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MACROSCOPIC CONTINUUM THEORY OF FERROELECTRIC LIQUID CRYSTAL OF SMECTIC C^* TYPE

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Abstract. The paper presents the formulation of the theory of ferroelectric liquid crystals (smecticC*). In this formulation the formalism of bundle space has been applied. The used bundle space has a form of a Cartesian product of the three-dimensional Euclidean space E^3 (the base space) and a differentiable manifold M_s with a conical structure. The paper contains: the formulation of the kinematics of the continuous micropolar model, the local form of the conservation laws (the equations of the evolution of the medium), and the constitutive relations for chiral smectic C^*.

The kinematic in the fibre space is described by two vector fields: the director $\underline{d}$ and the normal to the smectic layers - $\underline{k}$. The vector $\underline{d}$ rotates around the vector $\underline{k}$- the axis of instantaneous rotation. From the integral principle of the energy conservation law, the equations of evolution of the mass, momentum and angular momentum densities are derived.
The set of the constitutive arguments is established and the integrity base or the set of invariants of the group of material symmetry is obtained. The constitutive relations for stresses and ininternal force are presented.

INTRODUCTION

It was R.B. Meyer [1], who for the first time, predicted in 1974 the existence of ferroelectric liquid crystals, and after a short period this fact was verified experimentally. Since then the interest in ferroelectric liquid crystals has been growing rapidly. It is due to the very effective possibility of their applications in display devices with a great speed of images registration and as a very fast memory in electronics. It is performed by means of a rapid changes of helical structure caused by changes of external electric field.
R.B. Meyer, as discovering the ferroelectric state in liquid crystals, made use of the earlier considerations by F.C. Frank concerning the

possibilities of realization of homogeneous states of different kinds of deformations of director field. It was established by him that the chiral smectic C^* is the medium in which ferroelectricity phenomenon should occur. In such a liquid crystal the elongated molecules are ordered in layers and all are tilted at the same angle ϑ against the normal $\underline{k}$ to the smectic layer.This structure causes that the medium may have a low monoclinic symmetry, which is described by four symmetry elements: two-fold axis of rotation laying in the plane of smectic layer, the mirror plane normal to the smectic layer, the center of inversion and the identity transformation. But this low symmetry is yet too high to induce ferroelectricity or spontaneous polarization, because due to the existing plane of mirror symmetry the permanent polar moments of molecules can be compensated in the liquid crystal la yer. The introduction of the chiral molecules into the medium breaks the mirror symmetry and allows for the non compensated spontaneous polarization to exist. Thus, according to R.B. Meyer, the sufficient conditions for ferroelectricity of smectic C^* to exist are the molecules to be polar and chiral. Such a medium has only two-fold axis of ro tation. It is monoclinic, spheroidal symmetry or symmetry of S capital letter.Moreover, the introduction of chiral molecules into the smectic C^* may produce the helical structure. This structure may be used for ra pid switching of the existing bistable state in devices for registration of fast processes.

After the discovery of the liquid crystal ferroelectricity many papers have appeared. PIKIN and INDENBOM [2] were the first to formulate the background of the macroscopic theory of ferroelectricity of liquid cry stals.It was based on the symmetry consideration.Some other successful macroscopic approaches taking into account the thermodynamics of the continuous medium and the principle of the material continuum may be found in [3-11]. Except of those publications, many other papers may be mentioned, devoted to the some special, practical problems, which occur in design and applications of display devices. In such cases some asymptotic approximations of general theories are used. Some examples of such approaches are presented in [12-15].

The aim of this paper is to present the formulation of a macrosco-

pic, microstructural theory capable to describe the physical phenomena which take place in ferroelectric liquid crystals. The theory will be formulated in the terms of the notions of the differentiable manifold It means that the concept of a bundle space will be applied, what is important for the generality of formulations.

In the paper the following subjects will be presented:

- the kinematics of the ferroelectric medium,
- the conservation laws and evolution equations,
- the constitutive relations.

