc.

Adding Eqs. (7.6)–(7.8), we readily obtain

$$\frac{1}{2}\frac{d}{dt}\int_\Omega \rho^\varepsilon\left|\frac{\partial \mathbf{u}^\varepsilon}{\partial t}\right|^2 dx + \frac{1}{2}\frac{d}{dt}\int_\Omega \overline{c}^\varepsilon_{ijkm}e_{km}(\mathbf{u}^\varepsilon)e_{ij}(\mathbf{u}^\varepsilon)\,dx + \frac{1}{2}\frac{d}{dt}\int_\Omega \overline{b}^\varepsilon|\Theta^\varepsilon|^2\,dx + \frac{d}{dt}\int_\Omega \overline{d}^\varepsilon\Theta^\varepsilon M^\varepsilon\,dx + \frac{1}{2}\frac{d}{dt}\int_\Omega \overline{a}^\varepsilon|M^\varepsilon|^2\,dx + \int_\Omega [(\lambda^\varepsilon_{ij}\Theta^\varepsilon_{,j} + L^\varepsilon_{ij}M^\varepsilon_{,j})\Theta^\varepsilon_{,i} + (L^\varepsilon_{ij}\Theta^\varepsilon_{,j} + D^\varepsilon_{ij}M^\varepsilon_{,j})M^\varepsilon_{,i}]\,dx = \int_\Omega \left(B_i\frac{\partial u^\varepsilon_i}{\partial t}\,dx + g_1\Theta^\varepsilon + g_2M^\varepsilon\right)dx.$$

On account of the initial conditions (7.5), integration in time yields

$$\begin{aligned}(7.9)\quad &\frac{1}{2}\frac{d}{dt}\int_{\Omega}\Big(\rho^{\varepsilon}\Big|\frac{\partial \mathbf{u}^{\varepsilon}}{\partial t}\Big|^{2} + \overline{c}^{\varepsilon}_{ijkm}e_{km}(\mathbf{u}^{\varepsilon})e_{ij}(\mathbf{u}^{\varepsilon}) + \overline{b}^{\varepsilon}|\Theta^{\varepsilon}|^{2}\\ &+2\overline{d}^{\varepsilon}\Theta^{\varepsilon}M^{\varepsilon} + \overline{a}^{\varepsilon}|M^{\varepsilon}|^{2}\Big)\,dx + \int_0^t\int_{\Omega}[(\lambda^{\varepsilon}_{ij}\Theta^{\varepsilon}_{,j} + L^{\varepsilon}_{ij}M^{\varepsilon}_{,j})\Theta^{\varepsilon}_{,i}\\ &+(L^{\varepsilon}_{ij}\Theta^{\varepsilon}_{,j} + D^{\varepsilon}_{ij}M^{\varepsilon}_{,j})M^{\varepsilon}_{,i}]\,dx\,ds\\ &= \frac{1}{2}\int_{\Omega}(\rho^{\varepsilon}|\mathbf{V}|^{2} + \overline{c}^{\varepsilon}_{ijkm}e_{km}(\mathbf{U})e_{ij}(\mathbf{U}) + \overline{b}^{\varepsilon}|\Theta_0|^{2}\\ &+2\overline{d}^{\varepsilon}\Theta_0M_0 + \overline{a}^{\varepsilon}|M_0|^{2})\,dx + \int_0^t\int_{\Omega}\Big(B_i\frac{\partial u^{\varepsilon}_i}{\partial t}\,dx + g_1\Theta^{\varepsilon} + g_2M^{\varepsilon}\Big)\,dx\,ds.\end{aligned}$$

The last relation plays an important role in mathematical developments, including existence problems. It also provides some useful hints for the study of correctors. Particularly, by using the assumptions (A_1)–(A_3), (H_4) and (H_5) combined with Gronwall lemma [150], from Eq. (7.9) we deduce that

$\{\mathbf{u}^{\varepsilon}\}_{\varepsilon>0}$ is bounded in $L^{\infty}(0,t_0;H^1_0(\Omega)^3)$,

$\left\{\dfrac{\partial \mathbf{u}^{\varepsilon}}{\partial t}\right\}_{\varepsilon>0}$ is bounded in $L^{\infty}(0,t_0;L^2(\Omega)^3)$,

$\{\Theta^{\varepsilon}\}_{\varepsilon>0}$ and $\{M^{\varepsilon}\}_{\varepsilon>0}$ are bounded in $L^{\infty}(0,t_0;L^2(\Omega))\cap L^2(0,t_0;H^1_0(\Omega))$.

Now we can formulate

THEOREM 7.1. *Under the assumptions* (A_1)–(A_3), (H_4) *and* (H_5) *there exists a unique solution* $(\mathbf{u}^{\varepsilon},\Theta^{\varepsilon},M^{\varepsilon})$ *of* (7.1)–(7.5) *and*

$$\mathbf{u}^{\varepsilon}\in L^{\infty}(0,t_0;H^1_0(\Omega)^3),\qquad \frac{\partial u^{\varepsilon}_i}{\partial t}\in L^{\infty}(0,t_0;L^2(\Omega)),$$
$$\Theta^{\varepsilon};M^{\varepsilon}\in L^{\infty}(0,t_0;L^2(\Omega))\cap L^2(0,t_0;H^1_0(\Omega)).$$

REMARK 7.1. Existence of the solutions $(\mathbf{u}^{\varepsilon},\Theta^{\varepsilon},M^{\varepsilon})$ holds in the smaller class:

$$\mathbf{u}^{\varepsilon}\in C^{0}(0,t_0;H^1_0(\Omega)^3),\qquad \frac{\partial u^{\varepsilon}_i}{\partial t}\in C^{0}(0,t_0;L^2(\Omega)),$$
$$\Theta^{\varepsilon};M^{\varepsilon}\in C^{0}(0,t_0;L^2(\Omega))\cap L^2(0,t_0;H^1_0(\Omega)).$$

THEOREM 7.2. *If the assumptions* (A_1)–(A_3), (H_4) *and* (H_5) *are satisfied (see Sec. 3), then there exists a subsequence* $(\mathbf{u}^{\varepsilon'},\Theta^{\varepsilon'},M^{\varepsilon'})$ *convergent to* $(\mathbf{u},\Theta,M)$ *in the following sense:*

$$\begin{aligned}\mathbf{u}^{\varepsilon'}&\to\mathbf{u} &&\textit{weak-* in } L^{\infty}(0,t_0;H^1_0(\Omega)^3),\\ \frac{\partial\mathbf{u}^{\varepsilon'}}{\partial t}&\to\frac{\partial\mathbf{u}}{\partial t} &&\textit{weak-* in } L^{\infty}(0,t_0;L^2(\Omega)^3),\\ \Theta^{\varepsilon'}&\to\Theta &&\textit{weak-* in } L^{\infty}(0,t_0;L^2(\Omega))\cap L^2(0,t_0;H^1_0(\Omega)),\\ M^{\varepsilon'}&\to M &&\textit{weak-* in } L^{\infty}(0,t_0;L^2(\Omega))\cap L^2(0,t_0;H^1_0(\Omega)).\end{aligned}$$

when $\varepsilon\to0$.

The triple $(\mathbf{u}, \Theta, M) = (\mathbf{u}^h, \Theta^h, M^h)$ is the unique solution to the homogenized system given by

$$(7.10) \quad \overset{0}{\rho}\frac{\partial^2 u_i}{\partial t^2} - \frac{\partial}{\partial x_j}(\overline{c}^h_{ijkl}e_{kl}(\mathbf{u}) - \overline{\gamma}^h_{ij}\Theta - \overline{\xi}^h_{ij}M) = B_i, \quad \text{in } \Omega \times (0, t_0),$$

$$(7.11) \quad (\overset{0}{b} + \kappa_1)\frac{\partial \Theta}{\partial t} + \overset{0}{d}\frac{\partial M}{\partial t} - \frac{\partial}{\partial x_i}\left(\lambda^h_{ij}\frac{\partial \Theta}{\partial x_j} + L^h_{ij}\frac{\partial M}{\partial x_j}\right) + \overline{\gamma}^h_{ij}\frac{\partial \dot{u}_i}{\partial x_j} = g_1, \quad \text{in } \Omega \times (0, t_0),$$

$$(7.12) \quad \overset{0}{d}\frac{\partial \Theta}{\partial t} + (\overset{0}{a} + \kappa_2)\frac{\partial M}{\partial t} - \frac{\partial}{\partial x_i}\left(L^h_{ij}\frac{\partial \Theta}{\partial x_j} + D^h_{ij}\frac{\partial M}{\partial x_j}\right) + \overline{\xi}^h_{ij}\frac{\partial \dot{u}_i}{\partial x_j} = g_2, \quad \text{in } \Omega \times (0, t_0),$$

$$(7.13) \quad \mathbf{u}(\mathbf{x}, t) = 0, \quad \Theta(\mathbf{x}, t) = 0, \quad M(\mathbf{x}, t) = 0, \quad \text{on } \partial\Omega \times (0, t_0),$$

$$(7.14) \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{U}(\mathbf{x}), \quad \dot{\mathbf{u}}(\mathbf{x}, 0) = \mathbf{V}(\mathbf{x}),$$

$$(7.15) \quad \Theta(\mathbf{x}, 0) = \Theta^h_0(\mathbf{x}) \neq \Theta_0, \quad M(\mathbf{x}, 0) = M^h_0(\mathbf{x}) \neq M_0(\mathbf{x}).$$

REMARK 7.2

(i) Theorem 7.2 is just a reformulation of Theorem 3.1 for the case of a solid with a microstructure characterized by ε. The proof of Theorem 7.2 is rather lengthy and will be given elsewhere.

(ii) As we already know from Secs. 5 and 6, even in the periodic case the homogenized coefficients $\overline{a}^h = \overset{0}{a}$, $\overline{b}^h = \overset{0}{b}$ and $\overline{d}^h = \overset{0}{d}$ are not equal to their mean values.

(iii) On account of (A_1), $\rho^{\varepsilon'} \to \overset{0}{\rho}$ weak-* in $L^\infty(\Omega)$. Here one has the liberty in the choice of a subsequence ε'.

(iv) In the general non-periodic case the effective coefficients $\overset{0}{\rho}$, c^h_{ijkl}, ... etc. are not necessarily constant but may depend on $\mathbf{x} \in \Omega$.

(v) The homogenized system (7.10)–(7.12) is of the same type as the primal one or (7.1)–(7.3).

Part 2. Correctors and examples

In Part 1 of our contribution the homogenization problem was solved for linear equations of thermodiffusion in a three-dimensional solid. The formal method of two-scale asymptotic expansions was justified by Theorem 7.2. Now we will continue our considerations; particularly in Sec. 8 the results concerning correctors will be given. Secs. 9 and 10 are more specific and illustrate the general developments of Part 1. The sense of introducing correctors follows from Theorems 8.1 and 8.2 below.

8. Correctors

For $\varepsilon > 0$ the initial conditions for the entropy and concentration are given by, see (2.38) and (2.39),

$$s^\varepsilon(\mathbf{x},0) = \overline{\gamma}^\varepsilon_{ij}(\mathbf{x})e_{ij}(\mathbf{u}^\varepsilon) + \overline{b}^\varepsilon(\mathbf{x})\Theta^\varepsilon(\mathbf{x},0) + \overline{d}^\varepsilon M^\varepsilon(\mathbf{x},0)\,, \tag{8.1}$$

$$c^\varepsilon(\mathbf{x},0) = \overline{\xi}^\varepsilon_{ij}(\mathbf{x})e_{ij}(\mathbf{u}^\varepsilon) + \overline{d}^\varepsilon(\mathbf{x})\Theta^\varepsilon(\mathbf{x},0) + \overline{a}^\varepsilon M^\varepsilon(\mathbf{x},0)\,. \tag{8.2}$$

We recall that now no periodicity assumption on the material coefficients is *a priori* imposed. Here $(\mathbf{u}^\varepsilon, \Theta^\varepsilon, M^\varepsilon)$ is the unique solution to the system (7.1)–(7.5). We still preserve the superscript h for some of the homogenized coefficients; they can be calculated explicitly for a periodic microstructure studied in Part 1, cf. [5].

The considerations which follow owe much to the papers by MURAT and TARTAR [151, 152], where scalar cases only are investigated.

Suppose that $(\mathbf{v}^{\varepsilon'}, \mathbf{z}^{\varepsilon'})$ be any functions such that, cf. Secs. 2 and 5,

$$\left.\begin{aligned} -\operatorname{div}[\overline{\mathbf{c}}^{\varepsilon'}\mathbf{e}(\mathbf{v}^{\varepsilon'}) - (\overline{\boldsymbol{\gamma}}^{\varepsilon'} - \overline{\boldsymbol{\gamma}}^h)] = 0, &\quad \text{in } \Omega \\ \mathbf{v}^{\varepsilon'} \to 0 &\quad \text{weakly in } H^1_0(\Omega)^3 \end{aligned}\right\} \quad \text{as } \varepsilon \to 0\,; \tag{8.3}$$

$$\left.\begin{aligned} -\operatorname{div}[\overline{\mathbf{c}}^{\varepsilon'}\mathbf{e}(\mathbf{z}^{\varepsilon'}) - (\overline{\boldsymbol{\xi}}^{\varepsilon'} - \overline{\boldsymbol{\xi}}^h)] = 0, &\quad \text{in } \Omega \\ \mathbf{z}^{\varepsilon'} \to 0 &\quad \text{weakly in } H^1_0(\Omega)^3 \end{aligned}\right\} \quad \text{as } \varepsilon \to 0\,. \tag{8.4}$$

Such a sequence $(\mathbf{v}^{\varepsilon'}, \mathbf{z}^{\varepsilon'})$ exists [40].

Next, we define (κ_1, κ_2) by extracting a subsequence, still denoted by ε', such that

$$\overline{\gamma}^{\varepsilon'}_{ij}(\mathbf{x})e_{ij}(\mathbf{v}^{\varepsilon'}) \to \kappa_1, \quad \text{weakly in } L^2(\Omega)\,, \tag{8.5}$$

$$\overline{\xi}^{\varepsilon'}_{ij}(\mathbf{x})e_{ij}(\mathbf{z}^{\varepsilon'}) \to \kappa_2, \quad \text{weakly in } L^2(\Omega)\,. \tag{8.6}$$

It can be shown that for $\alpha = 1, 2$

$$\kappa_\alpha \in L^\infty(\Omega) \quad \text{and} \quad \kappa_\alpha(\mathbf{x}) \geq 0 \quad \text{a.e.} \quad \mathbf{x} \in \Omega\,. \tag{8.7}$$

Further, we note that one can extract a subsequence, still indexed by ε', such that

$$\rho^{\varepsilon'} \to \overset{0}{\rho}, \quad \overline{b}^{\varepsilon'} \to \overset{0}{b}, \quad \overline{d}^{\varepsilon'} \to \overset{0}{d}, \quad \overline{a}^{\varepsilon'} \to \overset{0}{a} \quad \text{weak-* in } L^2(\Omega) \tag{8.8}$$

with

$$\lambda_1(e_1 + e_2) \leq [e_1, e_2]\begin{bmatrix} \overset{0}{b} & \overset{0}{d} \\ \overset{0}{d} & \overset{0}{a} \end{bmatrix}\begin{bmatrix} e_1 \\ e_2 \end{bmatrix} \leq \lambda_2(e_1^2 + e_2^2) \quad \text{a.e. } \mathbf{x} \in \Omega,\ \forall e_1, e_2 \in \mathbb{R}\,.$$

We observe that in the periodic case $\overset{0}{\rho} = \langle \rho \rangle$, etc. To find the homogenized coefficients $\overline{\boldsymbol{\gamma}}^h$ and $\overline{\boldsymbol{\chi}}^h$ one may use the corrector tensor $\mathbf{P}^\varepsilon = (P^\varepsilon_{ijkl})$ associated to $\overline{\mathbf{c}}^\varepsilon$. This tensor will be defined below.

Firstly, however, let us introduce the notion of H-convergence for $\overline{\mathbf{c}}^\varepsilon$, [151, 152].

The sequence $\overline{\mathbf{c}}^\varepsilon$ (strictly a subsequence $\overline{\mathbf{c}}^{\varepsilon'}$) is said to H-converge to $\overline{\mathbf{c}}^h$ if for any $\mathfrak{h}^\varepsilon \to \mathfrak{h}$ strongly in $H^{-1}(\Omega)^3$, the solutions $\mathbf{v}^{\varepsilon'}$ of the elliptic system

$$-\operatorname{div}[\overline{\mathbf{c}}^{\varepsilon'}\mathbf{e}(\mathbf{v}^{\varepsilon'})] = \mathfrak{h}^{\varepsilon'} \quad \text{in } \Omega, \quad \mathbf{v}^{\varepsilon'} \in H^1_0(\Omega)^3 \tag{8.9}$$

satisfy

$$\overline{\mathbf{c}}^{\varepsilon'}\mathbf{e}(\mathbf{v}^{\varepsilon'}) \to \overline{\mathbf{c}}^h\mathbf{e}(\mathbf{v}) \quad \text{weakly in } L^2(\Omega, \mathsf{E}^3_s)\,. \tag{8.10}$$

Here $\mathbf{v} \in H_0^1(\Omega)^3$ is the unique solution of

$$(8.11)\qquad -\operatorname{div}[\overline{\mathbf{c}}^h \mathbf{e}(\mathbf{v})] = \mathfrak{h}, \qquad \text{in } \Omega .$$

We note that for a general microstructure $\overline{\mathbf{c}}^h$ depends on $\mathbf{x} \in \Omega$.

The matrices $\boldsymbol{\lambda}^h$, $\mathbf{L}^h$ and $\mathbf{D}^h$ are defined similarly. More precisely, the matrices $\boldsymbol{\lambda}^{\varepsilon'}$, $\mathbf{L}^{\varepsilon'}$ and $\mathbf{D}^{\varepsilon'}$ are said to H-converge to $\boldsymbol{\lambda}^h$, $\mathbf{L}^h$ and $\mathbf{D}^h$, respectively, if for any sequence $(g^\varepsilon, \mathfrak{h}^\varepsilon) \to (g, \mathfrak{h})$ strongly in $H^{-1}(\Omega)^2$, the solution $(v^{\varepsilon'}, w^{\varepsilon'})$ of

$$(8.12)\qquad \begin{aligned} -\operatorname{div}(\boldsymbol{\lambda}^{\varepsilon'} \operatorname{grad} v^{\varepsilon'} + \mathbf{L}^{\varepsilon'} \operatorname{grad} w^{\varepsilon'}) &= g^{\varepsilon'}, \qquad \text{in } \Omega ,\\ -\operatorname{div}[(\mathbf{L}^{\varepsilon'})^T \operatorname{grad} v^{\varepsilon'} + \mathbf{D}^{\varepsilon'} \operatorname{grad} w^{\varepsilon'}] &= \mathfrak{h}^{\varepsilon'}, \qquad \text{in } \Omega ,\end{aligned}$$

where $(v^{\varepsilon'}, w^{\varepsilon'}) \in H_0^1(\Omega)^2$, satisfy

$$\begin{aligned} \boldsymbol{\lambda}^{\varepsilon'} \operatorname{grad} v^{\varepsilon'} &\to \boldsymbol{\lambda}^h \operatorname{grad} v ,\\ \mathbf{L}^{\varepsilon'} \operatorname{grad} w^{\varepsilon'} &\to \mathbf{L}^h \operatorname{grad} w ,\\ \mathbf{D}^{\varepsilon'} \operatorname{grad} w^{\varepsilon'} &\to \mathbf{D}^h \operatorname{grad} w ,\end{aligned}$$

weakly in $L^2(\Omega)^3$. Here $(v, w) \in H_0(\Omega)^2$ is the unique solution of

$$(8.13)\qquad \begin{aligned} -\operatorname{div}(\boldsymbol{\lambda}^h \operatorname{grad} v + \mathbf{L}^h \operatorname{grad} w) &= g , \qquad \text{in } \Omega ,\\ -\operatorname{div}[(\mathbf{L}^h)^T \operatorname{grad} v^{\varepsilon'} + \mathbf{D}^h \operatorname{grad} w] &= \mathfrak{h} , \qquad \text{in } \Omega .\end{aligned}$$

Let $\mathbf{E} \in \mathbb{E}_s^3$ (see Subsec. 2.2); particularly one may take $\mathbf{E} = \boldsymbol{\delta} = (\delta_{ij})$. Suppose that a sequence $\overline{\mathbf{c}}^{\varepsilon'}$ is H-convergent to $\overline{\mathbf{c}}^h$. Consider the function $\mathbf{w}_{\mathbf{E}}^{\varepsilon'} \in H^1(\Omega)^3$ such that

$$(8.14)\qquad \begin{aligned} \mathbf{w}_{\mathbf{E}}^{\varepsilon'} &\to (E_{ij} x_j) \qquad &&\text{weakly in } H^1(\Omega)^3 ,\\ \operatorname{div}(\overline{\mathbf{c}}^{\varepsilon'} \mathbf{e}(\mathbf{w}_{\mathbf{E}}^{\varepsilon'})) &\to \operatorname{div}(\overline{\mathbf{c}}^h \mathbf{E}) \qquad &&\text{strongly in } H^{-1}(\Omega)^3 .\end{aligned}$$

It is worth noting that for a periodic microstructure the function $\mathbf{w}_{\mathbf{E}}^{\varepsilon}$ can be determined explicitly by solving the local problem on the basic cell Y, cf. [5].

Now we define $\mathbf{P}^{\varepsilon'} = (P_{ijkl}^{\varepsilon'})$, $P_{ijkl}^{\varepsilon'} \in L^2(\Omega)$, by

$$(8.15)\qquad \mathbf{P}^{\varepsilon'} \mathbf{E} = \mathbf{e}(\mathbf{w}_{\mathbf{E}}^{\varepsilon'}) \qquad \text{in } \Omega .$$

If $(\mathbf{v}^{\varepsilon'}, \mathbf{z}^{\varepsilon'})$ are solutions to (8.3) and (8.4) then [151, 152]

$$(8.16)\qquad \left.\begin{aligned} \mathbf{e}(\mathbf{v}^{\varepsilon'}) &= \mathbf{P}^{\varepsilon'} \mathbf{e}(\mathbf{v}) + \mathbf{r}_1^{\varepsilon'} ,\\ \mathbf{e}(\mathbf{z}^{\varepsilon'}) &= \mathbf{P}^{\varepsilon'} \mathbf{e}(\mathbf{z}) + \mathbf{r}_2^{\varepsilon'} ,\end{aligned}\right\}$$

with $\mathbf{r}_\alpha^{\varepsilon'} \to 0$ strongly in $L^1(\Omega, \mathbb{E}_s^3)$, $(\alpha = 1, 2)$. $\mathbf{P}^{\varepsilon'}$ is called the *corrector tensor* associated to $\overline{\mathbf{c}}^{\varepsilon'}$.

The corrector matrices associated to $\boldsymbol{\lambda}^{\varepsilon'}$ and $\mathbf{L}^{\varepsilon'}$ are defined similarly (we recall that $(\mathbf{L}^{\varepsilon'})^T = \mathbf{L}^{\varepsilon'}$). More precisely, let $\Lambda_\alpha \in \mathbb{R}^3$ $(\alpha = 1, 2)$. Consider the functions $w_{\Lambda_\alpha}^{\varepsilon'} \in H^1(\Omega)$, such that

$$(8.17)\qquad \begin{aligned} w_{\Lambda_\alpha}^{\varepsilon'} &\to (\Lambda_\alpha, \mathbf{x}) = \Lambda_{i\alpha} x_i , \qquad &&\text{weakly in } H^1(\Omega) ,\\ \operatorname{div}(\boldsymbol{\lambda}^{\varepsilon'} \operatorname{grad} w_{\Lambda_1}^{\varepsilon'} + \mathbf{L}^{\varepsilon'} \operatorname{grad} w_{\Lambda_2}^{\varepsilon'}) &\to \operatorname{div}(\boldsymbol{\lambda}^h \Lambda_1 + \mathbf{L}^h \Lambda_2) , \qquad &&\text{strongly in } H^{-1}(\Omega) .\end{aligned}$$

We can now define the matrices $\mathbf{Q}^{\varepsilon'}, \mathbf{R}^{\varepsilon'} \in L^2(\Omega, \mathbb{E}^3_s)$ by

$$\mathbf{Q}^{\varepsilon'}\Lambda_1 = \operatorname{grad} w^{\varepsilon'}_{\Lambda_1}, \qquad \mathbf{R}^{\varepsilon'}\Lambda_2 = \operatorname{grad} w^{\varepsilon'}_{\Lambda_2}. \tag{8.18}$$

If $(v^{\varepsilon'}, w^{\varepsilon'})$ is a solution to (8.12) then

$$\left.\begin{aligned} \operatorname{grad} v^{\varepsilon'} &= \mathbf{Q}^{\varepsilon'} \operatorname{grad} v + \mathbf{r}^{\varepsilon'}_1, \\ \operatorname{grad} w^{\varepsilon'} &= \mathbf{R}^{\varepsilon'} \operatorname{grad} w + \mathbf{r}^{\varepsilon'}_2, \qquad \text{with } \mathbf{r}^{\varepsilon'}_\alpha \to 0 \quad \text{strongly in } L^1(\Omega)^3 \end{aligned}\right\}. \tag{8.19}$$

Suppose now that the tensor $\mathbf{P}^{\varepsilon'}$ is known. Then one can define the homogenized coefficients $\overline{\gamma}^h$ and $\overline{\xi}^h$ by extracting a subsequence, still indexed by ε', such that, cf. [151, Sec. 2, Prop. 5],

$$\mathbf{P}^{\varepsilon'}\overline{\gamma}^{\varepsilon'} \to \overline{\gamma}^h \quad \text{and} \quad \mathbf{P}^{\varepsilon'}\overline{\xi}^{\varepsilon'} \to \overline{\xi}^h \quad \text{weakly in } L^2(\Omega, \mathbb{E}^3_s). \tag{8.20}$$

Denoting the r.h.s. of (8.1) and (8.2) by $(D^\varepsilon_1, D^\varepsilon_2)$, we have (for a subsequence, say ε')

$$D^{\varepsilon'}_\alpha \to D^0_\alpha \quad \text{weakly in } L^2(\Omega). \tag{8.21}$$

By using (8.5) and (8.6) we define $(\Theta^h(\mathbf{x}, 0), M^h(\mathbf{x}, 0))$ by

$$\begin{aligned} \overline{\gamma}^h_{ij} e_{ij}(\mathbf{U}) + (\overset{0}{b} + \kappa_1)\Theta^h(\mathbf{x}, 0) + \overset{0}{d} M^h(\mathbf{x}, 0) &= D^0_1, \\ \overline{\xi}^h_{ij} e_{ij}(\mathbf{U}) + \overset{0}{d}\, \Theta^h(\mathbf{x}, 0) + (\overset{0}{a} + \kappa_2) M^h(\mathbf{x}, 0) &= D^0_2. \end{aligned} \tag{8.22}$$

On the other hand we have $\overline{\gamma}^{\varepsilon'}_{ij}, \overline{\xi}^{\varepsilon'}_{ij} \in L^\infty(\Omega) \subset L^2(\Omega)$, since Ω is a bounded domain. Hence, for some subsequence — still indexed by ε' — we have

$$\overline{\gamma}^{\varepsilon'}_{ij} \to \overset{0}{\gamma}_{ij}, \quad \overline{\xi}^{\varepsilon'}_{ij} \to \overset{0}{\xi}_{ij} \quad \text{weakly in } L^2(\Omega).$$

Thus we obtain:

$$\begin{aligned} \lim_{\varepsilon' \to 0} s^{\varepsilon'}(\mathbf{x}, 0) &= \lim_{\varepsilon' \to 0} [\overline{\gamma}^{\varepsilon'}_{ij} e_{ij}(\mathbf{U}) + \overline{b}^{\varepsilon'}(\mathbf{x})\Theta_0(\mathbf{x}) + \overline{d}^{\varepsilon'}(\mathbf{x}) M_0(\mathbf{x})] = \\ &= \overset{0}{\gamma}_{ij} e_{ij}(\mathbf{U}) + \overset{0}{b}(\mathbf{x})\Theta_0(\mathbf{x}) + \overset{0}{d}(\mathbf{x}) M_0(\mathbf{x}), \\ \lim_{\varepsilon' \to 0} c^{\varepsilon'}(\mathbf{x}, 0) &= \lim_{\varepsilon' \to 0} [\overline{\xi}^{\varepsilon'}_{ij} e_{ij}(\mathbf{U}) + \overline{d}^{\varepsilon'}(x)\Theta_0(\mathbf{x}) + \overline{a}^{\varepsilon'}(x) M_0(\mathbf{x})] = \\ &= \overset{0}{\xi}_{ij}(\mathbf{x}) e_{ij}(\mathbf{U}) + \overset{0}{d}(\mathbf{x})\Theta_0(\mathbf{x}) + \overset{0}{a}(\mathbf{x}) M_0(\mathbf{x}). \end{aligned} \tag{8.23}$$

From the systems of algebraic equations (8.22) and (8.23) one derives the initial value for the temperature $\Theta^h_0(\mathbf{x}) = \Theta^h(\mathbf{x}, 0)$ and chemical potential $M^h_0(\mathbf{x}) = M^h(\mathbf{x}, 0)$.

Following [40] and performing energetic considerations we introduce a solution $(\widetilde{\mathbf{u}}^\varepsilon, \widetilde{\Theta}^\varepsilon, \widetilde{M}^\varepsilon)$ corresponding to initial conditions $(\mathbf{U}^\varepsilon, \mathbf{V}, \Theta^\varepsilon_0, M^\varepsilon_0)$. The latter are defined by

$$\begin{aligned} -\operatorname{div}[\overline{\mathbf{c}}^\varepsilon \mathbf{e}(\mathbf{U}^\varepsilon) - \Theta^h_0(\overline{\boldsymbol{\gamma}}^\varepsilon - \overline{\boldsymbol{\gamma}}^h) - M^h_0(\overline{\boldsymbol{\xi}}^\varepsilon - \overline{\boldsymbol{\xi}}^h)] &= -\operatorname{div}[\overline{\mathbf{c}}^h \mathbf{e}(\mathbf{U}^\varepsilon)], \quad \text{in } \Omega, \\ \mathbf{U}^\varepsilon \in H^1_0(\Omega)^3, \quad \Theta^\varepsilon_0 = \Theta^h_0, &\quad M^\varepsilon_0 = M^h_0. \end{aligned} \tag{8.24}$$

After these preparations we define $(\widetilde{\mathbf{u}}^\varepsilon, \widetilde{\Theta}^\varepsilon, \widetilde{M}^\varepsilon)$ and $(\mathbf{v}^\varepsilon, \eta^\varepsilon, N^\varepsilon)$, where $(\mathbf{u}^\varepsilon, \Theta^\varepsilon, M^\varepsilon) = (\widetilde{\mathbf{u}}^\varepsilon + \widetilde{\mathbf{v}}^\varepsilon, \widetilde{\Theta}^\varepsilon + \eta^\varepsilon, \widetilde{M}^\varepsilon + N^\varepsilon)$, as solutions to the following initial-boundary value problems:

$$\rho^\varepsilon \frac{\partial^2 \widetilde{\mathbf{u}}^\varepsilon}{\partial t^2} - \operatorname{div}(\overline{\mathbf{c}}^\varepsilon \mathbf{e}(\widetilde{\mathbf{u}}^\varepsilon) - \overline{\gamma}^\varepsilon \widetilde{\Theta}^\varepsilon - \overline{\xi}^\varepsilon \widetilde{M}^\varepsilon = \mathbf{B}, \quad \text{in } \Omega \times (0, t_0),$$

$$\overline{b}^\varepsilon \frac{\partial \widetilde{\Theta}^\varepsilon}{\partial t} + \overline{d}^\varepsilon \frac{\partial \widetilde{M}^\varepsilon}{\partial t} - \operatorname{div}(\boldsymbol{\lambda}^\varepsilon \operatorname{grad} \widetilde{\Theta}^\varepsilon + \mathbf{L}^\varepsilon \operatorname{grad} \widetilde{M}^\varepsilon) + \overline{\gamma}^\varepsilon \mathbf{e}\left(\frac{\partial \widetilde{\mathbf{u}}^\varepsilon}{\partial t}\right) = g_1,$$

$$\overline{d}^\varepsilon \frac{\partial \widetilde{\Theta}^\varepsilon}{\partial t} + \overline{a}^\varepsilon \frac{\partial \widetilde{M}^\varepsilon}{\partial t} - \operatorname{div}((\mathbf{L}^\varepsilon)^T \operatorname{grad} \widetilde{\Theta}^\varepsilon + \mathbf{D}^\varepsilon \operatorname{grad} \widetilde{M}^\varepsilon) + \overline{\xi}^\varepsilon \mathbf{e}\left(\frac{\partial \widetilde{u}^\varepsilon}{\partial t}\right) = g_2,$$

$$\text{in } \Omega \times (0, t_0),$$

$$\widetilde{\mathbf{u}}^\varepsilon(\mathbf{x}, t) = 0, \quad \widetilde{\Theta}^\varepsilon(\mathbf{x}, t) = 0, \quad \widetilde{M}^\varepsilon(\mathbf{x}, t) = 0, \quad \text{on } \partial\Omega \times (0, t_0),$$

$$\widetilde{\mathbf{u}}^\varepsilon(\mathbf{x}, 0) = \mathbf{U}(\mathbf{x}), \quad \widetilde{\Theta}^\varepsilon(\mathbf{x}, 0) = \Theta_0^h(\mathbf{x}), \quad \widetilde{M}^\varepsilon(\mathbf{x}, 0) = M_0^h(\mathbf{x}), \quad \frac{\partial \widetilde{\mathbf{u}}^\varepsilon}{\partial t}(\mathbf{x}, 0) = \mathbf{V}(\mathbf{x}) \quad \text{in } \Omega;$$

and

$$\rho^\varepsilon \frac{\partial^2 \widetilde{\mathbf{v}}^\varepsilon}{\partial t^2} - \operatorname{div}(\overline{\mathbf{c}}^\varepsilon \mathbf{e}(\widetilde{\mathbf{v}}^\varepsilon) - \overline{\gamma}^\varepsilon \eta^\varepsilon - \overline{\xi}^\varepsilon N^\varepsilon) = 0, \quad \text{in } \Omega \times (0, t_0),$$

$$\overline{b}^\varepsilon \frac{\partial \eta^\varepsilon}{\partial t} + \overline{d}^\varepsilon \frac{\partial N^\varepsilon}{\partial t} - \operatorname{div}(\boldsymbol{\lambda}^\varepsilon \operatorname{grad} \eta^\varepsilon + \mathbf{L}^\varepsilon \operatorname{grad} N^\varepsilon) + \overline{\gamma}^\varepsilon \mathbf{e}\left(\frac{\partial \widetilde{\mathbf{v}}^\varepsilon}{\partial t}\right) = 0,$$

$$\overline{d}^\varepsilon \frac{\partial \eta^\varepsilon}{\partial t} + \overline{a}^\varepsilon \frac{\partial N^\varepsilon}{\partial t} - \operatorname{div}((\mathbf{L}^\varepsilon)^T \operatorname{grad} \eta^\varepsilon + \mathbf{D}^\varepsilon \operatorname{grad} N^\varepsilon) + \overline{\xi}^\varepsilon \mathbf{e}\left(\frac{\partial \widetilde{\mathbf{v}}^\varepsilon}{\partial t}\right) = 0,$$

$$\text{in } \Omega \times (0, t_0),$$

$$\widetilde{\mathbf{v}}^\varepsilon(\mathbf{x}, t) = 0, \quad \eta^\varepsilon(\mathbf{x}, t) = 0, \quad N^\varepsilon(\mathbf{x}, t) = 0, \quad \text{on } \partial\Omega \times (0, t_0),$$

$$\widetilde{\mathbf{v}}^\varepsilon(\mathbf{x}, 0) = \mathbf{U}(\mathbf{x}) - \mathbf{U}^\varepsilon(\mathbf{x}), \quad \eta^\varepsilon(\mathbf{x}, 0) = 0, \quad N^\varepsilon(\mathbf{x}, 0) = 0, \quad \frac{\partial \widetilde{\mathbf{v}}^\varepsilon}{\partial t}(\mathbf{x}, 0) = 0, \ \text{in } \Omega.$$

Now, we will formulate the basic result of this section.

THEOREM 8.1. *For $\varepsilon \to 0$ the following corrector result holds true:*

$$\frac{\partial \widetilde{\mathbf{u}}^\varepsilon}{\partial t} \to \frac{\partial \mathbf{u}}{\partial t} \quad \text{strongly in} \quad C^0(0, t_0; L^2(\Omega)^3),$$

$$\widetilde{\Theta}^\varepsilon \to \Theta \quad \text{strongly in} \quad C^0(0, t_0; L^2(\Omega)^3),$$

$$\widetilde{M}^\varepsilon \to M \quad \text{strongly in} \quad C^0(0, t_0; L^2(\Omega)^3),$$

$$\mathbf{e}(\widetilde{\mathbf{u}}^\varepsilon) - \mathbf{P}^\varepsilon \mathbf{e}(\mathbf{u}) - \Theta \mathbf{e}(\mathbf{v}^\varepsilon) - M \mathbf{e}(\mathbf{z}^\varepsilon) \to 0 \quad \text{strongly in } C^0(0, t_0; L^1(\Omega, \mathbb{E}_s^3)),$$

$$\operatorname{grad} \widetilde{\Theta}^\varepsilon - \mathbf{Q}^\varepsilon \operatorname{grad} \Theta \to 0 \quad \text{strongly in } L^2(0, t_0; L^1(\Omega)^3),$$

$$\operatorname{grad} \widetilde{M}^\varepsilon - \mathbf{R}^\varepsilon \operatorname{grad} M \to 0 \quad \text{strongly in } L^2(0, t_0; L^1(\Omega)^3).$$

where $\mathbf{v}^\varepsilon$ *and* $\mathbf{z}^\varepsilon$ *are defined by* (8.3) *and* (8.4), *respectively.*

■

We recall that in Theorem 8.1 the fields $\mathbf{u}$, Θ and M describe the homogenized solid. It is worth noting that the fields $\widetilde{\mathbf{v}}^\varepsilon$, η^ε and N^ε do not appear in the corrector theorem.

Deeper insight into the structure of $(\mathbf{u}^\varepsilon, \Theta^\varepsilon, M^\varepsilon)$, leads to the conclusion that the solution to (7.1)–(7.5) is provided by the following

THEOREM 8.2. *For* $\varepsilon \to 0$, *the solution* $(\mathbf{u}^\varepsilon, \Theta^\varepsilon, M^\varepsilon)$ *of the system (7.1)–(7.5) exibits the following structure*

$$\frac{\partial \mathbf{u}^\varepsilon}{\partial t} = \frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \widetilde{\mathbf{v}}^\varepsilon}{\partial t} + \mathbf{r}_1^\varepsilon ,$$

(8.25)
$$\Theta^\varepsilon = \Theta + \eta^\varepsilon + r_2^\varepsilon ,$$

$$M^\varepsilon = M + N^\varepsilon + r_3^\varepsilon ;$$

$$\mathbf{e}(\mathbf{u}^\varepsilon) = \mathbf{P}^\varepsilon \mathbf{e}(\mathbf{u}) + \Theta \mathbf{e}(\mathbf{v}^\varepsilon) + M \mathbf{e}(\mathbf{z}^\varepsilon) + \mathbf{e}(\widetilde{\mathbf{v}}^\varepsilon) + \mathbf{r}_4^\varepsilon ,$$

(8.26)
$$\operatorname{grad} \Theta^\varepsilon = \mathbf{Q}^\varepsilon \operatorname{grad} \Theta + \operatorname{grad} \eta^\varepsilon + \mathbf{r}_5^\varepsilon ,$$

$$\operatorname{grad} M^\varepsilon = \mathbf{R}^\varepsilon \operatorname{grad} M + \operatorname{grad} N^\varepsilon + \mathbf{r}_6^\varepsilon ,$$

where $(\mathbf{u}, \Theta, M)$ *is the solution of the homogenized system* (7.10)–(7.15), *whereas* $\mathbf{v}^\varepsilon$ *and* $\mathbf{z}^\varepsilon$ *are defined by (8.3) and (8.4), respectively;* $(\widetilde{\mathbf{v}}^\varepsilon, \eta^\varepsilon, N^\varepsilon)$ *satisfies*

$$\frac{\partial \widetilde{\mathbf{v}}^\varepsilon}{\partial t} \to 0 \quad \text{weak-* in } L^\infty(0, t_0; L^2(\Omega)^3) ,$$

$$\eta^\varepsilon, N^\varepsilon \to 0 \quad \text{weak-* in } L^\infty(0, t_0; L^2(\Omega)) ,$$

$$\mathbf{e}(\widetilde{\mathbf{v}}^\varepsilon) \to 0 \quad \text{weak-* in } L^\infty(0, t_0; L^2(\Omega, \mathbb{E}_s^3)) ,$$

$$\operatorname{grad} \eta^\varepsilon, \operatorname{grad} N^\varepsilon \to 0 \quad \text{weakly in } L^2(0, t_0; L^2(\Omega)^3) .$$

Moreover

$$\mathbf{r}_1^\varepsilon \to 0 \quad \text{strongly in} \quad C^0(0, t_0; L^2(\Omega)^3) ,$$

$$r_2^\varepsilon, r_3^\varepsilon \to 0 \quad \text{strongly in} \quad C^0(0, t_0; L^2(\Omega)) ,$$

$$\mathbf{r}_4^\varepsilon \to 0 \quad \text{strongly in} \quad C^0(0, t_0; L^1(\Omega, \mathbb{E}_s^3)) ,$$

$$\mathbf{r}_5^\varepsilon, \mathbf{r}_6^\varepsilon \to 0 \quad \text{strongly in} \quad L^2(0, t_0; L^1(\Omega)^3) .$$

REMARK 8.1. Under additional assumptions, stronger results can be obtained, cf. [40, p. 35].

9. Microperiodic layered composites

9.1. Specification of the general homogenization formulae

The formulae derived in Sec. 5 will now be applied to a composite made of periodically distributed two layers. The layers are assumed to be anisotropic. The material coefficients in both layers are denoted by

(9.1)
$$\overset{(1)}{c}_{ijkn}, \overset{(1)}{\gamma}{}^{\alpha}_{ij}, \overset{(1)}{L}{}^{\alpha\beta}_{ij}; \ \overset{(2)}{c}_{ijkn}, \overset{(2)}{\gamma}{}^{\alpha}_{ij}, \overset{(2)}{L}{}^{\alpha\beta}_{ij} .$$

Suppose that the layers are orthogonal to the Ox_1-axis. For simplicity we set $y = y_1$; thus the material coefficient depends now on y only, though the dependence on macroscopic variables x_2 and x_3 is not excluded:

$$\bar{c}_{ijkn}(y) = \begin{cases} \overset{(1)}{c}_{ijkn} & \text{for } y \in (0, \xi), \\ \overset{(2)}{c}_{ijkn} & \text{for } y \in (\xi, 1). \end{cases}$$

$$\gamma_{ij}^{\alpha}(y) = \begin{cases} \overset{(1)}{\gamma}{}_{ij}^{\alpha} & \text{for } y \in (0,\xi), \\ \overset{(2)}{\gamma}{}_{ij}^{\alpha} & \text{for } y \in (\xi,1), \end{cases} \qquad L_{ij}^{\alpha\beta}(y) = \begin{cases} \overset{(1)}{L}{}_{ij}^{\alpha\beta} & \text{for } y \in (0,\xi), \\ \overset{(2)}{L}{}_{ij}^{\alpha\beta} & \text{for } y \in (\xi,1). \end{cases}$$

Now the local equations (5.7) reduce to

$$\begin{aligned} \frac{d}{dy}\left(\bar{c}_{i1k1}(y)\frac{d\chi_k^{(pq)}}{dy}\right) &= -\frac{d}{dy}\bar{c}_{i1pq}(y)\,, \\ \frac{d}{dy}\left(\bar{c}_{i1k1}(y)\frac{d\Gamma_k^{\alpha}}{dy}\right) &= \frac{d}{dy}\bar{\gamma}_{i1}^{\alpha}(y)\,, \\ \frac{d}{dy}\left(L_{11}^{\alpha\gamma}(y)\frac{d\Theta_k^{\gamma\beta}}{dy}\right) &= \frac{d}{dy}L_{1k}^{\alpha\beta}(y)\,. \end{aligned} \tag{9.2}$$

According to (5.5), in order to determine the homogenized coefficients, one must find the following derivatives:

$$\frac{d\chi_k^{(pq)}}{dy}, \qquad \frac{d\Gamma_k^{\alpha}}{dy}, \qquad \frac{d\Theta_k^{\alpha\beta}}{dy}\,. \tag{9.3}$$

By assuming that the matrices $[c_{ik}] = [\bar{c}_{i1k1}]$ and $[L^{\alpha\beta}] = [L_{11}^{\alpha\beta}]$ are non-singular, from (9.2) we obtain

$$\begin{aligned} \frac{d\chi_k^{(pq)}}{dy} &= (c^{-1})^{ki}(-\bar{c}_{i1pq}(y) + \overset{0}{c}{}_{ipq})\,, \\ \frac{d\Gamma_k^{\alpha}}{dy} &= (c^{-1})^{ki}(\bar{\gamma}_{i1}^{\alpha}(y) - \overset{0}{\gamma}{}_{i}^{\alpha})\,, \\ \frac{d\Theta_k^{\alpha\beta}}{dy} &= (L^{-1})_{\beta\gamma}(L_{1k}^{\alpha\gamma}(y) - \overset{0}{L}{}_{k}^{\alpha\gamma})\,, \end{aligned} \tag{9.4}$$

where $(c^{-1})^{ki}$ and $(L^{-1})_{\beta\gamma}$ are components of matrices inverse to $[c_{ik}]$ and $[L^{\alpha\beta}]$, respectively; moreover $\overset{0}{c}{}_{ipq}$, $\overset{0}{\gamma}{}_{i}^{\alpha}$, $\overset{0}{L}{}_{k}^{\alpha\beta}$ are constants of integration which can be determined by using the periodicity conditions for $\chi_k^{(\alpha\beta)}$, Γ_k^{α}, $\Theta_k^{\alpha\beta}$ and continuity of these functions at $y = \xi$.

Solutions to the system (9.4) are sought in the following form:

$$\begin{aligned} \chi_k^{(pq)}(y) &= \begin{cases} \overset{(1)}{\chi}{}_{k}^{pq}(y) & \text{for } y \in (0.\xi), \\ \overset{(2)}{\chi}{}_{k}^{(pq)}(y) & \text{for } y \in (\xi,1), \end{cases} \\ \Gamma_k^{\alpha}(y) &= \begin{cases} \overset{(1)}{\Gamma}{}^{k\alpha}(y) & \text{for } y \in (0.\xi), \\ \overset{(2)}{\Gamma}{}^{k\alpha}(y) & \text{for } y \in (\xi,1), \end{cases} \\ \Theta_k^{\alpha\beta}(y) &= \begin{cases} \overset{(1)}{\Theta}{}_{k}^{\alpha\beta}(y) & \text{for } y \in (0.\xi), \\ \overset{(2)}{\Theta}{}_{k}^{\alpha\beta}(y) & \text{for } y \in (\xi,1). \end{cases} \end{aligned} \tag{9.5}$$

From (9.4), by taking into account (9.5) one has

(9.6)
$$\frac{d\overset{(1)}{\chi}{}_k^{(pq)}}{dy} = (\overset{(1)}{c}{}^{-1})^{ki}(-\overset{(1)}{c}{}_{i1pq} + \overset{0}{c}{}_{ipq}), \qquad \frac{d\overset{(2)}{\chi}{}_k^{pq}}{dy} = (\overset{(2)}{c}{}^{-1})^{ki}(-\overset{(2)}{c}{}_{i1pq} + \overset{0}{c}{}_{ipq}),$$
$$\frac{d\overset{(1)}{\Gamma}{}_k^{\alpha}}{dy} = (\overset{(1)}{c}{}^{-1})^{ki}(\overset{(1)}{\gamma}{}_{i1}^{\alpha} - \overset{(0)}{\gamma}{}_i^{\alpha}), \qquad \frac{d\overset{(2)}{\Gamma}{}_k^{\alpha}}{dy} = (\overset{(2)}{c}{}^{-1})^{ki}(\overset{(2)}{\gamma}{}_{i1}^{\alpha} - \overset{0}{\gamma}{}_i^{\alpha}),$$
$$\frac{d\overset{(1)}{\Theta}{}_k^{\alpha\beta}}{dy} = (\overset{(1)}{L}{}^{-1})_{\beta\gamma}(\overset{(1)}{L}{}_{1k}^{\alpha\gamma} - \overset{(0)}{L}{}_k^{\alpha\gamma}), \qquad \frac{d\overset{(2)}{\Theta}{}_k^{\alpha\beta}}{dy} = (\overset{(2)}{L}{}^{-1})_{\beta\gamma}(\overset{(2)}{L}{}_{1k}^{\alpha\gamma} - \overset{0}{L}{}_k^{\alpha\gamma}),$$

where $(\overset{(1)}{c}{}^{-1})^{ki}$, $(\overset{(2)}{c}{}^{-1})^{ki}$, $(\overset{(1)}{L}{}^{-1})_{\beta\gamma}$, $(\overset{(2)}{L}{}^{-1})_{\beta\gamma}$ are components of matrices inverse to $[\overset{(1)}{c}{}_{i1k1}]$, $[\overset{(2)}{c}{}_{i1k1}]$, $[\overset{(1)}{L}{}_{11}^{\alpha\beta}]$, $[\overset{(2)}{L}{}_{11}^{\alpha\beta}]$, respectively.

Let us pass now to the determination of the constants $\overset{0}{c}{}_{ipq}$. The remaining constants, that is $\overset{(1)}{\gamma}{}_i^{\alpha}$ and $\overset{0}{L}{}_k^{\alpha\gamma}$, are calculated similarly.

From (9.6) we obtain

(9.7)
$$\overset{(1)}{\chi}{}_k^{(pq)}(y) = (\overset{(1)}{c}{}^{-1})^{ki}(-\overset{(1)}{c}{}_{i1pq} + \overset{0}{c}{}_{ipq})y + \overset{(1)}{A}{}_{pq}^{k},$$
$$\overset{(2)}{\chi}{}_k^{(pq)}(y) = (\overset{(2)}{c}{}^{-1})^{ki}(-\overset{(2)}{c}{}_{i1pq} + \overset{0}{c}{}_{ipq})y + \overset{(2)}{A}{}_{pq}^{k}.$$

Here $\overset{(1)}{A}{}_{pq}^{k}$, $\overset{(2)}{A}{}_{pq}^{k}$ are integration constants which will be eliminated.

The periodicity and continuity conditions for $\chi_k^{(pq)}$ given by

$$\overset{(1)}{\chi}{}_k^{(pq)}(0) = \overset{(2)}{\chi}{}_k^{(pq)}(1), \qquad \overset{(1)}{\chi}{}_k^{(pq)}(\xi) = \overset{(2)}{\chi}{}_k^{(pq)}(\xi),$$

yield

$$\overset{(1)}{A}{}_{pq}^{k} = (\overset{(2)}{c}{}^{-1})^{ki}(-\overset{(2)}{c}{}_{i1pq} + \overset{0}{c}{}_{ipq}) + \overset{(2)}{A}{}_{pq}^{k},$$

and

$$(\overset{(1)}{c}{}^{-1})^{ki}(-\overset{(1)}{c}{}_{i1pq} + \overset{0}{c}{}_{ipq})\xi + \overset{(1)}{A}{}_{pq}^{k} = (\overset{(2)}{c}{}^{-1})^{ki}(-\overset{(2)}{c}{}_{i1pq} + \overset{0}{c}{}_{ipq})\xi + \overset{(2)}{A}{}_{pq}^{k},$$

respectively.

Subtracting we arrive at

$$(\overset{(1)}{c}{}^{-1})^{ki}(-\overset{(1)}{c}{}_{i1pq} + \overset{0}{c}{}_{ipq})\xi = (\overset{(2)}{c}{}^{-1})^{ki}(-\overset{(2)}{c}{}_{i1pq} + \overset{0}{c}{}_{ipq})(\xi - 1).$$

Hence

(9.8)
$$\overset{0}{c}{}_{ipq} = (B^{-1})_{ik}[\xi(\overset{(1)}{c}{}^{-1})^{kj}\overset{(1)}{c}{}_{j1pq} + (1-\xi)(\overset{(2)}{c}{}^{-1})^{kj}\overset{(2)}{c}{}_{j1pq}],$$

where $(B^{-1})_{ik}$ are components of the matrix inverse to the matrix $B = [B^{ki}]$; here

(9.9)
$$B^{ki} = \xi(\overset{(1)}{c}{}^{-1})^{ki} + (1-\xi)(\overset{(2)}{c}{}^{-1})^{ki}.$$

In a similar way one obtains the constants $\overset{0}{\gamma}{}_i^{\alpha}$, $\overset{0}{L}{}_k^{\alpha\beta}$

(9.10)
$$\overset{0}{\gamma}{}_i^{\alpha} = (B^{-1})_{ik}[\xi(\overset{(1)}{c}{}^{-1})^{kj}\overset{(1)}{\gamma}{}_{j1}^{\alpha} + (1-\xi)(\overset{(2)}{c}{}^{-1})^{kj}\overset{(2)}{\gamma}{}_{j1}^{\alpha}],$$

$$\overset{0}{L}{}_{k}^{\alpha\beta} = (K^{-1})^{\alpha\gamma}(\xi(\overset{(1)}{L}{}^{-1})_{\gamma\delta}\overset{(1)}{L}{}_{1k}^{\delta\beta} + (1-\xi)(\overset{(2)}{L}{}^{-1})_{\gamma\delta}\overset{(2)}{L}{}_{1k}^{\delta\beta}), \tag{9.11}$$

where $(K^{-1})^{\alpha\gamma}$ are components of the matrix $\mathbf{K}^{-1}$ inverse to $\mathbf{K}$ and

$$K_{\alpha\beta} = \xi(\overset{(1)}{L}{}^{-1})_{\alpha\beta} + (1-\xi)(\overset{(2)}{L}{}^{-1})_{\alpha\beta}.$$

Substituting the integration constants $\overset{0}{c}{}_{ipq}, \overset{0}{\gamma}{}_{i}^{\alpha}, \overset{0}{L}{}_{k}^{\alpha\beta}$ into Eq. (9.4) and taking into account (9.5), after simple algebraic manipulations we obtain

$$\frac{d\chi_k^{(pq)}}{dy} = \begin{cases} (1-\xi)(\widetilde{B}^{-1})^{kj}[\![c_{j1pq}]\!] & \text{for } y\in(0,\xi),\\ -\xi(\widetilde{B}^{-1})^{kj}[\![c_{j1pq}]\!] & \text{for } y\in(\xi,1),\end{cases}$$

$$\frac{d\Gamma_k^{\alpha}}{dy} = \begin{cases} -(1-\xi)(\widetilde{B}^{-1})^{kj}[\![\gamma_{j1}^{\alpha}]\!] & \text{for } y\in(0,\xi),\\ \xi(\widetilde{B}^{-1})^{kj}[\![\gamma_{j1}^{\alpha}]\!] & \text{for } y\in(\xi,1),\end{cases}$$

$$\frac{d\Theta_k^{\alpha\beta}}{dy} = \begin{cases} -(1-\xi)(\widetilde{K}^{-1})_{\beta\delta}[\![L_{1k}^{\delta\alpha}]\!] & \text{for } y\in(0,\xi),\\ \xi(\widetilde{K}^{-1})_{\beta\delta}[\![L_{1k}^{\delta\alpha}]\!] & \text{for } y\in(\xi,1),\end{cases}$$

where $[\![\cdot]\!]$ stands for a jump; for instance $[\![c_{ijpq}]\!] = \overset{(2)}{c}{}_{ijpq} - \overset{(1)}{c}{}_{ijpq}$; moreover $(\widetilde{B}^{-1})^{kj}$ and $(\widetilde{K}^{-1})_{\beta\delta}$ are components of matrices inverse to $[\widetilde{B}_{kj}] = [\xi\,\overset{(2)}{c}{}_{k1j1} + (1-\xi)\,\overset{(1)}{c}{}_{k1j1}]$ and $[\widetilde{K}^{\alpha\beta}] = [\xi\,\overset{(2)}{L}{}_{11}^{\alpha\beta} + (1-\xi)\,\overset{(1)}{L}{}_{11}^{\alpha\beta}]$, respectively.

Thus we eventually obtain the homogenized coefficients

$$\begin{aligned} \bar{c}_{ijpq}^{h} &= \langle\bar{c}_{ijpq}\rangle - \xi(1-\xi)(\widetilde{B}^{-1})^{ks}[\![c_{s1pq}]\!][\![c_{ijk1}]\!],\\ \bar{\gamma}_{ij}^{h} &= \langle\bar{\gamma}_{ij}^{\alpha}\rangle - \xi(1-\xi)(\widetilde{B}^{-1})^{ks}[\![c_{s1ij}]\!][\![\gamma_{k1}^{\alpha}]\!],\\ \bar{a}^{h\alpha\beta} &= \langle\bar{a}^{\alpha\beta}\rangle + \xi(1-\xi)(\widetilde{B}^{-1})^{ks}[\![\gamma_{k1}^{\alpha}]\!][\![\gamma_{s1}^{\beta}]\!],\\ L_{ij}^{h\alpha\beta} &= \langle L_{ij}^{\alpha\beta}\rangle - \xi(1-\xi)(\widetilde{K}^{-1})_{\gamma\delta}[\![L_{1j}^{\delta\beta}]\!][\![L_{i1}^{\alpha\gamma}]\!], \end{aligned} \tag{9.12}$$

where

$$\langle\bar{c}_{ijpq}\rangle = \xi\,\overset{(1)}{c}{}_{ijpq} + (1-\xi)\,\overset{(2)}{c}{}_{ijpq}.$$

By substituting the formulae (9.12) for the homogenized coefficients into (6.5) we obtain the following expressions for the initial temperature and chemical potential of the homogenized body

$$\Theta^h(x,0) = \Theta_0 + \xi(1-\xi)(\widetilde{B}^{-1})^{ks}(\bar{a}^h[\![\gamma_k]\!] - \bar{d}^h[\![\zeta_k]\!])(-[\![\gamma_s]\!]\Theta_0 - [\![\zeta_s]\!]M_0 + [\![\bar{c}_{s1pq}]\!]e_{pq}(\mathbf{U}))\frac{1}{\overline{\Delta}^h}, \tag{9.13}$$

$$M^h(x,0) = M_0 - \xi(1-\xi)(\widetilde{B}^{-1})^{ks}(\bar{b}^h[\![\zeta_k]\!] - \bar{d}^h[\![\gamma_k]\!])([\![\gamma_s]\!]\Theta_0 + [\![\zeta_s]\!]M_0 - [\![\bar{c}_{s1pq}]\!]e_{pq}(\mathbf{U}))\frac{1}{\overline{\Delta}^h}, \tag{9.14}$$

where

$$\overline{\Delta}^h = \bar{a}^h\bar{b}^h - (\bar{d}^h)^2,$$

$$[\![\gamma_R]\!] = \overset{(2)}{\gamma}_{k1} - \overset{(1)}{\gamma}_{k1},$$

$$[\![\zeta_k]\!] = \overset{(2)}{\xi}_{k1} - \overset{(1)}{\xi}_{k1}, \quad \text{cf. (2.56)}.$$

9.2. Example: Numerical results

By using the *formulae* (9.12) we will discuss the homogenized properties of a *periodically* layered *medium* composed of two isotropic materials. For an isotropic elastic body one has

$$c_{1111} = \frac{E}{1+\nu}\left(1 + \frac{\nu}{1-2\nu}\right),$$

where E stands for the Young's *modulus* and ν is the Poisson ratio. Let $\overset{(1)}{E}$ and $\overset{(2)}{E}$ (resp. $\overset{(1)}{\nu}$ and $\overset{(2)}{\nu}$) denote Young's *moduli* (resp. Poisson ratios) of both layers. We set

$$e = \frac{\overset{(2)}{E}}{\overset{(1)}{E}}, \qquad e \in (0,1),$$

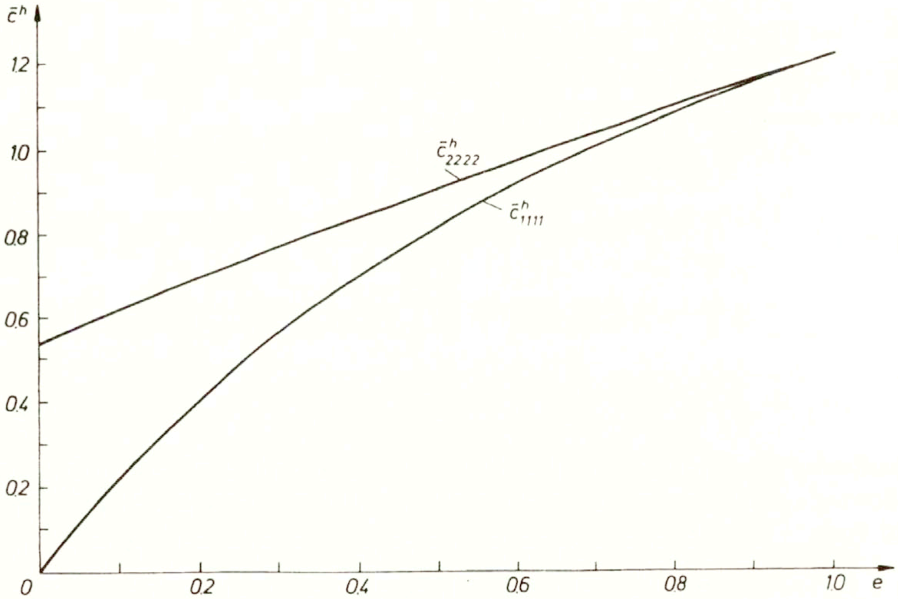

FIG. 1. Diagonal components $\bar{c}^h_{1111}$ and $\bar{c}^h_{2222}$ of the homogenized elasticity tensor as functions of $e = \overset{(2)}{E} / \overset{(1)}{E}$. Poisson ratio of both composite materials is the same: $\nu = 1/4$, and the thickness of both layers is also the same (i.e. $\xi = 1/2$).

Figures 1, 2 and 3 show diagonal components of the homogenized elasticity tensor, particularly Fig. 1 provides $\bar{c}^h_{1111}$ and $\bar{c}^h_{2222}$ as a function of e. Poisson ratio of both components is the same: $\nu = 1/4$, and the thickness of both layers of the considered medium is also the same (i.e. $\xi = 1/2$). The coefficient $\bar{c}^h_{3333}$ is identical with $\bar{c}^h_{2222}$, ($\bar{c}^h_{3333} = \bar{c}^h_{2222}$).

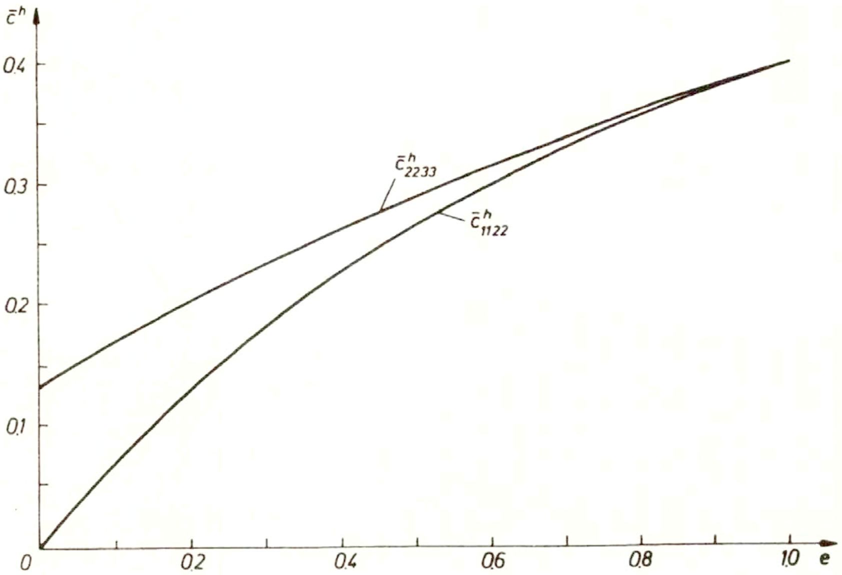

FIG. 2. Components $\bar{c}^h_{1122}$ and $\bar{c}^h_{2233}$ of the homogenized elasticity tensor as functions of $e = \overset{(2)}{E} / \overset{(1)}{E}$. Poisson ratio of both composite materials is the same: $\nu = 1/4$, and the thickness of both layers is the same (i.e. $\xi = 1/2$).

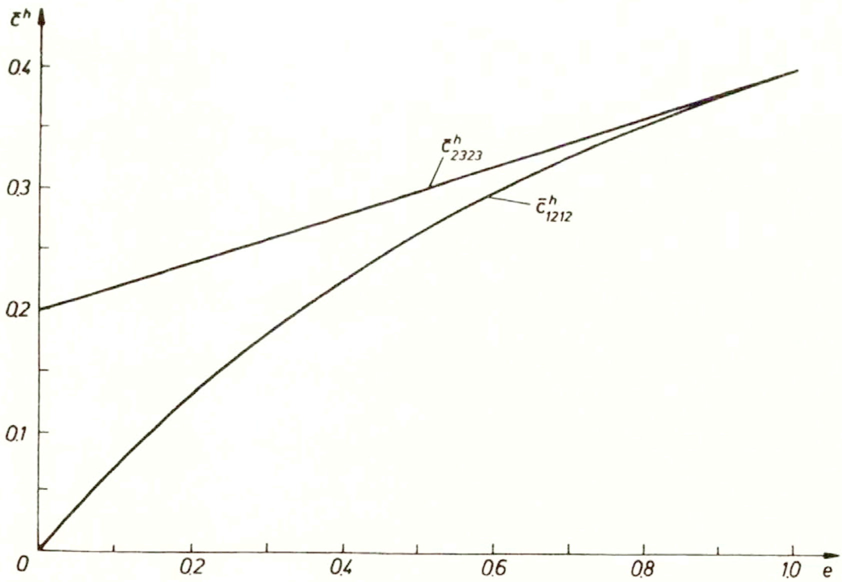

FIG. 3. Components $\bar{c}^h_{1212}$ and $\bar{c}^h_{2323}$ of the homogenized elasticity tensor as functions of $e = \overset{(2)}{E} / \overset{(1)}{E}$. Poisson ratio of both composite materials is $\nu = 1/4$ and the thickness of both layers is also the same (i.e. $\xi = 1/2$).

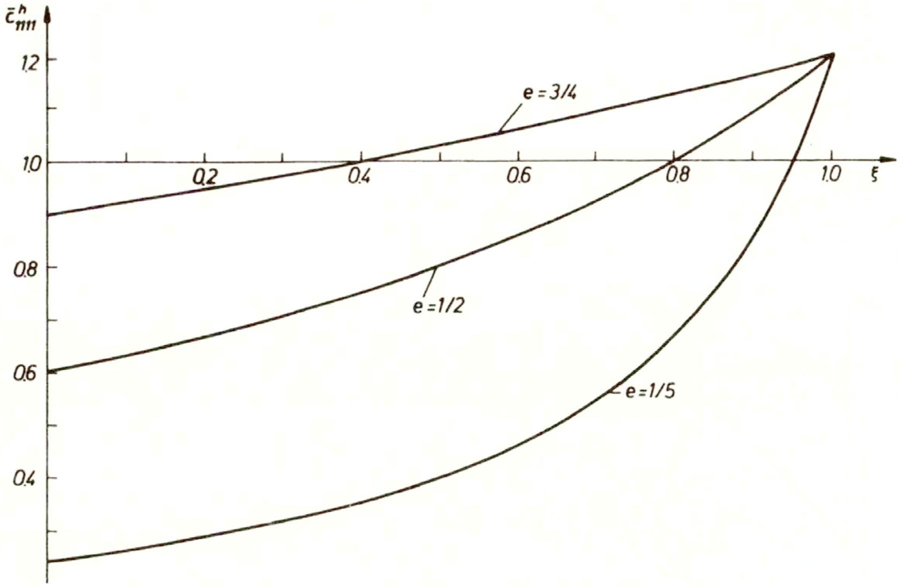

FIG. 4. Component $\bar{c}^h_{1111}$ as a function of the layers thickness ratio ξ, for $e = \overset{(2)}{E} / \overset{(1)}{E} = 1/5$, $1/2$ and $3/4$, while $\overset{(1)}{\nu} = \overset{(2)}{\nu} = 1/5$.

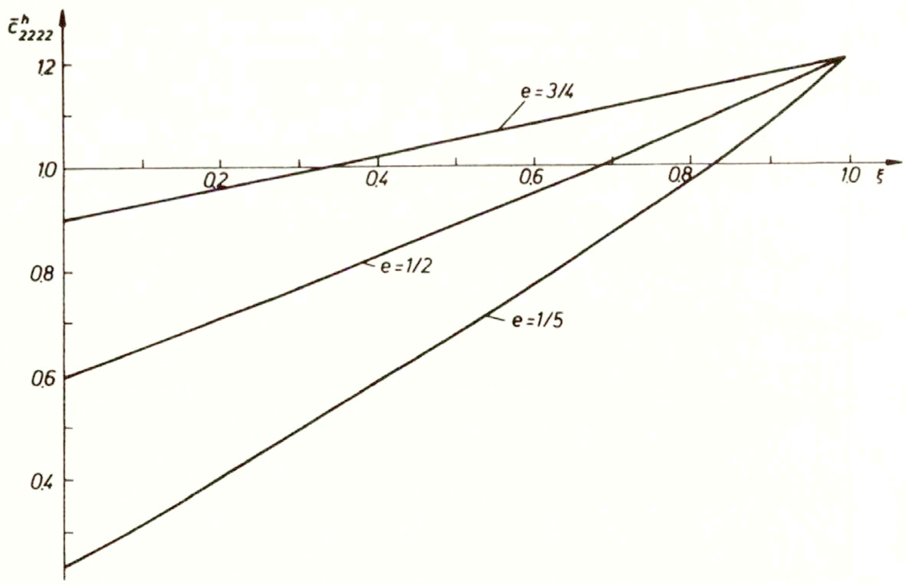

FIG. 5. Component $\bar{c}^h_{2222}$ as a function of the layers thickness ratio ξ, for $e = \overset{(2)}{E} / \overset{(1)}{E} = 1/5$, $1/2$ and $3/4$ while $\overset{(1)}{\nu} = \overset{(2)}{\nu} = 1/5$.

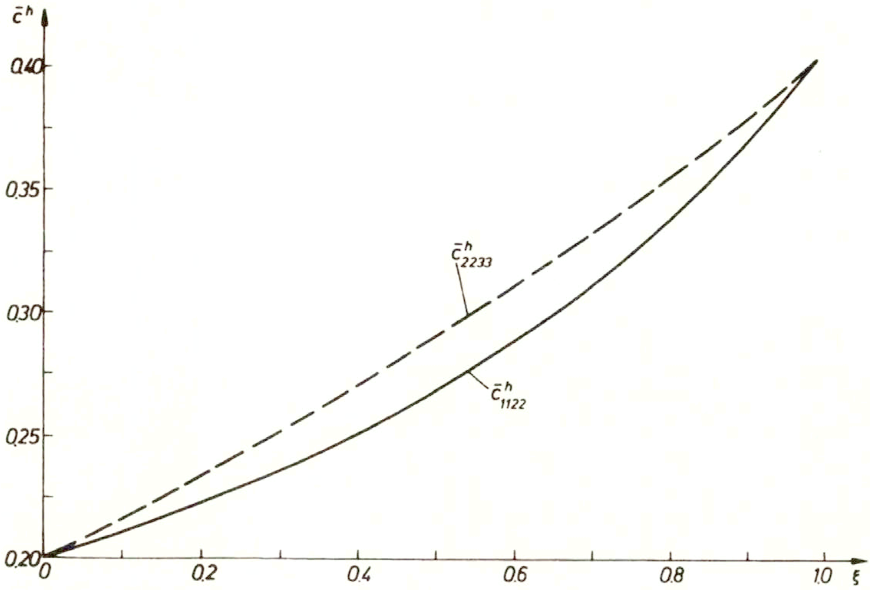

FIG. 6. Homogenized constants $\bar{c}^h_{1122}$ (solid line) and $\bar{c}^h_{2233}$ (dashed line) as a function of ξ for $e = \overset{(2)}{E} / \overset{(1)}{E} = 1/2$ and $\overset{(1)}{\nu} = \overset{(2)}{\nu} = 1/4$.

It is clear that the homogenized body is no longer an isotropic one.

The components $\bar{c}^h_{1122}$ and $\bar{c}^h_{2233}$ (resp. $\bar{c}^h_{2323}$ and $\bar{c}^h_{1212}$) are shown in Fig. 2 (resp. Fig. 3). Comments given for Fig. 1 still apply.

Figure 4 (resp. Fig. 5) show $\bar{c}^h_{1111}$ (resp. $\bar{c}^h_{2222}$) as a function of the layers thickness ratio ξ, for $e = 1/5, 1/2$ and $3/4$ while $\overset{(1)}{\nu} = \overset{(2)}{\nu} = 1/5$. Obviously, for $\xi = 1$ only the more stiff layer no. 1 exists.

Figure 6 shows homogenized constants $\bar{c}^h_{1122}$ (solid line) and $\bar{c}^h_{2233}$ (dashed line) as a functions of ξ for $e = 1/2$ and $\overset{(1)}{\nu} = \overset{(2)}{\nu} = 1/4$.

Figure 7 shows the thermoelatic coefficients $\bar{\gamma}^{1h}_{11}$ and $\bar{\gamma}^{1h}_{22}$ as functions of e, for $\overset{(1)}{\nu} = \overset{(2)}{\nu} = 1/4$. Remarks concerning homogenized coefficients $\bar{c}^h_{ijkl}$ (cf. Figs. 1–4) apply again.

In Fig. 8 the dependence of $\gamma^h_{11} := \gamma^{1h}_{11}$ on the thickness ratio ξ and the ratio $g = \overset{(1)}{\gamma}{}^1_{11} / \overset{(2)}{\gamma}{}^1_{11}$ is given. The following parameters are taken into account $e = \overset{(2)}{E} / \overset{(1)}{E} = 1/2$ and $\overset{(1)}{\gamma}{}^2_{11} / \overset{(2)}{\gamma}{}^2_{11} = 1/2$.

Figures 9 and 10 exhibit the influence of the homogenization on the coefficients $\bar{a}^{\alpha\beta}$, i.e. on the coefficients $\bar{a}$, $\bar{b}$ and $\bar{d}$(expressing the entropy s and concentration c in terms of the temperature Θ and chemical potential M). In these figures, performed for $\xi = 1/2$, the differences between the homogenized value of the coefficients and their mean values as functions of e are shown. The parameter g is defined by $g = \overset{(1)}{\gamma}{}_{11} / \overset{(2)}{\gamma}{}_{11}$; moreover $\bar{a}^{11h} = \bar{b}^h$.

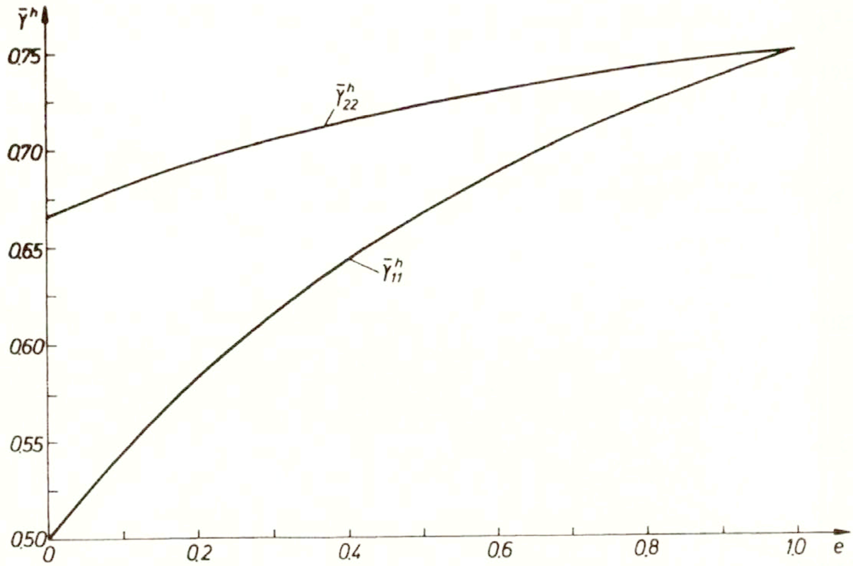

FIG. 7. Homogenized thermoelastic coefficients γ_{11}^h and γ_{22}^h as functions of $e = \overset{(2)}{E} / \overset{(1)}{E}$, for $\overset{(1)}{\nu} = \overset{(2)}{\nu} = 1/4$.

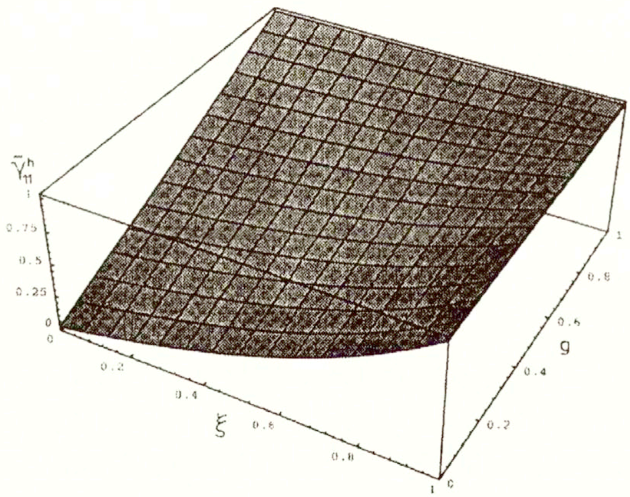

FIG. 8. Dependence of γ_{11}^h on thickness ratio ξ and ratio $g = \overset{(1)}{\gamma}{}^1_{11} / \overset{(2)}{\gamma}{}^1_{11}$, for parameters $e = \overset{(2)}{E} / \overset{(1)}{E} = 1/2$ and $\overset{(1)}{\gamma}{}^2_{11} / \overset{(2)}{\gamma}{}^2_{11} = 1/2$.

In Fig. 9 the difference $\overline{a}^{11h} - \langle \overline{a}^{11} \rangle = \overline{b}^h - \langle \overline{b} \rangle$ is shown, which at its turn is equal to $\overline{a}^{22h} - \langle \overline{a}^{22} \rangle = \overline{a}^h - \langle \overline{a} \rangle$. The same thickness of both layers is assumed ($\xi = 1/2$). Two ratios $\overset{(1)}{\gamma}{}^1_{11} / \overset{(2)}{\gamma}{}^1_{11}$, as parameters of the plot are taken.

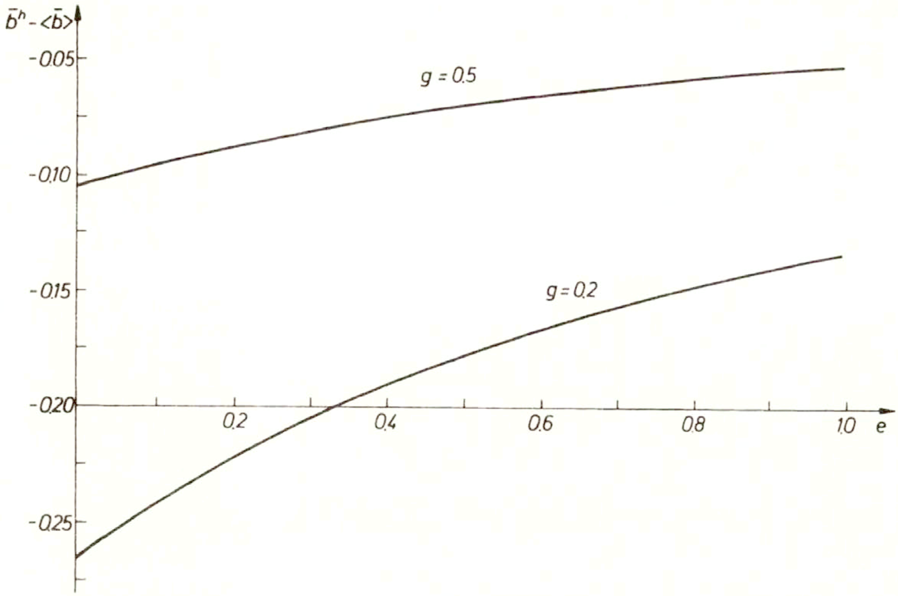

FIG. 9. $\bar{b}^h - \langle\bar{b}\rangle$ as the function of $e = \overset{(2)}{E} / \overset{(1)}{E}$ for two parameters $g = 0.2$ and $g = 0.5$, where $g = \overset{(1)}{\gamma}_{11} / \overset{(2)}{\gamma}_{11}$.

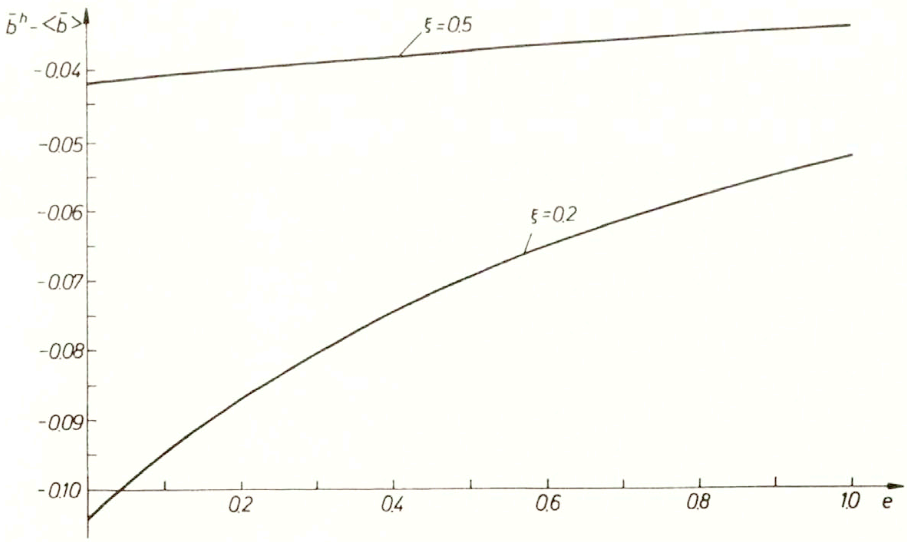

FIG. 10. $\bar{b}^h - \langle\bar{b}\rangle$ as the function of $e = \overset{(2)}{E} / \overset{(1)}{E}$ for two values of the parameter ξ: $\xi = 1/5$ and $\xi = 1/2$; ξ is the thickness ratio.

Figure 10 is analogous to the previous one. As a parameter of the plot ratio ξ is taken. The lower curve in Fig. 10 is identical with the upper one in Fig. 9 (note that the scale units in both figures are different).

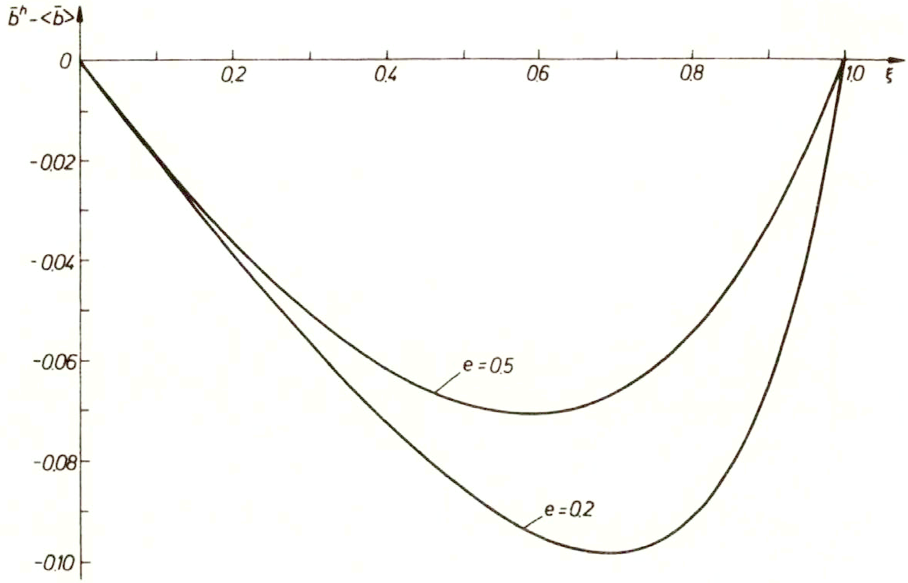

FIG. 11. $\overline{b}^h - \langle \overline{b} \rangle$ as the function of thickness ratio ξ for two values of the parameter $e = \overset{(2)}{E} / \overset{(1)}{E}$: $e = 1/5$ and $e = 1/2$.

In Fig. 11 the difference $\overline{a}^h - \langle \overline{a} \rangle = \overline{b}^h - \langle \overline{b} \rangle$ as a function of thickness ratio ξ with e as a parameter is shown. The lower curve corresponds to $e = 1/5$ and the upper one to $e = 1/2$.

Before the presentation of the results concerning homogenized transport coefficients, let us recall the notation introduced earlier: K_{11} and D_{11} denote heat and diffusion coefficients, and the other coefficients associated with them are:

$$L^{11}_{11} = K_{11}/T_0 = \lambda_{11} = \lambda, \qquad L^{22}_{11} = D_{11} = D\,.$$

For isotropic layers we have, e.g. $L^{11}_{\alpha\beta} = T_0 \lambda \delta_{\alpha\beta}$, $L^{22}_{\alpha\beta} = D\delta_{\alpha\beta}$.

Further we set:

$$\mathfrak{u} = \overset{(2)}{L}{}^{11}_{11} / \overset{(1)}{L}{}^{11}_{11} = \overset{(2)}{K}{}_{11} / \overset{(1)}{K}{}_{11} = \overset{(2)}{\lambda} / \overset{(1)}{\lambda}\,,$$
$$\mathfrak{v} = \overset{(2)}{L}{}^{22}_{11} / \overset{(1)}{L}{}^{22}_{11} = \overset{(2)}{D}{}_{11} / \overset{(1)}{D}{}_{11} = \overset{(2)}{D} / \overset{(1)}{D}\,.$$

In Figs. 12a and 12b the homogenized heat conductivity $L^{11h}_{11} = \lambda^h_{11}$ and diffusion coefficients $L^{22h}_{11} = D^h_{11}$ are shown as functions of ξ for $\mathfrak{u} = 1/2$ and $\mathfrak{v} = 1/5$ (Fig. 12a), and for $\mathfrak{u} = 1/2$ and $\mathfrak{v} = 1/2$ (Fig. 12b); in the last case plots of L^{11h}_{11} and L^{22h}_{11} coincide.

Figure 13 shows L^{11h}_{11} and L^{22h}_{11} as functions of ratio $\mathfrak{v}$ for $\mathfrak{u} = 1/2$. It is seen that the ratio $\mathfrak{v}$ does not influence the heat conductivity $L^{11h}_{11} = \lambda^h$. The diffusion coefficient $L^{22h}_{11} = D^h$ vanishes for $\mathfrak{v} = 0$ (no diffusion); the result for $\mathfrak{v} = 1$ is obvious.

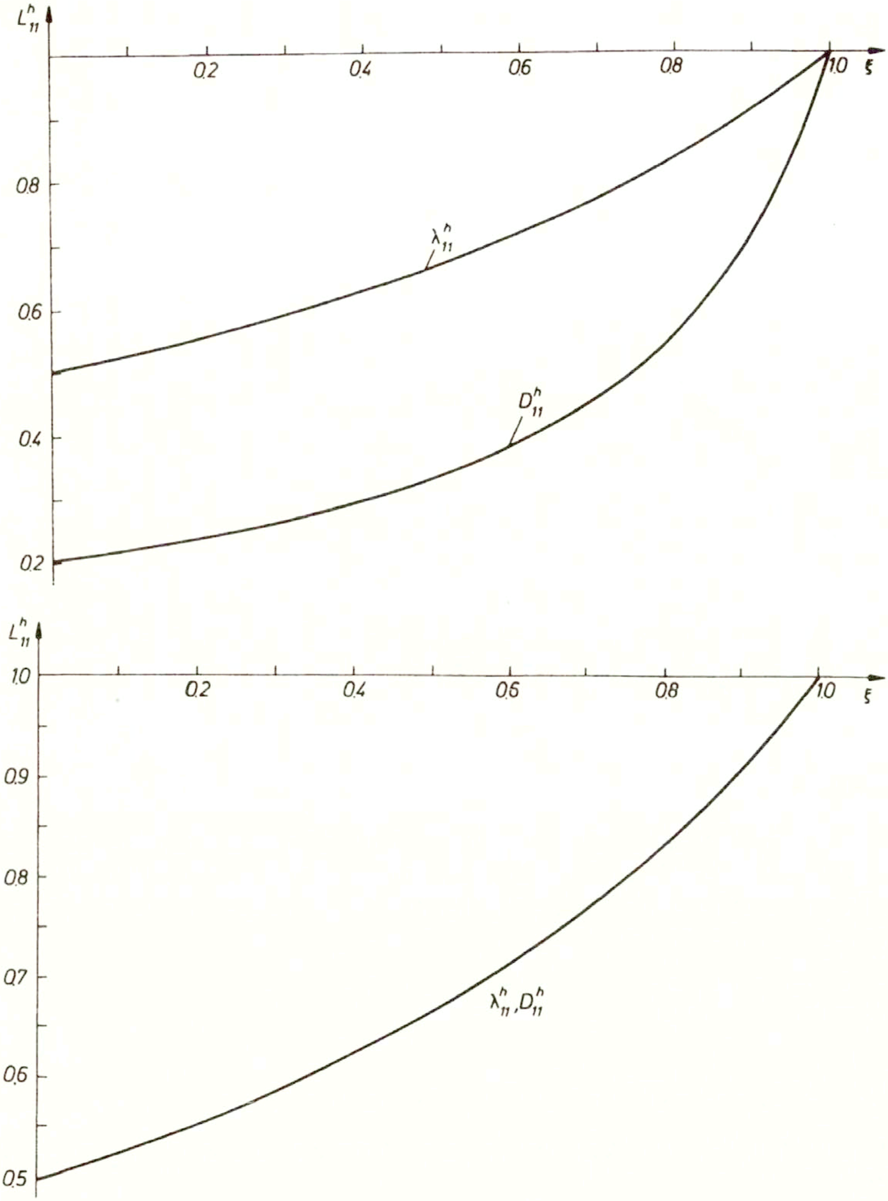

FIG. 12. a. Homogenized heat conductivity $L^{h11}_{11} = \lambda^h_{11}$ and diffusion $L^{h22}_{11} = D^h_{11}$ coefficients as the functions of ξ for $\mathfrak{u} = 1/2$ and $\mathfrak{v} = 1/5$, where

$$\mathfrak{u} = \overset{(2)}{L}{}^{11}_{11} / \overset{(1)}{L}{}^{11}_{11} = \overset{(2)}{K}{}_{11} / \overset{(1)}{K}{}_{11} = \overset{(2)}{\lambda} / \overset{(1)}{\lambda}, \quad \mathfrak{v} = \overset{(2)}{L}{}^{22}_{11} / \overset{(1)}{L}{}^{22}_{11} = \overset{(2)}{D}{}_{11} / \overset{(1)}{D}{}_{11} = \overset{(2)}{D} / \overset{(1)}{D};$$

b. Homogenized heat conductivity $L^{h11}_{11} = \lambda^h_{11}$ and diffusion $L^{h22}_{11} = D^h_{11}$ coefficients as the functions of ξ for $\mathfrak{u} = 1/2$ and $\mathfrak{v} = 1/2$; plots of L^{h11}_{11} and L^{h22}_{11} coincide. We have set:

$$\mathfrak{u} = \overset{(2)}{L}{}^{11}_{11} / \overset{(1)}{L}{}^{11}_{11} = \overset{(2)}{K}{}_{11} / \overset{(1)}{K}{}_{11} = \overset{(2)}{\lambda} / \overset{(1)}{\lambda}, \quad \mathfrak{v} = \overset{(2)}{L}{}^{22}_{11} / \overset{(1)}{L}{}^{22}_{11} = \overset{(2)}{D}{}_{11} / \overset{(1)}{D}{}_{11} = \overset{(2)}{D} / \overset{(1)}{D}.$$

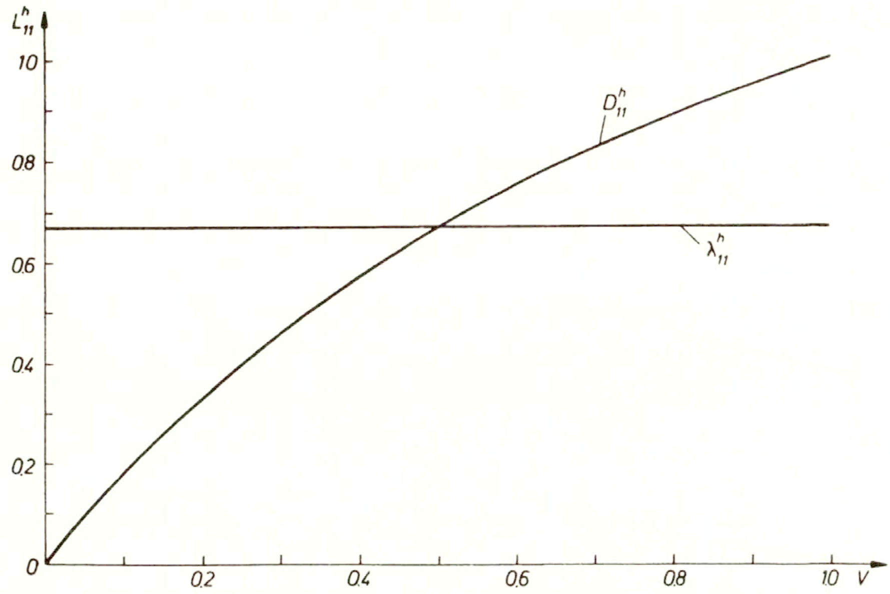

FIG. 13. Homogenized heat conductivity $L^{h11}_{11} = \lambda^h_{11}$ and diffusion $L^{h22}_{11} = D^h_{11}$ coefficients as the functions of ratio $\mathfrak{v}$ for $\mathfrak{u} = 1/2$, where

$$\mathfrak{u} = \overset{(2)}{L}{}^{11}_{11} / \overset{(1)}{L}{}^{11}_{11} = \overset{(2)}{K}{}_{11} / \overset{(1)}{K}{}_{11} = \overset{(2)}{\lambda} / \overset{(1)}{\lambda}, \quad \mathfrak{v} = \overset{(2)}{L}{}^{22}_{11} / \overset{(1)}{L}{}^{22}_{11} = \overset{(2)}{D}{}_{11} / \overset{(1)}{D}{}_{11} = \overset{(2)}{D} / \overset{(1)}{D}.$$

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Appendix

Comments on the constitutive equations and the study of the terms connected with ε^{-3}, ε^{-2}, ε^{-1} and ε^{0}

The form (2.40)–(2.42) of the constitutive realtions can be obtained from, cf. [34, 36, 135, 136],

$$\text{(A.1)} \qquad \sigma_{ij} = \frac{\partial \mathcal{U}}{\partial e_{ij}}, \qquad \Theta = \frac{\partial \mathcal{U}}{\partial s}, \qquad M = \frac{\partial \mathcal{U}}{\partial c},$$

where $\mathcal{U}(\mathbf{x}, \mathbf{e}, s, c)$ is the internal energy per unit volume. Obviously, to obtain (2.40)–(2.42) $\mathcal{U}$ has to be assumed as a general quadratic form in $\mathbf{e}$, s and c. Then it is reasonable to make the following assumption:

(A.2) $\mathcal{U}$ is a strictly convex and posistive function on $\mathbb{E}^3_s \times \mathbb{R} \times \mathbb{R}$.

The last assumption implies that the elasticity matrix $[\widetilde{c}_{ijkl}]$ is positive definite.

The free energy function $\mathcal{F}(\mathbf{x}, \mathbf{e}, \Theta, s)$ can be calculated as the partial concave conjugate of $\mathcal{U}$ with respect to s, cf. [153]

$$\mathcal{F}(\mathbf{x}, \mathbf{e}, \Theta, s) = \inf\{-\Theta s + \mathcal{U}(\mathbf{x}, \mathbf{e}, s, c) \mid s \in \mathbb{R}\}. \tag{A.3}$$

The function $\mathcal{F}$ is still strictly convex in $(\mathbf{e}, c)$, but strictly concave with respect to Θ. Consequently, the elasticity matrix $[c_{ijkl}]$ is positive definite. Eqs. (2.28)–(2.30) result from

$$\sigma_{ij} = \frac{\partial \mathcal{F}}{\partial e_{ij}}, \qquad s = -\frac{\partial \mathcal{F}}{\partial \Theta}, \qquad M = \frac{\partial \mathcal{F}}{\partial c}. \tag{A.4}$$

The partial concave conjugate of $\mathcal{U}$ with respect to (s, c) is

$$\mathcal{G}(\mathbf{x}, \mathbf{e}, \Theta, M) = \inf\{-\Theta s - Mc + \mathcal{U}(\mathbf{x}, \mathbf{e}, s, c) \mid (s, c) \in \mathbb{R} \times \mathbb{R}\}. \tag{A.5}$$

Under the assumption (A.2) the function $\mathcal{G}$ is strictly convex in $\mathbf{e}$ and jointly strictly concave in (Θ, M). Consequently, the elasticity matrix $[\overline{c}_{ijkl}]$ is positive definite and Eqs. (2.37)–(2.39) result from

$$\sigma_{ij} = \frac{\partial \mathcal{G}}{\partial e_{ij}}, \qquad s = -\frac{\partial \mathcal{G}}{\partial \Theta}, \qquad c = -\frac{\partial \mathcal{G}}{\partial M}. \tag{A.6}$$

Let us pass now to the asymptotic analysis. From the variational form of Eq. (4.11)

$$\int_Y \widetilde{c}_{ijkl}(\mathbf{y}) e_{ykl}(\mathbf{u}^{(0)}) e_{ykl}(\mathbf{v}) dy = 0 \qquad \forall \mathbf{v} \in H_{\text{per}}(Y, \mathbb{R}^3) \tag{A.7}$$

we immediately deduce that

$$e_{yij}(\mathbf{u}^{(0)}) = 0. \tag{A.8}$$

Consequently, $\mathbf{u}^{(0)}$ does not depend on $y \in Y$ and Eq. (4.9) is satisfied.