KINEMATICS OF FERROELECTRIC MEDIUM

The smectic C^* liquid crystals have a layered structure with the director $\underline{d}$ tilted at the angle ϑ against the normal $\underline{k}$ to the smectic layer Moreover, in ferroelectric liquid crystals the vector of spontaneous polarization $\underline{P}$ is defined as follows:

$$\underline{p} = \alpha(\underline{k}\times\underline{d}) \tag{2.1}$$

It means that the vector $\underline{p}$ is perpendicular to the director $\underline{d}$ and lies in the smectic layer,and α is the intensity of polarization. Moreover, the vectors $\underline{k}$, $\underline{d}$ are kinematically constrained as follows:

$$\underline{k}\cdot\underline{d} = \cos\vartheta\ , \quad \underline{d}\cdot\underline{d} = 1\ , \quad \underline{k}\cdot\underline{k} = 1 \tag{2.2}$$

The kinematics of the medium is described by three vector fields: velocity field $\underline{v}$ and two director fields $\underline{d}$, $\underline{k}$. Its motion is defined as follows;

$$(\kappa\times\gamma)_t : \beta \Rightarrow E^3\times M \tag{2.3}$$

which means the existence of one-parameter smooth transformations κ,γ of the defined differentiable manifold into the bundle space being the Cartesian product of the three-dimensional Euclidean space $E^3$and fi-

bre space M_s - the tangent space to the material manifold. M_s is defined as follows:

$$M_s = \left(\underline{d},\underline{k} \in \mathbf{V} : \underline{k}\cdot\underline{d} = \cos\vartheta \ , \ \underline{k}\cdot\underline{k} = 1, \ \underline{d}\cdot\underline{d} = 1 \right) \qquad (2.4)$$

where **V** is a vector (translational) space. The microstructural processes are defined on the tangent space. Because three vectors are defined, which are constrained by three relations (2.4), the processes are described by three degrees of freedom. These degrees of freedom treated as generalized coordinates of a Lagrangian microstructural system may be chosen in different ways. The most effective are those coordinates, which satisfy the constraint relations identically. To establish them, the structure of admissible deformations in the considered medium sholld be determined. The deformation of the layered smectic C^* may be divided into two steps:

- bending of the smectic layer (Fig.1b),
- rotation of the director $\underline{d}$ around the vector $\underline{k}$ with preservation of the tilt angle ϑ (Fig.1c).

These steps are presented in Fig.1a,b,c. We assume, for simplicity, that in indeformed state all directors $\underline{k}$ are parallel to the axis z and directors $\underline{d}$ are tilted on angle ϑ (see Fig.1a). In the first step (bending of the layer) the vector $\underline{k}$ rotates. This rotation is described by two angles μ,ϕ. Hence, after deformation we have

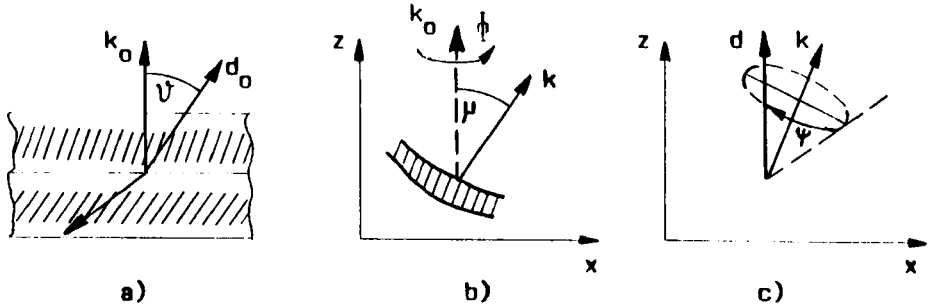

FIGURE 1 A.B.C

$$\underline{k} = \underline{\underline{Q}}_1(\mu,\phi)\underline{k}_0 \quad , \qquad \underline{k}_0 = (0,0,1) \quad , \tag{2.5}$$

where

$$\underline{\underline{Q}}_1(\mu,\phi) = \underline{\underline{c}}_3(\phi)\underline{\underline{c}}_1(\mu) \tag{2.6}$$

To preserve the constraint $\underline{k}\cdot\underline{d} = \cos\vartheta$, the director $\underline{d}$ should rotate in the same way as the vector $\underline{k}$.