Recalling that $\mathbf{u}^{(0)}$ depends on x and t only, Eq. (4.12) simplifies to

$$0 = \frac{\partial}{\partial y_i}\left\{ L_{ij}^{\alpha\beta} \frac{\partial}{\partial y_i}\left[-\widetilde{\gamma}_{mn}^{\beta}\left(\frac{\partial u_m^{(0)}}{\partial x_n} + \frac{\partial u_m^{(1)}}{\partial y_n}\right) + \widetilde{a}^{\beta\gamma} s^{(0)\gamma}\right]\right\}. \tag{A.9}$$

The coercivity of $[L_{ij}^{\alpha\beta}(y)]$ and periodic behaviour with respect to y imply

$$-\widetilde{\gamma}_{mn}^{\beta}\left(\frac{\partial u_m^{(0)}}{\partial x_n} + \frac{\partial u_m^{(1)}}{\partial y_n}\right) + \widetilde{a}^{\beta\gamma} s^{(0)\gamma} = C^{\beta}(\mathbf{x}, t), \tag{A.10}$$

where $C^{\beta}(\mathbf{x}, t)$, $\beta = 1, 2$ are unknown functions of x and t. Hence, cf. (4.14)

$$s^{(0)\alpha} = \overline{\gamma}_{mn}^{\alpha}(\mathbf{y})\left(\frac{\partial u_m^{(0)}}{\partial x_n} + \frac{\partial u_m^{(1)}}{\partial y_n}\right) + \overline{a}^{\alpha\beta}(\mathbf{y}) C^{\beta}(\mathbf{x}, t). \tag{A.11}$$

By virtue of (A.11) we obtain the following identity:

$$\begin{aligned}\widetilde{c}_{ijkl}\left(\frac{\partial u_k^{(0)}}{\partial x_l} + \frac{\partial u_k^{(1)}}{\partial y_l}\right) - \widetilde{\gamma}_{ij}^{\alpha} s^{(0)\alpha} &= (c_{ijkl} + \widetilde{\gamma}_{ij}\gamma_{kl})\left(\frac{\partial u_k^{(0)}}{\partial x_l} + \frac{\partial u_k^{(1)}}{\partial y_l}\right) \\ &\quad -\widetilde{\gamma}_{ij}\left[\gamma_{mn}\left(\frac{\partial u_m^{(0)}}{\partial x_n} + \frac{\partial u_m^{(1)}}{\partial y_n}\right) + \overline{\gamma}_{mn}^{\beta} C^{\beta}(\mathbf{x}, t)\right] \\ &= \overline{c}_{ijkl}\left(\frac{\partial u_k^{(0)}}{\partial x_l} + \frac{\partial u_k^{(1)}}{\partial y_l}\right) - \overline{\gamma}_{ij}^{\beta} C^{\beta}(\mathbf{x}, t),\end{aligned} \tag{A.12}$$

because $\widetilde{\gamma}^{\alpha}_{ij}\overline{a}^{\alpha\beta} = \overline{\gamma}^{\beta}_{ij}$, cf. (2.59), (2.60) and

$$\widetilde{\gamma}^{\alpha}_{ij}s^{(0)\alpha} = \widetilde{\gamma}^{\alpha}_{ij}\overline{\gamma}^{\alpha}_{mn}\left(\frac{\partial u^{(0)}_m}{\partial x_n} + \frac{\partial u^{(1)}_m}{\partial y_n}\right) + \overline{\gamma}^{\beta}_{ij}C^{\beta}(\mathbf{x}, t).$$

Terms associated with ε^{-1} in Eqs. (4.7) and (4.8) yield

$$\text{(A.13)}\quad \begin{aligned} 0 &= \frac{\partial}{\partial x_j}\left[\widetilde{c}_{ijkl}\frac{\partial u^{(0)}_k}{\partial y_l}\right] + \frac{\partial}{\partial y_j}\left[\widetilde{c}_{ijkl}\left(\frac{\partial u^{(0)}_k}{\partial x_l} + \frac{\partial u^{(1)}_k}{\partial y_l}\right) - \widetilde{\gamma}^{\alpha}_{ij}s^{(0)\alpha}\right], \\ 0 &= \frac{\partial}{\partial x_i}\left\{L^{\alpha\beta}_{ij}\frac{\partial}{\partial x_j}\left[-\widetilde{\gamma}^{\beta}_{mn}\frac{\partial u^{(0)}_m}{\partial y_n}\right]\right. \\ &\quad \left. + L^{\alpha\beta}_{ij}\frac{\partial}{\partial y_j}\left[-\widetilde{\gamma}^{\beta}_{mn}\left(\frac{\partial u^{(0)}_m}{\partial y_n} + \frac{\partial u^{(1)}_m}{\partial y_n}\right) + \widetilde{a}^{\beta\gamma}s^{(0)\gamma}\right]\right\} \\ &\quad + \frac{\partial}{\partial y_i}\left\{L^{\alpha\beta}_{ij}\frac{\partial}{\partial x_j}\left[-\widetilde{\gamma}^{\beta}_{mn}\left(\frac{\partial u^{(0)}_m}{\partial x_n} + \frac{\partial u^{(1)}_m}{\partial y_n}\right) + \widetilde{a}^{\beta\gamma}s^{(0)\gamma}\right]\right. \\ &\quad \left. + L^{\alpha\beta}_{ij}\frac{\partial}{\partial y_j}\left[-\widetilde{\gamma}^{\beta}_{mn}\left(\frac{\partial u^{(1)}_m}{\partial x_n} + \frac{\partial u^{(2)}_m}{\partial y_n}\right) + \widetilde{a}^{\beta\gamma}s^{(1)\gamma}\right]\right\}. \end{aligned}$$

Taking account of (A.10) and recalling that $\mathbf{u}^{(0} = \mathbf{u}^{(0)}(\mathbf{x}, t)$, from Eqs. (A.13) we have

$$\text{(A.14)}\quad \left|\; \begin{aligned} 0 &= \frac{\partial}{\partial y_j}\left[\widetilde{c}_{ijkl}\left(\frac{\partial u^{(0)}_k}{\partial x_l} + \frac{\partial u^{(1)}_k}{\partial y_l}\right) - \widetilde{\gamma}^{\alpha}_{ij}s^{(0)\alpha}\right], \\ 0 &= \frac{\partial}{\partial y_i}\left\{L^{\alpha\beta}_{ij}\frac{\partial}{\partial x_j}C^{\beta}(\mathbf{x})\right. \\ &\quad \left. + L^{\alpha\beta}_{ij}\frac{\partial}{\partial y_j}\left[-\widetilde{\gamma}^{\beta}_{mn}\left(\frac{\partial u^{(1)}_m}{\partial x_n} + \frac{\partial u^{(2)}_m}{\partial y_n}\right) + \widetilde{a}^{\beta\gamma}s^{(1)\gamma}\right]\right\}. \end{aligned}\right.$$

By substitution of (A.12) into $(\text{A.14})_1$ we obtain, cf. (4.15)–(4.16),

$$\text{(A.15)}\quad \left|\; \begin{aligned} &\frac{\partial}{\partial y_j}\left[\overline{c}_{ijkl}\left(\frac{\partial u^{(0)}_k}{\partial x_l} + \frac{\partial u^{(1)}_k}{\partial y_l}\right)\right] = \frac{\partial\overline{\gamma}^{\beta}_{ij}}{\partial y_j}C^{\beta}(\mathbf{x}, t), \\ &\frac{\partial}{\partial y_i}\left\{L^{\alpha\beta}_{ij}\frac{\partial}{\partial y_j}\left[-\widetilde{\gamma}^{\beta}_{mn}\left(\frac{\partial u^{(1)}_m}{\partial x_n} + \frac{\partial u^{(2)}_m}{\partial y_n}\right) + \widetilde{a}^{\beta\gamma}s^{(1)\gamma}\right]\right\} \\ &\qquad = -\left(\frac{\partial}{\partial y_i}L^{\alpha\beta}_{ij}\right)\frac{\partial}{\partial x_j}C^{\beta}(\mathbf{x}, t). \end{aligned}\right.$$

The local problems yields, cf. $(5.7)_{1,2}$,

$$\text{(A.16)}\quad \begin{aligned} \frac{\partial\overline{c}_{ijkl}}{\partial y_j} &= -\frac{\partial}{\partial y_j}\left(\overline{c}_{ijmn}\frac{\partial\chi^{(kl)}_m}{\partial y_n}\right), \\ \frac{\partial\overline{\gamma}^{\alpha}_{ij}}{\partial y_j} &= \frac{\partial}{\partial y_j}\left(\overline{c}_{ijmn}\frac{\partial\Gamma^{\alpha}_m}{\partial y_n}\right). \end{aligned}$$

Substituting (A.16) into (A.14)$_1$ we find

$$-\frac{\partial}{\partial y_j}\left(\bar{c}_{ijmn}\frac{\partial \chi_m^{(kl)}}{\partial y_n}\right)\frac{\partial u_k^{(0)}}{\partial x_l} + \frac{\partial}{\partial y_j}\left(\bar{c}_{ijkl}\frac{\partial u_k^{(1)}}{\partial y_l}\right) = \frac{\partial}{\partial y_j}\left(\bar{c}_{ijmn}\frac{\partial \Gamma_m^{\beta}}{\partial y_n}\right)C^{\beta}(\mathbf{x},t).$$

Hence we have

$$\text{(A.17)}\qquad \frac{\partial}{\partial y_j}\left[\bar{c}_{ijmn}\frac{\partial}{\partial y_n}\left(-\chi_m^{(kl)}\frac{\partial u_k^{(0)}}{\partial x_l} + u_m^{(1)} - \Gamma_m^{\beta}C\beta(\mathbf{x})\right)\right] = 0,$$

and consequently

$$-\chi_m^{(kl)}\frac{\partial u_k^{(0)}}{\partial x_l} + u_m^{(1)} - \Gamma_m^{\alpha}C^{\alpha}(\mathbf{x}) = w_m(\mathbf{x},t)$$

or

$$u_m^{(1)} = -\chi_m^{(pq)}(y)\frac{\partial u_p^{(0)}}{\partial x_q} + \Gamma_m C(\mathbf{x}) + w_m(\mathbf{x},t),$$

where $w_m(\mathbf{x},t)$ remains to be determined.

Equation (A.15)$_2$ can be integrated by use of the functions $\Theta_k^{\alpha\beta}$, cf. (5.7)$_3$

$$\text{(A.19)}\qquad \frac{\partial}{\partial y_i}\left(L_{ij}^{\alpha\beta}\frac{\partial \Theta_k^{\beta\gamma}}{\partial y_j}\right) = \frac{\partial L_{ik}^{\alpha\gamma}}{\partial y_i}.$$

On account of (A.19), Eq. (A.15)$_2$ takes the form

$$\text{(A.20)}\qquad \frac{\partial}{\partial y_i}\left\{L_{ij}^{\alpha\beta}\frac{\partial}{\partial y_j}\left[-\tilde{\gamma}_{mn}^{\beta}\left(\frac{\partial u_m^{(1)}}{\partial x_n} + \frac{\partial u_m^{(2)}}{\partial y_n}\right) + \tilde{a}^{\beta\gamma}s^{(1)\gamma} + \Theta_k^{\beta\gamma}\frac{\partial C^{\gamma}(\mathbf{x},t)}{\partial x_k}\right]\right\} = 0.$$

The coercivity of $[L_{ij}^{\alpha\beta}]$ yields

$$\text{(A.21)}\qquad -\tilde{\gamma}_{mn}^{\beta}\left(\frac{\partial u_m^{(1)}}{\partial x_n} + \frac{\partial u_m^{(2)}}{\partial y_n}\right) + \tilde{a}^{\beta\gamma}s^{(1)\gamma} + \Theta_k^{\beta\gamma}\frac{\partial C^{\gamma}(\mathbf{x},t)}{\partial x_k} = A^{\beta}(\mathbf{x},t)$$

where $A^{\beta}(\mathbf{x},t)$ is a new function. Hence

$$\text{(A.22)}\qquad s^{(1)\alpha} = \bar{\gamma}_{mn}^{\alpha}\left(\frac{\partial u_m^{(1)}}{\partial x_n} + \frac{\partial u_m^{(2)}}{\partial y_n}\right) + \bar{a}^{\alpha\beta}\left[A^{\beta}(\mathbf{x},t) - \Theta_k^{\beta\gamma}\frac{\partial C^{\gamma}(\mathbf{x},t)}{\partial x_k}\right].$$

The terms appearing in Eqs. (4.7)–(4.8) and associated with ε^0 yield, cf. (4.17) and (4.18)

$$\text{(A.23)}\qquad \rho\ddot{u}_i^{(0)} = \frac{\partial}{\partial x_j}\left[\tilde{c}_{ijkl}\left(\frac{\partial u_k^{(0)}}{\partial x_l} + \frac{\partial u_k^{(1)}}{\partial y_l}\right) - \tilde{\gamma}_{ij}^{\alpha}s^{(0)\alpha}\right] + \frac{\partial}{\partial y_j}\left[\tilde{c}_{ijkl}\left(\frac{\partial u_k^{(1)}}{\partial x_l} + \frac{\partial u_k^{(2)}}{\partial y_l}\right) - \tilde{\gamma}_{ij}^{\alpha}s^{(1)\alpha}\right],$$

and

$$\dot{s}^{(0)\alpha} = \frac{\partial}{\partial x_i}\Big\{ L^{\alpha\beta}_{ij}\frac{\partial}{\partial x_j}\Big[-\widetilde{\gamma}^{\beta}_{mn}\Big(\frac{\partial u^{(0)}_m}{\partial x_n} + \frac{\partial u^{(1)}_m}{\partial y_n}\Big) + \widetilde{a}^{\beta\gamma}s^{(0)\gamma}\Big] + L^{\alpha\beta}_{ij}\frac{\partial}{\partial y_j}\Big[-\widetilde{\gamma}^{\beta}_{mn}\Big(\frac{\partial u^{(1)}_m}{\partial x_n} + \frac{\partial u^{(2)}_m}{\partial y_n}\Big) + \widetilde{a}^{\beta\gamma}s^{(1)\gamma}\Big]\Big\} + \frac{\partial}{\partial y_i}\Big\{ L^{\alpha\beta}_{ij}\frac{\partial}{\partial x_j}\Big[-\widetilde{\gamma}^{\beta}_{mn}\Big(\frac{\partial u^{(1)}_m}{\partial x_n} + \frac{\partial u^{(2)}_m}{\partial y_n}\Big) + \widetilde{a}^{\beta\gamma}s^{(1)\gamma}\Big] - L^{\alpha\beta}_{ij}\frac{\partial}{\partial y_j}\Big[-\widetilde{\gamma}^{\beta}_{mn}\Big(\frac{\partial u^{(2)}_m}{\partial x_n} + \frac{\partial u^{(3)}_m}{\partial y_n}\Big) + \widetilde{a}^{\beta\gamma}s^{(2)\gamma}\Big]\Big\}. \tag{A.24}$$

Taking account of (A.12), after averaging of (A.23) we obtain

$$\langle\rho\rangle\ddot{u}^{(0)}_i = \frac{\partial}{\partial x_j}\Big\langle \overline{c}_{ijkl}\Big(\frac{\partial u^{(0)}_k}{\partial x_l} + \frac{\partial u^{(1)}_k}{\partial y_l}\Big) - \overline{\gamma}^{\beta}_{ij}C^{\beta}(\mathbf{x},t)\Big\rangle + \langle B_i\rangle , \tag{A.25}$$

while taking account of (A.10) and (A.21), after averaging of (A.24) we get

$$\dot{s}^{(0)\alpha} = \frac{\partial}{\partial x_i}\Big\langle L^{\alpha\beta}_{ij}\frac{\partial}{\partial x_j}[C^{\beta}(\mathbf{x},t)] + L^{\alpha\beta}_{ij}\frac{\partial}{\partial y_j}\Big[-\Theta^{\beta\gamma}_{k}\frac{\partial C^{\gamma}(\mathbf{x},t)}{\partial x_k}\Big]\Big\rangle . \tag{A.26}$$

Hence, by substituting (A.18) into (A.25) and taking account of (5.5) and (5.7), the homogenized equations of **TED** body (5.2) are arrived at.

Finally substituting (A.18) into (A.11) we get

$$s^{(0)\alpha} = \Big(\overline{\gamma}^{\alpha}_{mn} + \overline{\gamma}^{\alpha}_{rs}\frac{\partial\chi^{(mn)}_r}{\partial y_s}\Big)\frac{\partial u^{(0)}_m}{\partial x_n} + \Big(\overline{a}^{\alpha\beta} + \overline{\gamma}^{\alpha}_{rs}\frac{\partial\Gamma^{\beta}_r}{\partial y_s}\Big)C^{\beta}(\mathbf{x},t) . \tag{A.27}$$

Hence, again by use of (5.5) and (5.7), homogenized Eq. (5.3) is arrived at.

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Propagation of disturbances in an unbounded inhomogeneous linearly viscoelastic material with or without invariance conditions with respect to time translations

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AS AN EXTENSION of a result given in a previous paper [2], a general domain of dependence inequality is proved for isotropic but inhomogeneous linearly viscoelastic solids, which furnishes the explicit link between the maximum propagation speed of disturbances in the body and the memory functions of the material, and allows to prove a global uniqueness theorem for the mixed problem of viscoelasticity in an unbounded reference configuration Ω. The method of proof applies regardless of whether the memory functions are assumed or not to satisfy an invariance condition with respect to time translations, so that such a condition is not required.

1. Introduction

THE FINITENESS of the propagation speed of perturbations, and the uniqueness of the motion under the assigned body forces, initial past-history and boundary conditions, are the most important topics to be investigated in the framework of the linear theory of viscoelasticity (cf. [5, 8] for a complete exposition of the basic features of the theory), and have been deeply studied by J. BARBERÀN and I. HERRERA [1] and W. S. EDELSTEIN and M. E. GURTIN [6], whose results concerning these problems are so basic as to address the subsequent research on these problems. Nevertheless, in a previous paper [2], we raised the question whether it would be possible to deduce information about the finiteness of propagation speed of disturbances in a viscoelastic solid, and about the uniqueness of viscoelastic motions, from a general estimate of the "energy" of the motion in terms of body forces and initial past-history and boundary data. An estimate of such a kind (called "domain of dependence inequality") would involve as a consequence a "domain of influence theorem" analogous to the ones proved in linear elastodynamics (cf. [3, 4, 7]), which in turn would be a basic result, allowing us to find the explicit link between the maximum propagation speed and the memory functions of the material, and to deduce uniqueness theorems as simple corollaries.

In [2], as a first step towards an affirmative answer to the above question, we proved a domain of influence theorem for homogeneous and isotropic, linearly viscoelastic bodies. Though the result of [2], when compared with the ones proved in [1, 6], seemed to have been obtained under too restrictive conditions, we observed that the method of proof adopted there seemed to suggest by itself the way to extending its results to inhomogeneous and anisotropic bodies. In this connection, the current paper gives a proof of a domain of dependence inequality (and, as a consequence, the domain of influence theorem and the uniqueness of viscoelastic motions) for isotropic but inhomogeneous viscoelastic bodies. Moreover, the memory functions of the body are not assumed to satisfy an invariance condition with respect to time translations (cf. [1] and Sec. 2 below). From a purely physical viewpoint, this circumstance could seem to be of little interest, or even in contrast with the physical principles of continuum mechanics, since such an invariance condition is needed in order to satisfy the principle of objectivity. There are, instead, at least two reasons why the choice of giving up this assumption is quite meaningful: (1) it gives a result which is *mathematically* more general and useful in the framework of the study of integro-differential equations; (2) *not all the continuum theories take into account the principle of objectivity*: for instance, the *anisotropic* linearly elastic bodies (without memory) *do not* satisfy this principle, whose violation is implied in anisotropy (when a body $\mathcal{B}$ is assumed to be anisotropic, its response functions could appear, at least for some particular relative motions of two observers $\mathcal{O}$ and $\mathcal{O}'$, to be independent of time to $\mathcal{O}$ and *time-dependent* to $\mathcal{O}'$); as a consequence, if we had found our results for anisotropic viscoelastic bodies, even retaining the invariance of the memory functions with respect to time translations, we would still have violated the objectivity principle. (This, of course, would *not* be a good reason to reject all the continuum theories dealing with anisotropic materials).

We have, in short, two ways of violating objectivity, in the framework of the linear theory of viscoelasticity: (a) giving up the invariance condition of the memory functions with respect to time translations; (b) giving up the isotropy assumption. In the current paper, we have considered the former; the latter, it is hoped, will be considered in a future work.

Thus, the present paper is to be considered as a "second step" towards the desired general result. But it also has a feature which seems to be of some interest: it explicitly deals with *unbounded* viscoelastic bodies, and points out the link between the finite speed of propagation and the behaviour of the memory functions at *spatial infinity*. An information of this kind cannot be directly deduced from the *local* uniqueness theorems given in [1].

Furthermore, the main result of the paper, in virtue of its nature of an *explicit* "domain of dependence inequality", i.e. an *a priori* estimate of the solution with respect to the boundary and initial data and the initial past-history and the body force field, may be a very helpful and manageable tool to obtain stability and continuous dependence results (of course, with respect to suitable norms) for the motions of an unbounded viscoelastic system. This problem, however, will *not* be dealt with in the present paper.

The plan of the paper follows the same scheme as [2]: Section 2 is devoted to reformulate the mixed problem of linear viscoelasticity, and to list our basic assumptions on the regularity of data and solutions, and on the properties of the memory functions. Section 3 is entirely devoted to the statement and the proof of the main theorem (the "domain of dependence inequality"). Finally, in Section 4, we recall the definition given in [2] of the "domain of influence" in the framework of linear viscoelasticity, and apply the inequality proved in Section 2 to prove the domain of influence theorem and the uniqueness theorem.

NOTATION. Light-face letters denote real numbers or functions; bold-face sans-sérif lower case letters, such as x, x_0, etc., stand for *points* in a three-dimensional (real) point space E; bold-face lower case letters are *vectors* on E, i.e., the translations on E; bold-face upper case letters denote *second-order tensors*, i.e. linear mappings from the whole space of vectors into itself. The second-order tensor $\mathbf{I}$ maps every vector $\mathbf{v}$ onto itself.

We denote by $\boldsymbol{o}$ the origin of an (arbitrarily) assigned reference frame $(\boldsymbol{o}, \{\mathbf{e}_i\}_{1\leq i\leq 3})$ on E, and, for any $\mathsf{x} \in E$, we set $\mathsf{x} - \mathsf{o} = x^h\mathbf{e}_h$ (here and in the sequel, whenever the index notation will be used, the summation over repeated indexes is implied). We also set $|\mathbf{x}-\mathbf{o}| = \sqrt{\sum_{h=1}^{3}(x^h)^2}$. Moreover, for any pair of points $\mathbf{x}_0 = x_0^h\mathbf{e}_h$ and $\mathbf{x} = x^h\mathbf{e}_h$, $\mathbf{x}-\mathbf{x}_0$ is the vector $(x^i - x_0^i)\mathbf{e}_i$ and $|\mathbf{x}-\mathbf{x}_0| = \sqrt{\sum_i (x^i - x_0^i)^2}$. Finally $\mathbf{e}_r^{(0)} = |\mathbf{x}-\mathbf{x}_0|^{-1}(\mathbf{x}-\mathbf{x}_0)$.

For any $\mathbf{x}_0 \in E$, and for any $R > 0$, we denote by the symbol $B(\mathbf{x}_0, R)$ the ball centered at $\mathbf{x}_0$ of radius R. Its boundary will be referred to as $S(\mathbf{x}_0, R)$. For any open connected set $\Omega \subset E$, we set $\Omega(\mathbf{x}_0, R) = \Omega \cap B(\mathbf{x}_0, R)$ and $\Sigma(\mathbf{x}_0, R) = \Omega \cap S(\mathbf{x}_0, R)$. We denote by $\mathbf{n}$ the outer unit normal vector to the boundary $\partial\Omega$ of Ω at each point.

For any scalar function f of the couple $(\mathbf{x}, t) \in E \times \mathbb{R}$, we denote by $f_{,i} = \partial_i f$ its derivative with respect to the i-th coordinate x^i of $\mathbf{x}$ in $(o, \{\mathbf{e}_i\}_{1\le i\le 3})$, and by $\dot{f}$ its derivative with respect to the (time) variable t. If $f \equiv f(t,s)$ is a function on the set $\{(t,s) \in \mathbb{R}^2 : t \in \mathbb{R},\ s \in (-\infty, t]\}$, we use the symbol $\overline{f}$ to denote the partial derivative of f with respect to s. Furthermore

$$\dot{f}(\mathbf{x}, t, t) = \left.\frac{\partial f}{\partial t}(\mathbf{x}, t, s)\right|_{s=t},$$

$$\overline{f}(\mathbf{x}, t, t) = \left.\frac{\partial f}{\partial s}(\mathbf{x}, t, s)\right|_{s=t}$$

and

$$\dot{\overline{f}}(\mathbf{x}, t, s) = \frac{\partial^2 f}{\partial t \partial s}(\mathbf{x}, t, s).$$

At need, we shall also use the symbol

$$\mathring{f}(\mathbf{x}, t, t) \equiv \dot{f}(\mathbf{x}, t, t) + \overline{f}(\mathbf{x}, t, t).$$

If $\mathbf{v} = v^h\mathbf{e}_h$ is a vector field on $\Omega \times (a,b)$ (with $\Omega \subseteq E$ and $(a,b) \subseteq \mathbb{R}$), we have $\dot{\mathbf{v}} = \dot{v}^h\mathbf{e}_h$ and, as usual, $\nabla\mathbf{v} \equiv (\mathbf{v}^h_{,k})_{\substack{1\le h\le 3\\ 1\le k\le 3}}$, $\operatorname{div}\mathbf{v} = \sum_i v^i_{,i}$. For a tensor function $\mathbf{T} \equiv (T_{hk})_{\substack{1\le h\le 3\\ 1\le k\le 3}}$, $\operatorname{div}\mathbf{T} = T_{hk,k}e_h$.

2. Position of the problem. Hypotheses

Let $\mathcal{B}$ be a continuous solid body, identified with the open connected set $\Omega \subseteq E$ it occupies in an assigned reference configuration: as is well known, the motion of $\mathcal{B}$ in the time-interval $(0, \infty)$, obeys the system

$$\rho\ddot{\mathbf{u}} = \operatorname{div}\mathbf{T} + \rho\mathbf{b}, \qquad \text{on } Q = \Omega \times (0, \infty), \tag{2.1}$$

where $\rho = \rho(\mathbf{x})$ is the density field in the reference configuration, $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ is the (unknown) displacement vector field on Q, and $\mathbf{b} = \mathbf{b}(\mathbf{x}, t)$ is the (assigned) body force vector field on Q. The second-order tensor field $\mathbf{T} = \mathbf{T}(\mathbf{x}, t)$ is the *stress* field, which depends on the strain

$$\mathbf{E} = \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T). \tag{2.2}$$

The link between $\mathbf{T}$ and $\mathbf{E}$ is expressed by a *constitutive relation* $\mathbf{T} = \mathbf{T}(\mathbf{E})$, which defines the class of materials under consideration: we assume that $\mathcal{B}$ is an *inhomogeneous* but *isotropic* linearly viscoelastic solid, so that the functional $\mathbf{T}(\mathbf{E})$ is expressed by the relation

$$(2.3)\qquad \mathbf{T}(\mathbf{x},t) = \lambda(\mathbf{x},t,t)[\operatorname{div}\mathbf{u}(\mathbf{x},t)]\mathbf{I} + 2\mu(\mathbf{x},t,t)\mathbf{E}(\mathbf{x},t) + \int_{-\infty}^{t} \{\overline{\lambda}(\mathbf{x},t,s)[\operatorname{div}\mathbf{u}(\mathbf{x},s)]\mathbf{I} + 2\overline{\mu}(\mathbf{x},t,s)\mathbf{E}(\mathbf{x},s)\}\, ds$$

for $(\mathbf{x},t) \in \overline{Q}$. The functions $\lambda : (\mathbf{x},t,s) \in E \times \mathbb{R} \times (-\infty,t] \longrightarrow \lambda(\mathbf{x},t,s) \in (0,\infty)$ and $\mu : (\mathbf{x},t,s) \in E \times \mathbb{R} \times (-\infty,t] \longrightarrow \mu(\mathbf{x},t,s) \in (0,\infty)$ are *memory functions* of the material. Relation (2.3) simply tells us that the stress distribution on Ω at each instant $t \in \mathbb{R}$ depends not only on the deformation at the same instant, but also on the *history* of deformation in the whole time-interval $(-\infty,t)$, i.e. on all the deformations experienced by the body $\mathcal{B}$ in the past.

The assumption of invariance of λ and μ with respect to time translations is expressed by the conditions

$$(2.4)\qquad \lambda(\mathbf{x},\tau_1,\tau_1) = \lambda(\mathbf{x},\tau_2,\tau_2), \qquad \mu(\mathbf{x},\tau_1,\tau_1) = \mu(\mathbf{x},\tau_2,\tau_2)\,, \qquad \forall\tau_1,\tau_2 \in \mathbb{R}\,.$$

In the sequel, however, these conditions will *not* be assumed to be satisfied.

In order to determine the future evolution of the body, once the body forces acting on $\mathcal{B}$ and the contact actions on its boundary $\partial\mathcal{B}$ (when not empty) are assigned at each instant, and its past history is known, we have to find a solution $\mathbf{u}$ to System (2.1)–(2.2)–(2.3) satisfying the *initial past-history condition*

$$(2.5)\qquad \mathbf{u} = \mathbf{u}_0 \quad \text{on } \overline{\Omega} \times (-\infty,0]$$

and the *boundary conditions*

$$(2.6)\qquad \begin{aligned} \mathbf{u} &= \widehat{\mathbf{u}} \quad \text{on } \partial_1\Omega \times (0,\infty)\,,\\ \mathbf{Tn} &= \widehat{\mathbf{s}} \quad \text{on } \partial_2\Omega \times (0,\infty)\,, \end{aligned}$$

where

$$\partial_1\Omega \cup \partial_2\Omega = \partial\Omega \quad \text{and} \quad \partial_1\Omega \cap \partial_2\Omega = \emptyset\,.$$

We assume that the reference configuration Ω of $\mathcal{B}$ is *unbounded* and, if $\partial\Omega \neq \emptyset$, is so regular as to allow the application of the divergence theorem. The data are assumed to satisfy the conditions

(1) ρ is continuous and strictly positive on $\overline{\Omega}$, and $\mathbf{b}$ is continuous on $\overline{Q}$;

(2) $\mathbf{u}_0$ is twice continuously differentiable with respect to space and time on $\overline{\Omega} \times (-\infty,0]$;

(3) $\widehat{\mathbf{u}}$ is continuous on $\partial_1\Omega \times [0,\infty)$ together with its time derivative $\dot{\widehat{\mathbf{u}}}$;

(4) $\widehat{\mathbf{s}}$ is continuous on $\partial_2\Omega \times [0,\infty)$,

and we confine ourselves to consider only solutions $\mathbf{u}$ that are twice continuously differentiable on $\overline{Q}$ with respect to all the variables. Accordingly, in the sequel, the phrase "a solution to System (2.1)–. . .–(2.3)–(2.5)–(2.6)" will always denote a regular solution in the above specified sense.

As far as the memory functions are concerned, we assume that

A) the transformation $\mathbf{E} \longrightarrow \mathbf{T}(\mathbf{E})$ is *initially positive definite*, i.e.

$$\lambda(\mathbf{x},t,t) > 0 \quad \text{and} \quad \mu(\mathbf{x},t,t) > 0\,, \quad \forall t \in \mathbb{R};$$

B) $\lambda \in C^2(\overline{\Omega} \times [\bigcup_{t\in\mathbb{R}}(\{t\} \times (-\infty, t])])$ and $\mu \in C^2(\overline{\Omega} \times [\bigcup_{t\in\mathbb{R}}(\{t\} \times (-\infty, t])])$;

C) for any $\mathbf{x} \in \overline{\Omega}$, and for any $t \in \mathbb{R}$, the functions $\overline{\lambda}(\mathbf{x}, t, s)$ and $\overline{\mu}(\mathbf{x}, t, s)$ are summable on $(-\infty, t]$;

D) a smooth, increasing and convex function $q : \xi \in [0, \infty) \longrightarrow q(\xi) \in [0, \infty)$ and a smooth function $\kappa : t \in \mathbb{R} \longrightarrow \kappa(t) \in [0, \infty)$ exist such that

$$\lim_{\xi\to\infty} q(\xi) = \infty\,,$$

$$q'(|\mathbf{x} - \mathbf{o}|)U_L(\mathbf{x}, t) \leq \kappa(t), \qquad \forall(\mathbf{x}, t) \in \overline{\Omega} \times \mathbb{R}\,,$$

where, for any $\mathbf{x} \in \overline{\Omega}$ and for any $t \in \mathbb{R}$,

$$U_L(\mathbf{x}, t) = \sqrt{\frac{\lambda(\mathbf{x}, t, t) + 2\mu(\mathbf{x}, t, t)}{\rho(\mathbf{x})}}\,;$$

E) for any $T > 0$, the two functions

$$\overline{\ell}_T(\mathbf{x}) = \sup_{(0,T)}\left(\sup_{(0,t)} \frac{|\overline{\lambda}(\mathbf{x}, t, s)|}{\lambda(\mathbf{x}, s, s)}\right), \qquad \overline{m}_T(x) = \sup_{(0,T)}\left(\sup_{(0,t)} \frac{|\overline{\mu}(\mathbf{x}, t, s)|}{\mu(\mathbf{x}, s, s)}\right),$$

are bounded on $\overline{\Omega}$.

We must now observe that, by virtue of our assumptions A) and B), the four functions

$$\dot{\ell}_T(\mathbf{x}) = \sup_{(0,T)} \frac{|\dot{\lambda}(x, t, t)|}{\lambda(\mathbf{x}, t, t)}, \qquad \dot{m}_T(\mathbf{x}) = \sup_{(0,T)} \frac{|\dot{\mu}(\mathbf{x}, t, t)|}{\mu(\mathbf{x}, t, t)},$$

$$\dot{\overline{\ell}}_T(\mathbf{x}) = \sup_{(0,T)}\left(\sup_{(0,t)} \frac{|\dot{\overline{\lambda}}(\mathbf{x}, t, s)|}{\lambda(\mathbf{x}, s, s)}\right), \qquad \dot{\overline{m}}_T(\mathbf{x}) = \sup_{(0,T)}\left(\sup_{(0,t)} \frac{|\dot{\overline{\mu}}(\mathbf{x}, t, s)|}{\mu(\mathbf{x}, s, s)}\right),$$

are continuous on $\overline{\Omega}$ for any $T > 0$. Accordingly, if, for any $T > 0$, we agree to set

$$K = K(T) = \sup_{(0,T)} |\kappa(t)|\,,$$

$$k_1 = k_1(T) = \max\{\sup_{\Omega} \overline{\ell}_T(\mathbf{x})\,,\ \sup_{\Omega} \overline{m}_T(\mathbf{x})\}\,,$$

and, for any arbitrarily assigned $\varepsilon \in (0, 1)$,

$$c_\varepsilon = c_\varepsilon(T) = \frac{2(Tk_1(T) + 1)K(T)}{1 - \varepsilon}\,,$$

we are also allowed to consider, for any $\mathbf{x}_0 \in \overline{\Omega}$ and for any $R > 0$ and $T > 0$, the functions

$$k_0 = k_0(\mathbf{x}_0, T) = \max\{\sup_{\Omega(\mathbf{x}_0, q^{-1}(q(R+r_0)+c_\varepsilon T)-r_0)} \dot{\ell}_T(\mathbf{x})\,,\ \sup_{\Omega(\mathbf{x}_0, q^{-1}(q(R+r_0)+c_\varepsilon T)-r_0)} \dot{m}_T(\mathbf{x})\}\,,$$

$$k_2 = k_2(\mathbf{x}_0, T) = \max\{\sup_{\Omega(x_0, q^{-1}(q(R+r_0)+c_\varepsilon T)-r_0)} \dot{\overline{\ell}}_T(\mathbf{x})\,,\ \sup_{\Omega(x_0, q^{-1}(q(R+r_0)+c_\varepsilon T)-r_0)} \dot{\overline{m}}_T(\mathbf{x})\}\,,$$

where $r_0 = |\mathbf{x}_0 - \mathbf{o}|$.

3. The main result

This Section is devoted to the statement and the proof of our main result, namely, a *domain of dependence inequality*, which, as already pointed out in [2], will be the basic tool in the study of the propagation speed of perturbations in $\mathcal{B}$. To this aim, following step by step the method used in [2], we first re-write Eq. (2.1) and Relation (2.3) in a more convenient form: we set

$$\mathbf{T}_t(\mathbf{x},t) = \lambda(\mathbf{x},t,t)[\operatorname{div}\mathbf{u}(\mathbf{x},t)]\mathbf{I} + 2\mu(\mathbf{x},t,t)\mathbf{E}(\mathbf{x},t),$$

$$\mathbf{T}_{(0,t)}(\mathbf{x},t) = \int_0^t \{\overline{\lambda}(\mathbf{x},t,s)[\operatorname{div}\mathbf{u}(\mathbf{x},s)]\mathbf{I} + 2\overline{\mu}(\mathbf{x},t,s)\mathbf{E}(\mathbf{x},s)\}\,ds,$$

$$\mathbf{T}_0(\mathbf{x},t) = \int_{-\infty}^0 \{\overline{\lambda}(\mathbf{x},t,s)[\operatorname{div}\mathbf{u}(\mathbf{x},s)]\mathbf{I} + 2\overline{\mu}(\mathbf{x},t,s)\mathbf{E}(\mathbf{x},s)\}\,ds,$$

so that Relation (2.3) is equivalent to

$$\mathbf{T}(\mathbf{x},t) = \mathbf{T}_0(\mathbf{x},t) + \mathbf{T}_{(0,t)}(\mathbf{x},t) + \mathbf{T}_t(\mathbf{x},t), \qquad \forall(\mathbf{x},t) \in Q,$$

and we are allowed to write Eq. (2.1) in the form

$$\rho\ddot{\mathbf{u}} = \operatorname{div}\mathbf{T}_t + \operatorname{div}\mathbf{T}_{(0,t)} + \operatorname{div}\mathbf{T}_0 + \rho\mathbf{b}, \qquad \text{on } Q. \tag{3.1}$$

Next, we set

$$\eta(\mathbf{x},\tau) = \frac{1}{2}\Big(\rho\dot{\mathbf{u}}^2 + \lambda(\mathbf{x},\tau,\tau)[\operatorname{div}\mathbf{u}(\mathbf{x},\tau)]^2 + 2\mu(\mathbf{x},\tau,\tau)\mathbf{E}^2(\mathbf{x},\tau)\Big) \equiv \frac{1}{2}\Big(\rho\dot{\mathbf{u}}^2 + \mathbf{T}_\tau\cdot\nabla\mathbf{u}\Big), \tag{3.2}$$

and take the inner product of both sides of Eq. (3.1) by $\dot{\mathbf{u}}$: taking also into account the identity

$$\mathbf{T}_\tau(\mathbf{x},\tau)\cdot\nabla\dot{\mathbf{u}}(\mathbf{x},\tau) = (\mathbf{T}_\tau\cdot\nabla\mathbf{u})\dot{}(\mathbf{x},\tau) - \mathring{\lambda}(\mathbf{x},\tau,\tau)[\operatorname{div}\mathbf{u}(\mathbf{x},\tau)]^2 + 2\mathring{\mu}(\mathbf{x},\tau,\tau)|\mathbf{E}(\mathbf{x},\tau)|^2 - \mathbf{T}_\tau(\mathbf{x},\tau)\cdot\nabla\dot{\mathbf{u}}(\mathbf{x},\tau),$$

we find at once

$$\dot{\eta}(\mathbf{x},\tau) = \operatorname{div}(\mathbf{T}_\tau\dot{\mathbf{u}})(\mathbf{x},\tau) + \frac{1}{2}\{\mathring{\lambda}(\mathbf{x},\tau,\tau)[\operatorname{div}\mathbf{u}(\mathbf{x},\tau)]^2 + 2\mathring{\mu}(\mathbf{x},\tau,\tau)|\mathbf{E}(\mathbf{x},\tau)|^2\} + \operatorname{div}(\mathbf{T}_{(0,\tau)}\dot{\mathbf{u}})(\mathbf{x},\tau) - (\mathbf{T}_{(0,\tau)}\cdot\nabla\mathbf{u})\dot{}(\mathbf{x},\tau) + (\dot{\mathbf{T}}_{(0,\tau)}\cdot\nabla\mathbf{u})(\mathbf{x},\tau) + (\boldsymbol{\delta}_0\cdot\dot{\mathbf{u}})(\mathbf{x},\tau), \tag{3.3}$$

for any $(\mathbf{x},\tau) \in Q$, where, as in [2],

$$\boldsymbol{\delta}_0(\mathbf{x},\tau) = \operatorname{div}\mathbf{T}_0(\mathbf{x},\tau) + \rho\mathbf{b}(\mathbf{x},\tau).$$

It should be carefully noted that $\boldsymbol{\delta}_0$ is a vector independent of the solution of problem (2.1)–. . .–(2.5), since it is obviously fully determined by the (assigned) initial past-history and the (assigned) body force field. As a consequence, we may simply treat it as a "source term". In this connection, we also explicitly notice that the initial-past history $\mathbf{u}_0$ is assumed to be assigned suitably, so that $\mathbf{T}_0$ turns out to be a well-defined C^2 tensor function on $\overline{\Omega}\times[0,\infty)$.

This stated, we are in a position to prove the following

THEOREM 1 (Domain of dependence inequality). *Let* $\mathbf{u}$ *be any solution to System* (2.1)–. . .–(2.5), *and let assumptions* (1)–. . .–(4), *A*)–. . .–*C*) *of Sec. 2 be fulfilled. Then,*

$\forall\varepsilon \in (0,1)$, $\forall T > 0$, $\forall R > 0$ and $\forall \mathbf{x}_0 \in \Omega$, two continuous functions $H(t) = H(\mathbf{x}_0, T, t)$ and $\varphi(t) = \varphi(\varepsilon; \mathbf{x}_0, T, t)$ on $\mathbb{R}$ exist such that

$$(3.4)\quad \int_0^T \Bigg(\int_0^t d\tau \int_{\Omega(\mathbf{x}_0, q^{-1}(q(R+r_0)+c_\varepsilon(T-\tau))-r_0)} \eta(\mathbf{x},\tau)\,dv \Bigg) dt$$

$$\le \exp[\varphi(T)] \int_0^T \exp[H(t)-\varphi(t)] \Bigg(\int_0^t \Bigg\{ 2 \int_{\Omega(\mathbf{x}_0, q^{-1}(q(R+r_0)+c_\varepsilon T)-r_0)} \eta(\mathbf{x},0)\,dv$$

$$+2 \int_0^T \Bigg[\int_{\partial\Omega\cap B(\mathbf{x}_0, q^{-1}(q(R+r_0)+c_\varepsilon(T-s))-r_0)} (\mathbf{n}\cdot\mathbf{T}_s\dot{\mathbf{u}})(\mathbf{x},s)\,da$$

$$+ \int_{\partial\Omega\cap B(\mathbf{x}_0, q^{-1}(q(R+r_0)+c_\varepsilon(T-s))-r_0)} (\mathbf{n}\cdot\mathbf{T}_{(0,s)}\dot{\mathbf{u}})(\mathbf{x},s)\,da$$

$$+T \int_{\Omega(\mathbf{x}_0, q^{-1}(q(R+r_0)+c_\varepsilon(T-s))-r_0)} (\rho^{-1}[\div\mathbf{T}_0]^2 + \rho\mathbf{b}^2)(\mathbf{x},s)\,dv \Bigg] ds \Bigg\} d\tau \Bigg) dt\,. \quad \square$$

P r o o f. Throughout the whole proof, $R > 0$ and $T > 0$ will be hold fixed and treated as constants.

Let $w : \lambda \in \mathbb{R} \longrightarrow w(\lambda) \in \mathbb{R}$ be any smooth and increasing function such that

$$w(\lambda) = 0, \qquad \forall\,\lambda \in (-\infty, 0]\,,$$
$$w(\lambda) = 1, \qquad \forall\,\lambda \in [1, +\infty)\,,$$

and, for fixed R and T in $(0,\infty)$, set

$$g(\mathbf{x}_0; \mathbf{x}, \tau) = w\Big(\frac{1}{c_\varepsilon\delta}(q(R+r_0) + c_\varepsilon(T-\tau) - q(|\mathbf{x}-\mathbf{x}_0| + r_0)) \Big)\,.$$

It is readily seen that g has a compact support in $E \times [0,\infty)$, namely, the set

$$\mathcal{S} = \bigcup_{\tau\in[0,T]} B(\mathbf{x}_0, q^{-1}(q(R+r_0) + c_\varepsilon(T-\tau)) - r_0) \times \{\tau\}\,.$$

Furthermore, we must observe that $g \equiv 1$ on the whole set

$$\bigcup_{\tau\in[0,T]} B(\mathbf{x}_0, q^{-1}(q(R+r_0) + c_\varepsilon(T-\tau-\delta)) - r_0) \times \{\tau\}\,,$$

so that $\nabla g \equiv 0$ on this set, and g turns out to be smooth on the whole of E even if its derivative with respect to $|\mathbf{x}-\mathbf{x}_0|$ is not defined on the time axis $\mathbf{x} = \mathbf{x}_0$.

Throughout the remainder of the proof, in order to simplify the notation, and to avoid lengthy and complicated formulae, we shall set

$$R^\star_\tau = q^{-1}(q(R+r_0) + c_\varepsilon(T-\tau)) - r_0\,,$$

so that $R^\star_0 = q^{-1}(q(R+r_0)+c_\varepsilon T) - r_0$ and $R^\star_{\tau+\delta} = q^{-1}(q(R+r_0)+c_\varepsilon(T-\tau-\delta)) - r_0$.

Multiply both sides of (3.3) by $g(\mathbf{x}_0; \mathbf{x}, \tau)$, to get

$$(g\eta)^{\cdot}(\mathbf{x},\tau) = (\dot{g}\eta)(\mathbf{x},\tau) + \operatorname{div}(g\mathbf{T}_\tau\dot{\mathbf{u}})(\mathbf{x},\tau) - (\nabla g\cdot\mathbf{T}_\tau\dot{\mathbf{u}})(\mathbf{x},\tau) + \frac{g}{2}\{\mathring{\lambda}(\mathbf{x},\tau,\tau)[\operatorname{div}\mathbf{u}(\mathbf{x},\tau)]^2$$
$$+2\mathring{\mu}(\mathbf{x},\tau,\tau)|\mathbf{E}(\mathbf{x},\tau)|^2\} + \operatorname{div}(g\mathbf{T}_{(0,\tau)}\dot{\mathbf{u}})(\mathbf{x},\tau) - (\nabla g\cdot\mathbf{T}_{(0,\tau)}\dot{\mathbf{u}})(\mathbf{x},\tau)$$
$$-(g\mathbf{T}_{(0,\tau)}\cdot\nabla\mathbf{u})^{\cdot}(\mathbf{x},\tau) + (\dot{g}\mathbf{T}_{(0,\tau)}\cdot\nabla\mathbf{u})(\mathbf{x},\tau) + (g\dot{\mathbf{T}}_{(0,\tau)}\cdot\nabla\mathbf{u})(\mathbf{x},\tau) + (g\boldsymbol{\delta}_0\cdot\dot{\mathbf{u}})(\mathbf{x},\tau);$$

integration over Ω leads to

$$\frac{d}{d\tau}\int_\Omega (g\eta)(\mathbf{x},\tau)\,dv = \int_\Omega(\dot{g}\eta)(\mathbf{x},\tau)\,dv + \int_{\partial\Omega}(g\mathbf{n}\cdot\mathbf{T}_\tau\dot{\mathbf{u}})(\mathbf{x},\tau)\,da$$
$$+\int_\Omega\frac{g}{2}\{\mathring{\lambda}(\mathbf{x},\tau,\tau)[\operatorname{div}\mathbf{u}(\mathbf{x},\tau)]^2 + 2\mathring{\mu}(\mathbf{x},\tau,\tau)|\mathbf{E}(\mathbf{x},\tau)|^2\}\,dv - \int_\Omega(\nabla g\cdot\mathbf{T}_\tau\dot{\mathbf{u}})(\mathbf{x},\tau)\,dv$$
$$+\int_{\partial\Omega}(g\mathbf{n}\cdot\mathbf{T}_{(0,\tau)}\dot{\mathbf{u}})(\mathbf{x},\tau)\,da - \int_\Omega(\nabla g\cdot\mathbf{T}_{(0,\tau)}\dot{\mathbf{u}})(\mathbf{x},\tau)\,dv$$
$$-\frac{d}{d\tau}\int_\Omega(g\mathbf{T}_{(0,\tau)}\cdot\nabla\mathbf{u})(\mathbf{x},\tau)\,dv + \int_\Omega(\dot{g}\mathbf{T}_{(0,\tau)}\cdot\nabla\mathbf{u})(\mathbf{x},\tau)\,dv$$
$$+\int_\Omega(g\dot{\mathbf{T}}_{(0,\tau)}\cdot\nabla\mathbf{u})(\mathbf{x},\tau)\,dv + \int_\Omega(g\boldsymbol{\delta}_0\cdot\dot{\mathbf{u}})(\mathbf{x},\tau)\,dv;$$

so that, taking into account that

$$\dot{g}(\mathbf{x}_0;\mathbf{x},\tau) = -\frac{1}{\delta}w'(q(R+r_0) + c_\varepsilon(T-\tau) - q(|\mathbf{x}-\mathbf{x}_0| + r_0)),$$
$$\nabla g(\mathbf{x}_0;\mathbf{x},\tau) = -\frac{1}{c_\varepsilon\delta}w'(q(R+r_0) + c_\varepsilon(T-\tau) - q(|\mathbf{x}-\mathbf{x}_0| + r_0))e_r^{(0)},$$

by virtue of the inequalities

$$\frac{1}{2}\{\mathring{\lambda}(\mathbf{x},\tau,\tau)[\operatorname{div}\mathbf{u}(\mathbf{x},\tau)]^2 + 2\mathring{\mu}(\mathbf{x},\tau,\tau)|\mathbf{E}(\mathbf{x},\tau)|^2\} \le (k_0+k_1)\eta(\mathbf{x},\tau)$$

and

$$\mathbf{T}_\tau\dot{\mathbf{u}} \le 2U_L\eta;$$

$$|\mathbf{T}_{(0,\tau)}\dot{\mathbf{u}}| = \left|\int_0^\tau \overline{\lambda}(\mathbf{x},\tau,s)[\operatorname{div}\mathbf{u}(\mathbf{x},s)]\dot{\mathbf{u}}(\mathbf{x},\tau)\,ds + 2\int_0^\tau\overline{\mu}(\mathbf{x},\tau,s)\mathbf{E}(\mathbf{x},s)\dot{\mathbf{u}}(\mathbf{x},\tau)\,ds\right|$$
$$\le \int_0^\tau|\overline{\lambda}(\mathbf{x},\tau,s)|\,|\operatorname{div}\mathbf{u}(\mathbf{x},s)|\,|\dot{\mathbf{u}}(\mathbf{x},\tau)|\,ds + 2\int_0^\tau|\overline{\mu}(\mathbf{x},\tau,s)|\,|\mathbf{E}(\mathbf{x},s)|\,|\dot{\mathbf{u}}(\mathbf{x},\tau)|\,ds$$
$$\le k_1U_L\left(\frac{\tau}{T}\int_0^\tau\eta(\mathbf{x},s)\,ds + 2T\eta(\mathbf{x},\tau)\right);$$

$$\text{(3.5)}\qquad \mathbf{T}_{(0,\tau)}\cdot\nabla\mathbf{u} = \nabla\mathbf{u}\cdot\int_0^\tau\{\overline{\lambda}(\mathbf{x},\tau,s)[\operatorname{div}\mathbf{u}(\mathbf{x},s)]\mathbf{I} + 2\overline{\mu}(\mathbf{x},\tau,s)\mathbf{E}(\mathbf{x},s)\}\,ds$$
$$\le \varepsilon\eta + k_1^2\tau\varepsilon^{-1}\int_0^\tau\eta(\mathbf{x},s)\,ds;$$

(3.5) [cont.]
$$\dot{\mathbf{T}}_{(0,\tau)}\cdot\nabla\mathbf{u} = \overline{\lambda}(\mathbf{x},\tau,\tau)[\operatorname{div}\mathbf{u}(\mathbf{x},\tau)]^2 + 2\overline{\mu}(\mathbf{x},\tau,\tau)\mathbf{E}^2(\mathbf{x},\tau)$$
$$+\nabla\mathbf{u}\cdot\int_0^\tau\{\dot{\overline{\lambda}}(\mathbf{x},\tau,s)[\operatorname{div}\mathbf{u}(\mathbf{x},s)]\mathbf{I} + 2\dot{\overline{\mu}}(\mathbf{x},\tau,s)\mathbf{E}(\mathbf{x},s)\}\,ds$$
$$\le (k_1 + k_2T)\eta + k_2\frac{\tau}{T}\int_0^\tau \eta(\mathbf{x},s)\,ds;$$
$$\boldsymbol{\delta}_0\cdot\dot{\mathbf{u}} \le \frac{1}{2}\frac{T}{\rho}\boldsymbol{\delta}_0^2 + T^{-1}\eta,$$

we arrive at

$$\frac{d}{d\tau}\int_\Omega (g\eta)(\mathbf{x},\tau)\,dv \le \frac{1}{\delta}\int_\Omega\Big[\Big(-1+\varepsilon+\frac{2(k_1T+1)K}{c_\varepsilon}\Big)\eta\Big](\mathbf{x},\tau)\,dv + \int_{\partial\Omega}(g\mathbf{n}\cdot\mathbf{T}_\tau\dot{\mathbf{u}})(\mathbf{x},\tau)\,da$$
$$+\int_{\partial\Omega}(g\mathbf{n}\cdot\mathbf{T}_{(0,\tau)}\dot{\mathbf{u}})(\mathbf{x},\tau)\,da + \frac{k_1K\tau}{c_\varepsilon T\delta}\int_0^\tau ds\int_\Omega w'\eta(\mathbf{x},s)\,dv$$
$$-\frac{d}{d\tau}\int_\Omega (g\mathbf{T}_{(0,\tau)}\cdot\nabla\mathbf{u})(\mathbf{x},\tau)\,dv + \frac{k_1^2\tau}{\varepsilon\delta}\int_0^\tau ds\int_\Omega w'\eta(\mathbf{x},s)\,dv$$
$$+(k_0+2k_1+k_2T)\int_\Omega (g\eta)(\mathbf{x},\tau)\,dv + k_2\frac{\tau}{T}\int_0^\tau ds\int_\Omega (g\eta)(\mathbf{x},s)\,dv$$
$$+\frac{1}{2}T\int_\Omega (g\rho^{-1}\boldsymbol{\delta}_0^2)(\mathbf{x},\tau)\,dv + T^{-1}\int_\Omega (g\eta)(\mathbf{x},\tau)\,dv.$$

Recalling the definition of c_ε,

$$\frac{d}{d\tau}\int_\Omega (g\eta)(\mathbf{x},\tau)\,dv \le -\frac{d}{d\tau}\int_\Omega (g\mathbf{T}_{(0,\tau)}\cdot\nabla\mathbf{u})(\mathbf{x},\tau)\,dv + (k_0+2k_1+k_2T+T^{-1})$$
$$\times\int_\Omega (g\eta)(\mathbf{x},\tau)\,dv + \frac{1}{\delta}\Big(\frac{k_1K\tau}{c_\varepsilon T}+\frac{k_1^2\tau}{\varepsilon}\Big)\int_0^\tau ds\int_\Omega w'\eta(\mathbf{x},s)\,dv$$
$$+k_2\frac{\tau}{T}\int_0^\tau ds\int_\Omega (g\eta)(\mathbf{x},s)\,dv + \int_{\partial\Omega}(g\mathbf{n}\cdot\mathbf{T}_\tau\dot{\mathbf{u}})(\mathbf{x},\tau)\,da$$
$$+\int_{\partial\Omega}(g\mathbf{n}\cdot\mathbf{T}_{(0,\tau)}\dot{\mathbf{u}})(\mathbf{x},\tau)\,da + \frac{1}{2}T\int_\Omega (g\rho^{-1}\boldsymbol{\delta}_0^2)(\mathbf{x},\tau)\,dv,$$

whence, integrating over $(0,t)$ $(0<t<T)$, it follows that

$$\int_\Omega (g\eta)(\mathbf{x},t)\,dv \le 2\int_\Omega (g\eta)(\mathbf{x},0)\,dv + 4k_1^2t\int_0^t ds\int_\Omega g(\mathbf{x}_0;\mathbf{x},t)\eta(\mathbf{x},s)\,dv \tag{3.6}$$
$$+2(k_0+2k_1+k_2T+T^{-1})\int_0^t d\tau\int_\Omega (g\eta)(\mathbf{x},\tau)\,dv$$
$$+\frac{2}{\delta}\Big(\frac{k_1K}{c_\varepsilon T}+\frac{k_1^2}{\varepsilon}\Big)\int_0^t \tau\,d\tau\int_0^\tau ds\int_\Omega w'\eta(\mathbf{x},s)\,dv$$

(3.6) [cont.]

$$+\frac{2k_2}{T}\int_0^t \tau\, d\tau \int_0^T ds \int_\Omega (g\eta)(\mathbf{x}, s)\, dv$$

$$+2\int_0^t \Big\{ \int_{\partial\Omega} (g\mathbf{n}\cdot \mathbf{T}_\tau \dot{\mathbf{u}})(\mathbf{x},\tau)\, da + \int_{\partial\Omega} (g\mathbf{n}\cdot \mathbf{T}_{(0,\tau)}\dot{\mathbf{u}})(\mathbf{x},\tau)\, da$$

$$+\frac{1}{2}T\int_\Omega (g\rho^{-1}\delta_0^2)(\mathbf{x},\tau)\, dv\Big\}\, d\tau\,,$$

where we have used inequality $(3.5)_3$ with $\varepsilon = 1$.

Set now

$$F(t) = \int_0^t d\tau \int_\Omega (g\eta)(\mathbf{x},\tau)\, dv\,,$$

$$h(t) = \frac{k_2}{T}t^2 + 4k_1^2 t + 2\Big(k_0 + 2k_1 + k_2 T + \frac{1}{T}\Big)\,,$$

$$H(t) = \int_0^t h(s)\, ds$$

and

$$\Delta_0(t) = 2\int_\Omega (g\eta)(\mathbf{x},0)\, dv + 2\int_0^t \Big\{ \int_{\partial\Omega} (g\mathbf{n}\cdot \mathbf{T}_\tau \dot{\mathbf{u}})(\mathbf{x},\tau)\, da$$

$$+\int_{\partial\Omega} (g\mathbf{n}\cdot \mathbf{T}_{(0,\tau)}\dot{\mathbf{u}})(\mathbf{x},\tau)\, da + \frac{1}{2}T\int_\Omega (g\rho^{-1}\delta_0^2)(\mathbf{x},\tau)\, dv\Big\}\, d\tau\,.$$

Bearing in mind that

$$\int_0^t ds \int_\Omega g(\mathbf{x}_0;\mathbf{x},t)\eta(\mathbf{x},s)\, dv \le \int_0^t d\tau \int_\Omega (g\eta)(\mathbf{x},\tau)\, dv\,,$$

inequality (3.6) may be written in the form

$$\dot F(t) \le h(t)F(t) + \frac{2}{\delta}\Big(\frac{k_1 K}{c_\varepsilon T} + \frac{k_1^2}{\varepsilon}\Big)\int_0^t \tau\, d\tau \int_0^T ds \int_\Omega w'\eta(\mathbf{x},s)\, dv + \Delta_0(t)\,.$$

Hence, a standard integration method leads to

$$(3.7)\qquad F(t) \le \exp[H(t)]\Big\{\frac{2}{\delta}\Big(\frac{k_1 K}{c_\varepsilon T} + \frac{k_1^2}{\varepsilon}\Big)$$

$$\times\int_0^t \exp[-H(\sigma)]\Big(\int_0^\sigma \tau\, d\tau \int_0^T ds \int_\Omega w'\eta(\mathbf{x},s)\, dv\Big) d\sigma$$

$$+\int_0^t \exp[-H(\sigma)]\Delta_0(\sigma)\, d\sigma\Big\}\,,$$

for any $t < T$.

Now, as $\delta \to 0$, g tends boundedly to the characteristic function of the set S, so that we are allowed to let $\delta \to 0$ in the last inequality. Then, by virtue of Lebesgue's dominated convergence theorem, and in view of the relation

$$\lim_{\delta\to 0}\frac{1}{\delta}\int_{\Omega} w'\eta(\mathbf{x},s)\,dv = \lim_{\delta\to 0}\frac{1}{\delta}\int_{R^\star_{\tau+\delta}}^{R^\star_\tau} dr \int_{\Sigma(\mathbf{x}_0,r)} w'\eta(\mathbf{x},s)\,da$$

$$= c_\varepsilon[q'(R^\star_\tau + r_0)]^{-1}\int_{\Sigma(\mathbf{x}_0,R^\star_\tau)} w'\eta(\mathbf{x},s)\,da \le w'(\theta)c_\varepsilon[q'(R^\star_\tau + r_0)]^{-1}\int_{\Sigma(\mathbf{x}_0,R^\star_\tau)} \eta(\mathbf{x},s)\,da,$$

letting $\delta\to 0$ in (3.7), we obtain

$$G(t) \le \exp[H(t)]\Big\{2w'(\theta)c_\varepsilon\Big(\frac{k_1K}{c_\varepsilon T} + \frac{k_1^2}{\varepsilon}\Big) \times \int_0^t \exp[-H(\sigma)]\Big(\int_0^\sigma \tau[q'(R^\star_\tau + r_0)]^{-1}\,d\tau\int_0^\tau ds\int_{\Sigma(\mathbf{x}_0,R^\star_\tau)}\eta(\mathbf{x},s)\,da\Big)d\sigma + \int_0^t \exp[-H(\sigma)]\widehat{\Delta}_0(\sigma)\,d\sigma\Big\}, \tag{3.8}$$

where

$$G(t) = \int_0^t d\tau \int_{\Omega(\mathbf{x}_0,R^\star_\tau)} \eta(\mathbf{x},\tau)\,dv,$$

$$\widehat{\Delta}_0(t) = 2\int_{\Omega(\mathbf{x}_0,R^\star_\tau)} \eta(\mathbf{x},0)\,dv + 2\int_0^t\Big\{\int_{\partial\Omega\cap B(\mathbf{x}_0,R^\star_\tau)} (\mathbf{n}\cdot\mathbf{T}_\tau\dot{\mathbf{u}})(\mathbf{x},\tau)\,da + \int_{\partial\Omega\cap B(\mathbf{x}_0,R^\star_\tau)} (\mathbf{n}\cdot\mathbf{T}_{(0,\tau)}\dot{\mathbf{u}})(\mathbf{x},\tau)\,da + \frac{1}{2}T\int_{\Omega(\mathbf{x}_0,R^\star_\tau)} \rho^{-1}\delta_0^2(\mathbf{x},\tau)\,dv\Big\}\,d\tau$$

and $\theta\in(0,1)$.

We observe now that

$$\frac{d}{d\tau}\int_{\Omega(\mathbf{x}_0,R^\star_\tau)} \eta(\mathbf{x},s)\,dv = -c_\varepsilon[q'(R^\star_\tau + r_0)]^{-1}\int_{\Sigma(\mathbf{x}_0,R^\star_\tau)} \eta(\mathbf{x},s)\,da,$$

so that (3.8) becomes

$$G(t) \le \exp[H(t)]\Big\{-2w'(\theta)\Big(\frac{k_1K}{c_\varepsilon T} + \frac{k_1^2}{\varepsilon}\Big) \times \int_0^t \exp[-H(\sigma)]\Big(\int_0^\sigma \tau\,d\tau\int_0^\tau ds\frac{d}{d\tau}\int_{\Omega(\mathbf{x}_0,R^\star_\tau)}\eta(\mathbf{x},s)\,dv\Big)d\sigma + \int_0^t \exp[-H(\sigma)]\widehat{\Delta}_0(\sigma)\,d\sigma\Big\}.$$

Hence, taking into account the relation

$$
\begin{aligned}
-\int_0^\sigma \tau\, d\tau \int_0^\tau ds \frac{d}{d\tau} \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},s)\, dv &= -\int_0^\sigma \tau\, d\tau \frac{d}{d\tau} \int_0^\tau ds \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},s)\, dv \\
&+ \int_0^\sigma \tau\, d\tau \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},\tau)\, dv = -\int_0^\sigma \frac{d}{d\tau}\left(\tau \int_0^\tau ds \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},s)\, dv\right) d\tau \\
&+ \int_0^\sigma d\tau \int_0^\tau ds \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},s)\, dv + \int_0^\sigma \tau\, d\tau \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},\tau)\, dv \\
&= -\sigma \int_0^\sigma d\tau \int_{\Omega(\mathbf{x}_0,R_\sigma^\star)} \eta(\mathbf{x},\tau)\, dv + \int_0^\sigma d\tau \int_0^\tau ds \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},s)\, dv \\
&+ \int_0^\sigma \tau\, d\tau \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},\tau)\, dv \le \int_0^\sigma d\tau \int_0^\tau ds \int_{\Omega(\mathbf{x}_0,R_s^\star)} \eta(\mathbf{x},s)\, dv \\
&+ \int_0^\sigma \tau\, d\tau \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},\tau)\, dv \le 2\sigma \int_0^\sigma d\tau \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},\tau)\, dv\,,
\end{aligned}
$$

it follows that

$$
\begin{aligned}
G(t) \le \exp[H(t)]\Bigg\{&4w'(\theta)\left(\frac{k_1 K}{c_\varepsilon T} + \frac{k_1^2}{\varepsilon}\right) \\
&\times t \int_0^t \left(\int_0^\sigma d\tau \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},\tau)\, dv\right) d\sigma + \int_0^t \widehat{\Delta}_0(\sigma)\, d\sigma\Bigg\}.
\end{aligned}
\tag{3.9}
$$

We set again

$$
\varphi(t) = 4w'(\theta)\left(\frac{k_1 K}{c_\varepsilon} + \frac{k_1^2}{\varepsilon}\right) \int_0^t \exp[H(s)] s\, ds
$$

and

$$
\Phi(t) = \int_0^t \left(\int_0^\sigma d\tau \int_{\Omega(\mathbf{x}_0,R_\tau^\star)} \eta(\mathbf{x},\tau)\, dv\right) d\sigma = \int_0^t G(\sigma)\, d\sigma\,,
$$

to write inequality (3.9) in the form

$$
\dot{\Phi}(t) \le \dot{\varphi}(t)\Phi(t) + \exp[H(t)] \int_0^t \widehat{\Delta}_0(\sigma)\, d\sigma\,.
$$

A simple integration yields then

$$
\Phi(t) \le \exp[\varphi(t)] \int_0^t \exp[H(s) - \varphi(s)]\left(\int_0^s \widehat{\Delta}_0(\sigma)\, d\sigma\right) ds\,. \tag{3.10}
$$

Since the last relation holds for any $t < T$, the continuity of functions $\Phi(t)$ and $\widehat{\Delta}_0(t)$ on $\Omega \times [0, \infty)$ allows us to let $t \to T$ in (3.10). This gives the desired relation (3.4). □

4. The domain of influence theorem. Uniqueness

By virtue of the domain of dependence inequality proved in Sec. 3, we are in a position to give, for System (2.1)–. . .–(2.3), a definition of the "domain of influence of the data" at each instant, which is quite analogous to the ones given in [2–4, 7]. We can also prove that, when the data have a compact support, the domain of influence thus defined is still, at each instant, the largest subset of Ω, in which the solution may be different from zero (at the same instant), and is in turn a *compact subset* of Ω.

As in [2–4, 7] we first introduce the *support of the data* at instant $T > 0$, as the set $D(T)$ of all the points $\mathbf{x} \in \overline{\Omega}$ such that

1. $\mathbf{x} \in \Omega \Rightarrow \exists \tau \in (-\infty, 0] : \mathbf{u}_0(\mathbf{x}, \tau) \neq 0$ or $\exists \tau \in [0, T] : \mathbf{b}(\mathbf{x}, \tau) \neq 0$;
2. $\mathbf{x} \in \partial_1\Omega \Rightarrow \exists \tau \in (-\infty, 0] : \mathbf{u}_0(\mathbf{x}, \tau) \neq 0$ or $\exists \tau \in [0, T] : \widehat{\mathbf{u}}(\mathbf{x}, \tau) \neq 0$;
3. $\mathbf{x} \in \partial_2\Omega \Rightarrow \exists \tau \in (-\infty, 0] : \mathbf{u}_0(\mathbf{x}, \tau) \neq 0$ or $\exists \tau \in [0, T] : \widehat{\mathbf{s}}(\mathbf{x}, \tau) \neq 0$.

Then, we may give the following

DEFINITION 1. *The domain of influence of the data at instant $T > 0$ is the set*

$$D^*(T) = \{\mathbf{x}_0 \in \overline{\Omega} \,:\, D(T) \cap \overline{B}(\mathbf{x}_0, q^{-1}(q(r_0) + c(T)T) - r_0) \neq \emptyset\},$$

where, for any $T > 0$,

$$c(T) = \lim_{\varepsilon \to 0} c_\varepsilon(T) = 2(k_1(T) + 1)K(T). \tag{4.1}$$ □

We may then also prove the following

THEOREM 2. (Domain of influence theorem). *Let* $\mathbf{u}$ *be any solution to System* (2.1)–. . .–(2.5), *and let assumptions* (1)–. . .–(4), A)–. . .–C) *of Sec.* 2 *be fulfilled. Then, for any* $T > 0$,

$$\mathbf{u} = \mathbf{0} \quad \text{on} \quad \overline{\{\overline{\Omega} \setminus \overline{D^*(T)}\}} \times [0, T].$$ □

P r o o f. To begin with, let $\varepsilon > 0$ be arbitrarily small, and define

$$D^*_\varepsilon(T) = \{\mathbf{x}_0 \in \overline{\Omega} \,:\, D(T) \cap \overline{B}(\mathbf{x}_0, q^{-1}(q(r_0) + c_\varepsilon(T)T) - r_0) \neq \emptyset\}.$$

Next, with $T > 0$ assigned, let $\mathbf{x}_0 \in \{\overline{\Omega} \setminus \overline{D^*_\varepsilon(T)}\} \times [0, T]$. Then, applying inequality (3.4) with this choice of $\mathbf{x}_0$ and with $R = 0$, we find that all the integrals at left-hand side of (3.4) vanish, so that

$$\int_0^T \left(\int_0^t d\tau \int_{\Omega(\mathbf{x}_0, q^{-1}(q(r_0) + c_\varepsilon(T-\tau)) - r_0)} \eta(\mathbf{x}, \tau)\, dv \right) dt \leq 0.$$

Then, the definition of η, by virtue of the regularity assumptions on $\mathbf{u}$, yields at once

$$\mathbf{u} = \mathbf{0} \quad \text{on} \quad \{\overline{\Omega} \setminus \overline{D^*_\varepsilon(T)}\} \times [0, T].$$

This relation holds for any choice of $\varepsilon \in (0, 1)$, so that we are allowed to state that

$$\mathbf{u} = \mathbf{0} \quad \text{on} \quad \{\overline{\Omega} \setminus \overline{D^*(T)}\} \times [0, T].$$

Finally, the continuity of $\mathbf{u}$ completes the proof of the theorem. □

According to the result expressed by this theorem, we may state that relation (4.1) *defines* the maximum speed of propagation of perturbations in an inhomogeneous but isotropic viscoelastic body whose stress-strain relation is given by (2.3), with memory functions satisfying conditions A)-. . .-E).

As a trivial corollary of Theorem 4.1, we have the following uniqueness theorem.

COROLLARY 4.1 (Uniqueness theorem). *Let* $\mathbf{u}$ *be any solution to System* (2.1)–...–(2.5) *corresponding to zero data and body forces, and let assumptions* A)–...–E) *of Sec. 2 be fulfilled. Then*

$$\mathbf{u} = 0 \quad \text{on} \quad \overline{\Omega} \times (-\infty, \infty). \qquad \square$$

Proof. Obvious: indeed, under the assumptions of the theorem, $\mathbf{u} = 0$ on $\overline{\Omega} \times (-\infty, 0]$, and $D(T) = \emptyset$ for any $T > 0$. □

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On the lack of structure of Defay–Prigogine 2D-continua

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IN THIS PAPER it is proved that the bidimensional continua modelling the interfaces between fluid phases have to be endowed with a shell-like structure. Indeed (generalizing the result due to TOLMAN [1]) the Gibbs–Tolman formula is proved to be universally valid for the class of fluid interfaces introduced by DEFAY and PRIGOGINE in [3]. The starting assumption is that (following DELL'ISOLA and ROMANO [2]) the interfaces between different phases can be modelled by nonmaterial bidimensional ($2D$-)continua, whose independent constitutive variables are the temperature and the interfacial mass density. Moreover, for this class of $2D$-continua (their introduction is suggested in [3]) we prove the Gibbs phase rule, Kelvin relation between interfacial curvature and vapour pressure, and propose a formula which could allow for experimental evaluation of the surface mass density for plane and curved interfaces. Unfortunately, as discussed in ADAMSON [4], the dependence of surface tension on the curvature which is experimentally measured is inconsistent with the Tolman formula. Our result implies that, in order to supply theoretical forecasting consistent with experimental data, it is useless to look for new constitutive equations for interfacial free energy: therefore, the conjecture formulated by DEFAY and PRIGOGINE in [3] seems to be not true. Instead, to account experimental evidence, it is necessary to construct $2D$-continua endowed with a more complex structure. The minimal set of independent constitutive variables which seem to be necessary to this aim is determined in the epilogue.

1. Introduction

IN HIS FUNDAMENTAL series of paper [1, 5, 6] TOLMAN, developing the ideas of GIBBS [7], could obtain a formula (then generalized by KOENIG [8] to the case of mixtures) which relates the equilibrium surface tension acting on a liquid drop surrounded by its vapour to its radius. The fundamental assumptions accepted by Tolman are:

T1. The vapour is a Van der Waals gas.

T2. The liquid phase incompressible.

T3. The interface is a mixture between liquid and vapour: all properties of this mixture are postulated on a heuristic ground.(1)

The utility of this formula, which in the literature is sometimes called also Gibbs–Tolman formula, has been tested in many experimental conditions. ADAMSON [4], while underlining its conceptual importance, quotes many papers, for example LAMER and POUND [13], in which is shown that the dependence of the surface tension on curvature, as predicted from Tolman's results, is in poor agreement with experimental data. The first attempt to point out the theoretical reasons of the quoted failure is due to DEFAY and PRIGOGINE [3]; they conjecture that Tolman's results have to be improved by taking into account the dependence of the equilibrium surface mass density at the interface upon the curvature. We remark explicitly here that if one decides to model the interface by a bidimensional ($2D$-)nonmaterial continuum, this conjecture clearly implies that the

(1) In our opinion it is possible to deduce the quoted properties in the framework of the theories of the second gradient (see for instance SEPPECHER [9] or the series of papers CASAL–GOUIN [10, 11, 12]). Indeed, these theories provide a unique constitutive description for all the three phases (including the interface) coexisting in the systems considered.

constitutive assumption

$$\gamma = \gamma(\vartheta), \tag{1.1}$$

where γ is the surface tension and ϑ the interfacial temperature, which seems to be generally accepted in the literature, has to be generalized as follows:

$$\gamma = \gamma(\vartheta, \rho_\sigma), \tag{1.2}$$

where ρ_σ is the interfacial surface mass density.

We will call the $2D$-continua for which Eq. (1.2) is accepted Defay–Prigogine continua. The results experimentally found by KAYSER [14], once Eq. (1.2) is assumed, should be reinterpreted: he actually measured the values of the following function

$$\gamma_P^*(\vartheta) := \gamma(\vartheta, \rho_{\sigma P}^*(\vartheta)), \tag{1.3}$$

where $\rho_{\sigma P}^*(\vartheta)$ is the equilibrium surface mass density for plane interfaces. The aim of this paper is to prove, by modelling the interface between different phases of the same material as proposed in [2], that:

R0. The function $\rho_{\sigma P}^*(\vartheta)$ is determined when the functions $\gamma_P^*(\vartheta)$ and $E_{\sigma P}^*(\vartheta)$ (the equilibrium surface tension and the surface inner energy per unit area for plane interface) are known.

R1. (1.1) is not consistent with the Gibbs phase rule.

R2. (1.2) implies Gibbs phase rule and enables, once a constitutive choice of interfacial free energy is made, a theoretical evaluation, in terms of the function $\rho_{\sigma P}^*(\vartheta)$, of the function $\rho_\sigma^*(\vartheta, H)$, i.e. the equilibrium interfacial surface mass density corresponding to curvature H and fixed temperature ϑ (obviously $\rho_{\sigma P}^*(\vartheta) = \rho_\sigma^*(\vartheta, 0)$).

R3. The Gibbs–Tolman formula is universally valid for the interfaces modelled in [2].

We explicitly remark here that we supply a proof of Gibbs–Tolman which:

H1 — is independent of the assumptions T1 and T2: the only hypothesis we need is that both liquid and vapour are perfect fluids;

H2 — is independent also of the "physically grounded" assumption T3: we only accept that the interface between phases is a perfect (Defay–Prigogine) $2D$-continuum;

H3 — is almost independent of the classical one supplied by Tolman: since the model used carefully ignores the concepts of Gibbs surface excess and Gibbs dividing surface, our proof is simpler.

The results quoted in statement R0 and R2 seems to supply an experimental method for evaluating the interfacial mass density. Statement R3 implies that the models proposed in [2] need to be improved in order to produce a theoretical approach to the problem of curvature depending on surface tension which is consistent with experimental evidence. Indeed, in this paper we prove that a perfect Defay–Prigogine $2D$-continuum is not endowed with sufficient structure to see, in equilibrium conditions, the difference between nonmaterial and material interfaces. In the epilogue some hints of future developments are sketched: following the ideas stemming from the work of CAPRIZ and PODIO-GUIDUGLI [15] (generalized to $2D$-nonmaterial continua), the introduction of further independent constitutive variables to describe the state of the interface seems unavoidable. It has to be cleared up how many of these variables should be introduced: indeed, there are many possible choices. We list here the two which are subject to our investigations: i) one could generalize the model proposed by DICARLO, GURTIN and PODIO-GUIDUGLI [16], introducing the curvature itself as a further independent variable (this approach implies the introduction of interfacial couple stresses) or ii) if the ideas exposed by CHOI *et al.* [17] or by FISHER and ISRAELACHVILI [18, 19] in their comments to their experimental data are founded) one could, using the results found in DELL'ISOLA and KOSIŃSKI [20], introduce a surface scalar field modelling the thickness of the interface.

2. Constitutive equations for Defay–Prigogine $2D$-continua. Gibbs' phase rule

Following [2] we assume that the independent constitutive variable characterizing the state of the interface are ϑ and ρ_σ, i.e. the temperature and the surface mass density.

Therefore the interfacial free energy per unit mass ϑ_σ has to be determined as a function of (ϑ, ρ_σ). Once this function is known, the entropy principle implies that all the other constitutive laws are determined. Indeed, in [2] the following relations are proved:

$$(2.1) \qquad \eta_\sigma = -\frac{\partial \psi_\sigma}{\partial \psi}, \qquad \varepsilon_\sigma = \vartheta_\sigma + \psi \eta_\sigma, \qquad \gamma = -\rho_\sigma^2 \frac{\partial \psi_\sigma}{\partial \rho_\sigma},$$

where η_σ and ε_σ denote the interfacial entropy and inner energy per unit mass. If we define the interface Gibbs' potential per unit mass as follows

$$(2.2) \qquad g_\sigma = \psi_\sigma - \frac{\gamma}{\rho_\sigma}$$

and if we assume that

HYPOTHESIS 1. *Once ϑ is fixed, Eq.* (2.1)$_3$ *determines a one-to-one correspondence between γ and ρ_σ;*

then the Eq. (2.1) trivially implies that (if instead of ρ_σ we choose γ as independent variable)

$$(2.3) \qquad \frac{\partial g_\sigma}{\partial \gamma} = -\frac{1}{\rho_\sigma}.$$

On the other hand, if we assume that the interface is incompressible, i.e. if we assume that

IC1) ρ_σ is independent of the tension γ and is given as a function of the variable ϑ alone;

IC2) all the other thermomechanical quantities are functions of the variables γ and ϑ;

then the Eq. (2.3), with reasoning completely analogous to those one can find in [2], can be proved to start from the entropy principle.

DEFINITION 1. *We will call Defay–Prigogine continua those bidimensional nonmaterial continua whose free energy satisfies Hypothesis* 1 *and whose entropy, inner energy and surface tension satisfy Eq.* (2.1).

We will prove that Gibbs' Phase Rule holds for Defay–Prigogine continua in all the cases of planar or spherical interfaces.

We start from the equilibrium condition deduced in [2] from the reduced entropy inequality, specified to the case of plane and spherical interfaces:

$$(2.4) \qquad 2H\gamma = p_l - p_v, \qquad g_v = g_l, \qquad g_v = g_\sigma,$$

where H is the curvature of the interface, p_l and g_l, p_v and g_v, are, respectively, the pressure and Gibbs' potential in the liquid and in the vapour phases: in what follows g_l and g_v are assumed to be, respectively, function of ϑ and of p_l and p_v.

The set $\mathcal{S}$ of the parametres which describe the equilibrium of a liquid and its vapour, when capillarity phenomena can't be neglected and the interface is plane or spherical, is

$$\mathcal{S} = \{\vartheta, H, p_l, \rho_l, p_v, \rho_v, \rho_\sigma, \gamma\}\,. \tag{2.5}$$

We explicitly remark that, in view of H1 and H2, the constitutive relations for the vapour, liquid and interfacial phases reduce to the five independent variables appearing in $\mathcal{S}$.

Gibbs phase rule

If $H = 0$, i.e. if the interface is plane, the four independent quantities appearing in (2.5) are constrained by the three equations (2.4). If these equations are independent, then there is a one-to-one correspondence between one parameter chosen in $\mathcal{S}$ and the equilibrium states of the system. In what follows this parameter will always be the temperature ϑ: all the other quantities in $\mathcal{S}$ will become function of ϑ, these functions we will denote by the same letter with the superscript $*$ and the subscript p.

On the other hand, if H is not vanishing then there are two degrees of freedom of the system. This is exactly what was forecast by the suitably generalized form of Gibbs' Rule (for more details cf. ADAMSON [4], LEVINE [21] or GIBBS [7]).

We prove now the following

PROPOSITION 1. The assumption γ independent of ρ_σ is

i) a consequence of the relation (which is often accepted in the literature)

$$\gamma = \rho_\sigma \psi_\sigma\,; \tag{2.6}$$

ii) not consistent with the Gibbs' Phase Rule.

To prove ii) we remark that the hypothesis $\gamma = \gamma(\vartheta)$ implies (because of $(2.1)_3$) the following relation

$$\psi_\sigma = \frac{\gamma(\vartheta)}{\rho_\sigma} + \widehat{\psi}_\sigma(\vartheta), \tag{2.7}$$

where $\widehat{\psi}_\sigma(\vartheta)$ is a function of the variable ϑ alone which does not depend on γ.

Equation (2.7) implies, together the definition (2.2), that

$$g_\sigma(\psi, \rho_\sigma) = \widehat{\psi}_\sigma(\vartheta). \tag{2.8}$$

The consequences of (2.8) are remarkably inconsistent with the Gibbs' Phase Rule: indeed, even if one could always believe that ρ_σ is very small or vanishing or negligible, so that he is not interested in determining its value at the equilibrium states, he could never ignore $(2.4)_3$ (which was established by Gibbs himself) which, together with (2.8), states that

a) in the case of planar interfaces there exists an unique equilibrium state characterized by a fixed couple of values for temperature and pressure;

b) in the case of spherical interfaces there exists for every temperature a unique equilibrium radius.

Both the statements a) and b) are in obvious disagreement with the experimental evidence which supports Gibbs' Phase Rule.

To prove i) it is sufficient to remark that Eq. (2.6) together with Eq. $(2.1)_3$ leads to the following implications

$$\left(\psi_\sigma = -\rho_\sigma \frac{\partial \psi_\sigma}{\partial \rho_\sigma}\right) \Rightarrow \left(\psi_\sigma = \frac{k(\vartheta)}{\rho_\sigma}\right) \Rightarrow \gamma \text{ depends only on } \vartheta.$$

We remark explicitly that the relation (2.6) implies that

$$g_\sigma(\vartheta, \rho_\sigma) = 0. \tag{2.9}$$

The last equation is equivalent, because of $(2.1)_1$ and (2.2), to

$$-\rho_\sigma \eta_\sigma = \frac{\partial \gamma}{\partial \vartheta},$$

which is Eq. III-5 in ADAMSON [4]. The validity of the last equation and of Eq. (2.6) is therefore really doubtful.

3. Proof of Gibbs–Tolman formula

In this section we assume that

H1) both vapour and the liquid phase are perfect fluids, therefore the following equalities hold:

$$\frac{\partial g_v}{\partial p_v} = \frac{1}{\rho_v}, \qquad \frac{\partial g_l}{\partial p_l} = \frac{1}{\rho_l}; \tag{3.1}$$

H2) the set of equilibrium equations (2.4) is independent: therefore once the temperature ϑ is fixed, the choice of the variable p_v, determines the equilibrium state of the system and therefore all the equilibrium values of the other quantities in $\mathcal{S} - \{\vartheta\}$; we will denote H^*, γ^*, p_l^*, ρ_l^*, ρ_v^* and ρ_σ^* the functions which map (p_v, ϑ) onto the corresponding equilibrium values.

In what follows we do not indicate the functional dependence on ϑ.

According to our notation, Eqs. (2.3), $(2.4)_3$ and (3.1), we have the following chain of implications:(2)

$$(g_\sigma(\gamma^*(p_v)) = g_v(p_v)) \Rightarrow \left(\frac{\partial g_\sigma}{\partial \gamma}\frac{d\gamma^*}{dp_v} = \frac{\partial g_v}{\partial p_v}\right) \Rightarrow \left(\frac{d\gamma^*}{dp_v} = -\frac{\rho_\sigma^*}{\rho_v^*}\right). \tag{3.2}$$

Moreover, starting from Eqs. $(2.3)_{1,2}$ we establish the hypothesis of the following implication, its thesis being obtained by making use of Eq. (3.1) and the last equality in (3.2)

$$\left\{\begin{aligned} \frac{\partial g_v}{\partial p_v} &= \frac{\partial g_l}{\partial p_l}\frac{dp_l^*}{dp_v} \\ \frac{dp_l^*}{dp_v} &= 1 + 2\frac{dH^*}{dp_v}\gamma^* + 2H^*\frac{d\gamma^*}{dp_v} \end{aligned}\right\} \Rightarrow \left(\frac{dH^*}{dp_v} = \frac{(\rho_l^* - \rho_v^*) + 2H^*\rho_\sigma^*}{2\gamma^*\rho_v^*}\right). \tag{3.3}$$

Finally, the Gibbs'–Tolman formula is obtained by evaluating the ratio of the last equalities appearing in (3.2) and (3.3), after having observed that the nonvanishing expression we have obtained for the derivative dH^*/dp_v allows us to chose, instead of p_v, the variable H in order to characterize the equilibrium states:

$$\frac{d\widetilde{\gamma}}{dH} = -\frac{2\widetilde{\gamma}\delta}{1 + 2H\delta}, \tag{3.4}$$

where $\delta(H) := \widetilde{\gamma}_\sigma / (\widetilde{\gamma}_l - \widetilde{\gamma}_v)$ and where the upper tilde indicates the generic composite function $\widetilde{f}(H) := f^*(p_v(H))$.

(2) This relation seems to represent a reasonable reformulation of Eq. (III-22) on p. 56 in ADAMSON [4].

Trivial integration by parts allows us to obtain the following equivalent expression, which can be more easily compared with those found in literature, and in particular in TOLMAN [1]:

$$\widetilde{\gamma} = \gamma_0 \frac{e^{\Delta(H)}}{1 + 2\delta(H)H}, \tag{3.5}$$

where

$$\Delta(H) := \int (1 + 2H\delta(H))^{-1}\left(2H\frac{d\delta}{dH}\right) dH.$$

4. Interfacial free energy and the dependence of interfacial mass density on temperature and curvature

Once Eq. (3.5) is obtained, the problem of determining the function $\delta(H)$ arises. It is easy to forecast, simply by observing Eq. (2.4), that $\delta(H)$, which is the ratio of the functions $\widetilde{\rho}_\sigma$ and $\widetilde{\rho}_l - \widetilde{\rho}_v$, has not many chances to be independent of the constitutive law assigning the interfacial free energy ψ_σ.

We remark explicitly here that the classical treatment due to Tolman hides this circumstance behind some Gibbsian reasoning which seems to be neither logically nor physically well grounded. However, it is our belief that these "Gibbsianism" could be made understandable (and the dependence of $\delta(H)$ on the constitutive law for ψ_σ explicit) once that the theory of the second gradient or interstitial working (see for instance SEPPECHER [9] or CASAL–GOUIN [10, 11] or DUNN–SERRIN [22]) is introduced to describe the behaviour of the interfacial phase.

4.1 Determination of surface mass density for plane interfaces. The case of compressible Defay–Prigogine $2D$-continua

In this subsection we aim to determine a relation between equilibrium surface mass density, surface tension and surface inner energy per unit area, which is valid in the case of plane interfaces and which we could not find in the literature. In our opinion it could be very useful in determining experimentally the magnitude of interface mass density involved in capillarity phenomena.

We start with the remark that, because of our definition, Eqs. (2.1) and Eq. $(2.4)_3$ we obtain (recall that the subscript P refers to the circumstance that all equilibrium functions which we consider are related to plane interfaces, and that all the functions considered have a unique variable, the temperature ϑ)

$$E^*_{\sigma P} = \rho^*_{\sigma P}\varepsilon^*_{\sigma P} = \rho^*_{\sigma P}\psi^*_{\sigma P} - \rho^*_{\sigma P}\vartheta\left(\frac{\partial\psi_\sigma}{\partial\vartheta}\right)^*_P, \tag{4.1}$$

$$\gamma^*_P = -(\rho^*_{\sigma P})^2\left(\frac{\partial\psi_\sigma}{\partial\rho_\sigma}\right)^*_P, \tag{4.2}$$

$$\psi^*_{\sigma P} + \rho^*_{\sigma P}\left(\frac{\partial\psi_\sigma}{\partial\rho_\sigma}\right)^*_P = g^*_{vP} = g^*_{lP}; \tag{4.3$_1$}$$

here we used the notations

$$g^*_{vP}(\vartheta) := g_v(p^*_{vP}(\vartheta), \vartheta); \qquad g^*_{lP}(\vartheta) := g_l(p^*_{lP}(\vartheta), \vartheta) \tag{4.3$_2$}$$

and the relations (resulting from $(2.4)_{1,2}$)

$$(4.3)_3 \qquad p^*_{vP}(\vartheta) = p^*_{lP}(\vartheta) \Rightarrow g_v(p^*_{vP}(\vartheta), \vartheta) = g_l(p^*_{lP}(\vartheta), \vartheta).$$

On the other hand, using the chain rule for the derivation of composed functions, we obtain

$$(4.4) \qquad \left(\frac{\partial \psi_\sigma}{\partial \vartheta}\right)^*_P = \frac{d\psi^*_{\sigma P}}{d\vartheta} - \left(\frac{\partial \psi_\sigma}{\partial \rho_\sigma}\right)^*_P \frac{d\rho^*_{\sigma P}}{d\vartheta}.$$

Then, from Eqs. (4.2) and (4.3), using simple algebra we obtain

$$(4.5) \qquad \psi^*_{\sigma P} = g^*_{vP} + \gamma^*_P (\rho^*_{\sigma P})^{-1},$$

$$(4.6) \qquad -\gamma^*_P (\rho^*_{\sigma P})^{-2} = \left(\frac{\partial \psi_\sigma}{\partial \rho_\sigma}\right)^*_P.$$

Finally one has to

i) substitute the LHS of Eq. (4.6) in the RHS of Eq. (4.4),

ii) substitute the derivative of RHS of Eq. (4.5) again in the RHS of Eq. (4.4),

iii) substitute the RHS of the so transformed Eq. (4.4) in the RHS of Eq. (4.1),

iv) substitute the RHS of Eq. (4.5) again in RHS of Eq. (4.1), in order to obtain the following relation

$$(4.7) \qquad \rho^*_{\sigma P}\left(g^*_{vP} - \vartheta \frac{dg^*_{vP}}{d\vartheta}\right) = -\gamma^*_P + \vartheta \frac{d\gamma^*_P}{d\vartheta} + E^*_{\sigma P}.$$

In order to compare Eq. (4.7) with the experimental data available in the literature, it is necessary to evaluate the second factor on LHS. We start by calculating the derivative appearing in (4.7),

$$(4.8) \qquad \frac{dg^*_{vP}}{d\vartheta} = (\rho^*_{lP} - \rho^*_{vP})^{-1}\left(\rho_l \frac{\partial g_l}{\partial \vartheta} - \rho_v \frac{\partial g_v}{\partial \vartheta}\right)^*_P.$$

The last expression is easily obtained by differentiating both expressions appearing in $(4.3)_2$ and recalling Eq. (3.1) and $(2.4)_2$. In order to make the final step of our derivation clear it is useful to recall that the partial derivatives appearing in Eq. (4.8) are evaluated at fixed variables p_l and p_v. Indeed, as a consequence of Eq. (3.1), if ε_1 and ε_v denote the inner energy per unit mass in the liquid and vapour phase, we have

$$(4.9) \qquad g_l - \vartheta \frac{\partial g_l}{\partial \vartheta} = \varepsilon_l + p_l/\rho_l, \qquad g_v - \vartheta \frac{\partial g_v}{\partial \vartheta} = \varepsilon_v + p_v/\rho_v$$

and therefore (using (4.8) and again recalling $(2.4)_2$) we obtain

$$(4.10) \qquad \left(g^*_{vP} - \vartheta \frac{dg^*_{vP}}{d\vartheta}\right) = (\rho^*_{lP}\varepsilon^*_{lP} - \rho^*_{vP}\varepsilon^*_{vP})(\rho^*_{lP} - \rho^*_{vP})^{-1}$$

and (here the enthalpy per unit mass h is introduced in both phases)

$$(4.11) \qquad \rho^*_{lP}\varepsilon^*_{lP} - \rho^*_{vP}\varepsilon^*_{vP} = \rho^*_{lP}h^*_{lP} - \rho^*_{vP}h^*_{vP}.$$

In conclusion Eq. (4.7) becomes

$$\rho^*_{\sigma P}(\rho^*_{lP}h^*_{lP} - \rho^*_{vP}h^*_{vP} = \left(-\gamma^*_P + \vartheta\frac{d\gamma^*_P}{d\vartheta} + E^*_{\sigma P}\right)(\rho^*_{lP} - \rho^*_{vP}), \tag{4.12}$$

which is the relation announced at the beginning of the section.

We underline that some tables of measures for all equilibrium quantities which appear in this equation, except the interfacial mass density, are available in the literature: therefore it is possible to use it to determine indirectly the interfacial mass density. Before discussing shortly the numerical information which could be drawn from Eq. (4.12), it is necessary to compare it with the theoretical results found in the literature in order to warn the reader about a danger which one should avoid. Indeed in the literature (see for example ADAMSON [4]) sometimes a little approximation (cf. 50, the lines between Eq. (III-6) and Eq. (III-7) in [4]) is made: *"as a good approximation surface enthalpy per unit area and surface inner energy per unit area are not distinguished"*. The reasons for this statement, its explanation being left to those readers which are familiar with Gibbsian thermodynamics, most likely can be found in the papers of GIBBS himself [7]. We limit ourselves to remark that, as a consequence of this statement, we obtain (Eq. (III-8) at p. 50 in [4])

$$E^*_{\sigma P} = \gamma^*_P - \vartheta\frac{d\gamma^*_P}{d\vartheta}, \tag{4.13}$$

which trivially implies that, because of Eq. (4.12),

$$\rho^*_{\sigma P} = 0. \tag{4.14}$$

We can conclude that the approximation quoted by Adamson consists in neglecting the interfacial mass density. Two problems now arise:

1. It is not clear to us if Tolman in his papers accepts or not the quoted approximation, but it is certain that he needs to evaluate equilibrium surface mass density as it appears in the definition of the function $\delta(H)$.

2. When the tables of measurements are to be used, one should check if the interfacial inner energy has been measured directly or indirectly by means of (4.13) (as it seems to be the case, for instance, in case of the measures listed in WOLF [23]).

If we make use of tables of measurements which apparently do not use (4.13) (for instance see [24]), we can obtain some interesting results, when organizing the data following Eq. (4.12). Indeed,

i) we can observe that the second factor on its RHS is negative (what is physically obvious in view of the meaning of enthalpy);

ii) its LHS is also always negative (we believe that this circumstance is related to the nonlinearities in the dependence of the equilibrium γ on the temperature, measured by KAYSER [14]);

iii) the numerical value obtained for water at 20°C are of the order of magnitude of $10^{-8} - 10^{-7}$ g/cm^2, which is the order of magnitude generally accepted as the most likely in the literature (for a detailed discussion of this point see the series of papers of ALTS and HUTTER [25]).

However, we do not believe it would be wise to rely much on Eq. (4.12) since we are aware of simplicity of the model which allowed for its deduction; together with the Tolman formula it should be generalized to a more reliable one, once a more sophisticated model for the interface will be available.

4.2 Spherical interfaces. The Kelvin formula for vapour pressure and the influence of surface free energy on surface mass density

In order to simplify the comparison between the theoretical results and experimental data, in the literature instead of the vapour pressure p_v all equilibrium quantities are often expressed as functions of the variable H. While this choice is legitimate (at least in the framework of the model we use in this paper, see considerations following Eq. (3.3)) it leads, even when the simplest constitutive assumptions are made, to some technical problems in the explicit calculation of the quoted equilibrium function. A typical example of this situation is represented by the relationship between the curvature H and the vapour pressure, which in the literature is named after Kelvin.

Differentiating Eqs. $(2.4)_{1,2}$ with respect to the variable H and using Eqs. (3.1), we obtain

$$\left(1-\frac{\rho_l}{\rho_v}\right)\frac{d\widetilde{p}_v}{dH} = -\frac{d}{dH}(2H\widetilde{\gamma}). \tag{4.15}$$

If we assume that

C1. The liquid phase is incompressible.

C2. The vapour is a perfect gas so that the following relation holds:

$$p_v = R_v\vartheta\rho_v, \tag{4.16}$$

then from (4.15) we obtain

$$\frac{d}{dH}(-\rho_l R_v\vartheta\ln(\widetilde{p}_v) + \widetilde{p}_v + 2H\widetilde{\gamma}) = 0 \tag{4.17}$$

which becomes (as $\widetilde{p}_v(0,\vartheta) = p^*_{vP}(\vartheta)$)

$$\rho_l R_v\vartheta\ln\left(\frac{\widetilde{p}_v}{p^*_{vP}}\right) = -(p^*_{vP}-\widetilde{p}_v) + 2H\widetilde{\gamma}\,. \tag{4.18}$$

Equation (4.18) is exactly the Kelvin formula: it is seen that already under the particular constitutive assumption C1–C2 the function mapping H into p_v is transcendental. Moreover, in (4.18) the unknown function δ appears, since $\widetilde{\gamma}$ depends on it.

When more general constitutive equations are to be introduced, we can regard (4.15) as an equation which generalizes the Kelvin formula.

Let us now briefly consider the system of equations which governs the equilibrium of drops separated from their vapour by compressible Defay–Prigogine $2D$-continua (we do not indicate the dependence on the temperature ϑ which is assumed to be fixed),

$$\begin{aligned} p_l &= p_v + 2H\gamma\,,\\ g_l(p_l) &= g_v(p_v)\,,\\ g_\sigma(\rho_\sigma) &= g_v(p_v)\,, \end{aligned} \tag{4.19}$$

to which we must add the constitutive relation

$$\gamma = \gamma(\rho_\sigma)/\frac{\partial\gamma}{\partial\rho_\sigma} > 0\,, \tag{4.20}$$

which is invertible, so that we can regard the Gibbs potential also as a function of γ.

Now we recall that ROMANO in [26], using the consequences of the second principle of thermodynamics together with some well-grounded physical assumptions on the Gibbs potential, could prove the existence and the uniqueness of the solutions of the system $(4.19)_{1,2}$. Therefore, to complete the proof of the validity of Gibbs phase rule we started in Sec. 2, we only need to prove the existence and uniqueness of the surface density ρ_σ^* which is a solution of $(4.19)_3$ when $p_v = p_v^*$.