$$\underline{d}' = \underline{\underline{Q}}_1\underline{d}_0 \quad , \qquad \underline{d}_0 = (0.-\sin\vartheta,\cos\vartheta) \tag{2.7}$$

and moreover the vector of polarization

$$\underline{p}' = \underline{\underline{Q}}_1\underline{p}_0 \quad , \qquad \underline{p} = a(\underline{k}_0\times\underline{d}_0) \tag{2.8}$$

In the second step the tilted director $\underline{d}$ rotates around the instantaneous axis of rotation $\underline{k}$ on the angle ψ. According to the known formula we get for the second step of deformation (rotation)

$$\underline{d} = \underline{d}'\cos\psi + (1-\cos\psi)(\underline{k}\cdot\underline{d}')\underline{k} + \sin\psi(\underline{k}\times\underline{d}') \tag{2.9}$$

$$\underline{p} = \underline{p}'\cos\psi + (1-\cos\psi)(\underline{k}\cdot\underline{p}')\underline{k} + \sin\psi(\underline{k}\times\underline{d}') \tag{2.10}$$

In case of helical structure

$$\psi(x,y,z) = \psi(x,y)\sin(qz) \tag{2.11}$$

After deformation the components of vectors $\underline{d}$, $\underline{k}$ can be expressed by angles ϕ,μ,ψ as follows:

$$d_1 = \sin\phi\cos\psi\cos\mu\sin\vartheta + \sin\psi\cos\phi\sin\vartheta + \\ + \sin\phi\sin\mu\cos\vartheta \tag{2.12}$$

$$d_2 = \sin\phi \sin\psi \sin\vartheta - \cos\phi \cos\psi \cos\mu \sin\vartheta - \\ - \cos\phi \sin\mu \cos\vartheta \tag{2.13}$$

$$d_3 = \cos\vartheta \cos\mu - \cos\phi \sin\vartheta \sin\mu \tag{2.14}$$

$$k_1 = \sin\phi \sin\mu \tag{2.15}$$

$$k_2 = -\cos\phi \sin\mu \tag{2.16}$$

$$k_3 = \cos\mu \tag{2.17}$$

It can by easily verify that:

- the constraint relations in (2.4) are satisfied identically,
- the angles ϕ,μ,ψ are the Euler angles, since

$$\underline{d} = \underline{\underline{Q}}\, \underline{d}_0 \quad , \tag{2.18}$$

where

$$\underline{\underline{Q}} = \underline{\underline{c}}_3(\phi)\underline{\underline{c}}_1(\mu)\underline{\underline{c}}_3(\psi) \quad , \tag{2.19}$$

presents the opposite sequence of rotations as usual. Hence, the Euler angles ϕ,μ,ψ are generalized coordinates of Lagrangian system in fibre space M_s.

Since, in practice, many simplified kinematics are applied, we will discuss the main ones.

1. When $\mu = 0$, what means that there is no bending of the layers

$$d_1 = \sin\vartheta \sin(\phi+\psi) = \sin\vartheta \sin\alpha \tag{2.20}$$

$$d_2 = -\sin\vartheta \cos(\phi+\psi) = -\sin\vartheta \cos\alpha \tag{2.21}$$

$$d_3 = \cos\vartheta \tag{2.22}$$

In this case we have the microstructure with only one degree of free-

dom. Thus we should have only one equation describing microstructure. This equation will be obtained from the proper Lagrangian system. This way the using of Lagrangian systems for the description of the microstructural dynamics instead of equation, which comes out from angular momentum conservation law, allows us to be free from the troubles with the improper numbers of degrees of freedom.

2. When the bending of the layers is small (μ,ϕ are small) we get the following relations for $\underline{d}$, $\underline{k}$

$$d_1 = (\cos\psi \sin\vartheta)\ \phi + (\cos\vartheta)\ \phi\ \mu + \sin\psi \sin\vartheta \tag{2.23}$$

$$d_2 = -\cos\psi \sin\vartheta + (\sin\vartheta \sin\psi)\ \phi - (\cos\vartheta)\ \mu \tag{2.24}$$

$$d_3 = \cos\vartheta - (\sin\vartheta)\ \mu \tag{2.25}$$

$$k_1 = \phi\ \mu, \quad k_2 = -\mu\ , \quad k_3 = 1 \tag{2.26}$$

In this approximation the constraints are satisfied with the accuracy

$$\underline{d}\cdot\underline{d} = 1 + O(\mu),\ \underline{k}\cdot\underline{k} = 1 + \mu^2,\ \ \underline{k}\cdot\underline{d} = \cos\vartheta + O(\mu) \tag{2.27}$$