To this aim we assume (as done in the second part of the hypothesis iii) on p. 261 in [26]) that

$$\lim_{\rho_\sigma \to \infty} g_\sigma(\rho_\sigma) = \infty\,, \qquad \lim_{\rho_\sigma \to 0} g_\sigma(\rho_\sigma) = -\infty\,. \tag{4.21}$$

Moreover, we remark that we do not need to introduce any hypothesis similar to that formulated in [26] (cf. Eq. (3.7) there): indeed, starting from the thermodynamical relations (2.1) we can easily prove that *for every* $\vartheta \in]\vartheta_*, \vartheta_c[$ (ϑ_* *— temperature of the triple point*, ϑ_c *— critical temperature*) there exists a unique solution $\rho_{\sigma P}^*$ for $(4.19)_3$ once the value p_{vP}^* is substituted on its RHS. When (4.21) is accepted, the proof parallels step-by-step that presented in [26] to which we refer. In principle, therefore, once all constitutive assumptions for liquid, vapour and interfacial phases are made and, in particular, when the interfacial free energy is chosen in such a way that the hypotheses (4.20)–(4.21) are respected, the equilibrium functions $\delta(p_v)$, $\gamma^*(p_v)$, $\rho_v^*(p_v)$ and $\rho_l^*(p_v)$ can be determined. Using the thesis in (3.3) and the definition of δ, the function $\delta(H)$ can also be found. In order to obtain some suggestions concerning the dependence of surface mass density on vapour pressure and an interesting expression for $d\delta/dH$ we assume C1, C2, and

C3. The interface is a linearly compressible bidimensional fluid, and its Gibbs potential is given by

$$g_\sigma(\vartheta, \rho_\sigma) = g_v(p_{vP}^*(\vartheta), \vartheta) + \alpha(\vartheta) \ln\left(\frac{\rho_\sigma}{\rho_{\sigma P}^*(\vartheta)}\right). \tag{4.22}$$

The function $\alpha(\vartheta)$, to our knowledge, was never introduced in the literature, neither we could find any experimental data which could, suitably reinterpreted, allow for its determination. However, (4.22) is clearly related, via the thermodynamical relationships (2.1), to Eötvös relation (III-10) in ADAMSON [4]. Because of C2 we have

$$g_v(\vartheta, p_v) = g_v(p_{vP}^*(\vartheta), \vartheta) + R_v\vartheta \ln\left(\frac{p_v}{p_{vP}^*(\vartheta)}\right), \tag{4.23}$$

so that Eq. $(2.4)_3$ implies that:

$$\left(\frac{\rho_\sigma^*}{\rho_{\sigma P}^*(\vartheta)}\right)^{\frac{\alpha(\vartheta)}{R_v\vartheta}} = \left(\frac{p_v}{p_{vP}^*(\vartheta)}\right). \tag{4.24}$$

Finally we add the following assumption (cf. the experimental data listed by FISHER-ISRAELACHVILI in [18, 19]) that in the range of considered measures

C4. The vapour mass density is negligible with respect the liquid mass density (i.e. $\rho_v \ll \rho_l$); therefore because of the definition of δ and the constitutive equation (4.16), we have

$$\frac{d\delta}{dH} = \frac{1}{\tilde{\rho}_l}\left(\left(\frac{d\tilde{\rho}_\sigma}{dH}\right) + \tilde{\rho}_\sigma (R_v\vartheta)^{-1}\frac{d\tilde{p}_v}{dH}\right). \tag{4.25}$$

Owing to (4.15), $(2.4)_3$ and (4.22), this becomes

$$\frac{d\delta}{dH} = \frac{1}{\widetilde{\rho}_l}(\alpha + \widetilde{\rho}_v(R_v\vartheta)^{-1})\frac{d\widetilde{\gamma}}{dH} \tag{4.26}$$

which, taking account of (3.5), (4.16) and (4.18) (in which the first term on RHS can be neglected in the range of measurements performed by Fisher–Israelachvili), represents an equation which determines δ. Indeed,

$$\delta(0) = \frac{\widetilde{\rho}_{\sigma P}}{\widetilde{\rho}_{lP} - \widetilde{\rho}_{vP}}. \tag{4.27}$$

5. Epilogue. Comments and program for further investigations

In this paper some classical results of chemical physics are generalized making use of the simple model for the interface between different phases of a single material proposed in [2].

In our opinion, the relative simplicity of our deduction compared with those proposed by TOLMAN [1] or ADAMSON [4] is due to our use of the methods of Rational Thermodynamics exposed by TRUESDELL in his classical work [27].

Therefore we expect that a further improvement in the modellization of the interfacial structure leading to the introduction of directed bidimensional nonmaterial continua could allow for the theoretical deduction of a relation between the equilibrium surface tension, surface mass and curvature, consistent with available experimental data. Moreover, we urge (cf. our discussion in subsec. 4.1) for the development of a more precise theoretical framework for the study of capillarity phenomena, as, in our opinion, the actual state of the art is pretty confuse. Too many theoretical prejudices make the appropriate interpretation of experimental evidence very defficult.

We can indicate here two improvements of the model proposed in [2] which could modify our understanding of the quoted phenomena, at least for what concerns the influence of capillarity on curvature.

i. Following the ideas developed by DICARLO–PODIO–GUIDUGLI–GURTIN [16], one could introduce nonmaterial constrained bidimensional continua, similar to those material bidimensional continua introduced in the theory of shells. Together with surface stress tensor, a couple-stress tensor and a suitable complex family of directors (spins, etc.) describe the state of the interface. One of these directors could model the direction of the flux of mass through the interface: the first formulation of the model could assume that this vector always coincides with the direction normal to the interface, thus introducing some unknown reaction terms of both surface stress and couple-stress tensor. In this model (contrary to the model we used in this paper), the dependence of interfacial free energy on curvature is allowed by the second principle of thermodynamics: therefore it seems possible to obtain, by a suitable selection of a constitutive equation for it, a generalized Tolman formula more consistent with the experimental evidence. This approach seems more reasonably founded for describing the interfaces, for instance, between solid and melted crystals.

ii. In the literature (see for instance [13, 17, 18, 19]) it is often stated that an influence of the thickness of the interface on equilibrium surface tension is possible. For this reason CHOI *et al.* [17] develop a theoretical method (using statistical mechanics) to define a dividing thickness between different phases of some carbon compound, and an experimental method to determine the thickness so defined. However these results, when used together with Tolman's data, lead to some results inconsistent with the experimental data. In [20] a heuristic method is proposed to add a more detailed structure to bidimensional nonmaterial continua used to describe capillarity phenomena. In this approach a concept of thickness is also introduced, which plays a relevant role in determining the behaviour of continua considered. However, we think that its physical nature is different from that introduced by CHOI *et al.* Indeed, the spatial region in which in [20] the interface is localized can be identified with the region in which the material in consideration shows a behaviour of the Korteweg type (see [22]) or of the second grade type (see [9, 10, 11, 12]).

The interfacial region so identified is more likely macroscopic than those introduced by means of the methods of statistical mechanics, and it could be defined as that region in which the constitutive equations for the Stokes–Navier simple materials cannot be considered to be valid.

To make the set of equations proposed in [20] complete from a physical point of view, it is necessary to specify the properties of the interfacial layer. This is done by

a) introducing one further surface scalar field modelling the thickness of the thin but macroscopic capillarity region (such a region is studied for instance by SEPPECHER in [9]), and

b) postulating (or deducing in the sense of [20]) the evolution equation for such a field.

The interfacial free energy for bidimensional continua endowed with this structure will depend also on the thickness, and this circumstance could lead to a solution of the proposed problem.

This approach seems more suitable for the description of the behaviour of the interfaces between fluid phases.

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Growth of spherical voids in shear bands

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BASED ON MACROSCOPIC constitutive relations for nonlinearly viscous voided materials, the spherical void growth law in shear bands is investigated through the upper bound approach. A unit cell isolated from shear bands is considered for studies. Microscopic velocity fields are developed by incompressibility of the matrix material and the velocity boundary condition. From the velocity fields, the macroscopic potential and corresponding constitutive relations are found. Then, a relative void growth rate is obtained as an implicit function of the stress triaxiality, void volume fraction and strain rate sensitivity. When the matrix is a perfectly plastic material, we obtain an approximate analytical expression. When the matrix becomes a linearly viscous material, an exact expression is obtained. The special case corresponding to an isolated void is also discussed. Comparisons of the growth rates for three-dimensional ($3D$) spherical voids with those for two-dimensional ($2D$) cylindrical voids are made. Results show that the growth rates for $2D$ voids are larger than those for $3D$ voids. The void growth rates are also influenced strongly by the degree of damage and nonlinearity of the material.

1. Introduction

FRACTURE by shear bands has been observed in ductile materials in a lot of experiments. The mechanism of the fracture is growth and coalescence of microvoids, which was also observed by experiments [1]. However, studies for void growth in shear bands are relatively little known. The early work on such a problem was made by MCCLINTOCK *et al.* [1] in 1966. They studied the isolated $2D$ cylindrical voids with circular or elliptical cross-sections in shear bands for a linearly viscous solid using Muskhelishvili methods. Later, in 1986, FLECK and HUTCHINSON [2] expanded the results of McClintock *et al.* to a nonlinear power-law viscous solid using a potential function and obtained some numerical results. Their work is significant since it reveals the void growth and the void shape evolution in shear bands for the first time. These studies are only restricted to an isolated void in an infinite matrix material. However, void interaction may occur in shear bands especially at the stage of void coalescence. To account for void interaction effects, we usually assume the voids to be arranged in a space filling array since this allows a simple "unit cell" to be isolated for study. In this way, a micromechanical quantity, the void volume fraction, can be introduced. The pioneering work using this method was given by GURSON [3] who obtained constitutive models for solids containing circular-cylindrical or spherical voids through an upper bound approach. Other studies on such methods were given by TRACEY [4] and NEEDLEMAN [5] who modelled the response of an array of circular-cylindrical voids, and by LICHT and SUQUET [6] who gave a simple model for cylindrical void growth in a nonlinearly viscous material at arbitrary void volume fractions. Some authors extended Gurson's results by numerical calculations. For example, TVERGAARD [7] has attempted to improve the accuracy of the Gurson model by adjusting some of its numerical coefficients so that the model is more accurate for a voided material, and MEAR [8] has obtained an exact numerical result for the stress-strain response of an elastic-plastic material containing a cubic array of spherical voids. Studies for void growth in a finite body were also given by DUVA [9], and WORSWICK and PICK [10]. The comprehensive review descriptions on this subject were given by GILORMINI *et al.* [11] and NEEDLEMAN *et al.* [12]. Recently, PAN and HUANG [13] considered effects of void growth on constitutive relations for viscoplastic materials containing circular-cylindrical voids. PAN [14] studied cylindrical void growth in shear bands for nonlinear power-law viscous solids.

This paper expands the previous work [14] to $3D$ spherical voids by analyzing a unit cell isolated from shear bands in a nonlinearly viscous material through an upper bound approach. This method has been employed by Gurson and some others to develop constitutive models for porous ductile materials, as described above. Experiments have shown that, in shear bands, there is not only the shear stress but also the transverse compressive stress components [1]. To obtain the macroscopic constitutive relations, a boundary condition of simple shearing with superimposed triaxial loading is considered. From such a boundary condition and incompressibility of the matrix material, the microscopic velocity field, equivalent strain rate, macroscopic potential function and the corresponding constitutive relations are obtained. Then, based on the constitutive relations, the stress triaxiality can be defined under simple shearing and hydrostatic tension (or pressure) states. The relative void growth rate can be found numerically as an implicit function of the stress triaxiality, void volume fraction and strain rate sensitivity exponent. From the general expression for the void growth rate, some special cases such as perfectly plastic matrix material, Newtonian matrix material and infinite matrix material are discussed in details, and in these cases some analytical expressions can be obtained. Finally, comparisons of the present results with previous results of $2D$ model and Fleck–Hutchinson model are made. The results show similar behaviors of void growth in $3D$ and in $2D$. However, the latter is larger than the former under the same conditions (the same loading condition, void volume fraction and strain rate sensitivity exponent). The investigated results also predict that void growth in shear bands is governed mainly by the stress triaxiality and the degree of damage and nonlinearity of the material.

2. Macroscopic constitutive relations

A unit cell containing a spherical traction-free void and outer velocity field are shown in Fig. 1. The radii of the void and the cell are a and b, respectively. Volumes of the void and the matrix are V_v and V_m, respectively. The volume of the cell is then $V = V_v + V_m$. The macroscopic and microscopic quantities employed throughout the paper are denoted, respectively, by upper-case letters and lower-case letters. For example, Σ_{ij} and $\dot{E}_{ij}$ are macroscopic stress and strain rate. σ_{ij} and $\dot{\varepsilon}_{ij}$ are microscopic stress and strain rate. With these conventions, the outer velocity field can be expressed as simple shearing with superimposed triaxial loading

$$v_1 = \dot{E}_{11}x_1 + \dot{\Gamma}x_2, \qquad v_2 = \dot{E}_{22}x_2, \qquad v_3 = \dot{E}_{33}x_3, \tag{2.1}$$

where $x_1 = x$, $x_2 = y$, $x_3 = z$ are rectangular coordinates, $\dot{\Gamma}$ is shear strain rate and its corresponding tensorial components are

$$\dot{E}_{12} = \dot{E}_{21} = \dot{\Gamma}/2. \tag{2.2}$$

For convenience, we assume $\dot{E}_{ij} \geq 0$. The case $\dot{E}_{ij} \leq 0$ can be treated in the same way.

The matrix is assumed to be an incompressible and nonlinearly viscous material. In simple tension, the stress and strain rate are related by a power-law formula

$$\sigma = \mu\dot{\varepsilon}^n,$$

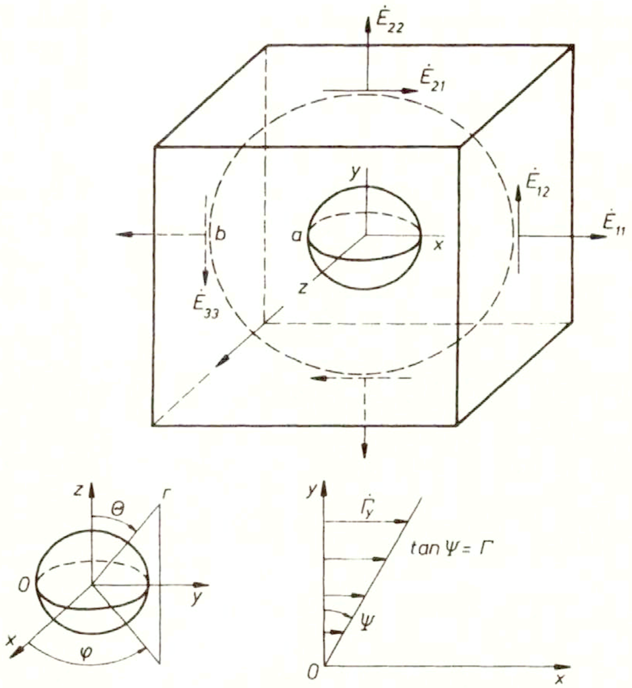

FIG. 1. A unit cell and outer loading.

where n $(0 \leq n \leq 1)$ is a strain rate sensitivity exponent and μ is a viscous constant defined by

$$\mu = \sigma_0/\dot{\varepsilon}_0^n,$$

whereas σ_0 and $\dot{\varepsilon}_0$ are reference stress and strain rate.

For multiaxial states, a microscopic potential can be introduced to describe the relation of the stress and strain rate in the matrix material

$$\varphi(\dot{\epsilon}) = \mu(n+1)^{-1}\dot{\varepsilon}_e^{(n+1)}, \tag{2.3}$$

so that the stress is

$$s_{ij} = (2\mu/3)(\dot{\varepsilon}_e)^{n-1}\dot{\varepsilon}_{ij}, \tag{2.4}$$

where s is the stress deviator and $\dot{\varepsilon}_e = (2\dot{\varepsilon}_{ij}\dot{\varepsilon}_{ij}/3)^{1/2}$ is the equivalent strain rate. The macroscopic potential is related to a distribution of the microscopic potential by

$$\Phi(\dot{\mathbf{E}}) = V^{-1}\int\limits_{V_m}\varphi\, dV. \tag{2.5}$$

The macroscopic, or overall stress is given by

$$\Sigma_{ij} = \partial\Phi/\partial\dot{E}_{ij}. \tag{2.6}$$

The key element for finding macroscopic constitutive relations is the velocity field in the matrix material, from which the equivalent strain rate, both microscopic and macroscopic potentials and then macroscopic constitutive relations can be found by Eqs. (2.3)–(2.6).

The velocity field should satisfy the velocity boundary condition and incompressibility of the matrix material. For this purpose, we divide the velocity field into three parts

$$\mathbf{v} = \mathbf{v}' + \mathbf{v}^v + \mathbf{v}^*,$$

where $\mathbf{v}'$ and $\mathbf{v}^v$ correspond, respectively, to the deviatoric part and the dilatational part of the field $\dot{\epsilon}$, and each satisfies its corresponding velocity boundary condition as well as incompressibility. $\mathbf{v}^*$ should satisfy zero boundary condition and incompressibility. If only the first two terms in the velocity field are considered, an upper bound solution will be obtained. The boundary conditions corresponding to $\mathbf{v}'$ and $\mathbf{v}^v$ can be expressed as follows under spherical coordinates (r, θ, φ) (see Fig. 1):

$$\begin{aligned} v'_r|_{r=b} &= b(\dot{E}'_{11}\cos^2\varphi + \dot{E}'_{22}\sin^2\varphi)\sin^2\theta + b\dot{E}'_{33}\cos^2\theta + \frac{1}{2}b\dot{\Gamma}\sin^2\theta\sin 2\varphi, \\ v'_\theta|_{r=b} &= \frac{1}{2}b(\dot{E}'_{11}\cos^2\varphi + \dot{E}'_{22}\sin^2\varphi - \dot{E}'_{33})\sin 2\theta + \frac{1}{4}b\dot{\Gamma}\sin 2\theta\sin 2\varphi, \\ v'_\varphi|_{r=b} &= \frac{1}{2}b(\dot{E}'_{22} - \dot{E}'_{11})\sin\theta\sin 2\varphi - b\dot{\Gamma}\sin\theta\sin^2\varphi; \end{aligned} \tag{2.7}$$

$$v^v_r|_{r=b} = b\dot{E}, \qquad v^v_\theta|_{r=b} = 0, \qquad v^v_\varphi|_{r=b} = 0, \tag{2.8}$$

where $\dot{E}'_{ij} = \dot{E}_{ij} - \dot{E}$ is the deviator of $\dot{E}_{ij}$, and $\dot{E} = \dot{E}_{kk}/3$ is the overall mean stress. It can be proved that $\mathbf{v}'$ satisfies the incompressibility condition $\dot{\varepsilon}'_{kk} = 0$. $\mathbf{v}^v$ can be found from the incompressibility equation

$$\dot{\varepsilon}^v_{kk} = \partial v^v_r/\partial r + 2r^{-1}v^v_r = 0$$

and the boundary condition (2.8), which gives

$$v^v_r = \dot{E}b^3/r^2, \qquad v^v_\theta = 0, \qquad v^v_\varphi = 0.$$

Then, we have the microscopic velocity field

$$\begin{aligned} v_r &= v'_r + v^v_r = r\dot{E}_e h_1 + r\dot{E}' h_2\cos 2\varphi + \frac{1}{2}r\dot{\Gamma}h_2\sin 2\varphi + Ar^{-2}, \\ v_\theta &= v'_\theta + v^v_\theta = \frac{1}{4}r\sin 2\theta(3\dot{E}_e + 2\dot{E}'\cos 2\varphi + \dot{\Gamma}\sin 2\varphi), \\ v_\varphi &= v'_\varphi + v^v_\varphi = -r\sin\theta(\dot{E}'\sin 2\varphi + \dot{\Gamma}\sin^2\varphi), \end{aligned} \tag{2.9}$$

where

$$A = \dot{E}b^3, \qquad \dot{E}_e = \dot{E} - \dot{E}_{33}, \qquad \dot{E}' = (\dot{E}_{11} - \dot{E}_{22})/2,$$
$$h_1 \equiv h_1(\theta) = (1 - 3\cos^2\theta)/2, \qquad h_2 \equiv h_2(\theta) = \sin^2\theta.$$

The strain rate components can be expressed by the velocity components in Eq. (2.9) as follows:

$$\dot{\varepsilon}_{rr} = \frac{\partial}{\partial r}v_r = \dot{E}_e h_1 + \dot{E}' h_2\cos 2\varphi + \frac{1}{2}\dot{\Gamma}h_2\sin 2\varphi - 2Ar^{-3},$$

$$\dot{\varepsilon}_{\theta\theta} = \frac{\partial}{r\partial\theta}v_\theta + \frac{1}{r}v_r = \dot{E}_e h_3 + \dot{E}' h_4 \cos 2\varphi + \frac{1}{2}\dot{\Gamma} h_4 \sin 2\varphi + Ar^{-3},$$

$$\dot{\varepsilon}_{\varphi\varphi} = \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}v_\varphi + \frac{\operatorname{ctan}\theta}{r}v_\theta + \frac{1}{r}v_r = \frac{1}{2}\dot{E}_e - \dot{E}'\cos 2\varphi - \frac{1}{2}\dot{\Gamma}\sin 2\varphi + Ar^{-3},$$

$$\dot{\varepsilon}_{r\theta} = \frac{1}{2}\left(\frac{\partial}{r\partial\theta}v_r + \frac{\partial}{\partial r}v_\theta - \frac{1}{r}v_\theta\right) = \frac{1}{2}\sin 2\theta\left(\frac{3}{2}\dot{E}_e + \dot{E}'\cos 2\varphi + \frac{1}{2}\dot{\Gamma}\sin 2\varphi\right),$$

$$\dot{\varepsilon}_{r\varphi} = \frac{1}{2}\left(\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}v_r + \frac{\partial}{\partial r}v_\varphi - \frac{1}{r}v_\varphi\right) = \sin\theta\left(-\dot{E}'\sin 2\varphi + \frac{1}{2}\dot{\Gamma}\cos 2\varphi\right),$$

$$\dot{\varepsilon}_{\theta\varphi} = \frac{1}{2}\left(\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}v_\theta + \frac{\partial}{r\partial\theta}v_\varphi - \frac{\operatorname{ctan}\theta}{r}v_\varphi\right) = \cos\theta(-\dot{E}'\sin 2\varphi + \frac{1}{2}\dot{\Gamma}\cos 2\varphi),$$

where

$$h_3 \equiv h_3(\theta) = -(2 - 3\cos^2\theta)/2, \qquad h_4 \equiv h_4(\theta) = \cos^2\theta.$$

Then, the equivalent strain rate can be found as

$$\dot{\varepsilon}_e = H^{1/2}, \tag{2.10}$$

where

$$H \equiv \dot{E}_e^2 + \frac{4}{3}\dot{E}'^2 + 4\dot{E}^2x^2 - 4\dot{E}_e\dot{E}xh_1 - 4\dot{E}'\dot{E}xh_2\cos 2\varphi - 2\dot{\Gamma}\dot{E}xh_2\sin 2\varphi + \frac{1}{3}\dot{\Gamma}^2$$

and the variable $x = b^3/r^3$ has been introduced for convenience.

Substituting Eq. (2.10) into Eqs. (2.3) and (2.5) and then into Eq. (2.6), we can find macroscopic constitutive relations

$$\Sigma_{ij} = \frac{\mu}{8\pi}\int_0^{2\pi}\int_0^{\pi}\int_1^{1/f} H^{(n-1)/2}H_{ij}\sin\theta x^{-2}\,dx\,d\theta\,d\varphi, \tag{2.11}$$

where

$$H_{11} = \frac{2}{3}\dot{E}_e + \frac{4}{3}\dot{E}' + \frac{8}{3}\dot{E}x^2 - \frac{4}{3}(2\dot{E} - \dot{E}_{33})xh_1 - \frac{2}{3}(3\dot{E} + 2\dot{E}')xh_2\cos 2\varphi - \frac{2}{3}\dot{\Gamma}xh_2\sin 2\varphi,$$

$$H_{22} = \frac{2}{3}\dot{E}_e - \frac{4}{3}\dot{E}' + \frac{8}{3}\dot{E}x^2 - \frac{4}{3}(2\dot{E} - \dot{E}_{33})xh_1 + \frac{2}{3}(3\dot{E} - 2\dot{E}')xh_2\cos 2\varphi - \frac{2}{3}\dot{\Gamma}xh_2\sin 2\varphi,$$

$$H_{33} = -\frac{4}{3}\dot{E}_e + \frac{8}{3}\dot{E}x^2 + \frac{4}{3}(2\dot{E} - \dot{E}_e)xh_1 - \frac{4}{3}\dot{E}'xh_2\cos 2\varphi - \frac{2}{3}\dot{\Gamma}xh_2\sin 2\varphi,$$

$$H_{12} = -2\dot{E}xh_2\sin 2\varphi + \frac{2}{3}\dot{\Gamma}.$$

In Eq. (2.11), the integral limit f is defined by

$$f \equiv V_v/V = a^3/b^3 \tag{2.12}$$

and is called the void volume fraction which is a damage variable and can be used to describe the isotropic damage of ductile materials. In this way, some account is taken of the void interaction. The criterion of the void volume fraction in shear bands may be determined by experiments. Here we assume that the evolution of the void volume fraction and the rate of macroscopic volume expansion have the following relation:

$$\dot{f} = (1 - f)\dot{E}_{kk}. \tag{2.13}$$

With Eq. (2.13) and the definition of $\dot{E}_{kk}$, we can obtain a relation between the rate of macroscopic volume expansion and the voids' logarithmic growth rate $\dot{V}_v/V_v$

$$\dot{E}_{kk} = f\dot{V}_v/V_v. \tag{2.14}$$

This relation can also be obtained by consideration of incompressibility of the material.

From the above discussions in this section, we conclude that for any given macroscopic strain rates $\dot{E}_{ij}$, the macroscopic stresses Σ_{ij} can be determined by Eq. (2.11) using numerical integration.

3. Void growth in shear bands

The void growth law in shear bands can be investigated by constitutive relations in Eq. (2.11) and the velocity boundary condition

$$\dot{\Gamma} \neq 0 \quad \text{and} \quad \dot{E}_{11} = \dot{E}_{22} = \dot{E}_{33} \neq 0. \tag{3.1}$$

They correspond to stresses Σ_{12} and $\Sigma_m = \Sigma_{kk}/3$. All possible overall stress states can be described by the ratio of Σ_m and Σ_{12}. This gives a definition of the stress triaxiality

$$\chi \equiv 2\Sigma_m/\sqrt{3}\Sigma_{12}, \tag{3.2}$$

where Σ_m and Σ_{12} are found by the constitutive equation (2.11) with the boundary condition (3.1) in non-dimensional forms:

$$\begin{aligned} \Sigma_m &= \int_0^{2\pi}\int_0^{\pi}\int_{\omega}^{\omega^*} \overline{H}^{(n-1)/2}\overline{H}_m \sin\theta t^{-2}\,dt\,d\theta\,d\varphi, \\ \Sigma_{12} &= \int_0^{2\pi}\int_0^{\pi}\int_{\omega}^{\omega^*} \overline{H}^{(n-1)/2}\overline{H}_{12} \sin\theta t^{-2}\omega\,dt\,d\theta\,d\varphi, \end{aligned} \tag{3.3}$$

whereas

$$\begin{aligned} \overline{H}_m &\equiv \overline{H}_m(t,\theta,\varphi) = t^2 - th, \\ \overline{H}_{12} &\equiv \overline{H}_{12}(t,\theta,\varphi) = 1 - th, \\ \overline{H} &\equiv \overline{H}(t,\theta,\varphi) = 1 + t^2 - 2th, \\ h &\equiv h(\theta,\varphi) = \frac{1}{2}\sqrt{3}\sin^2\theta\sin 2\varphi. \end{aligned}$$

The constants in front of the integrals for Σ_m and Σ_{12} have been omitted for they have no effect on the ratio χ. In Eq. (3.3), a new quantity, the relative void growth rate

$$\lambda = \dot{V}_v/(\dot{\Gamma}V_v) \tag{3.4}$$

and substitutions

$$t = \omega x, \quad \omega = 2\lambda f/\sqrt{3}, \quad \omega^* = 2\lambda/\sqrt{3}$$

have been introduced using the relation (2.14). To obtain the integrals in Eq. (3.3), we expand $\overline{H}^{(n-1)/2}$ into the series of h since $|h| < 1$

$$\overline{H}^{(n-1)/2} = P^{(n-1)/2}\left[1 + \sum_{k=1}^{\infty} \frac{(2k-1-n)!!}{(2k)!!}\left(\frac{2t}{P}h\right)^{k}\right],$$

where

$$P \equiv P(t) = 1 + t^2.$$

Noting the following integrals:

$$\int_0^{2\pi}\int_0^{\pi} \sin\theta \, d\theta \, d\varphi = 4\pi,$$

$$\int_0^{2\pi}\int_0^{\pi} h^k \sin\theta \, d\theta \, d\varphi = \begin{cases} 0, & \text{for } k = 2m-1, \\ 4\pi I_m & \text{for } k = 2m \quad (m = 1,2,3,\ldots), \end{cases}$$

where

$$I_m = \frac{(4m)!!(2m-1)!!}{(2m)!!(4m+1)!!}\left(\frac{\sqrt{3}}{2}\right)^{2m},$$

we can perform the integrals in Eq. (3.3) with respect to variables θ and φ, which leads to

$$\text{(3.5)} \qquad \begin{aligned} \Sigma_m &= 4\pi \int_{\omega}^{\omega^*} (F_1 + F_m)\, dt, \\ \Sigma_{12} &= 4\pi \int_{\omega}^{\omega^*} (G_1 + G_m) t^{-2} \omega \, dt, \end{aligned}$$

where

$$F_1 = P^{(n-1)/2} + \frac{1}{10}(1-n)[(1-n)P^{(n-3)/2} - (3-n)P^{(n-5)/2}],$$

$$G_1 = P^{(n-1)/2} - \frac{1}{10}(1-n)[2(1-n)P^{(n-3)/2} - (3-n)P^{(n-5)/2}]t^2,$$

$$F_m = \sum_{m=2}^{\infty}\left(g_{1m} - \frac{1}{2}g_{2m}Pt^{-2}\right)(2t)^{2m}P^{(n-1-4m)/2}I_m,$$

$$G_m = \sum_{m=2}^{\infty}\left(g_{1m} - \frac{1}{2}g_{2m}P\right)(2t)^{2m}P^{(n-1-4m)/2}I_m,$$

and

$$g_{1m} = \frac{(4m-1-n)!!}{(4m)!!}, \qquad g_{2m} = \frac{(4m-3-n)!!}{(4m-2)!!}.$$

Then, from Eq. (3.2) the stress triaxiality can be expressed by

$$\text{(3.6)} \qquad \chi \equiv \chi(\lambda, f, n, m) = 2\Sigma_m/\sqrt{3}\Sigma_{12}.$$

With variables λ, f, n and m, the values of function χ are listed in Table 1.

Table 1. Values of χ as a function of λ, f, n and m.

	$n = 0$, $\lambda = 10$,	$f = 0.1$, 20,	$m = 7$ 30	$n = 0$, $f = 0.1$,	$\lambda = 10$, 0.25,	$m = 7$ 0.4	$f = 0.1$, $n = 0$,	$\lambda = 10$, 0.3,	$m = 7$ 0.6
χ_1	2.20	2.28	2.29	2.20	1.37	0.91	2.20	3.40	5.40
$\chi_{2(10^{-2})}$	3.09	0.72	0.19	3.09	0.35	0.06	3.09	3.82	4.79
$\chi_{3(10^{-1})}$	3.55	1.84	1.22	3.55	1.39	7.76	3.55	4.65	6.20
$\chi_{4(10^{-2})}$	−2.78	−1.46	−0.59	−2.78	−0.91	−0.27	−2.78	−3.21	−3.75

	$m = 5$,	6,	7,	8,	9	$(\lambda = 10, n = 0, f = 0.1)$
$\chi_{2(10^{-2})}$	3.087	3.090	3.091	3.092	3.092	
$\chi_{4(10^{-2})}$	−2.795	−2.799	−2.780	−2.780	−2.780	

where $\chi_1 = \int_\omega^{\omega^*} F_1\,dt$, $\chi_2 = \int_\omega^{\omega^*} F_m\,dt$, $\chi_3 = \int_\omega^{\omega^*} G_1 t^{-2}\omega\,dt$, $\chi_4 = \int_\omega^{\omega^*} G_m t^{-2}\omega\,dt$.

It is found that χ_2 and χ_4 are convergent functions since they are almost constant for given λ, f, n and m ($m \geq 7$). Table 1 also predicts that the terms χ_2 and χ_4 have little contribution to χ. Comparing χ_2 and χ_4 with their corresponding main terms χ_1 and χ_3, we find that χ_2 and χ_4 are high order infinitesmall quantities and the quantities become much smaller with increased λ and f, but decreased n. Therefore, for large void growth rate λ and void volume fraction f (e.g., $\lambda \geq 10$, $f \geq 0.1$), we have a better approximate, but simple expression for the stress triaxiality

$$\chi = 2\chi_1/\sqrt{3}\chi_3. \tag{3.7}$$

Equation (3.7) will be analytical for $n = 0$ and $n = 1$. For $n = 0$, we have

$$\chi = \frac{2}{\sqrt{3}}\,\frac{\ln\left[\dfrac{\omega^* + \sqrt{(1+\omega^{*2})}}{\omega + \sqrt{(1+\omega^2)}}\right] - \dfrac{1}{10}\left[\dfrac{\omega^*(2+\omega^{*2})}{\sqrt{(1+\omega^{*2})^3}} - \dfrac{\omega(2+\omega^2)}{\sqrt{(1+\omega^2)^3}}\right]}{\sqrt{(1+\omega^2)} - f\sqrt{(1+\omega^{*2})} + \dfrac{\omega}{10}\left[\dfrac{\omega^*}{\sqrt{(1+\omega^{*2})^3}} - \dfrac{\omega}{\sqrt{(1+\omega^2)^3}}\right]}. \tag{3.8}$$

For $n = 1$, we have

$$\chi = \frac{4}{3}\lambda. \tag{3.9}$$

In fact, Eq. (3.9) is an exact expression for we can obtain it directly from Eq. (3.2) using $n = 1$, which is true for a linearly viscous Newtonian matrix material. For small λ and f, there are some deviations between Eqs. (3.6) and (3.7), which are plotted in Figs. 2 and 3 for several f and n.

For the case $f = 0$, we will have a detailed discussion in the next section. The lines of $n = 0$ and $n = 1$ in Fig. 3 come from Eqs. (3.8) and (3.9). It is found that λ increases with decreasing f and n when χ is fixed. The largest rate of void growth is for $f = 0$ (without void interaction effects) and $n = 0$ (perfectly plastic material). To compare the present results for $3D$ spherical voids in shear bands with those for $2D$ circular-cylindrical voids, we also give relations of the stress triaxiality and the relative void growth rate for $2D$ voids from the previous work [14] as follows:

$$\chi = \int_{\lambda f}^{\lambda} F_1(t)\,dt \Big/ \int_{\lambda f}^{\lambda} G_1(t) t^{-2}\lambda f\,dt, \tag{3.10}$$

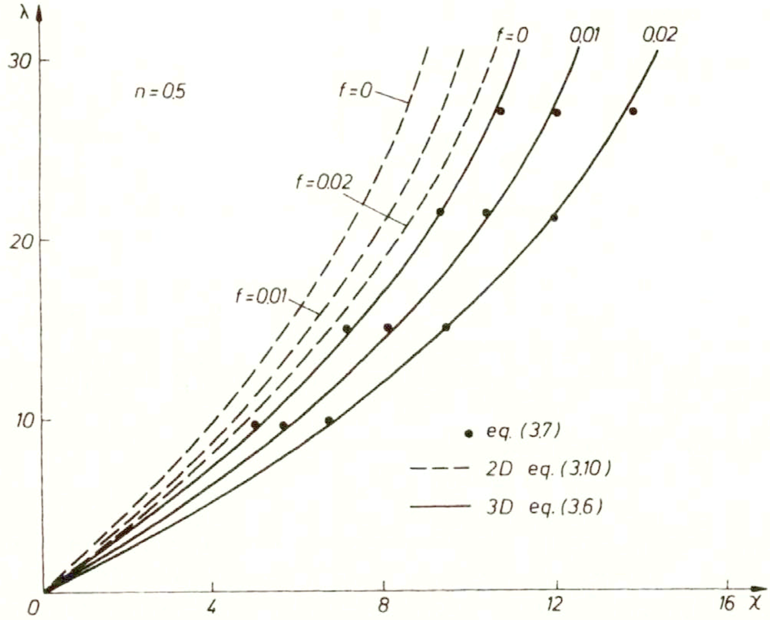

FIG. 2. Relation between void growth rate λ and triaxiality χ at several values of void fraction f ($n = 0.5$).

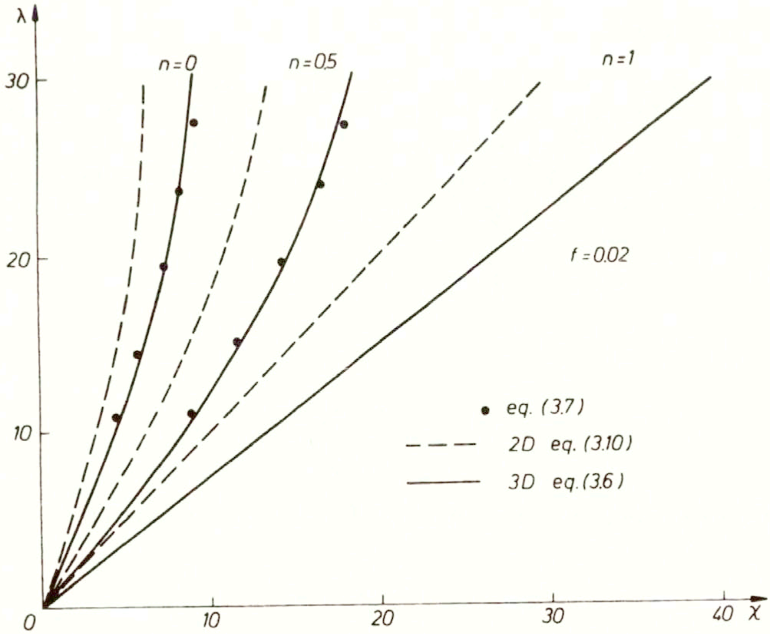

FIG. 3. Relation between void growth rate λ and triaxiality χ at several values of strain rate sensitivity exponent n ($f = 0.02$).

where

$$F_1 = P^{(n-1)/2} + \frac{1}{4}(1-n)[(1-n)P^{(n-3)/2} - (3-n)P^{(n-5)/2}],$$

$$G_1 = P^{(n-1)/2} - \frac{1}{4}(1-n)[(2P^{(n-3)/2} - (3-n)P^{(n-5)/2}]t^2.$$

When $n = 0$ and $n = 1$, Eq. (3.10) also gives analytical expressions

(3.11)
$$\chi = \frac{\ln\left[\dfrac{\lambda + \sqrt{(1+\lambda^2)}}{\omega + \sqrt{(1+\omega^2)}}\right] - \dfrac{1}{4}\left[\dfrac{\lambda(2+\lambda^2)}{\sqrt{(1+\lambda^2)^3}} - \dfrac{\omega(2+\omega^2)}{\sqrt{(1+\omega^2)^3}}\right]}{\sqrt{(1+\omega^2)} - f\sqrt{(1+\lambda^2)} + \dfrac{\omega}{4}\left[\dfrac{\lambda}{\sqrt{(1+\lambda^2)^3}} - \dfrac{\omega}{\sqrt{(1+\omega^2)^3}}\right]},$$

where $\omega = \lambda f$ (for $2D$ voids), and

(3.12)
$$\chi = \lambda.$$

These results are also plotted in Fig. 2 for several void volume fraction f, and in Fig. 3 for several strain rate sensitivity exponent n as compared with $3D$ voids. From these diagrams, we can conclude that $2D$ voids in shear bands increase more quickly than $3D$ voids under the same loading condition and the same material behavior (the same damage and nonlinearity of the material).

4. An isolated void model

At the initial stage of void growth in shear bands, it can be assumed that voids are relatively far apart. In this case an isolated void model can be employed as that given by FLECK and HUTCHINSON [2] for $2D$ cylindrical voids. This consideration results in an infinite matrix material. We can obtain the solution of the problem by setting $f = 0$ in the present results (3.5)–(3.9). In this limiting case $f = 0$, we have $\omega = 0$ and

$$\Sigma_{12} = 4\pi \int_{\omega}^{\omega^*} (G_1 + G_m)t^{-2}\,dt \Big/ \frac{1}{\omega} \to 4\pi.$$

Then, Eq. (3.6) becomes

(4.1)
$$\chi \equiv \chi(\lambda, n, m) = \frac{2}{\sqrt{3}} \int_0^{\omega^*} (F_1 + F_m)\,dt.$$

The approximate expression corresponding to Eq. (3.7) can be given by

$$\chi = \frac{2}{\sqrt{3}} \int_0^{\omega^*} F_1\,dt$$

which has the following closed form for $n = 0$

$$\chi = \frac{2}{\sqrt{3}}\left[\mathrm{sh}^{-1}(\omega^*) - \frac{1}{10}\omega^*(2+\omega^{*2})(1+\omega^{*2})^{-3/2}\right].$$

For large λ, we have

$$\chi \simeq \frac{2}{\sqrt{3}}[\ln(2\omega^*) - 0.1]. \tag{4.2}$$

When $n = 0$, Eq. (4.1) also gives an analytical expression

$$\chi = \frac{2}{\sqrt{3}}\{\ln[\omega^* + \sqrt{(1 + \omega^{*2})}] + c\}, \tag{4.3}$$

where

$$c = -\frac{1}{10}\omega^*(2 + \omega^{*2})(1 + \omega^{*2})^{-3/2} + \int\limits_0^{\omega^*} F_m|_{n=0}\, dt. \tag{4.4}$$

As discussed in the case $f \neq 0$, the function c is convergent for large λ. Table 2 gives the numerical results of c for variable m with large λ (e.g., $\lambda \geq 10$. In fact, for large λ, c can be expressed by the series as shown in Appendix).

Table 2. Numerical results of Eq. (4.4).

m	c	m	c
2	−0.1833	6	−0.2277
3	−0.2172	7	−0.2279
4	−0.2250	8	−0.2280
5	−0.2271	9	−0.2280

It is clear $c = -0.228$. Then, we have

$$\frac{\sqrt{3}}{2}\chi \simeq \ln(2\omega^*) - 0.228$$

or

$$\lambda = 0.544 \exp\left(\frac{\sqrt{3}}{2}\chi\right). \tag{4.5}$$

The similar results for $2D$ voids were given by PAN [14], FLECK *et al.* [2] and MCCLINTOCK *et al.* [1], which are listed here

$$\lambda = 0.68 \exp(\chi), \quad \text{from PAN or FLECK } et\ al., \tag{4.6}$$

$$\lambda = 0.50 \exp(\chi), \quad \text{from MCCLINTOCK } et\ al. \tag{4.7}$$

For comparison, these results are plotted in Fig. 4.

As expected, the lines for $2D$ voids are higher than those for $3D$ voids, which means that $2D$ voids grow more quickly than $3D$ voids in an infinite matrix material. It seems that MC CLINTOCK model overestimates the void growth rate. The approximate expression (4.2) underestimates the void growth rate. In the last section, we have pointed out that the void growth rate is larger in an infinite ($f = 0$), perfectly plastic ($n = 0$) matrix material than in other materials. Now we know that the growth rate for $2D$ circular-cylindrical voids is larger than that for $3D$ spherical voids. So we conclude that the growth of circular-cylindrical voids in an inifnite, perfectly plastic matrix material is larger than in any other cases under shearing deformation.

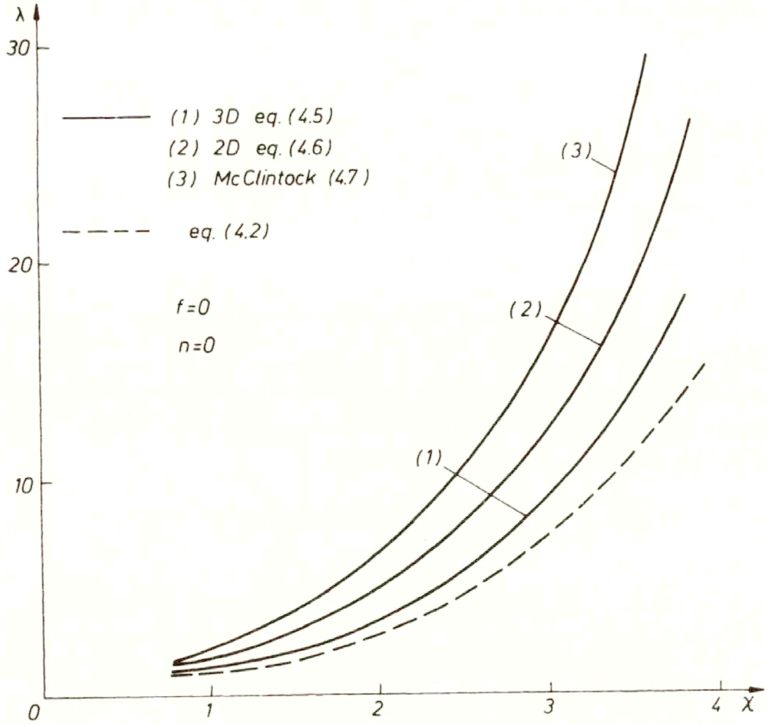

FIG. 4. Comparison of present results for $3D$ voids with those for $2D$ voids from an isolated void model ($f = 0$).

5. Conclusion remarks

The void interaction effects on void growth in shear bands are considered by introducing arbitrary void volume fractions. Numerical and analytical results show that the void growth rate is a strong function of the void volume fraction and the strain rate sensitivity. The former gives the degree of damage of the material, and the latter corresponds to the degree of nonlinearity of the material. Relatively simple approximate analytical formulae are obtained for perfectly plastic materials.

Apart from void interaction effects, the other phenomenon in shear bands is the void shape evolution. This problem may be discussed in the forthcoming paper.

Appendix. Calculation of the constant c in Eq. (4.4)

Substituting the expression F_m in Eq. (3.5) for $n = 0$ into Eq. (4.4), we have

$$c = c_1 + c_m, \tag{A.1}$$

where

$$c_1 = -\frac{1}{10}\omega^*(2+\omega^{*2})(1+\omega^{*2})^{-3/2},$$

$$c_m = \sum_{m=2}^{\infty} I_m \int_0^{\omega^*} \left(g_{1m} - \frac{1}{2} g_{2m} P t^{-2}\right)(2t)^{2m} P^{-(1+4m)/2}\, dt.$$

The following recurrence formulae are useful to obtain the integral in Eq. (A.1):

$$\text{(A.2)} \qquad \int \frac{t^M dt}{P^{N/2}} = \frac{t^{M-1}}{(M-N+1)P^{(N-2)/2}} + \frac{M-1}{N-M-1} \int \frac{t^{M-2}}{P^{N/2}}\, dt,$$

$$\text{(A.3)} \qquad \int \frac{dt}{P^{N/2}} = \frac{t}{(N-2)P^{(N-2)/2}} + \frac{N-3}{N-2} \int \frac{1}{P^{(N-2)/2}}\, dt.$$

When λ is large, the first term of the right-hand side in Eqs. (A.2) and (A.3) is about

$$\frac{t^{M-1}}{P^{(N-2)/2}} \sim t^{(M-N+1)}, \qquad \frac{t}{P^{(N-2)/2}} \sim t^{(3-N)}.$$

In our problem, $N = 1+4m$, $M = 2m$, so that $M-N+1 = -2m$ and $3-N = 2-4m$, $(m \geq 2)$. It is obvious that the first term at the right-hand side in Eqs. (A.2) and (A.3) is an infinitesmall quantity of λ^{-2m}. For example, when $\lambda = 10$ and $m = 2$, we have $\lambda^{-4} = 10^{-4}$, but $\int P^{-9/2}\, dt \sim 10^{-1}$, $\int t^4 P^{-9/2}\, dt \sim 10^{-2}$. Therefore this term is negligible. In this case, we have

$$I_{1m} \equiv \int_0^{\omega^*} t^{2m} P^{-(1+4m)/2}\, dt = \left(\prod_{j=0}^{m-1} \frac{2m-2J-1}{2m+2J}\right)\left(\prod_{J=0}^{2m-2} \frac{4m-2J-2}{4m-2J-1}\right),$$

$$I_{2m} \equiv \int_0^{\omega^*} t^{2m-2} P^{(1-4m)/2}\, dt = \left(\prod_{J=0}^{m-2} \frac{2m-2J-3}{2m+2J}\right)\left(\prod_{J=0}^{2m-3} \frac{4m-2J-4}{4m-2J-3}\right).$$

Thus, from Eq. (A.1), c can be expressed by the series

$$c = -0.1 + \sum_{m=2}^{\infty} \left(g_{1m} I_{1m} - \frac{1}{2} g_{2m} I_{2m}\right) (2)^{2m} I_m.$$

It is convergent to a constant $c = -0.228$ as shown in Table 2.

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Wave pulses in one-dimensional randomly defected thermoelastic media

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IN THE PAPER the propagation of wave pulses in a one-dimensional thermoelastic medium is considered. The problem is described by the transition matrix method. The transition matrix for such a wave problem is obtained and then the equation for the reflected and transmitted wave field is derived. Finally, the effective thermoelastic constants are derived with the use of the law of large numbers for the product of random matrices.

1. Introduction

THERMOMECHANICAL phenomena in elastic media conducting heat are usually modelled by the equations of thermoelasticity (see [31]). Using such a theory, many authors have attempted to solve both the stationary (harmonic) wave problems and non-stationary wave problems (wave pulses). In this short review let us confine the analysis to the problems of one-dimensional (or planar) thermoelastic waves.

In the paper [37] the problem of harmonic wave propagation in a semi-infinite and infinite bar has been considered for various boundary conditions and, consequently, various excitations generating the waves. Analogous problems for the thermoelastic medium have been considered in [31], where the effect of planar mass forces in an infinite space and the effect of planar heat sources acting on the layer was studied.

The non-stationary problems of thermoelasticity are more complicated from the mathematical point of view; since here the additional, time variable appears, they need more involved computations. The most effective method used in such problems is the application of the Fourier transformation with respect to spatial variables and (or) the Laplace transform with respect to time. As an example of the nonstationary thermoelastic problem, we can present the propagation of plane wave generated by a sudden heating of the plane boundary of the half-space (the Danilovskaya problem). Such a problem has been considered in [5, 11, 12, 29]. Another example can be the propagation of the longitudinal wave in infinite and semi-infinite bar, considered in [13, 37]. In the paper by IGNACZAK [13] the method of spatial Fourier transformation of the thermoelastic wave equation was applied to the analysis of the problem.

In the literature, thermomechanical phenomena have been mostly analyzed in the homogeneous spaces. The description of the problem in spatially non-homogeneous case is not simple, because then one must analyze the equations with spatially variable coefficients. However, considering the stratified media we can apply the methods known from the homogeneous media theory, using equations with constant coefficients and applying the suitable continuity conditions. The stratified models can be approximations of the continuously variable media, as well as they can describe physical situations where the stratified scheme is natural, like wave processes in layered soils, defected or compound elements of structures, etc.

The mathematical description of the thermoelastic wave processes in stratified media and the methods of solution of the problems are analogous to the methods of analysis of the purely thermal or elastic problems. In the literature there is a number of papers where such problems are considered. In this short introduction we only mention the most important of them, and give the references to the literature where more information about the state of art can be found.

The problems of heat transmission through multi-layered structures and their interactions with environment are presented, among others, in the papers [2, 6, 7, 32]. The most effective methods proved to be the transition matrix method and the thermal factors method.

The first method of the analysis of heat transfer in layered bodies with periodic boundary conditions is shown in [6, 32].

The thermal factors method, originally presented in [27], is discussed in [7, 30, 15, 16]. Applying this method, the processes of heat transfer through multi-layered walls is analyzed in [17]. Analogously, using the factors method, the computer simulation of heat transmission in the solar wall is performed in [18, 19].

The literature concerning elastic waves propagation in stratified media is very rich (see e.g. [14]). In this presentation we restrict ourselves to the presentation of the transition matrix method, widely applied as the method of analysis of this problem. The earliest papers where the method was used for the surface harmonic waves are [34, 36]. Later the method was applied to SH [9] and P + SV [10] waves. The method proved to be useful for the stochastic models: one-dimensional [39, 3, 20, 21] and two-dimensional [22, 23]. It was also effective in the case of wave pulses propagation in stratified media: deterministic [1, 28] and stochastic [24, 25, 26].

In this paper we apply the transition matrix method to the analysis of the dynamic problem of thermoelastic wave pulse propagation in a randomly segmented one-dimensional medium. Starting from the one-dimensional equations of thermoelasticity ([31]) and the appropriate continuity conditions, we obtain the transfer matrices for the randomly stratified medium. We apply two methods: we use either the Legendre interpolation polynomials, or alternatively, solve the appropriate system of continuity equations. Then we are able to write the solution of the wave problem applying the derived matrices. Finally, using the limit theorem (see [4]), we obtain the equation for the homogenized problem.

2. Governing equations

2.1. The equations of motion

Consider the linear thermoelastic wave propagating in a one-dimensional medium. The equations describing the changes of the displacement of the medium $u(t,x)$ and the temperature fluctuations of the medium $\vartheta(t,x)$ are the following (see [31]):

$$\rho\frac{\partial^2 u}{\partial t^2} = (\lambda+2\mu)\frac{\partial^2 u}{\partial x^2} - (3\lambda+2\mu)\alpha\frac{\partial\vartheta}{\partial x}, \tag{2.1}$$

$$\rho c_\varepsilon\frac{\partial\vartheta}{\partial t} = \beta\frac{\partial^2\vartheta}{\partial x^2} - T_0(3\lambda+2\mu)\alpha\frac{\partial}{\partial t}\frac{\partial u}{\partial x}, \tag{2.2}$$

where λ, μ — Lamé elastic constants, T_0 — the reference temperature, c_ε — the specific heat at constant strain for the unit of mass, ρ — the density of the material, β — the heat conductivity coefficient, α — the coefficient of linear expansion of the medium.

The system of equations (2.1)–(2.2) can be alternatively written in the form of two following continuity equations:

the principle of the conservation of linear momentum:

(2.3)
$$\rho\frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma}{\partial x},$$

and the heat equation:

(2.4)
$$\rho c_\varepsilon\frac{\partial \vartheta}{\partial t} = \frac{\partial \varphi}{\partial x},$$

where we have introduced, as new variables, the stress σ and the heat flux φ, defined as

(2.5)
$$\sigma = (\lambda + 2\mu)\frac{\partial u}{\partial x} - (3\lambda + 2\mu)\alpha\vartheta$$

and

(2.6)
$$\varphi = \beta\frac{\partial \vartheta}{\partial x} - T_0(3\lambda + 2\mu)\alpha\frac{\partial}{\partial t}u.$$

Using Eqs. (2.3)–(2.6) we can write the following system of thermoelastic equations:

(2.7)
$$\frac{\partial u}{\partial x} = \frac{1}{(\lambda + 2\mu)}\sigma + \frac{(3\lambda + 2\mu)\alpha}{(\lambda + 2\mu)}\vartheta,$$

(2.8)
$$\frac{\partial \sigma}{\partial x} = \rho\frac{\partial^2 u}{\partial t^2},$$

(2.9)
$$\frac{\partial \vartheta}{\partial x} = \frac{1}{\beta}\varphi + \frac{T_0(3\lambda + 2\mu)\alpha}{\beta}\frac{\partial u}{\partial t},$$

(2.10)
$$\frac{\partial \varphi}{\partial x} = \rho c_\varepsilon\frac{\partial \vartheta}{\partial t}.$$

Introducing new definitions of constants,

(2.11)
$$A_1 = \frac{1}{(\lambda + 2\mu)},$$

(2.12)
$$A_2 = \frac{(3\lambda + 2\mu)\alpha}{(\lambda + 2\mu)},$$

(2.13)
$$A_3 = \rho,$$

(2.14)
$$B_1 = \frac{T_0(3\lambda + 2\mu)\alpha}{\beta},$$

(2.15)
$$B_2 = \frac{1}{\beta},$$

(2.16)
$$B_3 = \rho c_\varepsilon,$$

we can write the system of equations (2.7)–(2.10) in the following vector-matrix form:

$$\frac{\partial}{\partial x}\begin{bmatrix} u \\ \sigma \\ \vartheta \\ \varphi \end{bmatrix} = \begin{bmatrix} 0 & A_1 & A_2 & 0 \\ A_3\dfrac{\partial^2}{\partial t^2} & 0 & 0 & 0 \\ B_1\dfrac{\partial}{\partial t} & 0 & 0 & B_2 \\ 0 & 0 & B_3\dfrac{\partial}{\partial t} & 0 \end{bmatrix}\begin{bmatrix} u \\ \sigma \\ \vartheta \\ \varphi \end{bmatrix}. \tag{2.17}$$

Applying the Fourier transforms to the system of equations with respect to the time variable t, according to the following definition:

$$\widehat{s}(\omega) = \int \exp\{-i\omega t\} s(t)\, dt, \tag{2.18}$$

$$\frac{\partial \widehat{s}}{\partial t} = i\omega\widehat{s}, \tag{2.19}$$

we obtain the following system of linear ordinary differential equations:

$$\frac{\partial}{\partial x}\begin{bmatrix} \widehat{u} \\ \widehat{\sigma} \\ \widehat{\vartheta} \\ \widehat{\varphi} \end{bmatrix} = \begin{bmatrix} 0 & A_1 & A_2 & 0 \\ -\omega^2 A_3 & 0 & 0 & 0 \\ i\omega B_1 & 0 & 0 & B_2 \\ 0 & 0 & i\omega B_3 & 0 \end{bmatrix}\begin{bmatrix} \widehat{u} \\ \widehat{\sigma} \\ \widehat{\vartheta} \\ \widehat{\varphi} \end{bmatrix}, \tag{2.20}$$

where the variable of the Fourier transformation ω is now the parameter.

Let us define the matrix of the system of equations (2.20) as

$$\mathcal{A} = \begin{bmatrix} 0 & A_1 & A_2 & 0 \\ -\omega^2 A_3 & 0 & 0 & 0 \\ i\omega B_1 & 0 & 0 & B_2 \\ 0 & 0 & i\omega_3 B_3 & 0 \end{bmatrix}. \tag{2.21}$$

Then the eigenvalues of the matrix $\mathcal{A}$ of the system of equations are the solutions of the characteristic equation

$$\det(A - r\mathbf{Id}) = 0, \tag{2.22}$$

(**Id** is a 4×4 identity matrix), or explicitly

$$r^4 - r^2\omega[-A_1A_3\omega + (A_2B_1 + B_2B_3)i] - B_2B_3A_1A_3 i\omega^3 = 0. \tag{2.23}$$

The solutions of the characteristic equation are

$$r_{1,2} = \pm\frac{\sqrt{\omega}}{\sqrt{2}}\sqrt{bi - a\omega + \sqrt{a^2\omega^2 - b^2 + 2id\omega}} \tag{2.24}$$

and

$$r_{3,4} = \pm\frac{\sqrt{\omega}}{\sqrt{2}}\sqrt{bi - a\omega - \sqrt{a^2\omega^2 - b^2 + 2id\omega}}, \tag{2.25}$$

where the following notations have been introduced:

$$a = A_1 A_3, \tag{2.26}$$

$$b = A_2 B_1 + B_2 B_3, \tag{2.27}$$

$$d = A_1 A_3 (A_2 B_1 - B_2 B_3). \tag{2.28}$$

2.2. Discontinuity surfaces and continuity conditions

The governing equations (2.1)–(2.2) are valid for the homogeneous media, that is for such media where the coefficients in the equations are constants. If the medium is built of several regions where the coefficients are constant, in every region the suitable governing equation of the form (2.1)–(2.2) is valid. If the solution of the wave problem exists in the entire medium, then on the interfaces of the homogeneous subregions (being the surfaces of discontinuity) some continuity conditions must be satisfied. The conditions are: the mechanical variables — displacements (u) and normal stresses (σ), and two thermal variables — temperature (ϑ) and normal heat flux (φ), are continuous across the surface of discontinuity of the medium.

2.3. Excitation, initial and boundary conditions

The complete description of the thermoelastic problem necessitates the governing equation and, additionally, appropriately described excitations acting on the system, and initial and boundary conditions. Usually one defines the mechanical excitations acting on the structure (displacements or stresses) and heat sources distributed in the medium. Analogously, one defines the initial displacements, stresses and the temperature fluctuations over the body.

In this paper we assume there are no external excitations acting on the body in the x-direction. Moreover, we assume that at $t = 0$ the medium is in equilibrium (homogeneous initial conditions).

The wave processes analyzed in the paper are one-dimensional; we consider the wave pulse in the (stratified) slab or bar. The pulse is generated by suitable changes of the boundary conditions. The boundary conditions of thermoelastic problems are of two types: mechanical and thermal. In the literature authors usually assume known displacements or normal stresses (on non-overlapping surfaces of the boundary), and known temperature and normal projections of the heat flux (also on non-overlapping surfaces). Some combinations of the above conditions are also possible.

In our wave problem, since we consider a one-dimensional model, we should assume only one mechanical and one thermal boundary condition on the whole surface of the slab. The wave problem considered requires precise specification of the boundary conditions (being in our model the excitations generating the thermoelastic wave pulse in the slab or bar).

3. Continuity equations and transition matrix

To construct the transition matrix for the solution of Eq. (2.20), we postulate the form of two components of the solution as

$$\widehat{u}(x) = \sum_{i=1}^{4} C_i^u \exp(r_i x), \tag{3.1}$$

$$\widehat{\vartheta}(x) = \sum_{i=1}^{4} C_i^\vartheta \exp(r_i x). \tag{3.2}$$

Then the spatial derivatives of the functions are

$$\frac{d\widehat{u}(x)}{dx} = \sum_{i=1}^{4} C_i^u r_i \exp(r_i x), \tag{3.3}$$

$$\frac{d\widehat{\vartheta}(x)}{dx} = \sum_{i=1}^{4} C_i^\vartheta r_i \exp(r_i x), \tag{3.4}$$

where $r_i, i = 1,2,3,4$ are the eigenvalues of the matrix $\mathcal{A}$ of the system of equations (2.20), given by formulae (2.24), (2.25), and the constants C_i^u and C_i^ϑ, $i = 1,2,3,4$, must be determined from the boundary conditions. Then the value of the solution of Eq. (2.20) at the plane $x = 0$ is

$$\widehat{u}(0) \equiv \widehat{u}_0 = \sum_{i=1}^{4} C_i^u, \tag{3.5}$$

$$\widehat{\vartheta}(0) \equiv \widehat{\vartheta}_0 = \sum_{i=1}^{r} C_i^\vartheta, \tag{3.6}$$

$$\widehat{\sigma}(0) \equiv \widehat{\sigma}_0 = \frac{1}{A_1} \sum_{i=1}^{4} C_i^u r_i - \frac{A_2}{A_1} \sum_{i=1}^{4} C_i^\vartheta, \tag{3.7}$$

$$\widehat{\varphi}(0) \equiv \widehat{\varphi}_0 = \frac{1}{B_1} \sum_{i=1}^{4} C_i^\vartheta r_i - \frac{B_2}{B_1} i\omega \sum_{i=1}^{4} C_i^u \tag{3.8}$$

and the value for $x = L$ is

$$\widehat{u}(L) \equiv \widehat{u}_L = \sum_{i=1}^{4} C_i^u \exp(r_i L), \tag{3.9}$$

$$\widehat{\vartheta}(L) \equiv \widehat{\vartheta}_L = \sum_{i=1}^{4} C_i^\vartheta \exp(r_i L), \tag{3.10}$$

$$\widehat{\sigma}(L) \equiv \widehat{\sigma}_L = \frac{1}{A_1} \sum_{i=1}^{4} C_i^u r_i \exp(r_i L) - \frac{A_2}{A_1} \sum_{i=1}^{4} C_i^\vartheta \exp(r_i L), \tag{3.11}$$

$$\widehat{\varphi}(L) \equiv \widehat{\varphi}_L = \frac{1}{B_1} \sum_{i=1}^{4} C_i^\vartheta r_i \exp(r_i L) - \frac{B_2}{B_1} i\omega \sum_{i=1}^{4} \exp(r_1 L). \tag{3.12}$$

Our purpose is to express the values of the solution at $x = 0$ in terms of its value at $x = L$. To do this we must eliminate from the equations (3.5)–(3.12) constants C_i^u and C_i^ϑ, $i = 1,2,3,4$. From the above equations we obtain the following matrix equation for the constants C_i^u, $i = 1,2,3,4$:

$$\begin{bmatrix} \widehat{u}_0 \\ \widehat{u}_L \\ \widehat{\sigma}_0 + \dfrac{A_2}{A_1}\widehat{\vartheta}_0 \\ \widehat{\sigma}_L + \dfrac{A_2}{A_1}\widehat{\vartheta}_L \end{bmatrix} = \mathbf{A}^u \begin{bmatrix} C_1^u \\ C_2^u \\ C_3^u \\ C_4^u \end{bmatrix}, \tag{3.13}$$

where matrix $\mathbf{A}^u$ has the following form:

$$\mathbf{A}^u = \begin{bmatrix} 1 & 1 & 1 & 1 \\ \exp(r_1 L) & \exp(r_2 L) & \exp(r_3 L) & \exp(r_4 L) \\ \dfrac{1}{A_1} r_1 & \dfrac{1}{A_1} r_2 & \dfrac{1}{A_1} r_3 & \dfrac{1}{A_1} r_4 \\ \dfrac{1}{A_1} r_1 \exp(r_1 L) & \dfrac{1}{A_1} r_2 \exp(r_2 L) & \dfrac{1}{A_1} r_3 \exp(r_3 L) & \dfrac{1}{A_1} r_4 \exp(r_4 L) \end{bmatrix}. \tag{3.14}$$

Now we can obtain the following formula for the coefficients C_i^u:

$$\begin{bmatrix} C_1^u \\ C_2^u \\ C_3^u \\ C_4^u \end{bmatrix} = [\mathbf{A}^u]^{-1} \begin{bmatrix} \widehat{u}_0 \\ \widehat{u}_L \\ \widehat{\sigma}_0 + \dfrac{A_2}{A_1}\widehat{\vartheta}_0 \\ \widehat{\sigma}_L + \dfrac{A_2}{A_1}\widehat{\vartheta}_L \end{bmatrix}. \tag{3.15}$$

Analogously we can obtain the following matrix equation for the constants C_i^ϑ, $i = 1,2,3,4$:

$$\begin{bmatrix} \widehat{\vartheta}_0 \\ \widehat{\vartheta}_L \\ \widehat{\varphi}_0 + \dfrac{B_2}{B_1} i\omega \widehat{u}_0 \\ \widehat{\varphi}_L + \dfrac{B_2}{B_1} i\omega \widehat{u}_L \end{bmatrix} = \mathbf{A}^\vartheta \begin{bmatrix} C_1^\vartheta \\ C_2^\vartheta \\ C_3^\vartheta \\ C_4^\vartheta \end{bmatrix}, \tag{3.16}$$

where matrix $\mathbf{A}^\vartheta$ has the form

$$\mathbf{A}^\vartheta = \begin{bmatrix} 1 & 1 & 1 & 1 \\ \exp(r_1 L) & \exp(r_2 L) & \exp(r_3 L) & \exp(r_4 L) \\ \dfrac{1}{B_1} r_1 & \dfrac{1}{B_1} r_2 & \dfrac{1}{B_1} r_3 & \dfrac{1}{B_1} r_4 \\ \dfrac{1}{B_1} r_1 \exp(r_1 L) & \dfrac{1}{B_1} r_2 \exp(r_2 L) & \dfrac{1}{B_1} r_3 \exp(r_3 L) & \dfrac{1}{B_1} r_4 \exp(r_4 L) \end{bmatrix}. \tag{3.17}$$

Now we can obtain the following formula for the coefficients C_i^{ϑ}:

$$
(3.18) \qquad \begin{bmatrix} C_1^{\vartheta} \\ C_2^{\vartheta} \\ C_3^{\vartheta} \\ C_4^{\vartheta} \end{bmatrix} = [\mathbf{A}^{\vartheta}]^{-1} \begin{bmatrix} \widehat{\vartheta}_0 \\ \widehat{\vartheta}_L \\ \widehat{\varphi}_0 + \dfrac{B_2}{B_1} i\omega \widehat{u}_0 \\ \widehat{\varphi}_L + \dfrac{B_2}{B_1} i\omega \widehat{u}_L \end{bmatrix}.
$$

The formulae for the derivatives are

$$
(3.19) \qquad \left.\frac{d\widehat{\sigma}}{dx}\right|_{x=0} = -A_3\omega^2 \widehat{u}_0 = \frac{1}{A_1}\sum_{i=1}^{4} C_i^u r_i^2 - \frac{A_2}{A_1}\sum_{i=1}^{4} C_i^{\vartheta} r_i,
$$

$$
(3.20) \qquad \left.\frac{d\widehat{\sigma}}{dx}\right|_{x=L} = -A_3\omega^2 \widehat{u}_L = \frac{1}{A_1}\sum_{i=1}^{4} C_i^u r_i^2 \exp(r_i L) - \frac{A_2}{A_1}\sum_{i=1}^{4} C_i^{\vartheta} r_i \exp(r_i L),
$$

$$
(3.21) \qquad \left.\frac{d\widehat{\varphi}}{dx}\right|_{x=0} = B_3 i\omega \widehat{\vartheta}_0 = \frac{1}{B_1}\sum_{i=1}^{4} C_i^{\vartheta} r_i^2 - \frac{B_2}{B_1}\sum_{i=1}^{4} C_i^u r_i,
$$

$$
(3.22) \qquad \frac{d\widehat{\varphi}}{dx}|_{x=L} = B_3 i\omega \widehat{\vartheta}_L = \frac{1}{B_1}\sum_{i=1}^{4} C_i^{\vartheta} r_i^2 \exp(r_i L) - \frac{B_2}{B_1}\sum_{i=1}^{4} C_i^u r_i \exp(r_i L).
$$

Now we can obtain the expressions for the functions sought for at the front plane $x = 0$,

$$
(3.23) \qquad \widehat{u}_0, \ \widehat{\sigma}_0, \ \widehat{\vartheta}_0, \ \widehat{\varphi}_0,
$$

under the given values of the functions at the rear plane $x = L$:

$$
(3.24) \qquad \widehat{u}_L, \ \widehat{\sigma}_L, \ \widehat{\vartheta}_L, \ \widehat{\varphi}_L.
$$

The formulae constitute the following system of linear algebraic equations:

$$
(3.25) \qquad A_3\omega^2 \widehat{u}_0 = -\frac{1}{A_1}\sum_{i=1}^{4} C_i^u r_i^2 + \frac{A_2}{A_1}\sum_{i=1}^{4} C_i^{\vartheta} r_i,
$$

$$
(3.26) \qquad A_3\omega^2 \widehat{u}_L = -\frac{1}{A_1}\sum_{i=1}^{4} C_i^u r_i^2 \exp(r_1 L) + \frac{A_2}{A_1}\sum_{i=1}^{4} C_i^{\vartheta} r_i \exp(r_i L),
$$

$$
(3.27) \qquad B_3 i\omega \widehat{\vartheta}_0 = \frac{1}{B_1}\sum_{i=1}^{4} C_i^{\vartheta} r_i^2 - \frac{B_2}{B_1}\sum_{i=1}^{4} C_i^u r_i,
$$

$$
(3.28) \qquad B_3 i\omega \widehat{\vartheta}_L = \frac{1}{B_1}\sum_{i=1}^{4} C_i^{\vartheta} r_i^2 \exp(r_i L) - \frac{B_2}{B_1}\sum_{i=1}^{4} r_i \exp(r_i L).
$$

where the constants C_i^u and C_i^{ϑ} are the solutions of Eq. (3.13) and (3.16), respectively.

The above system of equations can be written in the following matrix form:

$$
(3.29) \qquad \begin{bmatrix} \widehat{u}_0 \\ \widehat{\sigma}_0 \\ \widehat{\vartheta}_0 \\ \widehat{\varphi}_0 \end{bmatrix} = \mathbf{T}^{-1} \begin{bmatrix} \widehat{u}_L \\ \widehat{\sigma}_L \\ \widehat{\vartheta}_L \\ \widehat{\varphi}_L \end{bmatrix},
$$

where matrix $\mathbf{T}^{-1}$ is the inverse of the transition matrix for a single layer. It can be represented in the following form:

(3.30)
$$\mathbf{T}^{-1} = [\mathbf{P}]^{-1}\mathbf{Q},$$

where matrices **P** and **Q** are defined by the formulae

(3.31)
$$\mathbf{P} = [\mathbf{P}_{ij}], \qquad i,j = 1,2,3,4,$$

(3.32)
$$\mathbf{P}_{11} = -A_3\omega^2 - \frac{1}{A_1}\sum_{k=1}^{4}\mathbf{A}_{k1}^{u}r_k^2 + \frac{A_2}{A_1}\frac{B_2}{B_1}i\omega\sum_{k=1}^{4}\mathbf{A}_{k3}^{\vartheta}r_k,$$

(3.33)
$$\mathbf{P}_{21} = -\frac{1}{A_1}\sum_{k=1}^{4}\mathbf{A}_{k1}^{u}r_k^2\exp(r_kL) + \frac{A_2}{A_1}\frac{B_2}{B_1}i\omega\sum_{k=1}^{4}\mathbf{A}_{k3}^{\vartheta}r_k\exp(r_kL),$$

(3.34)
$$\mathbf{P}_{31} = -\frac{B_2}{b_1^2}i\omega\sum_{k=1}^{4}\mathbf{A}_{k3}^{\vartheta}r_k^2 + \frac{B_2}{B_1}i\omega\sum_{k=1}^{4}\mathbf{A}_{k1}^{u}r_k,$$

(3.35)
$$\mathbf{P}_{41} = -\frac{B_2}{B_1^2}i\omega\sum_{k=1}^{4}\mathbf{A}_{k3}^{\vartheta}r_k^2\exp(t_kL) + \frac{B_2}{B_1}i\omega\sum_{k=1}^{4}\mathbf{A}_{k1}^{u}r_k\exp(r_kL),$$

(3.36)
$$\mathbf{P}_{12} = -\frac{1}{A_1}\sum_{k=1}^{4}\mathbf{A}_{k3}^{u}r_k^2,$$

(3.37)
$$\mathbf{P}_{22} = -\frac{1}{A_1}\sum_{k=1}^{4}\mathbf{A}_{k3}^{u}r_k^2\exp(r_kL),$$

(3.38)
$$\mathbf{P}_{32} = \frac{B_2}{B_1}\sum_{k=1}^{4}\mathbf{A}_{k3}^{u}r_k^2,$$

(3.39)
$$\mathbf{P}_{42} = \frac{B_2}{B_1}\sum_{k=1}^{4}\mathbf{A}_{k3}^{u}r_k^2\exp(r_kL),$$

(3.40)
$$\mathbf{P}_{13} = -\frac{A_2}{A_1^2}\sum_{k=1}^{4}\mathbf{A}_{k3}^{u}r_k^2 + \frac{A_2}{A_1}\sum_{k=1}^{4}\mathbf{A}_{k1}^{\vartheta}r_k,$$

(3.41)
$$\mathbf{P}_{23} = -\frac{A_2}{A_1^2}\sum_{k=1}^{4}\mathbf{A}_{k3}^{u}r_k^2\exp(r_kL) + \frac{A_2}{A_1}\sum_{k=1}^{4}\mathbf{A}_{k1}^{\vartheta}r_k\exp(r_kL),$$

(3.42)
$$\mathbf{P}_{33} = B_3i\omega - \frac{1}{B_1}\sum_{k=1}^{4}\mathbf{A}_{k1}^{\vartheta}r_k^2 + \frac{A_2}{A_1}\frac{B_2}{B_1}i\omega\sum_{k=1}^{4}\mathbf{A}_{k3}^{u}r_k,$$

(3.43)
$$\mathbf{P}_{43} = -\frac{1}{B_1}\sum_{k=1}^{4}\mathbf{A}_{k1}^{\vartheta}r_k^2\exp(r_kL) + \frac{A_2}{A_1}\frac{B_2}{B_1}i\omega\sum_{k=1}^{4}\mathbf{A}_{k3}^{u}r_k\exp(r_kL),$$

(3.44)
$$\mathbf{P}_{14} = \frac{A_2}{A_1}\sum_{k=1}^{4}\mathbf{A}_{k3}^{\vartheta}r_k^2,$$

(3.45) $$\mathbf{P}_{24} = \frac{A_2}{A_1}\sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k3} r_k^2 \exp(r_k L),$$

(3.46) $$\mathbf{P}_{34} = -\frac{1}{B_1}\sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k3} r_k^2,$$

(3.47) $$\mathbf{P}_{44} = -\frac{1}{B_1}\sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k3} r_k^2 \exp(r_k L)$$

and

(3.48) $$\mathbf{Q} = [\mathbf{Q}_{ij}], \qquad i,j = 1,2,3,4,$$

(3.49) $$\mathbf{Q}_{11} = \frac{1}{A_1}\sum_{k=1}^{4}\mathbf{A}^{u}_{k2} r_k^2 - \frac{A_2}{A_1}\frac{B_2}{B_1} i\omega \sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k4} r_k,$$

(3.50) $$\mathbf{Q}_{21} = A_3\omega^2 + \frac{1}{A_1}\sum_{k=1}^{4}\mathbf{A}^{u}_{k2} r_k^2 \exp(r_k L) - \frac{A_2}{A_1}\frac{B_2}{B_1} i\omega \sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k4} r_k \exp(r_k L),$$

(3.51) $$\mathbf{Q}_{31} = \frac{B_2}{B_1} i\omega \sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k4} r_k^2 - \frac{B_2}{B_1} i\omega \sum_{k=1}^{4}\mathbf{A}^{u}_{k2} r_k,$$

(3.52) $$\mathbf{Q}_{41} = \frac{B_2}{B_1^2} i\omega \sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k4} r_k^2 \exp(r_k L) - \frac{B_2}{B_1} i\omega \sum_{k=1}^{4}\mathbf{A}^{u}_{k2} r_k \exp(r_k L),$$

(3.53) $$\mathbf{Q}_{12} = \frac{1}{A_1}\sum_{k=1}^{4}\mathbf{A}^{u}_{k4} r_k^2,$$

(3.54) $$\mathbf{Q}_{22} = \frac{1}{A_1}\sum_{k=1}^{4}\mathbf{A}^{u}_{k4} r_k^2 \exp(r_k L),$$

(3.55) $$\mathbf{Q}_{32} = -\frac{B_2}{B_1}\sum_{k=1}^{4}\mathbf{A}^{u}_{k4} r_k^2,$$

(3.56) $$\mathbf{Q}_{42} = -\frac{B_2}{B_1}\sum_{k=1}^{4}\mathbf{A}^{u}_{k4} r_k^2 \exp(r_k L),$$

(3.57) $$\mathbf{Q}_{13} = \frac{A_2}{A_1^2}\sum_{k=1}^{4}\mathbf{A}^{u}_{k4} r_k^2 - \frac{A_2}{A_1}\sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k2} r_k,$$

(3.58) $$\mathbf{Q}_{23} = \frac{A_2}{A_1^2}\sum_{k=1}^{4}\mathbf{A}^{u}_{k4} r_k^2 \exp(r_k L) - \frac{A_2}{A_1}\sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k2} r_k \exp(r_k L),$$

(3.59) $$\mathbf{Q}_{33} = \frac{1}{B_1}\sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k2} r_k^2 - \frac{A_2}{A_1}\frac{B_2}{B_1} i\omega \sum_{k=1}^{4}\mathbf{A}^{u}_{k4} r_k,$$

(3.60) $$\mathbf{Q}_{43} = -B_3 i\omega + \frac{1}{B_1}\sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k2} r_k^2 \exp(r_k L) - \frac{A_2}{A_1}\frac{B_2}{B_1} i\omega \sum_{k=1}^{4}\mathbf{A}^{u}_{k4} r_k \exp(r_k L),$$

$$\mathbf{Q}_{14} = -\frac{A_2}{A_1}\sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k4}r_k^2, \tag{3.61}$$

$$\mathbf{Q}_{24} = -\frac{A_2}{A_1}\sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k4}r_k^2\exp(r_kL), \tag{3.62}$$

$$\mathbf{Q}_{34} = \frac{1}{B_1}\sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k4}r_k^2, \tag{3.63}$$

$$\mathbf{Q}_{44} = \frac{1}{B_1}\sum_{k=1}^{4}\mathbf{A}^{\vartheta}_{k4}r_k^2\exp(r_kL). \tag{3.64}$$

4. The Legendre polynomial and transition matrix

In this section we present the alternative method of calculating the transition matrix through a single layer of thermoelastic material. The method is based on the spectral representation of the matrix and the Legendre interpolation formula.

The transition matrix through a single layer of thickness L is the solution (taken at point L) of the ordinary differential equation of the form

$$\frac{d}{dx}\mathbf{T} = \mathcal{A}\mathbf{T}, \tag{4.1}$$

with the initial condition

$$\mathbf{T}(0) = \mathbf{Id}, \tag{4.2}$$

where $\mathcal{A}$ is the matrix of the system of equations defined in (2.21). The solution of Eq. (4.1) can be represented by

$$\mathbf{T}(L) = \exp(\mathcal{A}L). \tag{4.3}$$

Since the eigenvalues of the matrix A are known, we can calculate its exponent using the Legendre interpolation polynomial method (see [35]):

$$\begin{aligned}\exp\{\mathcal{A}L\} = {} & \frac{(\mathcal{A}-r_2\mathbf{Id})(\mathcal{A}-r_3\mathbf{Id})(\mathcal{A}-r_4\mathbf{Id})}{(r_1-r_2)(r_1-r_3)(r_1-r_4)}e^{r_1L} \\ & + \frac{(\mathcal{A}-r_1\mathbf{Id})(\mathcal{A}-r_3\mathbf{Id})(\mathcal{A}-r_4\mathbf{Id})}{(r_2-r_1)(r_2-r_3)(r_2-r_4)}e^{r_2L} \\ & + \frac{(\mathcal{A}-r_1\mathbf{Id})(\mathcal{A}-r_2\mathbf{Id})(\mathcal{A}-r_4\mathbf{Id})}{(r_3-r_1)(r_3-r_2)(r_3-r_4)}e^{r_3L} + \frac{(\mathcal{A}-r_1\mathbf{Id})(\mathcal{A}-r_2\mathbf{Id})(\mathcal{A}-r_3\mathbf{Id})}{(r_4-r_1)(r_4-r_2)(r_4-r_3)}e^{r_4L}.\end{aligned} \tag{4.4}$$

Substituting the matrix $\mathcal{A}$ in Eq. (4.4) and performing calculations, we obtain the explicit expressions for the transition matrix $\mathbf{T}$:

$$\begin{aligned}\mathbf{T}_{11}(L) = {} & (\operatorname{ch} r_3L(r_1^2 - i\omega A_2B_1 + \omega^2A_1A_3) \\ & + \operatorname{ch} r_1L(-r_3^2 + i\omega A_2B_1 - \omega^2A_1A_3))/(PD\omega), \\ \mathbf{T}_{12}(L) = {} & (r_3 \operatorname{sh} r_1L(-r_3^2 - \omega^2A_1A_3 + i\omega A_2B_1) \\ & + r_1 \operatorname{sh} r_3L(r_1^2 + \omega^2A_1A_3 - i\omega A_2B_1))A_1/(r_1r_3PD\omega), \\ \mathbf{T}_{13}(L) = {} & (r_3 \operatorname{sh} r_1L(-r_3^2 - \omega^2A_1A_3 + i\omega(A_2B_1 + B_2B_3))\end{aligned} \tag{4.5}$$

(4.5) [cont.]
$$+ r_1 \operatorname{sh} r_3L(r_1^2 + \omega^2 A_1A_3 - i\omega(A_2B_1 + B_2B_3)))A_2/(r_1r_3PD\omega),$$

$$\begin{aligned}
\mathbf{T}_{14}(L) &= (\operatorname{ch} r_1L - \operatorname{ch} r_3L)A_2B_2/(PD\omega),\\
\mathbf{T}_{21}(L) &= (r_3 \operatorname{sh} r_1L(r_3^2 + \omega^2 A_1A_3 - i\omega A_2B_1)\\
&\quad + r_1 \operatorname{sh} r_3L(-r_1^2 - \omega^2 A_1A_3 + i\omega A_2B_1))A_3\omega/(r_1r_3PD),\\
\mathbf{T}_{22}(L) &= (\operatorname{ch} r_3L(r_1^2 + \omega^2 A_1A_3) - \operatorname{ch} r_1L(r_3^2 + \omega^2 A_1A_3))/(PD\omega),\\
\mathbf{T}_{23}(L) &= (-\operatorname{ch} r_1L + \operatorname{ch} r_3L)\omega A_2A_3/PD,\\
\mathbf{T}_{24}(L) &= (-r_3 \operatorname{sh} r_1L + r_1 \operatorname{sh} r_3L)\omega A_2A_3B_2/(r_1r_3PD),\\
\mathbf{T}_{31}(L) &= (-r_3 \operatorname{sh} r_1L(ir_3^2 + i\omega^2 A_1A_3 + \omega(A_2B_1 + B_2B_3))\\
&\quad + r_1 \operatorname{sh} r_3L(ir_1^2 + i\omega^2 A_1A_3 + \omega(A_2B_1 + B_2B_3)))B_1/(r_1r_3PD),\\
\mathbf{T}_{32}(L) &= (\operatorname{ch} r_1L - \operatorname{ch} r_3L)iA_1B_1/PD,\\
\mathbf{T}_{33}(L) &= (\operatorname{ch} r_3L(r_1^2 - i\omega(A_2B_1 + B_2B_3))\\
&\quad - \operatorname{ch} r_1L(r_3^2 - i\omega(A_2B_1 + B_2B_1)))/(PD\omega),\\
\mathbf{T}_{34}(L) &= (r_3 \operatorname{sh} r_1L(-r_3^2 + i\omega(A_2B_1 + B_2B_3))\\
&\quad + r_1 \operatorname{sh} r_3L(r_1^2 - i\omega(A_2B_1 + B_2B_3)))B_2/(r_1r_3PD\omega),\\
\mathbf{T}_{41}(L) &= (-\operatorname{ch} r_1L + \operatorname{ch} r_3L)\omega B_1B_3/PD,\\
\mathbf{T}_{42}(L) &= (-r_3 \operatorname{sh} r_1L + r_1 \operatorname{sh} r_3L)\omega A_1B_1B_3/(r_1r_3PD),\\
\mathbf{T}_{43}(L) &= (-r_3 \operatorname{sh} r_1L(r_3^2 i + \omega(A_2B_1 + B_2B_3))\\
&\quad + r_1 \operatorname{sh} r_3L(r_1^2 i + \omega(A_2B_1 + B_2B_3)))B_3/(r_1r_3PD),\\
\mathbf{T}_{44}(L) &= (\operatorname{ch} r_3L(r_1^2 - i\omega B_2B_3) - \operatorname{ch} r_1L(r_3^2 - i\omega B_2B_3))/(PD\omega),
\end{aligned}$$

where ch, sh are the hyperbolic cosine and sine functions,

(4.6)
$$\operatorname{ch} x = \frac{e^x + e^{-x}}{2},$$

(4.7)
$$\operatorname{sh} x = \frac{e^x - e^{-x}}{2}$$

and

(4.8)
$$PD = \sqrt{a^2\omega^2 - b^2 + 2i\omega d} = \sqrt{A_1^2A_3^2\omega^2 - (A_2B_1 + B_2B_3)^2 + 2i\omega A_1A_3(A_2B_1 - B_2B_3)},$$

r_i, $i = 1, 2, 3, 4$ are defined in (2.24), (2.25), a, b, d are defined in (2.26)–(2.28), and the constants A_i, B_i, $i = 1, 2, 3$, are defined in (2.11)–(2.16).

5. The layered thermoelastic medium

The transition matrices obtained in the previous section enable us to describe the passage of the thermoelastic wave through a multi-layered medium. In such a case, knowing the transition matrices through individual layers, we can obtain the transition matrix through all the stratified medium as the product of the matrices. The transition matrix

$\mathbf{T}(.)$ enables us to express the wave field $\mathbf{U}$,

$$\mathbf{U} = \begin{bmatrix} \widehat{u} \\ \widehat{\sigma} \\ \widehat{\vartheta} \\ \widehat{\varphi} \end{bmatrix}, \tag{5.1}$$

at any point x in a homogeneous medium, provided the boundary condition $\mathbf{U}_0 = \mathbf{U}(0)$ at $x = 0$ is known, in the following form:

$$\mathbf{U}(x) = \mathbf{T}(x)\mathbf{U}_0. \tag{5.2}$$

Consider now the multi-layered medium (slab) consisting of N layers of thermoelastic materials, with thicknesses $\triangle_j, j = 1, 2, \ldots, N$. Assume that the stratified medium is surrounded by a homogeneous thermoelastic environment, located at $x < 0$ and $x > d = \sum_{i=1}^{N} \triangle_j$. Since the wave field $\mathbf{U}$ must be continuous at the interfaces of the layers in the stratified medium, we can express the wave satisfying some boundary conditions $\mathbf{U}_0$ at $x = 0$, after it reaches the plane $x = d$:

$$\mathbf{U}(d) = \mathbf{T}_N(\triangle_N)\mathbf{T}_{N-1}(\triangle_{N-1}) \ldots \mathbf{T}_2(\triangle_2)\mathbf{T}_1(\triangle_1)\mathbf{U}_0, \tag{5.3}$$

or, in a more compact form:

$$\mathbf{U}(d) = \prod_{j=1}^{N} \mathbf{T}_j(\triangle_j)\mathbf{U}_0. \tag{5.4}$$

In the above equation all the material properties of the multi-layered medium are completely described by the 4×4 matrix $\mathcal{T}$, being the product of the transition matrices through the individual layers and interpreted as the transition matrix through the slab built of N layers of homogeneous materials,

$$\mathcal{T} = \prod_{j=1}^{N} \mathbf{T}_j(\triangle_j). \tag{5.5}$$

Let us remark that the boundary condition $\mathbf{U}_0$ represents jointly the initial wave pulse, going along the positive direction x and measured at $x = 0$, as well as all the pulses generated due to multiple reflections and transmissions of the initial wave pulse at the surfaces of discontinuity inside the slab, going in the opposite direction and also measured at $x = 0$. The vector $\mathbf{U}(d)$ represents all the transmitted wave pulses generated inside the stratified slab, going to plus infinity and measured at $x = d$.

6. The limiting case — homogenization

Assume that the slab is built of $2K$ layers of the thicknesses $l_1(\gamma), l_2(\gamma), \ldots, l_{2K}(\gamma)$, where $l_i(\gamma), i = 1, 2, \ldots, 2K$ are random variables. In the above $\gamma \in \Gamma$ is an elementary event and (Γ, F, P) is the complete probabilistic space (cf. [38]). Assume additionally that the material parameters of the layers and their thicknesses $(\rho_{2j-1}(\gamma), \lambda_{2j-1}(\gamma), \mu_{2j-1}(\gamma), \alpha_{2j-1}(\gamma), \beta_{2j-1}(\gamma), c_{\varepsilon,2j-1}(\gamma), l_{2j-1}(\gamma), \rho_{2j}(\gamma), \lambda_{2j}(\gamma), \mu_{2j}(\gamma), \alpha_{2j}(\gamma), \beta_{2j}(\gamma), c_{\varepsilon,2j}(\gamma), l_{2j}(\gamma))$ are, as the vector random variables, independent and identically distributed for $j = 1, 2, \ldots, K$. Moreover, we assume that the thicknesses of the layers have the following particular property:

$$(6.1)\qquad (l_{2j-1}(\gamma), l_{2j}(\gamma)) = \left(\frac{L_{2j-1}(\gamma)}{2K}, \frac{L_{2j}(\gamma)}{2K}\right),$$

for $j = 1, 2, \ldots, K$, are independent, identically distributed two-dimensional random variables with the given mean values:

$$(6.2)\qquad E\{L_{2j-1}(\gamma)\} = L^1, \quad E\{L_2(\gamma)\} = L^2,$$

independent of j. In this particular case the periodically repeated segments of the bar are built of the couples of elements with the lengths $l_{2j-1}(\gamma)$, $l_{2j}(\gamma)$, $j = 1, 2, \ldots, K$. For such segments the transition matrices $\mathbf{M}_j(\gamma)$ are the products of the pairs of the transition matrices through the individual layers

$$(6.3)\qquad \mathbf{M}_j(\gamma) = \mathbf{T}_{2j-1}(l_{2j-1}(\gamma))\mathbf{T}_{2j}(l_{2j}(\gamma)), \quad j = 1, 2, \ldots, K,$$

and Eq. (5.4) for the Fourier transform of the amplitudes takes the following form ($2K = N$):

$$(6.4)\qquad \mathbf{U}(d) = \prod_{j=1}^{K} \mathbf{M}_j(\gamma)\mathbf{U}_0,$$

where $d = d(\gamma) = \sum_{j=1}^{N} l_j(\gamma)$.

To study the asymptotic behavior of the randomized equation for the amplitudes of the waves we apply the law of large numbers for the products of random matrices obtained in [4]. This theorem can be written in the following form:

Consider the sequence of the products of real random matrices

$$(6.5)\qquad \mathbf{P}_K(\gamma) = \prod_{j=1}^{K} \mathbf{M}_{j,K}(\gamma).$$

It is assumed that for K tending to infinity the matrices $\mathbf{M}_{j,K}$ *can be represented by*

$$(6.6)\qquad \mathbf{M}_{j,K}(\gamma) = \mathbf{Id} + \frac{1}{K}\mathbf{B}_{j,K}(\gamma) + \mathbf{R}_j(K, \gamma),$$

where $\mathbf{B}_{j,K}(\gamma)$ *for* $j = 1, 2, \ldots, K$, *are independent, identically distributed random matrices, integrable with respect to probability measure* $\mathcal{P}$ *and* $|\mathbf{R}_j(K, \gamma)| = o(K^{-1})$ *for large K. Under these conditions the law of large numbers takes place and*

$$(6.7)\qquad \lim_{K\to\infty} \mathbf{P}_K(\gamma) = \exp(E\{\mathbf{B}_{j,K}(\gamma)\}),$$

in the sense of convergence in distribution of all the vectors obtained by multiplication of the random matrix by an arbitrary deterministic vector.

To analyze the limit case of Eq. (6.4) when K tends to infinity, we decompose, at the beginning, the transition matrix defined in (4.5) under the assumption (6.1) on the thickness of the layers, with respect to the powers of $1/K$:

$$(6.8)\qquad \mathbf{T}_j\left(\frac{L_j}{K}\right) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} + \frac{L_j}{K}\begin{bmatrix} 0 & A_{1,j} & A_{2,j} & 0 \\ -\omega^2 A_{3,j} & 0 & 0 & 0 \\ i\omega B_{1,j} & 0 & 0 & B_{2,j} \\ 0 & 0 & i\omega B_{3,j} & 0 \end{bmatrix} + o\left(\frac{L_j}{K}\right).$$

Multiplying the matrices $\mathbf{T}_1(L_1)$, corresponding to the transition matrices with odd indices and $\mathbf{T}_2(L_2)$ — even indices we obtain that the matrices $\mathbf{B}_j$ required in formula (6.7) are given by (we have changed the numbering of the random variables being the material parameters and the thicknesses of the layers according to the following rule: $p_{2j-1} = p_j^1$, $p_{2j} = p_j^2$ for any parameter p and $j = 1, 2, \ldots, K$, so the parameters with identical superscripts — 1 or 2 — have the identical distribution):

(6.9) $$\mathbf{B}_j = \\ = \begin{bmatrix} 0 & A^1_{1,j}L^1_j + A^2_{1,j}L^2_j & A^1_{2,j}L^1_j + A^2_{2,j}L^2_j & 0 \\ -\omega^2(A^1_{3,j}L^1_j + A^2_{3,j}L^2_j) & 0 & 0 & 0 \\ i\omega(B^1_{1,j}L^1_j + B^2_{1,j}L^2_j) & 0 & 0 & B^1_{2,j}L^1_j + B^2_{2,j}L^2_j \\ 0 & 0 & i\omega(B^1_{3,j}L^1_j + B^2_{3,j}L^2_j) & 0 \end{bmatrix}.$$

The common average value of the matrices $\mathbf{B}_j$ is

(6.10) $$E\{\mathbf{B}_j\} = \\ = \begin{bmatrix} 0 & E\{A^1_1L^1 + A^2_1L^2\} & E\{A^1_2L^1 + A^2_2L^2\} & 0 \\ -\omega^2 E\{A^1_3L^1 + A^2_3L^2\} & 0 & 0 & 0 \\ i\omega E\{B^1_1L^1 + B^2_1L^2\} & 0 & 0 & E\{B^1_2L^1 + B^2_2L^2\} \\ 0 & 0 & i\omega E\{B^1_3L^1 + B^2_3L^2\} & 0 \end{bmatrix}.$$

Here the parameters and the thicknesses under the expectation are the random variables with the distribution common for all couples of layers.

The matrix $e^{E\{\mathbf{B}_j\}}$ is of the form analogous to (4.5), where instead of the parameters $A_1(\gamma)$, $A_2(\gamma)$, $A_3(\gamma)$, $B_1(\gamma)$, $B_2(\gamma)$, $B_3(\gamma)$, being random variables, one has the effective constant parameters A_1^{eff}, A_2^{eff}, A_3^{eff}, B_1^{eff}, B_2^{eff}, B_3^{eff}, defined as:

(6.11) $$A_1^{\text{eff}} = \frac{E\{A_1^1(\gamma)L^1(\gamma) + A_1^2(\gamma)L^2(\gamma)\}}{d},$$

(6.12) $$A_2^{\text{eff}} = \frac{E\{A_2^1(\gamma)L^1(\gamma) + A_2^2(\gamma)L^2(\gamma)\}}{d},$$

(6.13) $$A_3^{\text{eff}} = \frac{E\{A_3^1(\gamma)L^1(\gamma) + A_3^2(\gamma)L^2(\gamma)\}}{d},$$

(6.14) $$B_1^{\text{eff}} = \frac{E\{B_1^1(\gamma)L^1(\gamma) + B_1^2(\gamma)L^2(\gamma)\}}{d},$$

(6.15) $$B_2^{\text{eff}} = \frac{E\{B_2^1(\gamma)L^1(\gamma) + B_2^2(\gamma)L^2(\gamma)\}}{d},$$

(6.16) $$B_3^{\text{eff}} = \frac{E\{B_3^1(\gamma)L^1(\gamma) + B_3^2(\gamma)L^2(\gamma)\}}{d},$$

where

(6.17) $$d = L^1 + L^2.$$

Summarizing this section we can say that the effective (homogenized) medium is also thermoelastic, with the material parameters defined in (6.11)–(6.16). It is seen that the statistical relations between the constants inside each layer make the form of the effective material parameters rather complicated.