These two kinds of approximation are the most frequently used in technical applications. In further consideration we will use the d_1 as general degrees of freedom.They are single-valued functions (in local sense) of Euler angles ϕ,ψ,μ and are very convenient in general considerations.For any numerical calculations the Euler angles can be prefe red.

CONSERVATION LAWS AND EVOLUTIONARY EQUATIONS

The energy conservation law plays the central role since all other conservation laws can be derived from this one. For the considered medium it has the following form:

$$\frac{d}{dt}\int_V \left[-\frac{1}{2}\rho v_i v_i + \frac{1}{2} I \dot{d}_i \dot{d}_i + \rho e \right] dv = \int_V \left[\rho f_i v_i^2 + G_i \dot{d}_i + \rho q \right] d v +$$

$$+ \int_S \left[t_i v_i + s_i \dot{d}_i - h_i \right] ds \qquad (3.1)$$

with the left-hand side, the time derivative of the total energy density appears, consisting of the internal energy density, the kinetic energy densities in the base (Euclidean) space and in the fibre (micro structural) space M_s. The integrals appearing on the right-hand side of (3.1) correspond to the generalized power of the external body and sur face actions applied to the medium; G_i is an external generalized body force, s_i-external generalized surface force acting on microstructural (fibre) space. The term $\dot{p}_i E_i$ corresponds to the power of the external electric field.

The other conservation laws and evolutionary equations result from the energy conservation law (3.1). From the translational invariance of (3.1) under the velocity field change

$$\underline{v}' = \underline{v} + \underline{a} \quad , \qquad (3.2)$$

where $\underline{a}$ is a constant vector, the mass conservation law and momentum conservation law are derived. The local forms of them or evolution equations have the known classical form

$$\frac{d\rho}{dt} + \rho \mathrm{div}(\underline{v}) = 0 \qquad (3.3)$$

$$\rho \frac{d}{dt} v_i = \rho f_i + t_{ji,j} = 0 \qquad (3.4)$$

The angular momentum conservation law will be considered later. It results from the requirement of the energy conservation law to be invariant under rigid rotation. In the fibre space M_s the following generalized momentum conservation law is formulated

$$\int_V \left(\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{d}_i} \right) - \frac{\partial T}{\partial d_i} \right) dv = \int_V \left(G_i - g_i \right) dv + \int_S s_i \, ds \qquad (3.5)$$

where T is the density of the kinetic energy of micromotion

$$T = \frac{1}{2} I \dot{d}_i \dot{d}_i \qquad (3.6)$$

The local form of the Eq.(3.5) is following:

$$I \ddot{d}_i = G_i - g_i + s_{ji,j} \qquad (3.7)$$

The energy conservation law, after transformations and application of the Eq.(3.4),takes the form of the equation of the rate of the change of the internal energy density

$$\rho \dot{e} = t_{ji} v_{i,j} + s_{ji} \dot{d}_{i,j} + p_i \dot{E}_i +$$

$$+ (I\ddot{d}_i - G_i - s_{ji,j}) \dot{d}_i \qquad (3.8)$$

From the Eq. (3.7) it follows that

$$(I\ddot{d}_i - G_i - s_{ji,j}) \dot{d}_i = -g_i \dot{d}_i \qquad (3.9)$$

and the Eq. (3.8) takes the form

$$\rho \dot{e} = t_{ji} v_{i,j} + s_{ji} \dot{d}_{i,j} - g_i \dot{d}_i + p_i \dot{E}_i \qquad (3.10)$$

From the general condition of invariance, the rate of change of the internal energy density under rigid rotation in space $E^3 \times M_s$ should be equal to zero. Hence,

$$t_{ji} \omega_{ij} + s_{ji} \dot{d}^R_{i,j} - g_i \dot{d}^R_i + p_i \dot{E}^R_i = 0 \qquad (3.11)$$

where $\omega_{ij} = v_{[i,j]}$ and $\dot{d}_i^R$ is the velocity of rigid rotation of the director $\underline{d}$. Generally for rigid rotation

$$\dot{d}_i^R = a_{ij}d_j \,, \quad \dot{p}_i^R = a_{ij}p_j \,, \quad a_{ij} = -a_{ji} \tag{3.12}$$

The rigid rotation in micropolar medium means the stiff rotation of both continua E^3, M_s or the state without relative rotation of both continua. Hence $a_{ij} = \omega_{ij}$ and

$$[t_{ji} + d_{j,p}s_{pi} - g_j d_i + p_j E_i]\ \omega_{ij} = 0 \tag{3.13}$$

It can be easily shown that the obtained relation (3.13) is equivalent to the equation coming out from the angular momentum conservation law. But here it has a form of a constitutive constraint relating micro and macro phenomena running in both spaces, Euclidean and fibre space. Because the relation (3.13) should be satisfied for arbitrary ω_{ij}, the relation in brackets should be equal to zero. It allows to express the non symmetrical part of stress tensor t_{ij} by the microstresses s_{ij}, internal body force g_i and polarization vector p_i as follows:

$$t_{ji} - t_{ij} = p_i E_j - p_j E_i + g_j d_i - g_i d_j +$$

$$+ d_{i,p}s_{pj} - d_{j,p}s_{pi} \tag{3.14}$$

It comes out from this considerations that two different ways of formulation of a theory of microstructural media are possible:

- introduction of a momentum conservation law in fibre space; then the angular momentum conservation law plays a role of a constitutive constraint relating Cauchy stresses with microstresses s_{ij} and internal body forces g_i,
- using of the angular momentum conservation law for derivation of the equation describing combined phenomena in base and fibre space.

In the formulation of the theory of the liquid crystals the first approache was used by Ericksen-Leslie-Parodi, and the second one-by Eringen-Lee.

CONSTITUTIVE RELATIONS

Very important problem is here a proper choice of constitutive arguments. Since some arbitrariness is here possible we assume the following sets of arguments:

- for deformation: k_i, d_i, $k_{i,j}$, $d_{i,j}$,
- for rate of deformation: $\dot{k}_i$, $\dot{d}_i$, $\dot{k}_{i,j}$, $\dot{d}_{i,j}$, $v_{i,j}$.

Because the liquid crystals are, as usual,dissipative media the stresses and internal force should be divided into non dissipative and dissipative ${}_E t_{ij}$, ${}_E s_{ij}$, ${}_E g_i$; ${}_D t_{ij}$, ${}_D s_{ij}$, ${}_D g_i$. It results from general considerations that this medium should have a potential for non-dissipative stresses. It can be shown that the free energy density f is such a potential

$$f = e - \eta T \tag{4.1}$$

where η is the entropy density, T - temperature. This scalar single-valued function depends on the constitutive arguments presented above, mass density ρ and, moreover,on a set of structural tensors M_i. They model the anisotropy of the considered liquid crystalline medium. Wishing to obtain the ferroelectricity in liquid crystal or non-compensated spontaneous polarization, the material symmetry of the medium should be lowered to the monoclinic, sphenoidal one.The symmetry group contains only two elements: identity transformation and two-fold axis of rotation

$$G_m = \left(I, C^2 \right) \tag{4.2}$$

All structural tensors $\underline{\underline{M}}^i$ should be invariants of this group, what means that

$$\underline{\underline{S}}_p \underline{\underline{M}}^i \underline{\underline{S}}_p^T = \underline{\underline{M}}^i \qquad \underline{\underline{S}}_p \in G_m \tag{4.3}$$

It can be easily verified that in the considered case the set of $\underline{\underline{M}}^i$ contains five structural tensors of the following form:

$$\underline{\underline{M}}^1 = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{vmatrix} \quad \underline{\underline{M}}^2 = \begin{vmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{vmatrix} \quad \underline{\underline{M}}^3 = \begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

$$\underline{\underline{M}}^4 = \begin{vmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{vmatrix} \quad \underline{\underline{M}}^5 = \begin{vmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{vmatrix} \tag{4.4}$$