7. Closing remarks

The formulae for the transition matrices in the thermoelastic wave problem make it possible to analyze certain wave problems. To define them accurately, one must assume the particular kind of excitation at the front boundary of the stratified medium. The excitation is included in the boundary condition $\mathbf{U}_0$, in the matrix evolution equation (5.4). Since the boundary condition contains also the reflected wave pulses, one must separate two waves: the ones going to the right (excitation), and to the left (reflected pulses). This is possible by postulating the specific form of the solution of the equation analogous to (3.1)–(3.2). Then the terms with positive exponents represent the waves going to the left, while the terms with negative ones — that going to the right (excitation). Assuming the known excitation, we can obtain from (5.4) the system of algebraic equations for the coefficients, what makes it possible to calculate the amplitudes of the reflected and transmitted waves. Substituting them into the formulae analogous to (3.1)–(3.2) and calculating the inverse Fourier transforms (using for example the Fast Fourier Transform numerical algorithm — see [33]), one can obtain the shape of the reflected and transmitted waves. The analysis of some particular thermoelastic wave problems will be the subject of our future research.

The wave problem considered in this paper is an example of a wide class of dynamic problems that can be called the coupled field problems. The applied transition matrix method proved to be very effective in the analysis of elastic, thermal and thermoelastic wave problems. The method seems to be applicable to more complicated coupled field problems, for example those including electromagnetic effects.

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Internal geometry, general covariance and generalized Born–Infeld models
Part I. Scalar fields

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DISCUSSED IS the geometric structure of nonlinearities of the Born–Infeld type, known from electrodynamics. It is shown that this kind of nonlinearity is strictly related to the demand of general covariance combined with an appropriate group of internal symmetries. Multiplets of scalar and covector fields are analyzed in more details, with special stress on the status of internal geometry. Models suggested here may be useful in relativistic mechanics of continua, alternative approaches to gravitation, and unified field-theoretical treatments.

1. Introduction and motivation

A CORNER STONE of general relativity was the experimental coincidence of the inertial and heavy masses. According to A. Einstein, the most natural explanation of this mysterious coincidence is achieved when one interprets the metric structure of the space-time continuum as a carrier of gravitational interactions. In this way, the metric tensor, which in specially-relativistic theories was a purely geometrical parameter of the matter Lagrangians, becomes a physical field subject to the variational procedure, on the same footing with all other fields. If one modifies matter Lagrangians by adding to them the Einstein-Hilbert Lagrangian of the gravitational field, one obtains field equations compatible with experimental data. The total Lagrangian of matter and gravitation is invariant under the group of all diffeomorphisms of the spatio-temporal continuum. This was a very essential novelty in physics, and the general covariance has become a new fundamental principle. This principle states that, on the level of fundamental interactions, there are no absolute spatio-temporal objects. Geometry disappears and becomes physics.

Nevertheless, some special, so to speak post-geometric status of the metric tensor survives in dynamical structure of the Einstein theory of gravitation. Metric tensor is the central member of the family of all physical fields. It is self-interacting and all other fields interact through it even if there is no other interaction between them. Any system of fields which includes the metric tensor, admits a generally-covariant variational principle of the first differential order. And one often claims incorrectly, that any generally-covariant model must include the metric tensor as one of fundamental physical variables (roughly speaking, the metric tensor is to be necessary for the very existence of other fields).

Some philosophical objections may be raised against this non-democratic scheme. The bundle of symmetric second-order tensors is not any special element of the universe of all associated bundles of the principal bundle of linear frames. From the purely mathematical point of view this scheme is not necessary for the general covariance of a theory. And physically, the Einstein–Hilbert principle of general covariance seems to be independent of the particular, metric model of gravitation; probably it is much more general and fundamental.

Nevertheless, it is true that geometric objects admitting nontrivial, generally covariant variational principles are rather exceptional. It is instructuve to review simple examples. First of all, the number of dependent variables N must exceed the number n of independent variables, i.e., there must be more field components than space-time coordinates. Indeed, the general-covariance group is "parametrized" by n arbitrary functions of n variables, thus, at least to some extent, any system of $k \leq n$ field variables may be transformed by an appropriate diffeomorphism to any a priori given form. This implies that, if $N \leq n$ and Lagrangian is generally covariant, then, either any or no field is a solution, i.e., the theory is either trivial or empty. Let us quote two examples of such trivial schemes with $N = n$.

(i) Let A denote a contravariant vector density of weight one. The only scalar density of weight one, built of A alone, has the form

$$L = \frac{\partial A^{\mu}}{\partial x^{\mu}}. \tag{1.1}$$

The divergence structure of this generally-covariant "Lagrangian" implies that the resulting Euler–Lagrange equations are trivial, $0 = 0$.

(ii) Let A denote a differential one-form; put $F := dA$. We can interpret A as an electromagnetic potential and F as the corresponding field strength. In terms of coordinates: $F_{\mu\nu} = \dfrac{\partial A_{\nu}}{\partial x^{\mu}} - \dfrac{\partial A_{\mu}}{\partial x^{\nu}}$. The only scalar density of weight one we can construct of A alone, has the form:

$$L = \sqrt{|\det[F_{\mu\nu}]|}. \tag{1.2}$$

It is implicitly assumed that $\det[F_{\mu\nu}] \neq 0$; otherwise we would have been dealing with a differential singularity of the type $\sqrt{0}$. It is clear that Lagrangian (1.2) is generally-covariant, thus, the resulting Euler–Lagrange equations must be either inconsistent or trivial, because there are as many dynamical variables as coordinates. Indeed, one can show that L may be represented as a total divergence,

$$\sqrt{|\det[F_{\mu\nu}]|} = \frac{2}{n}\frac{D}{Dx^{\nu}} A_{\mu} F^{\mu\nu} \sqrt{|\det[F_{\mu\nu}]|}, \tag{1.3}$$

where $F^{\mu\nu}F_{\nu\varkappa} = \delta^{\mu}{}_{\varkappa}$, and n is the "space-time" dimension. Therefore, the corresponding Euler–Lagrange equations are trivial identities $0 = 0$.

The field of symmetric and non-degenerate second-order tensors (twice covariant, or twice contravariant) provides the simplest and oldest-known example of an irreducible geometric object admitting a generally-covariant variational principle of the first differential order. Let us remind that irreducible linear objects in an n-dimensional manifold are defined as quantities the components of which transform according to irreducible representations of the group $GL(n, \mathbb{R})$, when the local reference n-leg is deformed. Thus, scalars, vectors, covectors, symmetric and skew-symmetric second-order tensors are irreducible, whereas the multiplets of the above objects, as well as general (asymmetric) second-order tensors, are reducible. It is a nice feature of symmetric non-degenerate T^0_2- and T^2_0-tensors g that, the very geometry of their degrees of freedom determines almost uniquely the structure of generally covariant variational principle of the first differential order in g. Namely, the most general Lagrangian leading to second-order field equations is a combination of Hilbert Lagrangian and cosmological term,

$$L = \frac{1}{k} R[g]\sqrt{|g|} + \Lambda\sqrt{g}, \tag{1.4}$$

$R[g]$ denotes the curvature scalar built of g, Λ — the cosmological constant, and k — gravitational constant.

The peculiarity of non-degenerate symmetric T^0_2- and T^2_0-tensors is that they provide a universal tool for constructing scalars and scalar densities from arbitrary tensorial objects. This justifies to some extent the special status of the metric field and Hilbert–Einstein model among the family of all generally covariant theories. It is natural to ask what is the position of another inhabitants of the second floor of the tensor algebra, namely, the mixed second-order tensors (T^1_1-tensors). A distinguishing geometric feature of such tensors is that they are linear mappings of tangent spaces into themselves and define local automorphisms of the full tensor algebra. They are not irreducible geometric objects, but their trace-less parts are irreducible. In spite of its special geometric status, the T^1_1-field has not yet found any direct physical applications; none of the recently known fundamental interactions or matter fields is representable in terms of mixed second-order tensors. Nevertheless, it is interesting that such tensors admit generally-covariant variational principles. To construct them, we must use the Nijenhuis torsion concept. Let us remind that the Nijenhuis torsion $S(X,Y)$ of two T^1_1-tensor fields X, Y is defined as the following skew-symmetric T^1_2-tensor:

$$\begin{aligned} S(X,Y)^{\mu}{}_{\nu\lambda} := {} & X^{\varrho}{}_{\nu}Y^{\mu}{}_{\lambda,\varrho} + Y^{\varrho}{}_{\nu}X^{\mu}{}_{\lambda,\varrho} - Y^{\varrho}{}_{\lambda}X^{\mu}{}_{\nu,\varrho} - X^{\varrho}{}_{\lambda}Y^{\mu}{}_{\nu,\varrho} \\ & - X^{\mu}{}_{\varrho}Y^{\varrho}{}_{\lambda,\nu} - Y^{\mu}{}_{\varrho}X^{\varrho}{}_{\lambda,\nu} + X^{\mu}{}_{\varrho}Y^{\varrho}{}_{\nu,\lambda} + Y^{\mu}{}_{\varrho}X^{\varrho}{}_{\nu,\lambda}. \end{aligned} \tag{1.5}$$

It may be represented in a coordinate-free form by means of its evaluation $S(X,Y)\cdot(A,B) = S(X,Y)^{\mu}{}_{\nu\lambda}A^{\nu}B^{\lambda}\dfrac{\partial}{\partial x^{\mu}}$ on vector fields A, B:

$$\begin{aligned} S(X,Y)\cdot(A,B) = {} & [XA, YB] + [YA, XB] + XY[A,B] + YX[A,B] \\ & - X[A, YB] - X[YA, B] - Y[A, XB] - Y[XA, B], \end{aligned} \tag{1.6}$$

where $[A, B]$ denotes the Lie bracket of vector fields,

$$[A,B]^{\mu} = A^{\lambda}B^{\mu}_{,\lambda} - B^{\lambda}A^{\mu}_{,\lambda}.$$

Apparently, the formula (1.6) involves the derivatives of A, B; nevertheless, it may be shown that the terms involving derivatives cancel each other, thus as a matter of fact, the expression (1.6) is algebraic in A, B and may be correctly used for defining the T^1_2-tensor field $S(X,Y)$.

With any second-order mixed tensor X we can associate the torsion $S(X) := S(X,X)$. Obviously, the expressions $S^{k,l}(X) := S(X^k, X^l)$ are also possible, including negative powers k, l when X is non-degenerate; however, they are much more complicated. Using S we can construct the following metric-like object based on the Killing prescription:

$$G_{\mu\nu} = G_{\nu\mu} := S^{\lambda}{}_{\mu\varkappa}S^{\varkappa}{}_{\nu\lambda}. \tag{1.7}$$

It is quadratic in derivatives of X. The most general twice-covariant second order tensor built algebraically of S alone and quadratic in derivatives of X has the form

$$T_{\mu\nu} := AS^{\lambda}{}_{\mu\varkappa}S^{\varkappa}{}_{\nu\lambda} + BS^{\lambda}{}_{\mu\lambda}S^{\varkappa}{}_{\nu\varkappa} + CS^{\lambda}{}_{\varkappa\lambda}S^{\varkappa}{}_{\mu\nu}, \tag{1.8}$$

A, B, C, being constants. Let us observe that the quantity

$$L := \sqrt{|\det[T_{\mu\nu}]|} \tag{1.9}$$

is a Weyl density of weight one, thus, in principle, it may be used as a generally-covariant Lagrangian for the field X.

Lagrangian (1.9) is more complicated than the Hilbert–Einstein Lagrangian (1.4). Namely, the latter is quadratic in derivatives $g_{\mu\nu,\lambda}$ (with coefficients built algebraically of $g_{\alpha\beta}$), and the resulting field equations are quasilinear. The expression (1.9) is irrational in derivatives. The resulting Euler-Lagrange equations are essentially rational (become rational after dividing by $\sqrt{|T|}$), however, the coefficients at second derivatives of X depend not only on X itself, but also on its first derivatives.

Any generally-covariant theory must be nonlinear, however, the nonlinearity of the model based on Eq. (1.9) is much stronger than the nonlinearity of Einstein equations. It resembles the Born–Infeld nonlinearity in electrodynamics. Indeed, Lagrangian (1.9) is obtained by square-rooting the determinant of the tensor T quadratic in derivatives. Let us remind that the Born–Infeld electrodynamical Lagrangian has the form

$$(1.10) \qquad \sqrt{|\det[g_{\mu\nu} + aF_{\mu\nu}]|},$$

thus, the tensor under the square-root and determinant symbol is a first order polynomial of field derivatives $A_{\mu,\nu}$. There are also certain modifications based on second-order polynomials,

$$(1.11) \qquad \sqrt{|\det[g_{\mu\nu} + aF_{\mu\nu} + bg^{\varkappa\varrho}F_{\mu\varkappa}F_{\varrho\nu}}.$$

Thus, perhaps the most essential structural feature of the Born–Infeld nonlinearity is that Lagrangian has the form (1.9), where T is a low-order polynomial of field derivatives. Let us remind, incidentally, that the square-rooting of twice-covariant tensors is a standard tool for constructing Weyl densities of weight one. Thus, one can reasonably expect that generalized Born–Infeld models are geometrically and physically distinguished within the family of all possible Lagrangians. Another, much more familiar class of physically privileged models consists of traditional Lagrangians, quadratic in derivatives, and factorized as in Eq. (1.4) into dynamical scalar factor comprising all derivatives, and some Weyl density depending on the field variables in a purely algebraic way. There are certain weak-field correspondences between these two kinds of models; they seem to indicate that generalized Born–Infeld models $L = \sqrt{|\det[T_{\mu\nu}]|}$, with T quadratic in derivatives, are particularly promising and reasonable. For any kinds of fields they are the simplest possible generally-covariant models. For example, as we have just seen, the second-order mixed tensor field X admits such models, but does not admit any model quadratic in derivatives. Lagrangians (1.9), (1.8) do not exhaust the class of all generally-covariant models for the T^1_1-field X. More general and much more complicated models are obtained by replacing the constants A, B, C by functions of basic scalars built of X; the expression (1.9) also may be multiplied by a factor depending on basic scalars. If the field G Eq. (1.7) is non-degenerate, the basic scalars may be obtained, e.g., with the help of Weitzenböck prescription:

$$J_1 = G_{\mu\alpha}G^{\nu\beta}G^{\lambda\gamma}S^{\mu}{}_{\nu\lambda}S^{\alpha}{}_{\beta\gamma}, \qquad J_2 = G^{\mu\nu}S^{\alpha}{}_{\mu\beta}S^{\beta}{}_{\nu\alpha}, \qquad J_3 = G^{\mu\nu}S^{\alpha}{}_{\mu\alpha}S^{\beta}{}_{\nu\beta}.$$

It is easy to see that all such scalars are zeroth-degree homogeneous functions of derivatives, thus, all generally-covariant Lagrangians for X are homogeneous of degree n in derivatives (n equals the "space-time" dimension).

It is not well known that the affine connection field also admits generally-covariant variational principle. Let $\Gamma^{\lambda}{}_{\mu\nu}$ be a symmetric affine connection, $R^{\lambda}{}_{\mu\varkappa\nu}$ — its curvature tensor, and $R_{\mu\nu} = R^{\lambda}{}_{\mu\lambda\nu}$ — the Ricci tensor of Γ. The twice covariant tensor $R_{\mu\nu}$ gives rise to the scalar Weyl density of weight one,

$$L := \sqrt{|\det[R_{\mu\nu}]|}. \tag{1.13}$$

This density is built algebraically of $\Gamma^{\lambda}{}_{\mu\nu}$ and its derivatives $\Gamma^{\lambda}{}_{\mu\nu,\alpha}$, thus, at least formally, it looks acceptable as a Lagrangian for $\Gamma^{\lambda}{}_{\mu\nu}$. This Lagrangian was suggested many years ago by EDDINGTON and SCHRÖDINGER [15], who expected to formulate an alternative gravitation theory. More recently, KIJOWSKI showed that the resulting scheme is essentially equivalent to the Einstein theory; the metric field appears, roughly speaking, as a momentum conjugate to Γ, [8]. This physical equivalence of the Born–Infeld scheme (1.13) and the quadratic in derivatives model (1.4) is interesting in itself. Let us observe, incidentally, that (1.13) differs in one essential respect from Eqs. (1.1), (1.2), (1.4), (1.5); namely, $\Gamma^{\lambda}{}_{\mu\nu}$ is a geometric object ruled by the affine group $GAf(n,\mathbb{R}) = GL(n,\mathbb{R}) \underset{s}{\times} \mathbb{R}^n$, whereas the tensorial objects A_{μ}, A_{μ}, $g_{\mu\nu}$, $X^{\mu}{}_{\nu}$ are ruled by the linear group $GL(n,\mathbb{R})$.

This short review seems to exhaust the list of low-dimensional irreducible objects admitting reasonable generally-covariant variational principles. However, there exist reducible objects, first of all — multiplets of scalar and covector fields, which admit reasonably looking and physically promising Lagrangians invariant under the group of all spatio-temporal diffeomorphisms.

All non-gravitational interactions are described by scalar and covector fields, and anyway, it seems that differential forms are the best candidates for describing fundamental interactions in generally-covariant theories, because they can be intrinsically differentiated in the sense of exterior differentials [1, 2, 21, 22, 23]. This motivates the attempts of interpreting also gravitational interactions in terms of scalars and covectors. Moreover, one actually describes gravitation in this way, expressing the metric field through the tetrad (Vierbein), i.e., the quadruple of covector fields. This procedure is necessary when we introduce fermion fields into the treatment. Originally, in Einstein theory, tetrads were introduced as nonholonomic reference frames and there were no attempts to interpret them as genuine physical fields. There exists, however, a wider class of Vierbein-based theories of gravitation, known as metric-teleparallel theories [5, 9, 12, 13, 14]. This class includes the tetrad form of Einstein theory as a special case. There are certain theoretical arguments in favour of this generalization, and as yet there are no experimental arguments against it. In generic metric-teleparallel models, tetrad components acquire a microphysical individuality. They become fields and it is no longer possible to reduce their meaning to that of being axes of auxiliary non-holonomic frames.

Thus, at least formally, the whole boson sector may be described with the use of nothing but covector and scalar fields. Gauge fields also are representable as multiplets of differential one-forms ruled by appropriate groups of internal symmetries. Among covector fields there is a singled-out geometric quadruplet (Vierbein) responsible for gravitation and general covariance. This quadruplet absorbs the most essential nonlinearity of dynamical models. Thus, even after eliminating the metric tensor from the system of dynamical variables, we still have to do with "post-geometric" quantities. But, if we once decide to use only scalars and covectors as fundamental fields, and if we agree that the principle of general covariance and the particular metric or Vierbein model of gravitation are two different things, then it is natural to object against this picture and search for "democratic" models in which all covector and scalar fields occur in a completely symmetric way. In such models one does not distinguish a quadruplet of carriers of gravitational interactions. Moreover, on the fundamental level, characterized by the use of strongly nonlinear equations, there is no division of "duties" between covector fields, i.e., no assignment of special kinds of interaction (gravitational, electromagnetic, weak, strong, etc.) to particular multiplets of fields. Splitting of this interaction into a few kinds of forces and identification of covector fields as carriers of those forces should appear scarcely on the level of solutions, due to a mechanism like the spontaneous symmetry breaking. Thus, it will be characteristic for small perturbations of "vacuum" solutions. The latter, roughly speaking, will be "flat" or "constant", i.e., they will describe situations physically to be as non-excited as possible. Let us notice that in classical generally-covariant theories, the concept of energy is a rather delicate matter and one must be very careful with the energetic criterion of vacuums as solutions minimizing the energy functional. The point is that the formally introduced Hamiltonian vanishes in virtue of the general covariance. Performing the symplectic reduction of Dirac's primary and secondary constraints (ADM-procedure), one can obtain an effective Hamiltonian of the reduced dynamics; however, there are certain ambiguities in this procedure, and one is faced with computational difficulties increasing drastically together with the order of nonlinearity.

The aim of this paper is to review a family of generally-covariant Lagrangians for systems of scalar and covector fields. As yet I have not carried out a detailed mathematical analysis of the consistency of the resulting Euler–Lagrange field equations. It is expected that among those Lagrangians there are good candidates for unification models. We begin with some class of very ascetic field-theoretical models, involving only scalar fields as dynamical variables.

2. Generally covariant Lagrangians for multiplets of scalar fields

Let M and W be differential manifolds of dimensions n and N, respectively. Differentiable mappings $\Phi : M \to W$ will be interpreted as W-valued fields on the "space-time" continuum M. We shall consider first-order variational principles for such fields, thus, Φ are assumed to be at least twice continuously differentiable. Diffeomorphism groups $\operatorname{Diff} M$ and $\operatorname{Diff} W$ act on the fields Φ according to the formulas:

$$\begin{aligned} &\operatorname{Diff} M \ni \phi : \Phi \mapsto \Phi \circ \phi^{-1}, \\ &\operatorname{Diff} W \ni U : \Phi \mapsto U \circ \Phi. \end{aligned} \tag{2.1}$$

Formulas $(2.1)_1$ and $(2.1)_2$ describe, respectively, spatio-temporal and internal (isotopic) transformations. The rule $(2.1)_1$ expresses the scalar character of Φ.

Let x^μ, $\mu = 1, \ldots, n$, y^a, $a = 1, \ldots, N$ be local coordinates in M and W. The fields Φ and their tangent mappings $T\Phi : TM \to TW$ are analytically represented by their components,

$$\Phi^a = y^a \circ \Phi, \qquad \left(\Phi^a, \frac{\partial \Phi^a}{\partial x^\mu}\right).$$

We are interested in generally-covariant variational principles for Φ, thus, no geometric structure in M will be assumed. The isotopic space W, on the other hand, will be endowed with some absolute geometry. The simplest and most intuitive possibility is a nonsingular, twice covariant tensor field η on W.

Any field $\Phi : M \to W$ gives rise to the pull-back tensor field $g[\Phi]$ on M,

$$g[\Phi] = g(T\Phi) = \Phi^* \cdot \eta. \tag{2.2}$$

Analytically,

$$g[\Phi]_{\mu\nu} = \eta_{ab}(\Phi^1, \dots, \Phi^N) \frac{\partial \Phi^a}{\partial x^\mu} \frac{\partial \Phi^b}{x^\nu}. \tag{2.2'}$$

The assignment $\Phi \mapsto g[\Phi]$ is generally covariant in M,

$$g[\Phi \circ \phi] = \phi^* g[\Phi], \tag{2.3}$$

for any $\phi \in \mathrm{Diff}\, M$. It is also invariant under isotropic transformations preserving the structure (W, η), i.e.,

$$g[U \circ \Phi] = g[\Phi] \quad \text{if} \quad U^* \cdot \eta = \eta. \tag{2.4}$$

From $g[\Phi]$ we can construct the following scalar W-density of weight one on M [10]:

$$L[\Phi] = \sqrt{|g[\Phi]|} = \sqrt{|\det[\eta_{ab}(\Phi)\Phi^a{}_{,\mu}\Phi^b{}_{,\nu}]|}. \tag{2.5}$$

It is a homogeneous function of degree n of derivatives $\Phi^a{}_{,\mu}$. Algebraic values of Φ^a enter through the internal geometry η. The density (2.5) is generally covariant in M and invariant under symmetries of (W, η),

$$\begin{aligned} L[\Phi \circ \phi] &= \phi^* L[\Phi] \quad \text{for any} \quad \phi \in \mathrm{Diff}\, M, \\ L[U \circ \Phi] &= L[\Phi] \quad \text{if} \quad U^*\eta = \eta. \end{aligned} \tag{2.6}$$

We can interpret Eq. (2.5) as a Lagrangian for the nonlinear scalar multiplet $\Phi : M \to W$. Its shape is uniquely defined by the assumed invariance properties (2.6). There is, however, a wide class of Lagrangians invariant under $(2.6)_1$ alone. They have the following general form:

$$L[\Phi] := f(\Phi)\sqrt{|\det[g[\Phi]_{\mu\nu}]|} = \sqrt{|k(\Phi)\det[g[\Phi]_{\mu\nu}]|}, \tag{2.7}$$

where $f : W \to \mathbb{R}$ resp. $k : W \to \mathbb{R}$ is a sufficiently regular "potential" function. If f is non-constant, then Eq. (2.7) is not invariant in the sense of Eq. $(2.6)_2$ under the total group $\mathrm{Diff}(W, \eta)$ of isotopic isometries (diffeomorphisms of W preserving η).

Another convenient representation of Diff M — invariant Lagrangians is:

$$L[\Phi] = \sqrt{|\det[T[\Phi]_{\mu\nu}]|}, \qquad T[\Phi] = \omega(\Phi)\Phi^*\eta + \Phi^*(\alpha \otimes \beta), \tag{2.8}$$

α, β being differential one-forms on W. By an appropriate redefinition of k, g, ω, η, α, β we can formally identify expressions (2.7) and (2.8). Nevertheless, it may happen that the tensors η, α, β have a well-defined physical meaning (isotopic metric, directions in the isotopic space); in such situations (2.8) is more convenient.

Obviously, we must assume that $N > n$. Indeed, as mentioned in the Introduction, any generally covariant Lagrangian involving $N \leq n$ real field variables is trivial; its space of extremals is either empty or identical with the family of all kinematically admissible (sufficiently smooth) fields. The reason is that Diff M is controlled by n real functions of n variables (space-time coordinates), thus, any Diff M — invariant theory with N real field quantities involves $\min(n, N)$ gauge variables. If $N \leq n$, every field is a pure gauge. For example, $g[\Phi]$ Eq. (2.2) is singular for any $N < n$, and Lagrangian (2.5) identically vanishes. If $N = n$ and Φ is a local diffeomorphism, then $g[\Phi]$ is non-degenerate and Eq. (2.5) needs not vanish. Nevertheless, the corresponding variational principle is still trivial, because for any field Φ and for any domain Ω the action $I[\Phi, \Omega] = \int L[\Phi]$ depends only on the boundary conditions $\Phi \mid \partial\Omega$; more precisely, $I[\Phi, \Omega]$ equals the η-volume of the region contained within the closed hypersurface $\Phi(\partial\Omega) \subset W$. It is clear that this region, thus, also its volume, is uniquely determined by $\Phi|\partial\Omega$ and does not depend at all on $\Phi \mid \operatorname{Int}\Omega$. If L is given by Eq. (2.7) and f is non-constant, then $I[\Phi, \Omega]$ becomes functionally dependent on the behaviour of Φ within the interior of Ω. However, if, as assumed, f depends on Φ in an algebraic way, then, it is rather typical that the resulting Euler–Lagrange equations are inconsistent, because for $N = n$, the dependence of Eq. (2.7) on derivatives is artificial. It is impossible to introduce the derivatives of Φ to f without violating the general covariance of Eq. (2.7).

We conclude that $N > n$, and Φ^a are immersions, i.e., rank $\Phi = n$, except isolated singularities. For non-immersive Φ Lagrangians (2.5), (2.7) have differential singularity of the type $\sqrt{0}$.

The structure of Lagrangians (2.5), (2.7) is particularly intuitive when (W, η) is a Riemannian space, i.e., when η is symmetric and positive. For any immersion Φ the pair $(M, g[\Phi])$ also is a Riemannian structure. If L is given by Eq. (2.5) and $\Phi : \Omega \to W$ is an injection locally minimizing the functional $I[\cdot, \Omega]$ on the family of all injections with given boundary data $\Phi \mid \partial\Omega$, then the image $\Phi(\Omega) \subset W$ is a surface of locally minimal n-dimensional η-volume among all surfaces with the same boundary $\Phi(\partial\Omega) \subset W$. As an intuitive example let us realize a rubber membrane or a soap film stretched on a ring; $n = 2$, $N = 3$. If $n = 1$, the extremals of Eq. (2.5) are geodetic curves in (W, η). When (W, η) is a mechanical configuration space and $n = 1$, then Eq. (2.7) becomes the integrand of Jacobi–Maupertuis variational principle if we identify f with $\sqrt{2(E - V)}$, where E is a fixed energy value, V denotes the potential energy function, and the kinetic energy is understood in the sense of η. If η is normally-hyperbolic instead of elliptic, and $n = 1$, then the extremals of (2.7) are geodetic world-lines in (W, η). If $n = 2$, we obtain strings.

If M is interpreted as an n-dimensional space-time, then the model (2.7) describes the physical world as a vibrating n-dimensional "membrane" in N-dimensional isotopic space W endowed with some absolute geometry η. This absolute metric induces on the "membrane" the physical metric $g[\Phi]$ depending explicitly on the configuration Φ.

Minimizers of the action functional based on Lagrangians (2.5) with symmetric positively definite η are known in Riemannian geometry as "minimal surfaces". Their peculiarity is that they minimize the n-dimensional Riemannian volume of n-dimensional submanifolds of W spanned on a fixed $(n - 1)$-dimensional boundary. The corresponding Euler–Lagrange equations are equivalent to vanishing of the mean curvature vector, i.e., the first trace-like invariant of the second quadratic form of $\Phi(M) \subset W$.

Generally-covariant Lagrangians for multiplets of scalars are never quadratic in derivatives; we have seen that expressions (2.5), (2.7), (2.8) are homogeneous of degree n in derivatives of Φ. The corresponding field equations are essentially nonlinear. Nevertheless, it must be stressed that expressions (2.5), (2.7), (2.8) are, roughly speaking, "as quadratic as possible"; they are given by square roots of tensors quadratic in derivatives. Thus, we are dealing with a generalized Born–Infeld nonlinearity; the square-rooted tensor $T[\Phi]$ will be referred to as a Lagrange tensor. Variational principles with Lagrange tensors quadratic in derivatives (more generally — low order polynomials of derivatives) are interesting in themselves; it may be very instructive to investigate their general structure in some details.

We can also admit complex manifolds W and analytic isotopic metrics η. Then $g = \Phi^* \cdot \eta$ is a complex twice covariant tensor on the real manifold M. Its real part, $\mathrm{Re}\, g$, if symmetric, is a candidate for the spatio-temporal metric tensor. It suggests us to use Lagrangians

$$L = \sqrt{|\det[\mathrm{Re}\, g_{\mu\nu}]|}, \tag{2.5'}$$

nevertheless, the previous expression (2.5) is also a priori possible. Obviously, for complex fields Φ, the use of the absolute value symbol in Eq. (2.5) becomes more essential than for real fields; it is unavoidable even locally. Let us observe in this connection that if Φ is real and immersive, M orientable, and η-globally nonsingular in W, then the absolute value in Eq. (2.5) either acts trivially or reverses the overall negative sign of the determinant under the square-root expression.

When dealing with complex isotopic manifolds W, one uses rather sesquilinear, e.g., Hermitian, scalar products than the analytic ones; let us recall the defining property of sesquilinear metrics η:

$$\eta_w(\lambda_1 z_1 + \lambda_2 z_2, z) = \overline{\lambda_1}\eta_w(z_1, z) + \overline{\lambda_2}\eta_w(z_2, z),$$
$$\eta_w(z, \lambda_1 z_1 + \lambda_2 z_2) = \lambda_1\eta_w(z, z_1) + \lambda_2\eta_w(z, z_2),$$

for any $w \in W$, $z_1, z_2, z \in T_wW$. Thus, if $(\ldots, e_a, \ldots)$ is an ordered basis in T_wW and $z_i = z_i^a e_a$, $i = 1, 2$, then

$$\eta_w(z_1, z_2) = \eta_{ab}(w)\overline{z_1^a} z_2^b,$$

where

$$\eta_{ab}(w) = \eta_w(e_a, e_b).$$

The pull-back $g = \Phi^* \cdot \eta$ of a sesquilinear form η is analytically given by

$$g_{\mu\nu} = \eta_{ab}\overline{\Phi^a}_{,\mu}\Phi^b{}_{,\nu}. \tag{2.8'}$$

Usually in applications one deals with Hermitian isotopic metrics, when $\eta_w(z_1, z_2) = \overline{\eta_w(z_2, z_1)}$, i.e., $\eta_{ab} = \overline{\eta_{ba}}$. The corresponding spatio-temporal metric $g[\Phi]$ is also Hermitian, $g_{\mu\nu} = \overline{g_{\nu\mu}}$, its squared arc element $ds^2 = g_{\mu\nu}dx^\mu dx^\nu$ and determinant $\det[g_{\mu\nu}]$ are both real, thus, the use of the absolute value symbol in $L = \sqrt{|\det[g_{\mu\nu}]|}$ has the same status as for real-valued scalars.

In physical applications we usually deal with linear scalars, in which case W is a linear space, the field η is constant, i.e., identical with an algebraic tensor $\eta \in W^* \otimes W^*$, and $(\ldots, y^a, \ldots)$ is a linear basis in W^*. The quadratic form $v \mapsto \eta(v, v) = ||v||^2$ distinguishes a natural class of factors f in (2.7), namely, those depending on Φ through $||\Phi||^2 = \eta_{ab}\Phi^a\Phi^b$,

$$f(\Phi) = k(||\Phi||^2). \tag{2.9}$$

The corresponding Lagrangians (2.7) are invariant under transformations $(2.6)_2$ iff $U \in 0(W, \eta) \subset GL(W)$, i.e., iff U is a linear mapping preserving η; $U^* \cdot \eta = \eta \circ (U \times U) = \eta$. Let us observe that if η is symmetric and nonsingular, the group $\mathrm{Diff}(W, \eta)$ is not essentially wider than the η-orthogonal Lie group $0(W, \eta)$, because then $\mathrm{Diff}(W, \eta) = 0(W, \eta) \underset{s}{\times} W$. More generally, if the symmetric part of η is nonsingular, then $\mathrm{Diff}(W, \eta) =$

$G \underset{s}{\times} W$, G being a Lie subgroup of $0(W, \eta + \eta^T)$. If the potential term f is constant, then the "free" Lagrangian

$$L = \sqrt{|g|} = \sqrt{|\det[\eta_{ab}\Phi^a_{,\mu}\Phi^b_{,\nu}]|} \tag{2.10}$$

is also translationally invariant in W. Thus, if η is pseudo-Euclidean (constant, symmetric, nonsingular), then Eq. (2.10) is isotopically invariant under the non-compact Lie group $E(W, \eta) = 0(W, \eta) \underset{s}{\times} W$ — the group of affine transformations of W preserving η. Moreover, Eq. (2.10) is uniquely determined by the demand of invariance under Diff M and $E(W, \eta)$. If we give up the assumption of translational invariance in isotopic space, and retain the demand of invariance under Diff $M \times 0(W, \eta)$, then the class of admissible Lagrangians is given by

$$L = \sqrt{|\det(T_{\mu\nu}]|}, \tag{2.11}$$

where

$$T[\Phi] := \omega(||\Phi||^2)\Phi^*\eta + \varkappa(||\Phi||^2)d\left(\frac{1}{2}||\Phi||^2\right) \otimes d\left(\frac{1}{2}||\Phi||^2\right), \tag{2.11'}$$

ω, $\varkappa$ denoting scalar functions of the $0(W, \eta)$-invariant quantity $||\Phi||^2$. Analytically,

$$T_{\mu\nu} = \omega\eta_{ab}\frac{\partial\Phi^a}{\partial x^\mu}\frac{\partial\Phi^b}{\partial x^\nu} + \varkappa\lambda_\mu\lambda_\nu \tag{2.11''}$$

$$= \frac{1}{2}\frac{\partial||\Phi||^2}{\partial x^\mu} = \eta_{ab}\Phi^a\frac{\partial\Phi^b}{\partial x^\mu}.$$

Obviously, Eq. (2.11′) is a special case of Eq. (2.8) corresponding to $\alpha \otimes \beta = \varkappa\varrho \otimes \varrho$, where ϱ denotes the differential form on W obtained from the radius-vector field $w \mapsto w$ by means of the canonical isomorphism $W \ni u \mapsto \eta(u, \cdot) \in W^*$ — lowering of indices.

If W is complex and η — Hermitian, then, in virtue of Eq. (2.8′) we have

$$L = \sqrt{|g[\Phi]|} = \sqrt{\det[\eta_{ab}\overline{\Phi^a}_{,\mu}\Phi^b_{,\nu}]} \tag{2.12}$$

instead Eq. (2.10). The complex-Hermitian analogue of Eq. (2.11′) is given by

$$T_{\mu\nu} = \omega\eta_{ab}\overline{\Phi^a}_{,\mu}\Phi^b_{,\nu} + \varkappa\lambda_\mu\lambda_\nu, \tag{2.13}$$

obviously, the quantities λ_μ are real.

Lagrangians (2.10), (2.12) are simplest generally-covariant models for multiplets of scalar fields. Their position among all Diff M — invariant Lagrangians (2.7), (2.8), (2.11) may be compared with that of Klein–Gordon Lagrangians

$$L = \left(\frac{1}{2}\eta_{ab}G^{\mu\nu}\overline{\Phi^a}_{,\mu}\Phi^b_{,\nu} - \frac{m^2}{2}\eta_{ab}\overline{\Phi^a}\Phi^b\right)\sqrt{|G|} \tag{2.14}$$

among all models formulated on the basis of a fixed pesudo-Riemannian geometry (M, G). Obviously, when dealing with multiplets of scalars in a structureless manifold M, we have no fixed G at disposal, and because of this there are no quadratic models like (2.14). Expression (2.14) provides the simplest Lagrangian for immersive mappings acting between pseudo-Riemannian spaces (M, G), (W, η); Lagrangians of this kind are used in σ-models. In spite of the structural difference between Eqs. (2.5) and (2.14), there exists an interesting relationship between them, invented by Polyakov and used in certain problems of strings theory. For simplicity we assume that Φ is real and there is no mass term in (2.14), thus

$$L = \frac{1}{2}\eta_{ab}\Phi^a{}_{,\mu}\Phi^b{}_{,\nu}G^{\mu\nu}\sqrt{|G|}. \tag{2.14'}$$

Let us consider a reducible field system (G, Φ); the quantities G, Φ are to be independent dynamical variables. As a dynamical model for (G, Φ) we use the Lagrangian

$$L'[G,\Phi] = \frac{1}{2}\eta_{ab}\Phi^a{}_{,\mu}\Phi^b{}_{,\nu}G^{\mu\nu}\sqrt{|G|} + C\sqrt{|G|}, \tag{2.14''}$$

which differs from Eq. $(2.14)_1$ by the "cosmological" term $C\sqrt{|G|}$. The metric G enters L' in a purely algebraic way, just as in the gravitational Palatini Lagrangian. If $n \neq 2$, the equation $\dfrac{\delta L'}{\delta G_{\mu\nu}} = 0$ gives $G^{\mu\nu} = \dfrac{2C}{2-n}g^{\mu\nu}$. Substituting this result to $\dfrac{\delta L'}{\delta \Phi^a} = 0$, we obtain equations equivalent to those following from the Lagrangian (2.5), $\dfrac{\delta\sqrt{|g[\Phi]|}}{\delta\Phi^a} = 0$. If $n = 2$, then the equation $\dfrac{\delta L'}{\delta G_{\mu\nu}} = 0$ is consistent only if $C = 0$, and implies that $G^{\mu\nu} = fg^{\mu\nu}$, f being a completely undetermined function. Thus, the space-time metric G is now conformally-equivalent to $g[\Phi]$, but not necessarily identical with $g[\Phi]$. Substituting this result to $\dfrac{\delta L'}{\delta\Phi^a} = 0$, we again obtain the equations $\dfrac{\delta\sqrt{|g[\Phi]|}}{\delta\Phi^a} = 0$. Thus, if we introduce subsidiary dynamical variables $G_{\mu\nu}$, then irrational Lagrangian (2.5) becomes essentially equivalent to the Lagrangian $(2.14)_2$, quadratic in derivatives. This means that there exists an interesting kinship between quadratic models and generalized Born–Infeld models.

It is instructive to investigate field equations corresponding to Lagrangians (2.10), (2.11). For the model (2.10) we obtain the following Euler–Lagrange equations:

$$g^{\mu\nu}\overset{g}{\nabla}_\mu\overset{g}{\nabla}_\nu\Phi^a = 0, \qquad a = 1,\ldots,N, \tag{2.15}$$

where $\overset{g}{\nabla}_\mu$ denotes the covariant differentiation in the sense of the Levi–Civita connection induced by the metric g. Equations (2.15) have the form of nonlinear d'Alambert equations; their nonlinearity is due to the dependence of g and $\overset{g}{\nabla}$ on the fields $\Phi^1,\ldots,\Phi^N$. This nonlinearity is responsible for the mutual coupling of equations in (2.15), because the "Laplace–Beltrami" operator $\Delta[\Phi] := g^{\mu\nu}\overset{g}{\nabla}_\mu\overset{g}{\nabla}_\nu$ depends on the total system $\Phi^1,\ldots,\Phi^N$. It is possible to rewrite Eqs. (2.15) in the form:

$$g^{\mu\nu}\Phi^a{}_{,\mu\nu} + \Phi^a{}_{,\nu}\left(\frac{1}{2}g^{\mu\nu}g^{\alpha\beta} - g^{\mu\alpha}g^{\nu\beta}\right)g_{\alpha\beta,\mu} = 0. \tag{2.16}$$

Equations (2.15), (2.16) are equivalent to vanishing of the mean curvature of $\Phi(M)$.

The separate terms in Eq. (2.16) are evidently non-tensorial. The total expression is generally-covariant and we can simplify its form by an appropriate choice of coordinates. The most natural coordinate condition reads

$$\left(\frac{1}{2}g^{\mu\nu}g^{\alpha\beta} - g^{\mu\alpha}g^{\mu\beta}\right)g_{\alpha\beta,\mu} = 0. \tag{2.17}$$

The transversal gauge (2.17) reduces Eqs. (2.16) to the form

(2.18) $$g^{\mu\nu}\Phi^{a}{}_{,\mu\nu} = 0, \qquad a = 1, \ldots, N.$$

Let us observe that, locally, the simplest way to fulfil (2.17) and to visualize the dynamics of $(N - n)$ genuine degrees of freedom consists in identifying coordinates x^{μ}, $\mu = 1, \ldots, n$, with an n-tuple of fields Φ, e.g.,

(2.19) $$\Phi^{\varrho} = x^{\varrho}, \qquad \varrho = 1, \ldots, n.$$

The remaining fields Φ^{r}, $r = n + 1, \ldots, N$, represent the true, physical degrees of freedom. It is always possible to choose a basis in W in such a way that

(2.20) $$\eta_{\mu r} = 0, \qquad \mu = 1, \ldots, n, \qquad r = n + 1, \ldots, N.$$

Equations (2.19) and (2.20) imply that

(2.21) $$g_{\mu\nu} = \eta_{\mu\nu} + \eta_{rs}\Phi^{r}{}_{,\mu}\Phi^{s}{}_{,\nu}.$$

The true dynamics is expressed by equations

(2.22) $$g^{\mu\nu}\Phi^{r}{}_{,\mu\nu} = 0, \qquad r = n + 1, \ldots, N,$$

whereas the first n-tuple of Eq. (2.16) becomes an identity in virtue of Eqs. (2.22) and conditions $\Phi^{\varrho} = x^{\varrho}$, $\varrho = 1, \ldots, n$. One can obtain Eqs. (2.22) from the following effective Lagrangian:

(2.23) $$L_{\text{eff}} = \sqrt{|\det[\eta_{\mu\nu} + \eta_{rs}\Phi^{r}{}_{,\mu}\Phi^{s}{}_{,\nu}]|}.$$

Using the gauge (2.19), (2.20), we easily prove that all affine injections are solutions of Eq. (2.16). By affine injections we mean the mappings $\Phi : M \to W$ whose images $\Phi(M)$ are n-dimensional affine subspaces of W. Indeed, for such mappings we have

(2.24) $$\Phi^{r} = C^{r}{}_{\mu}x^{\mu} + C^{r}, \qquad g_{\mu\nu} = \eta_{\mu\nu} + \eta_{rs}C^{r}{}_{\mu}C^{s}{}_{\nu},$$

$[C^{r}{}_{\mu}]$ denoting an arbitrary constant matrix, C^{r} being also constants. Thus, $\Phi^{r}{}_{,\mu\nu} = 0$, $g^{\mu\nu}$ is finite, and Eqs. (2.22) are evidently satisfied. Obviously, in physical applications we are interested in fields well-behaving at infinity (up to a constant, if Lagrangian depends on Φ only through its derivatives). Thus, we put $C^{r}{}_{\mu} = 0$, i.e.,

(2.25) $$\Phi^{r} = C^{r}, \qquad g_{\mu\nu} = \eta_{\mu\nu}.$$

Affine injections are classical "vacuums" of our model. They represent physical situations to be as non-excited as possible (constant, thus non-oscillating functions without isolated nodes and stationary points). Besides, solutions (2.25) minimize the energy of the effective Lagrangian (2.23) interpreted as a model assuming some absolute background metric $\eta_{\mu\nu}$ in M. Obviously, this energetic interpretation of Eqs. (2.25) as a classical ground state of Eq. (2.23) is correct if the signature of $[\eta_{\mu\nu}]$ is normal-hyperbolic. Jacobi fields, i.e., small oscillations about vacuum solutions (2.25),

(2.26) $$\Phi^{r} = C^{r} + \phi^{r},$$

satisfy the usual, i.e., linear, d'Alambert equations

(2.27) $$\eta^{\mu\nu}\phi^{r}{}_{,\mu\nu} = 0, \qquad r = n + 1, \ldots, N.$$

Thus, they are ruled by the quadratic background Lagrangian

(2.28) $$\tfrac{1}{2}\eta_{rs}\eta^{\mu\nu}\phi^{r}{}_{,\mu}\phi^{s}{}_{,\nu}\sqrt{|\det[\eta_{\mu\nu}]|}.$$

Linearized system (2.27) is an $(N - n)$-tuple of mutually independent equations; the coupling between different Φ^r is an essentially nonlinear effect.

The square-root-determinant structure of Eq. (2.23) resembles the Born–Infeld electrodynamics. In some sense one can interpret Eq. (2.23) as a scalar version of the Born–Infeld theory. To demonstrate this, let us put $n = 4$, $N = 5$, $[\eta_{\mu\nu}] = \mathrm{diag}(1, -1, -1, -1)$, $\eta_{55} = \eta > 0$, i.e.,

$$L_{\mathrm{eff}} = \sqrt{|\det[\eta_{\mu\nu} + \eta\Phi_{,\mu}, \Phi_{,\nu}]|}. \tag{2.29}$$

One can show that stationary spherically-symmetric solutions are given by

$$\psi(r) = \pm\frac{\sqrt{C}}{\sqrt{\eta}} \int_0^r \frac{dx}{\sqrt{C + x^4}}, \tag{2.30}$$

where $C > 0$ is an integration constant. Expression (2.30) is identical with the formula for the electrostatic potential of point charges in Born–Infeld theory. In particular, ψ is asymptotically proportional to $1/r$ at spatial infinity ($r \to \infty$), and at the origin $r = 0$ ψ is finite, but non-differentiable.

Let us observe that if M is the one-dimensional time manifold, and (W, η) is the four-dimensional Minkowskian space-time, then, using appropriate coordinates in W and denoting $d\Phi^i/dt$ by v^i, we can rewrite Eqs. (2.23) in the form

$$L_{\mathrm{eff}} = \sqrt{1 - v^2} = \sqrt{1 - \delta_{ij}v^i v^j}. \tag{2.23'}$$

Apart from the mass-multiplier, this is the three-dimensional representation of the relativistic material point Lagrangian, written in the natural units, when $c = 1$. Its characteristic saturation property when $v \to 1$ was just one of primary motivations for the Born–Infeld model.

It seems to follow from the above remarks that the most essential geometric feature of the Born–Infeld type nonlinearity consists in a very peculiar link between general covariance in the argument space and internal geometry in the value-space.

Coordinate conditions (2.19) are reasonable only locally, in bounded domains of M. Indeed, in general the manifold M need not admit global coordinates. But even if M is diffeomorphic with $\mathbb{R}^n$, the global gauge (2.19) is meaningless if all the fields Φ^a, $a = 1, \ldots, N$, thus, also Φ^ϱ, $\varrho = 1, \ldots, n$, are to be interpretable as genuine physical fields propagating in space-time M and carrying energy, momentum and angular momentum. Obviously, from this point of view the linearly increasing behaviour of Φ^ϱ at infinity is unacceptable. The global gauge (2.19) would be equivalent to assuming from the very beginning that the n-tuple Φ^ϱ, $\varrho = 1, \ldots, n$ is essentially non-physical and that the true degrees of freedom are represented by cross-sections of an affine fibration $\pi : W \to W/H$, H being an $(N - n)$-dimensional linear subspace of W.

If all members of the multiplet $(\ldots, \Phi^a, \ldots)$ are to be dynamically interpretable as true fields on M, then one should use the general transversal gauge (2.17) together with appropriate asymptotic conditions for Φ^a at spatial infinity. When dealing with fields Φ vanishing, or, at least, bounded at infinity, we cannot separate n gauge parameters from $(N - n)$ physical degrees of freedom so simply as in Eq. (2.19); instead, any field Φ^a, $a = 1, \ldots, N$ involves both of them mixed in a rather complicated, non-algebraic way.

When discussing the scalar Born–Infeld model (2.29), we considered time-independent isotropic solutions for the gauge-free variable ψ, after identifying the remaining fields of the multiplet with spatio-temporal coordinates (including the time variable). In certain problems, however, it may be more convenient, or even necessary, to use another sense of stationarity, including, e.g., harmonic oscillations. The general Ansatz for such stationary fields will be

$$\Phi(x^0, x^i) = \Phi(t, x^i) = \exp(\Omega t)\psi(x^i), \tag{2.31}$$

where the linear mapping $\Omega \in L(W)$ is an element of the Lie algebra $so(W, \eta)$ of the η-orthogonal group $SO(W, \eta)$, i.e.,

$$\eta(\Omega u, v) + \eta(u, \Omega v) = 0 \tag{2.32}$$

for any $u, w \in W$, or, analytically,

$$\eta_{bc}\Omega^c{}_a + \eta_{ca}\Omega^c{}_b = 0.$$

In formula (2.31) we apply the usual relativistic conventions, thus, $x^0 = t$ is the "time" variable and x^i are "spatial" coordinates. Expressions of the form (2.31) comprise, in particular, the usual complex-valued stationary fields $e^{i\omega t}\psi(x^j)$ represented in terms of real-valued fields with doubled dimension. The factor $\exp(\Omega t)$ in Eq. (2.31) is η-orthogonal, thus, physically interpretable quantities built of Φ will be time-independent. Obviously, the coordinate gauge conditions $\Phi^\mu = x^\mu$ may be combined with the Ansatz (2.31) applied to the remaining $(N - n)$-tuple ($(N - 4)$-tuple in the physical case) of fields Φ^r; thus, roughly speaking, Ω will be an $(N - n) \times (N - n)$ matrix skew-symmetric in the sense of an $(N - n)$-dimensional part of η. General covariance implies that the "time" variable is always somehow involved in the total multiplet Φ^a, $a = 1, \ldots, N$. Therefore, if we subject all the fields Φ^a, $a = 1, \ldots, N$ to physical conditions of vanishing at spatial infinity, and, consequently, exclude the coordinate-type gauges (2.19), then it is impossible to use the trivial stationarity condition corresponding to $\Omega = 0$ in Eq. (2.31).