Their structure may be presented as follows:

$$M_{ij}^{pq} = \delta_{pi}\delta_{qj} \quad , \quad p,q = 1\text{-}5 \tag{4.5}$$

The function of the free energy density f has a general form

$$f = f(\rho, T;\ k_i, d_i, k_{i,j}, d_{i,j}, M_{ij}^{pq};\ k_i, d_i, k_{i,j}, d_{i,j}, v_{i,j}) \tag{4.6}$$

We should mention here that the vectors $\underline{d}$ and $\underline{k}$ are not independent since they are constrained by the relations (2.4)

$$d_i = B_{ij}k_j \quad \text{or} \quad k_i = A_{ij}d_j \tag{4.7}$$

But for the generality of considerations we will treat them as independent with a possibility to present stresses and internal force by k_i or d_i. The function f is an arbitrary single-valued function of its arguments. The restriction imposed on its form comes only from thermodynamical considerations that is from Clausius-Duhem inequality

$$\rho \frac{d\eta}{dt} - \frac{q}{T} + \frac{h_{i,i}}{T} - \frac{h_i T_i}{T^2} \geq 0 \tag{4.8}$$

where η is the entropy density, q -heat sources, $\underline{h}$ - heat flux. Taking king into account Eq.(3.8), Clausius-Duhen inequality after some transformations takes a form

$$t_{ji}v_{i,j} + s_{ji}\dot{d}_{i,j} - g_i\dot{d}_i + p_iE_i + \rho q - \frac{h_i T_{,i}}{T} -$$

$$- \rho\left(\frac{df}{dt} + \eta\frac{dT}{dt}\right) \geq 0 \qquad (4.9)$$

Omitting the heat effects ($q = 0$, $\underline{h}=0$) and due to the arbitrariness of $\dot{d}_i$, $\dot{k}_i$, $\dot{d}_{i,j}$, $\dot{k}_{i,j}$, $v_{i,j}$ the function f depends only on arguments of deformation. After further transformations and from the requirement that the Clausius-Duhem inequality should be satisfied for arbitrary arguments, a general form of constitutive equations for non-dissipative stresses t_{ij}, s_{ij} and internal body force are obtained

$$_E t_{ij} = -\rho^2 \frac{\partial f}{\partial \rho}\delta_{ij} - \rho\frac{\partial f}{\partial d_{k,j}} d_{k,i} \qquad (4.10)$$

$$_E s_{ji} = \rho\frac{\partial f}{\partial d_{i,j}} \qquad (4.11)$$

$$_E g_i = -\frac{\partial f}{\partial d_i} \qquad (4.12)$$

and moreover the following relations are valid

$$\frac{\partial f}{\partial k_{i,j}} = 0 \quad , \quad \frac{\partial f}{\partial k_i} = 0 \qquad (4.13)$$

Taking into account the relations (4.7) the above constitutive equations can be expressed also by components of director $\underline{k}$. It should be mentioned that the problem of the existence of internal body force ε_i still remains open. Here the question arises whether the directors $\underline{k}$, $\underline{d}$ are constitutive or structural arguments only.

In order to establish the exact forms of constitutive relations for $_E t_{ij}$, $_E s_{ij}$, $_E g_i$, the potential function f should depend on the invariants of the constitutive arguments and structural tensors. They are

invariants of the considered group of material symmetry

$$G = \left(I, C^2 \right) \tag{4.14}$$

In the presented level of approximation we will take into account only linear and square tensorial invariants. The set of linear invariants is following:

$$tr(\underline{\underline{M}}^{pq}\underline{\underline{D}}) \quad , \quad tr(\underline{\underline{M}}^{pq}\underline{d}\circ\underline{d}) \tag{4.15}$$

where $\underline{\underline{D}} = \nabla\underline{d}$ and $\circ$ denotes the external product of vectors $\underline{d}$. The set of square invariants is following:

$$tr(\underline{\underline{M}}^{pq}\underline{\underline{D}}\underline{\underline{D}}) \quad , \quad tr(\underline{\underline{M}}^{pq}\underline{\underline{D}}^{T}\underline{\underline{D}}) \quad , \quad tr(\underline{\underline{M}}^{pq}\underline{\underline{D}}\underline{\underline{D}}^{T}) \tag{4.16}$$