3. Natural models of internal geometry

Let us turn to the problem of the status of isotopic geometry (W, η). Formally, in the above treatment, the structure (W, η) is logically independent of the space-time M. The differential structure of M and geometry of (W, η) are unified into one framework in a completely artificial way. Obviously, it is a tempting idea to derive them both from some common principle, however, it is difficult to postulate a priori a convincing scheme. Let us quote two extreme possibilities: (i) M is a fundamental entity, and W is implied by M, or at least, suited to M in a natural way; (ii) (W, η) is a primary entity, and physical situations are represented by n-dimensional surfaces in W. In (i) the general covariance is something very fundamental and expresses the fact that there are no absolute objects in M and that every quantity explicitly present in Lagrangian or field equations has the status of degrees of freedom and is subject to the variational procedure. In (ii), on the other hand, M is merely a parametrization of surfaces in W, and the principle of general covariance simply expresses the fact that the particular choice of parametrization does not affect the physical content of equations. Obviously, there is also a whole spectrum of possibilities placed between two extrema (i), (ii).

If W is finite-dimensional, as it usually is in realistic models, then, without going into philosophical details of its origin, we can simply put $W = \mathbb{R}^N$ or $W = C^N$. The arbitrariness of isotopic structure is then reduced to the arbitrariness of N and the signature of η, when the latter is a real symmetric or a complex Hermitian scalar product. A neutral choice is $N = 2p$ for a sufficiently large natural number p, and sign $\eta = (p(+), p(-))$. To avoid a non-motivated choice of N, we can assume $n = \infty$, i.e., admit potentially denumerably infinite multiplets (in typical situations only a few components being noticeably excited).

There are certain geometric hints concerning the choice of candidates for internal structures (W, η). Namely, there exist linear spaces which, due to certain details of their structure, are endowed with natural bilinear forms, e.g., metric structures. We shall now quote a few examples.

(i) Let U be an arbitrary linear space and U^* its dual. We take the self-dual space $W = U \times U^*$. There are two natural non-degenerate scalar products on W, namely, the skew-symmetric (symplectic) bilinear from Γ and the symmetric form η, given by:

(3.1)
$$\begin{aligned} \Gamma((x_1, p_1), (x_2, p_2)) &= \langle p_1, x_2\rangle - \langle p_2, x_1\rangle, \\ \eta((x_1, p_2), (x_2, p_2)) &= \langle p_1, x_2\rangle + \langle p_2, x_1\rangle. \end{aligned}$$

The symplectic structure (W, Γ) is used in mechanics; U is then interpreted as the configuration space of a system, W as its phase space, and the elements of U^* are canonical moments. Poisson bracket of functions on W is given by

$$\{f, g\} = \Gamma^{ab}\frac{\partial f}{\partial w^a}\frac{\partial g}{\partial w^b},$$

w^a being linear coordinates on W, Γ_{ab} — components of Γ with respect to w^a, and $\Gamma^{ac}\Gamma_{cb} = \delta^a{}_b$.

If U is a real p-dimensional space, then η is a pseudo-Euclidean scalar product of signature $(p(+), p(-))$.

Let $\Phi = (Q, P) : M \to W = U \times U^*$ be a W-valued scalar field on M, thus, Q, P are scalar fields with values respectively in U and U^*. Introducing a pair of mutually dual bases $(\ldots, e_A, \ldots)$, $(\ldots, e^A, \ldots)$ in U and U^*, we can represent $\Phi = (Q, P)$ with the help of $2n$ real-valued functions Q^A, P_A on M, where $Q = Q^A e_A$, $P = P_A e^A$. The metric $g[\Phi] = \Phi^*\eta$ is then represented as follows:

(3.2)
$$g_{\mu\nu} = Q^A{}_{,\mu}P_{A,\nu} + Q^A{}_{,\nu}P_{A,\mu}.$$

It is clear that the group $GL(U)$ is naturally imbedded in $O(W, \eta) = O(U \times U^*, \eta)$. This imbedding is given by

(3.3)
$$GL(U) \ni L \mapsto L \times \widetilde{L},$$

where $\widetilde{L} \in GL(U^*)$ denotes the mapping contragradient to $L \in GL(U)$; $\widetilde{L} := L^{*-1} = L^{-1*}$. Explicitly:

(3.3')
$$(L \times \widetilde{L})(q, p) = (Lq, p \circ L^{-1}).$$

It is obvious that such transformations belong to $O(U \times U^*, \eta)$, thus, in particular, the metric tensor $g[Q, P]$ and Lagrangian $L = \sqrt{|g[Q, P]|}$ are invariant under $GL(U)$ acting through the above prescription. If U is a model space of M, e.g., $U = \mathbb{R}^n$, one obtains the scheme invariant under $GL(n, \mathbb{R})$, the structural group of FM — the principal bundle of linear frames over M.

(ii) Again let U be an auxiliary linear space and $W := L(U) \simeq U \otimes U^*$ — the algebra of endomorphisms of U. Another natural possibility is $sl(U) \subset L(U)$ — Lie algebra of trace-less endomorphisms; obviously, $L(U) = sl(U) \oplus \mathbb{R}Id_U$. There is a natural family of symmetric scalar products on W:

$$\eta(A, B) = \langle A \mid B\rangle_{\lambda,\mu} = \lambda \operatorname{tr}(AB) + \mu \operatorname{tr} A \operatorname{tr} B, \tag{3.4}$$

λ, μ being free parameters. If this scalar product is to be non-singular, then there is essentially only one free parameter μ, because one cannot put $\lambda = 0$ without violating the nonsingularity. Thus, we can normalize Eq. (2.4) in such a way that $\lambda = 1$. If we restrict ourselves to $sl(U)$, then the only surviving term is $\operatorname{tr}(AB)$. Scalar products of this type are closely related to the Killing metric of $L(U)$ as a Lie algebra of $GL(U)$. Killing form is given by

$$(A \mid B) = \operatorname{tr}(ad_A ad_B), \tag{3.5}$$

where $ad_A : W \to W$ acts as follows: $ad_A X = [A, X] = AX - XA$. One can easily show that

$$(A|B) = 2p \operatorname{tr}\left(\left(A - \frac{1}{p}\operatorname{tr} A Id_U\right)\left(B - \frac{1}{p}\operatorname{tr} B Id_U\right)\right) = 2p \operatorname{tr}(AB) - 2 \operatorname{tr} A \operatorname{tr} B, \tag{3.5'}$$

where $p = \dim U$. Thus, Killing product is the special case of Eq. (3.4) with $\lambda = 2p$, $\mu = -2$. It is degenerate, and its one-dimensional singularity consists of all dilatations, $\mathbb{R}Id_U$.

No doubt, the main term in Eq. (3.4) is $\operatorname{tr}(AB)$. If U is real, then the signature of $\operatorname{tr}(AB)$ is $(\frac{1}{2}p(p-1)-, \frac{1}{2}p(p+1)+)$; the minus signs corresponding to compact dimensions in $L(U)$, i.e., infinitesimal rotations, and the plus signs corresponding to non-compact dimensions, i.e., infinitesimal deformations.

The metric tensor $g[\Phi] = \Phi^* \cdot \eta$ induced by Φ from $W = L(U)$ has the form

$$g_{\mu\nu} = \lambda(\operatorname{tr} \Phi_{,\mu}\Phi_{,\nu}) + \mu \operatorname{tr} \Phi_{,\mu} \operatorname{tr} \Phi_{,\nu} = \lambda \Phi^A{}_{B,\mu}\Phi^B{}_{A,\nu} + \mu \Phi^A{}_{A,\mu}\Phi^B{}_{B,\nu}. \tag{3.6}$$

Just as in (i), the group $GL(U)$ is canonically mapped into $O(W, \eta) = O(L(U), \eta)$ and acts through the adjoint representation,

$$GL(U) \ni L \mapsto Ad_L \in GL(L(U)), \tag{3.7}$$

where

$$Ad_L A = LAL^{-1}.$$

This representation is not faithful; its kernel consists of all dilatations λId_U, $\lambda \in \mathbb{R}/\{0\}$. It is clear that the metric η is invariant under $\{Ad_L : L \in GL(U)\}$. Thus, the spatio-temporal metric $g[\Phi]$ and Lagrangian $L = \sqrt{|g[\Phi]|}$ is invariant under $GL(U)$ acting through the above prescription. If U is a model space of M, e.g., $U = \mathbb{R}^n$, we again obtain the amorphous scheme invariant under $GL(n, \mathbb{R})$, the structural group of FM, [3, 4, 5, 16, 17, 18, 19, 20].

(iii) More generally, if W is a semisimple Lie algebra (semisimple commutator subalgebra of some $L(U)$), there is a natural isotopic metric η, namely, the Killing form,

$$\eta(X, Y) = \operatorname{tr}(ad_X ad_Y), \qquad ad_X Z := [X, Z]. \tag{3.8}$$

(iv) Let U be a complex linear space, U^* its dual, and $\overline{U}$ — the linear space of antilinear functionals on U. As denoted, elements of $\overline{U}^*$ are complex conjugates of linear functionals, i.e., elements of U^*. By analogy with example (i) we define the internal space as $V := U \times \overline{U}^*$. This space is endowed with two natural scalar products, $\eta : V \times V \to \mathbb{C}$,

$i\phi : V \times V \to \mathbb{C}$, namely,

$$\begin{aligned} \eta(w_1, w_2) &= \eta((x_1, p_1), (x_2, p_2)) = \overline{p_1(x_2)} + p_2(x_1), \\ \phi(w_1, w_2) &= \phi((x_1, p_1), (x_2, p_2)) = \overline{p_1(x_2)} - p_2(x_1). \end{aligned} \tag{3.9}$$

Obviously, the forms η, $i\phi$ are sesquilinears, i.e., antilinear in the first argument and linear in the second one. They are Hermitian,

$$\eta(w_1, w_2) = \overline{\eta(w_2, w_1)}, i\varphi(w_1, w_2) = \overline{i\varphi(w_2, w_1)},$$

and their signature is neutral, $\operatorname{sign}\eta = \operatorname{sign} i\varphi = (p(+), p(-))$, where, obviously, $p = \dim U$.

The Hermitian metric $g[\Phi] = \Phi^*\eta$ induced by $\Phi = (Q, P) : M \to U \times \overline{U}^*$ in the manifold M has the form

$$g_{\mu\nu} = \overline{P}_{A,\mu}\overline{Q}^A_{\ ,\nu} + P_{A,\nu}Q^A_{\ ,\mu}. \tag{3.10}$$

These objects are used in spinor theory. Namely, the Weyl spinors in four-dimensional space-time are analytically represented by scalar fields taking their values in a two-dimensional complex linear space U. That is usually considered as a non-scalar transformation rule of spinors under spatio-temporal Lorentz transformations, or, more rigorously, under the covering group $SL(2, \mathbb{C})$ is, as a matter of fact, a result of coupling between the Weyl field and the gravitational co-tetrad. Besides of U-valued spinors, one considers also $\overline{U}^*$-valued anti-Weyl fields; the latter may be interpreted as spatial reflections of the previous ones. Unifying them in a single object, we obtain V-valued Dirac bispinor fields. The sesquilinear form η is related to the Dirac's γ^0; it is necessary for the construction of the mass term in Dirac Lagrangian. Raising the index of $i\phi$ with the help of η, one obtains the γ^5-operator. The whole Clifford-algebraic structure is also an intrinsic element of the geometry of $U \times \overline{U}^*$.

(v) Let U again be a two-dimensional complex linear space of Weyl spinors. Its complex-conjugate space will be denoted by $\overline{U}$. As usual in the case of finite dimension, $\overline{U}$ may be canonically identified with the space of antilinear functions on U^*. Now, let us consider the space of twice contravariant Hermitian tensors on U,

$$W := \operatorname{herm} \overline{U} \otimes U \subset \overline{U} \otimes U. \tag{3.11}$$

It is canonically isomorphic with its own transpose

$$W^T := \operatorname{herm} U \otimes \overline{U} \subset U \otimes \overline{U}. \tag{3.11$'$}$$

Obviously, W, W^T are real four-dimensional spaces. We can construct also analogous spaces of Hermitian covariant tensors,

$$\begin{aligned} \widetilde{W} &:= \operatorname{herm} U^* \otimes \overline{U}^* \subset U^* \otimes \widetilde{U}^*, \\ \widetilde{W}^T &:= \operatorname{herm} \overline{U}^* \otimes U^* \subset \overline{U}^* \otimes U^*. \end{aligned} \tag{3.11$''$}$$

It is clear that the duals of W and W^T are canonically isomorphic with any of the linear spaces $\widetilde{W}$, $\widetilde{W}^T$. Linear space W is endowed with the natural Minkowskian-conformal structure. Indeed, let us fix an arbitrary basis $\{e_a, a = 1, 2\}$ in U. For any tensor $z = t^{\overline{a}b} e_{\overline{a}} \otimes e_b$ we define the quantity

$$Q[t] := \det[t^{\overline{a}b}]. \tag{3.12}$$

The peculiarity of dimension two is that the assignment $t \mapsto Q[t]$ is a quadratic form on $W = \operatorname{herm} \overline{U} \otimes U$. Polarizing it we obtain some bilinear form, i.e., scalar product $\eta \in W^* \otimes W^* \simeq \widetilde{W} \otimes \widetilde{W}$ on W. Its signature is normal-hyperbolic, thus (W, η) is a four-dimensional Minkowskian space. The quantities Q, η are unique modulo the normalization constant, because the change of basis $(e_a,\ a = 1, 2)$ results in multiplying them by a positive factor. Thus, Minkowskian-conformal structure is intrinsically built into the space $W = \operatorname{herm} \overline{U} \otimes U$. Another way of constructing η is based on fixing some symplectic form $\varepsilon \in U^* \wedge U^*$. It is unique modulo a complex multiplicative factor, because $\dim U = 2$. The form ε gives rise to Minkowskian metric η on W, namely

$$\eta_{AB} = \eta_{\bar{a}b\bar{c}d} = \overline{\varepsilon}_{\overline{ac}}\varepsilon_{bd}. \tag{3.13}$$

Its contravariant inverse, i.e., the dual metric η on $W^* \otimes W^* \simeq \widetilde{W} \otimes \widetilde{W}$ is given by

$$\eta^{AB} = \eta^{\bar{a}b\bar{c}d} = \varepsilon^{ac}\overline{\varepsilon}^{\overline{bd}}. \tag{3.14}$$

It is clear from this prescription that η is unique up to a positive factor equal to the squared modulus of the complex factor at ε.

If M is a four-dimensional manifold and the two-component complex Weyl fields $\phi : M \to U$ are assumed to be the most fundamental physical fields, then the normal-hyperbolic signature and conformal-Minkowskian geometry in tangent spaces of M become intrinsic, because the model space of M may be identified with $W = \operatorname{herm} \overline{U} \otimes U$.

There are also interesting examples of nonlinear internal spaces W with intrinsic metric structures.

(i) Let U be a linear space and $W \subset U \otimes U$ denote the manifold of nonsingular symmetric and twice contravariant tensors in U. The manifold W carries an almost canonical metrical structure. The corresponding arc element is given by

$$ds_g^2 = \eta_{ABCD}\, dg^{AC} \otimes dg^{BD}, \tag{3.15}$$

where

$$\eta_{ABCD}(g) = \lambda g_{AB} g_{CD} + \mu g_{AC} g_{BD}, \tag{3.15'}$$

λ, μ being constant parameters. The term $g_{AB}g_{CD}$ must be taken with a non-vanishing coefficient (we may put it equal one by convention), because otherwise η_{ABCD} would be singular. It decides about the structure of η_{ABCD}; the next term is a secondary one. Quite similarly we can use the space of nonsingular, symmetric, and twice covariant tensors, $W \subset U^* \otimes U^*$. Then, obviously,

$$ds_g^2 = \eta^{ABCD}(g)\, dg_{AC} \otimes dg_{BD}, \tag{3.16}$$

where

$$\eta^{ABCD} = \lambda g^{AB} g^{CD} + \mu g^{AC} g^{BD}. \tag{3.16'}$$

Let us observe that, although the manifold W is an open subset of a linear space, the above metrics are not flat. They have nontrivial curvature tensors and are not translationally invariant in $U \otimes U$ or $U^* \otimes U^*$.

The spatio-temporal metric tensor $g[\Phi]$ induced by $\Phi : M \to W$ has the form:

$$g[\Phi]_{\mu\nu}(x) = \eta_{ABCD}(\Phi(x))\frac{\partial\Phi^{AC}}{\partial x^{\mu}}\frac{\partial\Phi^{BD}}{\partial x^{\nu}} = (\lambda\Phi_{AB}(x)\Phi_{CD}(x) + \mu\Phi_{AC}(x)\Phi_{BD}(x))\frac{\partial\Phi^{AC}}{\partial x^{\mu}}\frac{\partial\Phi^{BD}}{\partial x^{\nu}}, \tag{3.17}$$

and, similarly, for covariantly-valued fields:

$$g[\Phi]_{\mu\nu}(x) = \eta^{ABCD}(\Phi(x))\frac{\partial\Phi_{AC}}{\partial x^{\mu}}\frac{\partial\Phi_{BD}}{\partial x^{\nu}} = (\lambda\Phi^{AB}(x)\Phi^{CD}(x) + \mu\Phi^{AC}(x)\Phi^{BD}(x))\frac{\partial\Phi_{AC}}{\partial x^{\mu}}\frac{\partial\Phi_{BD}}{\partial x^{\nu}}, \tag{3.18}$$

matrices $[\Phi^{AB}]$, $[\Phi_{AB}]$ being mutually reciprocal. Obviously, similar structures may be introduced for non-symmetric tensor-valued fields; however, they are more complicated, because their arbitrariness is stronger than that of the choice of λ, μ. If U is complex, then it is natural to define W as the space of Hermitan tensors in U. There exist obvious Hermitian counterparts of Eqs. (3.16)–(3.18); compare also (2.8′).

The above scheme is particularly natural, when U is a model space of M, e.g., $U = \mathbb{R}^n$.

The linear group $GL(U)$ acts in a natural way on the manifold W, namely,

$$L \in GL(U) : U \otimes U \ni g \mapsto L_* g \in U \otimes U,$$

where, analytically,

$$(L_* g)^{AB} = L^A_C L^B_D g^{CD}. \tag{3.19}$$

Similarly, when we deal with covariant tensors, then

$$L \in GL(U) : U^* \otimes U^* \ni g \mapsto L_* g \in U^* \otimes U^*,$$

where

$$(L_* g)_{AB} = g_{CD} L^{-1C}_{A} L^{-1D}_{B}. \tag{3.20}$$

Transformation group $\{L_* : L \in GL(U)\}$ preserves the metric tensor η on W, thus, it is a subgroup of the isometry group $\mathcal{E}(W, \eta)$ of the pseudo-Riemannian manifold (W, η).

As usual for generally-covariant models using multiplets of scalars, the metric (3.18) is quadratic in derivatives, and the Lagrangian $L[\Phi] = \sqrt{|g[\Phi]|}$ is homogeneous of degree n in derivatives. There are also, however, some new features following from the non-Euclidean character of η. Namely, the functional assignment $\Phi \mapsto g[\Phi]$ between the field Φ and the corresponding metric tensor $g[\Phi]$ is homogeneous of degree zero (it was quadratic when η was pseudo-Euclidean). Similarly, the functional dependence of the Lagrangian $L = \sqrt{|g[\Phi]|}$ on the field Φ is also homogeneous of degree zero (it was homogeneous of degree n when η was flat, i.e., pseudo Euclidean).

An interesting scheme is obtained when we consider scalar multiplets with values in $U \times U^* \otimes U^*$. Analytically, they are represented by the arrays (Φ^A, Φ_{AB}). Combining the structures (2.5), (3.18), we obtain Lagrangians of the form

$$L = \sqrt{|\det[g[\Phi^A, \Phi_{AB}]]|}, \tag{3.21}$$

where

$$(3.18') \quad g[\Phi^A, \Phi_{AB}] = a\Phi_{AB}\Phi^A{}_{,\mu}\Phi^B{}_{,\nu} + b\Phi^{CE}\Phi^{DF}\Phi_{CD,\mu}\Phi_{EF,\nu} + c\Phi^{CD}\Phi^{EF}\Phi_{CD,\mu}\Phi_{EF,\nu},$$

a, b, c being constants.

This means that the manifold $W = U \times U^* \otimes U^*$ is endowed with a curved, pseudo-Riemannian geometry wth the arc element:

$$(3.22) \quad ds^2_{(u,g)} = ag_{AB}du^A \otimes du^B + bg^{CE}g^{DF}dg_{CD} \otimes dg_{EF} + cg^{CD}g^{EF}dg_{CD} \otimes dg_{EF}.$$

(ii) Let us assume that the internal manifold W is identical with some Lie group G. To simplify notation we shall consider G as a linear group, e.g., $GL^+(U)$ or a subgroup of $GL^+(U)$; U denoting a finite-dimensional linear space.

One can distinguish a few natural groups of internal transformations in $W = G$, namely, left regular translations $X \to AX$, right regular translations $X \mapsto XA^{-1}$, two-sided regular translations $X \mapsto AXB^{-1}$, and inner automorphisms $X \mapsto AXA^{-1}$; A, B being arbitrary elements of G. Obviously, all these groups are subgroups of the group of double translations, $X \mapsto AXB^{-1}$. Left and right regular translations provide faithful realizations of the group G. If $G = GL^+(U)$, then, of course, the two-sided translations provide a non-faithful realization of $GL^+(U) \times GL^+(U)$; its kernel consists of elements $(\lambda Id_U, \lambda Id_U)$, $\lambda \in \mathbb{R}^+$. Similarly, the group of inner automorphisms provides a non-faithful realization of $GL^+(U)$, and its kernel consists of dilatations λId_U, $\lambda \in \mathbb{R}^+$.

The above groups act on G-valued fields as follows:

$$(3.23) \quad \begin{aligned} &\Phi \mapsto L\Phi, && (L\Phi)(x) := L\Phi(x),\\ &\Phi \mapsto \Phi L^{-1}, && (\Phi L^{-1})(x) := \Phi(x)L^{-1},\\ &\Phi \mapsto L\Phi K^{-1}, && (L\Phi K^{-1})(x) := L\Phi(x)K^{-1},\\ &\Phi \mapsto L\Phi L^{-1}, && (L\Phi L^{-1})(x) := L\Phi(x)L^{-1}. \end{aligned}$$

If, as assumed, $G \subset GL^+(U) \subset L(U)$, the field Φ takes its values in the linear space $L(U)$, thus, it may be invariantly differentiated in the sense of $L(U)$-valued differential forms, $d\Phi_x \in L(T_xM, L(U))$. Let us now define some auxiliary objects built of the field Φ and its differential $d\Phi$, namely, differential one-forms Ω, $\widehat{\Omega}$ on M taking values in $g = T_{Id_U}G \subset L(U)$ and acting on tangent vectors $u \in T_xM$ according to the prescription

$$(3.24) \quad \langle \Omega(x), u\rangle := \langle d\Phi_x, u\rangle \Phi(x)^{-1}, \qquad \langle \widehat{\Omega}(x), u\rangle := \Phi(x)^{-1}\langle d\Phi_x, u\rangle.$$

Their components with respect to local coordinates x^μ are given by

$$(3.24') \quad \Omega(x)_\mu = \frac{\partial \Phi}{\partial x^\mu}\Phi(x)^{-1}, \qquad \widehat{\Omega}(x)_\mu = \Phi(x)^{-1}\frac{\partial \Phi}{\partial x^\mu}.$$

Obviously, all multiplications in (3.24), $(3.24)_1$ are meant in the $L(U)$-sense.

REMARK. For simplicity, and having in view typical applications, we have assumed that $G \subset GL^+(U)$. Nevertheless, the above constructions are essentially valid for any Lie group G. The g-valued differential one-forms Ω, $\widehat{\Omega}$ on M are then defined as follows:

for any $x \in M$ and any $u \in T_x M$, we have:

$$(3.25)\qquad \begin{aligned} \langle \Omega(x), u \rangle &= (TR_{\Phi^{-1}(x)})(T\Phi(u)),\\ \langle \widehat{\Omega}(x), u \rangle &= (TL_{\Phi^{-1}(x)})(T\Phi(u)), \end{aligned}$$

where L_g, R_g denote, respectively, the left and right regular translations, $L_g(x) = gx$, $R_g(x) = xg$, and $T\Phi : TM \to TG$, $TL_g : TG \to TG$, $TR_g : TG \to TG$ are tangent mappings.

Differential one-forms Ω, $\widehat{\Omega}$ have the following transformation properties under left and right regular translations in the internal space G:

$$(3.26)\qquad \begin{aligned} \Phi &\mapsto L\Phi : \Omega_\mu \mapsto L\Omega_\mu L^{-1}, \quad \widehat{\Omega}_\mu \mapsto \widehat{\Omega}_\mu,\\ \Phi &\mapsto \Phi L : \Omega_\mu \mapsto \Omega_\mu, \quad \widehat{\Omega}_\mu \mapsto L^{-1}\widehat{\Omega}_\mu L. \end{aligned}$$

Thus, being Lie-algebraic objects, they are either Ad_G-covariant, or invariant, depending on, which kind of regular translations is applied. These transformation properties are helpful when we aim at constructing Lagrangians with appropriately postulated symmetry properties under the above internal groups. If we had at disposal a fixed metric G on M, then, on analogy of Eq. (2.14), we would be inclined to postulate Lagrangians like

$$(3.27)\qquad L = \frac{1}{2} G^{\mu\nu}\,\mathrm{tr}(\Omega_\mu \Omega_\nu)\sqrt{|G|} = \frac{1}{2} G^{\mu\nu}\,\mathrm{tr}(\widehat{\Omega}_\mu \widehat{\Omega}_\nu)\sqrt{|G|}.$$

The simplest Lagrangians built of $\Phi : M \to G$ alone, without using extrinsic elements like G, have the previously introduced form

$$(3.28)\qquad L = \sqrt{|g[\Phi]|},$$

where $g[\Phi]$ is an appropriately constructed spatio-temporal metric tensor. The prescription for $\Phi \mapsto g[\Phi]$ depends on the assumed symmetry properties.

If L is to be invariant under Eq. $(3.23)_1$, i.e., left regular translations, then we must put

$$(3.29)\qquad g_{\mu\nu} = \widehat{\Omega}^a{}_\mu \widehat{\Omega}^b{}_\nu N_{ab},$$

where $N \in g^* \otimes g^*$ is some metric tensor on g and $\widehat{\Omega}^c{}_\mu$, N_{ab} are components of $\widehat{\Omega}_\mu$, N with respect to some fixed basis in g, thus $N_{ab} = N_{ba}$ and $\det[N_{ab}] \neq 0$. If $g = L[U]$, i.e., $G = GL^+(U)$, then

$$(3.30)\qquad g_{\mu\nu} = \widehat{\Omega}^A{}_{B\mu} \widehat{\Omega}^C{}_{D\nu} N_A{}^B{}_C{}^D.$$

It is clear that Eq. (3.29) may be written as

$$(3.31)\qquad g[\Phi; N, l] = \Phi^* \eta[N, l],$$

where $\eta[N, l]$ denotes the left-invariant metric tensor on the manifold G, obtained from the algebraic metric $N \in g^* \otimes g^*$ with the help of left regular translations; thus

$$(3.32)\qquad \eta[N, l]_w(X, Y) := N(TL_w^{-1}(X), TL_w^{-1}(Y))$$

for any vectors $X, Y \in T_w G$.

If we assume that Lagrangian is to be invariant under right regular translations $(3.23)_2$, then

$$(3.33)\qquad g_{\mu\nu} = \Omega^a{}_\mu \Omega^b{}_\nu N_{ab},$$

with the same meaning of N as previously. This expression may be rewritten as

$$g[\Phi; N, r] = \Phi^* \eta[N, r], \tag{3.34}$$

where $\eta[N, r]$ denotes the extension of $N \in g^* \otimes g^*$ onto the manifold G through the right regular translations,

$$\eta[N, r]_w(X, Y) = N(TR_w^{-1}(X), TR_w^{-1}(Y)), \tag{3.35}$$

where X, Y are arbitrary vectors in $T_w M$.

If $G = GL^+(U)$, i.e., $g = L(U)$, then

$$g_{\mu\nu} = \Omega^A{}_{B\mu} \Omega^C{}_{D\nu} N_A{}^B{}_C{}^D. \tag{3.36}$$

If Lagrangian is to be invariant under $(3.23)_3$ with L running over the whole of $GL^+(U)$, and K restricted to the orthogonal subgroup $SO(U, \varkappa)$, $\varkappa \in U^* \otimes U^*$ denoting some fixed metric tensor in U, then

$$g_{\mu\nu} = \alpha \varkappa_{AC} \widehat{\Omega}^A{}_{B\mu} \widehat{\Omega}^C{}_{D\nu} \varkappa^{BD} + \beta \operatorname{tr}(\widehat{\Omega}_\mu \widehat{\Omega}_\nu) + \gamma \operatorname{tr} \widehat{\Omega}_\mu \operatorname{tr} \widehat{\Omega}_\nu, \tag{3.37}$$

α, β, γ being constants.

If Lagrangian is to be invariant under $(3.23)_3$ with L restricted to $SO(U, \varkappa)$ and K running over the whole $GL^+(U)$, then

$$g_{\mu\nu} = \alpha \varkappa_{AC} \Omega^A_{B\mu} \Omega^C_{D\nu} \varkappa^{BD} + \beta \operatorname{tr}(\Omega_\mu \Omega_\nu) + \gamma \operatorname{tr} \Omega_\mu \operatorname{tr} \Omega_\nu. \tag{3.38}$$

If Lagrangian is to be invariant under $(3.23)_3$ with L, K running over the whole $GL^+(U)$, then

$$g_{\mu\nu} = \beta \operatorname{tr}(\widehat{\Omega}_\mu \widehat{\Omega}_\nu) + \gamma \operatorname{tr} \widehat{\Omega}_\mu \operatorname{tr} \widehat{\Omega}_\nu = \beta \operatorname{tr}(\Omega_\mu \Omega_\nu) + \gamma \operatorname{tr} \Omega_\mu \operatorname{tr} \Omega_\nu. \tag{3.39}$$

If Φ takes values in a subgroup $G \subset GL^+(U)$ and Lagrangian is to be invariant under left and right regular translations $(3.23)_3$ with L, K running over the group G, then

$$g_{\mu\nu} = \widehat{\Omega}^a{}_\mu \widehat{\Omega}^b{}_\nu N_{ab} = \Omega^a{}_\mu \Omega^b{}_\nu N_{ab}, \tag{3.40}$$

where $N \in g^* \otimes g^*$ is some metric tensor on g, invariant under the adjoint group $Ad_G : g \to g$. This means that

$$g[\Phi, N] = \Phi^* \eta[N], \tag{3.41}$$

where the metric tensor $\eta[N]$ on G arises from N by extending it through the left or right regular translations. The assumed invariance of N under Ad_G implies that its extensions through the left and right regular translations give the same result $\eta[N]$, and the resulting pseudo-Riemannian structure is simultaneously left- and right-invariant. Thus, in particular, when G is semisimple, N is proportional to the Killing form on g.

Geometric meaning of quantities Ω_μ, $\widehat{\Omega}_\mu$ becomes more lucid, when we consider the special case of mechanics, $n = 1$, and the manifold M is interpreted as the time axis. Then Ω, $\widehat{\Omega}$ are non-holonomic velocities, i.e., so-called quasi-velocities, corresponding to the action of G on itself through the left and right regular translations. For example, when $G = SO(3, \mathbb{R})$, we are dealing with the mechanics of the rigid body, the matrix elements of Ω are components of the angular velocity with respect to the laboratory-fixed frame, and the matrix elements of $\widehat{\Omega}$ are projections of the angular velocity vector onto co-moving, i.e., body-fixed orthogonal axes. If $G = GL^+(3, \mathbb{R})$, we obtain the mechanics of the so-called affinely-rigid body [18].

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BRIEF NOTES

Convection effects in an inclined channel with highly permeable layers

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IN THE PRESENT investigation a coupled flow of a fluid between two inclined rigid walls with a highly permeable layer on the inner sides, is considered. The flow is governed by Navier–Stokes equations in the free fluid region, while in porous layers Brinkman equation is taken to govern the flow. A set of modified boundary conditions, discussed by KIM and RUSSEL [1], is applied at the fluid-porous interface, and the velocity, pressure, temperature distribution, the mass flow rate and its fractional increase are obtained and discussed.

1. Introduction

GERSHUNI [2] was first to discuss the stability of the conduction regime of natural convection in an inclined slot. In recent years the study of convection in an inclined layer bounded by solid walls heated uniformly from below has attracted considerable attention [3–5], as well as the study of convection in an inclined porous layer [6–9]. Convection in a fluid-saturated porous layer uniformly heated from below is of considerable geophysical interest. In general, convective flow problems involving porous media have many important applications in various disciplines of engineering and have intrinsic importance in many industrial problems. RUDRAIAH *et al.* [10] and RAMAKRISHNA *et al.* [11] studied convection in an inclined channel bounded by permeable material. They studied the coupled flow, taking Darcy's filter velocity inside the porous material and matching this to outer pure fluid flow by BEAVERS and JOSEPH [12] slip boundary conditions. In fact, the majority of existing studies on convection in porous media are based on the Darcy flow model. Darcy's law, however, is found to be inadequate for the formulation of fluid flow and heat transfer problems in porous media when there is a solid boundary. Therefore, it is necessary to incorporate the boundary and inertia terms into the momentum equation.

The model considered in this paper is based on the Brinkman equations which were developed to treat dense particle suspensions. The results of this paper might be applied to problems of water motion in geohydrology.

2. Formulation of the problem

The fluid is contained between two parallel, flat, rigid walls with a highly porous layer of thickness a on both inner sides. The walls are separated by a distance h and inclined at an angle θ to the horizontal direction. The temperature difference between the rigid walls is δt. A Cartesian coordinate system is taken as shown in Fig. 1. The flow is due to an imbalance between pressure and boundary forces when the Grashof number, Gr, is different from zero; however, at low Gr, this motion is described as a base flow in which the velocity is only in the axial direction and is a function of y and θ only. The heat transfer is assumed to occur by conduction only, therefore, the corresponding temperature is linear in y.

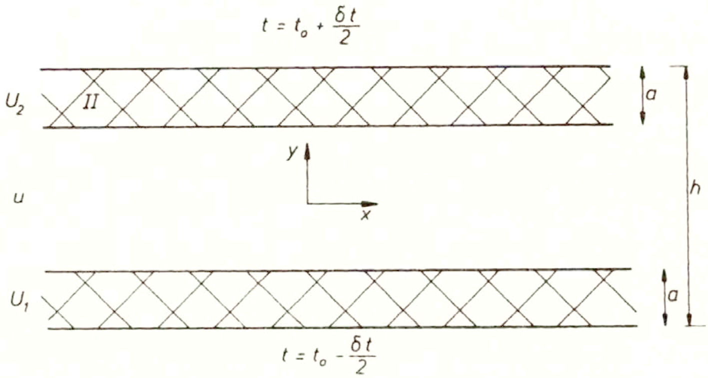

Fig. 1. Schematic diagram.

Using the following non-dimensional quantities:

$$u^* = \frac{u}{\nu/h}, \quad U_i^* = \frac{U_i}{\nu/h}, \quad x^* = \frac{x}{h}, \quad y^* = \frac{y}{h},$$

$$t^* = \frac{t}{\delta t}, \quad t_0^* = \frac{t_0}{\delta t}, \quad p^* = \frac{p}{\varrho_0 g h}, \quad K^* = \frac{K}{h^2},$$

$$a^* = \frac{a}{h}, \quad \text{and} \quad \frac{1}{2} - a^* = d,$$

the governing equations for the free and porous region flow (after dropping asterisks) are given in the following forms:

for free fluid region ($-d < y < d$):

$$\varrho = \varrho_0[1 - \beta(t - t_0)\delta t], \tag{2.1}$$

$$\frac{d^2u}{dy^2} - \eta\left(\frac{\partial p}{\partial x} + \sin\theta\right) + \mathrm{Gr}(t - t_0)\sin\theta = 0, \tag{2.2}$$

$$\frac{\partial p}{\partial y} + \left[1 - \frac{\mathrm{Gr}}{\eta}(t - t_0)\right]\cos\theta = 0, \tag{2.3}$$

$$\frac{d^2t}{dy^2} = 0, \tag{2.4}$$

and for porous regions — I($-\frac{1}{2} < y < -d$) and II($d < y < \frac{1}{2}$):

$$\frac{d^2U_i}{dy^2} - \phi^{-1}K^{-1}U_i - \phi^{-1}\eta\left(\frac{\partial p}{\partial x} + \sin\theta\right) + \phi^{-1}\,\mathrm{Gr}(t - t_0)\sin\theta = 0, \quad i = 1, 2,$$

under the assumption of the same pressure and temperature for the flow in the free fluid region.

Boundary conditions:

$$
\text{(2.6)}\qquad
\begin{aligned}
&\text{at } y=-d, \quad u=U_1 \quad\text{and}\quad \frac{\partial u}{\partial y}=\phi\frac{\partial U_1}{\partial y},\\
&\text{at } y=d, \quad u=U_2 \quad\text{and}\quad \frac{\partial u}{\partial y}=\phi\frac{\partial U_2}{\partial y},\\
&\text{at } y=-\frac{1}{2}, \quad U_1=0, \quad t=\left(t_0-\frac{1}{2}\right),\\
&\text{at } y=\frac{1}{2}, \quad U_2=0, \quad t=\left(t_0+\frac{1}{2}\right),\\
&\text{and at } \quad x=0, \quad y=0, \quad p(x,y)=0,
\end{aligned}
$$

where

$$
\mathrm{Gr}=\eta\beta\delta t, \qquad \eta=\frac{gh^3}{\nu^2}, \qquad \nu=\frac{\mu}{\varrho_0} \quad\text{and}\quad \phi=\frac{\overline{\mu}}{\mu}.
$$

Here u, U_i $(i=1,2)$ are the velocity components in the free fluid and the porous region, respectively, t is the temperature, p is the pressure, μ is the viscosity of the fluid, $\overline{\mu}$ is the effective viscosity of the fluid in porous medium, ν is the kinematic viscosity, K is the permeability of the porous medium, t_0 is the ambient temperature, ϱ is the density, ϱ_0 is the density at $t=t_0$, and β is the volume expansion coefficient.

3. Solutions

On solving equations (2.1)–(2.5), under the boundary conditions given in Eqs. (2.6), we obtain

$$
\text{(3.1)}\qquad t-t_0=-y,
$$

$$
\text{(3.2)}\qquad p=xp_0-\left(y+\frac{\mathrm{Gr}}{2\eta}y^2\right)\cos\theta,
$$

$$
\text{(3.3)}\qquad u=\frac{\mathrm{Gr}}{6}\sin\theta y^3-\frac{p}{2}y^2+Ay+B,
$$

and

$$
\text{(3.4)}\qquad U_i=A_i\exp(my)+B_i\exp(-my)-K(\mathrm{Gr}\sin\theta y-p), \qquad i=1,2,
$$

where p_0 is the pressure at $x=1$, $y=0$,

$$
m=(K\phi)^{-1/2} \quad\text{and}\quad p=-\eta(p_0+\sin\theta).
$$

The constants of integration A, B, A_i, B_i $(i=1,2)$ are given in Appendix.

4. Particular case

When $K\to 0$, we obtain

$$
\text{(4.1)}\qquad u=\left(\frac{\mathrm{Gr}}{6}\sin\theta y^3-\frac{\mathrm{Gr}}{6}\sin\theta d^2 y\right)+\frac{p}{2}(d^2-y^2),
$$

which is in agreement with the formula given by RUTH [5], when $d=1/2$ and $P=0$.

5. Mass flow rate

(i) The mass flow rate through the channel $(-1/2 < y < 1/2)$ with permeable layers on both inner sides is given by

$$(5.1)\quad M = \varrho_0[(A_1 + B_2)d_3 - (A_2 + B_1)d_4 + d_5] + \frac{\varrho_0 \,\mathrm{Gr}}{\eta}[(A_1 - B_2)d_1 - (A_2 - B_1)d_2 + d_6].$$

(ii) The mass flow rate through the free fluid channel $(-d < y < d)$ with permeable walls is given by

$$(5.2)\quad M_1 = \varrho_0\left(-\frac{pd^3}{3} + 2Bd\right) + \frac{\varrho_0 \,\mathrm{Gr}}{\eta}\left(\frac{\mathrm{Gr}}{15}\sin\theta d^5 + \frac{2A}{3}d^3\right).$$

(iii) The mass flow rate through the channel $(-d < y < d)$ with rigid walls is given by

$$(5.3)\quad M_2 = \varrho_0\left(\frac{2}{3}pd^3\right) - \frac{\varrho_0 \,\mathrm{Gr}}{\eta}\left(\frac{2}{45}Gr\sin\theta d^5\right),$$

where d_1, d_2, d_3, d_4, d_5 and d_6 are given in the Appendix.

The relative increase in the mass flow rate through the inclined channel with permeable walls over the one with rigid walls is given by

$$(5.4)\quad F = \frac{M_1 - M_2}{M_2},$$
$$= \left[-pd^2 + 2B + \frac{\mathrm{Gr}}{3\eta}\left(\frac{\mathrm{Gr}}{3}\sin\theta d^4 + 2Ad^2\right)\right] \Big/ \frac{2}{3}\left[pd^2 - \frac{\mathrm{Gr}^2}{15\eta}\sin\theta d^4\right].$$

6. Discussion

The effect of Brinkman flow with effective medium considerations in the porous layers, have been studied on the flow in the free fluid region of an inclined channel. The velocity distribution is numerically evaluated for different values of p, K and a, and the results are drawn in Fig. 2. The effect of the porous layers fixed to the inner sides of the bounding rigid walls is clearly seen, since in this case the fluid slips (depending upon the permeability and thickness of the porous layer) at the interface of fluid-saturated porous layer, unlike the case of rigid walls where the fluid clings and the velocity becomes zero. It is found that the flow in the channel increases by increasing permeability K and P; however, the flow decreases at increasing width of the porous layer, since when the width of the porous layer increases, the free fluid region becomes narrower. There is a backflow above the middle of the channel due to the momentum diffusion in the direction opposite to the flow. In fact, the adverse pressure gradient surpasses the action of the viscosity forces in this region. Due to this, an analogy can be seen in velocity profiles of this study and the other flows, e.g. when the walls of the channel are moving in the opposite directions with the same or different speeds.

The relative increase in mass flow rate is calculated (Table 1) in the free region channel over the corresponding values for a channel having rigid bounding walls. It is found that this mass flow rate grows at increasing permeability K of the porous layer. The same is true when the thickness of the porous layer increases.

Table 1. Relative increase in mass flow rate for $Gr = 50$, $\theta = \frac{\pi}{6}$, $\eta = 2$ and $\phi^{-1} = 0.8$.

$P \to$	0		1		2	
K	$a = 0.1$	$a = 0.2$	$a = 0.1$	$a = 0.2$	$a = 0.1$	$a = 0.2$
0.5	1.16623273	3.80000616	1.25356964	4.42321191	1.37833666	5.75865282
0.7	1.16783844	3.81825761	1.25527419	4.44329063	1.38018240	5.78264712
0.9	1.16873269	3.82848021	1.25622345	4.45452842	1.38121024	5.79606030
2.0	1.17045856	3.84832773	1.25805540	4.47632992	1.38319374	5.82204891
5.0	1.17130795	3.85815341	1.25895696	4.48711458	1.38416983	5.83488852

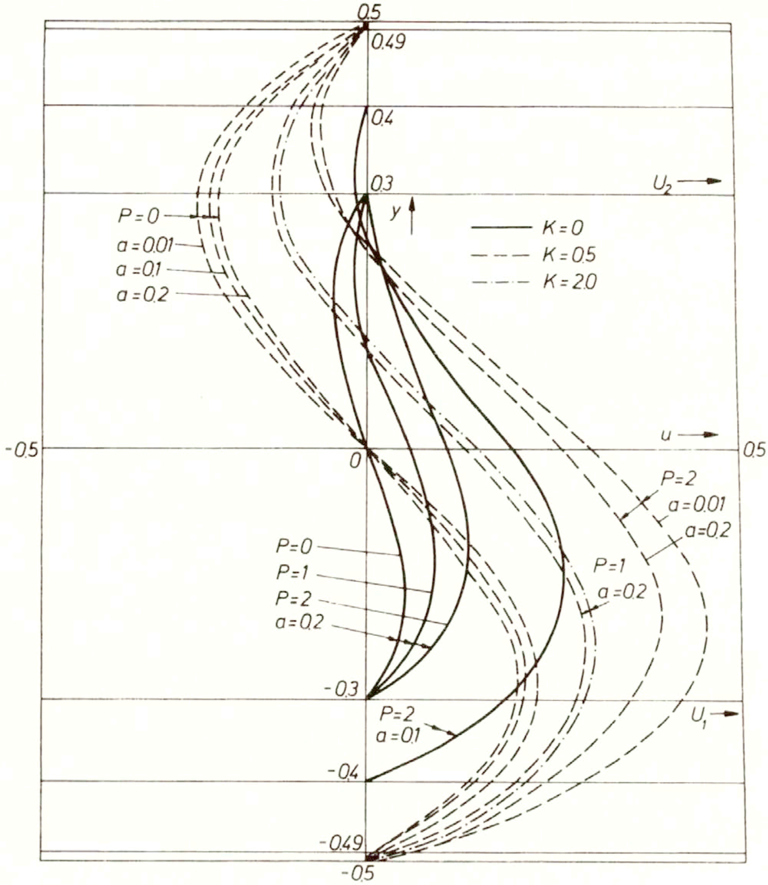

Fig. 2. Velocity profiles for Gr = 50, $\theta = \pi/6$, $\eta = 2$ and $\phi^{-1} = 0.8$.

This physical configuration may be used in many engineering devices for measurenents in the laboratory experiments, lubrication problems and to analyze the problems of vater motion in geohydrology.

Appendix

$$G = \mathrm{Gr}\sin\theta,$$

$$A = \frac{G}{6}\left(\frac{3Km - c_2 md\cosh c_1 + c_3\sinh c_1}{md\cosh c_1 - \phi^{-1}\sinh c_1}\right),$$

$$B = P\left(\frac{d^2}{2} - \frac{d\phi^{-1}}{m}\tanh c_1 + K - K\,\mathrm{sech}\, c_1\right),$$

$$A_1 = -c_5 A + c_4 B + c_{11},$$

$$B_1 = -c_{13} A + c_{12} B + c_{19},$$

$$
\begin{aligned}
A_2 &= c_{13}A + c_{12}B + c_{18},\\
B_2 &= c_5 A + c_4 B + c_{10},\\
c_1 &= m\left(d - \frac{1}{2}\right),\\
c_2 &= d^2 + 6K,\\
c_3 &= 3\left(d^2\phi^{-1} + 2K\right),\\
c_4 &= \frac{1}{2}\exp(md),\\
c_5 &= c_4\left(d - \frac{\phi^{-1}}{m}\right),\\
c_6 &= c_4\frac{G}{2}\left(\frac{d^3}{3} - \frac{d^2\phi^{-1}}{m}\right),\\
c_7 &= -c_4 P\left(\frac{d^2}{2} - \frac{d\phi^{-1}}{m}\right),\\
c_8 &= c_4 KG\left(d - \frac{1}{m}\right),\\
c_9 &= -KPc_4,\\
c_{10} &= c_6 + c_7 + c_8 + c_9,\\
c_{11} &= (c_7 + c_9) - (c_6 + c_8),\\
c_{12} &= \frac{1}{4c_4},\\
c_{13} &= c_{12}\left(d + \frac{\phi^{-1}}{m}\right),\\
c_{14} &= \frac{c_{12}G}{2}\left(\frac{d^3}{3} + \frac{d^2\phi^{-1}}{m}\right),\\
c_{15} &= -c_{12}P\left(\frac{d^2}{2} + \frac{d\phi^{-1}}{m}\right),\\
c_{16} &= c_{12}KG\left(d + \frac{1}{m}\right),\\
c_{17} &= -KPc_{12},\\
c_{18} &= c_{14} + c_{15} + c_{16} + c_{17},\\
c_{19} &= (c_{15} + c_{17}) - (c_{14} + c_{16}),\\
d_1 &= \left[\frac{\exp(-m/2)}{m^2} + \frac{\exp(-m/2)}{2m} - \frac{d\exp(-md)}{m} - \frac{\exp(-md)}{m^2}\right],\\
d_2 &= \left[\frac{\exp(m/2)}{m^2} - \frac{\exp(m/2)}{2m} + \frac{d\exp(md)}{m} - \frac{\exp(md)}{m^2}\right],\\
d_3 &= \frac{1}{m}[\exp(-md) - \exp(-m/2)],
\end{aligned}
$$

$$d_4 = \frac{1}{m}[\exp(md) - \exp(m/2)],$$

$$d_5 = KP(1 - 2d) - \frac{pd^3}{3} + 2Bd,$$

$$d_6 = \frac{KG}{3}\left(2d^3 - \frac{1}{4}\right) + \frac{Gd^5}{15} + \frac{2Ad^3}{3}.$$

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to be published quarterly starting in 1994

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