Moreover, such mixed tensorial and vectorial invariants should be taken into account

$$tr(\underline{\underline{M}}^{pq}\underline{\underline{D}}\underline{d}\underline{\underline{D}}\underline{d}) \quad , \quad tr(\underline{\underline{M}}^{pq}\underline{\underline{D}}^{T}\underline{d}\underline{\underline{D}}\underline{d}) \quad , \quad tr(\underline{\underline{M}}^{pq}\underline{\underline{D}}\underline{d}\underline{\underline{D}}^{T}\underline{d}) \tag{4.17}$$

where **tr** is the known " trace" operation. Bearing in mind the form of structural tensors (see Eq.(4.5)) the invariants are the components of constitutive tensor $\underline{\underline{D}}$ and vector $\underline{d}$.
The linear invariants of the tensor $\underline{\underline{D}}$ are following:

$$D_{11},\ D_{22},\ D_{33},\ D_{12},\ D_{21}$$

and square invariants are as follows:

$$D_{13}^2,\ D_{31}^2,\ D_{23}^2,\ D_{32}^2,\ D_{13}D_{31},\ D_{23}D_{32},\ D_{13}D_{23},\ D_{31}D_{32},$$

$$D_{31}D_{23},\ D_{31}D_{32}$$

Numbering invariants by I_k we have

$$f = f(I_1, I_2, \ldots, I_n) \tag{4.18}$$

and the constitutive equations can be presented according to the follo wing formulae:

$$t_{ji} = -\rho^2 \frac{\partial f}{\partial \rho} \delta_{ij} - \rho \left(\sum_k \frac{\partial f}{\partial I_k} \frac{\partial I_k}{\partial D_{ij}} \right) D_{ii} \tag{4.19}$$

$$s_{ij} = \rho \sum_k \frac{\partial f}{\partial I_k} \frac{\partial I_k}{\partial D_{ij}} \tag{4.20}$$

$$g_i = -\rho \sum_k \frac{\partial f}{\partial I_k} \frac{\partial I_k}{\partial d^k} \tag{4.21}$$

Because, according to the Eq.(4.19) the stress tensor t_{ij} is expressed by s_{ij} we focus the attention on determination of s_{ij} and g_i. Since the invariants are grouped into three subsets, the microstress tensor s_{ij} consists of three parts. Hence, for linear invariants

$$s^1_{ij} = \sum_{pq} \left(a_{1pq} + a_{2pq} \right) M^{pq}_{ij} \tag{4.22}$$

where

$$a_{1pq} = \frac{\partial f}{\partial \mathrm{tr}(\underline{\underline{M}}^{pq} \underline{\underline{D}})} \quad , \quad a_{2pq} = \frac{\partial f}{\partial \mathrm{tr}(\underline{\underline{M}}^{pq} \underline{\underline{D}}^T)} \tag{4.23}$$

for square invariants

$$s^2_{ij} = \sum_{pq} \left(b_{1pq} (\underline{\underline{M}}^{pq} \underline{\underline{D}} + \underline{\underline{D}} \underline{\underline{M}}^{pq})_{ij} + b_{2pq} ((\underline{\underline{M}} + \underline{\underline{M}}^T)^{pq} \underline{\underline{D}})_{ij} + \right.$$

$$\left. + b_{3pq} \underline{\underline{D}}^T (\underline{\underline{M}} + \underline{\underline{M}}^T)^{pq}_{ij} \right) \tag{4.24}$$

where

$$\underline{\underline{b}}_{1pq} = \frac{\partial f}{\partial \mathrm{tr}(M^{pq} D^2)} \quad , \qquad b_{2pq} = \frac{\partial f}{\partial \mathrm{tr}(M^{pq} D^T D)} \quad ,$$

$$b_{3pq} = \frac{\partial f}{\partial \mathrm{tr}(\underline{\underline{M}}^{pq}\underline{\underline{DD}}^{T})} \tag{4.25}$$

The stresses s^{3}_{ij} and internal forces g_i are calculated in similar way. Here we omit those calculations.

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