

**NOTE ON KINEMATICS, DYNAMICS, AND  
THERMODYNAMICS OF PLASTIC GLASSY MEDIA.**

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**ABSTRACT.** Unified geometric approach to describing kinematics of elastic and plastic deformations of continuous media is suggested. On the base of this approach we study mechanical deformations, viscous flow, and heat transport in glassy plastic media. As a result we derive appropriate differential equations for these phenomena in a form applicable to liquids, elastic solids, and to plastic solid materials as well.

1. INTRODUCTION.

AFM-assisted<sup>1</sup> electrostatic nanolithography (AFMEN) was suggested in [1] and [2]. It is new technique for nano-scale patterns formation on planar polymer films. By this paper we start series of papers aimed to prepare theoretical background for further numeric simulation of AFMEN process. First of all we consider kinematics (i. e. time-dependent geometry) of deformations and apply differential geometry to study it. Our main result is a method for separating elastic and plastic deformations within general nonlinear deformation tensor. Then we build this method into the standard framework of balance equations traditionally used to describe dynamics and thermodynamics of moving continuous media. Applying electrostatic field, surface phenomena, and phase transitions will be considered in separate papers.

As far as our technique is concerned, we use curvilinear coordinates from the very beginning. This looks a little bit tricky, but in this way we make transparent tensorial nature of all quantities we use. Moreover, the problem of AFMEN process simulation, which we are going to study numerically, has obvious cylindrical symmetry. So we prepare use of cylindrical coordinates in our future calculations. For reader's convenience in section 2 just below we resume some well-known facts concerning curvilinear coordinates.

2. MOVING FRAME OF CURVILINEAR COORDINATES.

Let  $x^1, x^2, x^3$  be three Cartesian coordinates of a point. Below we use both upper and lower indices, following traditions of tensorial analysis (see [3]). Curvilinear coordinates  $y^1, y^2, y^3$  of a point are usually introduced by functions

$$\begin{cases} x^1 = x^1(y^1, y^2, y^3), \\ x^2 = x^2(y^1, y^2, y^3), \\ x^3 = x^3(y^1, y^2, y^3). \end{cases} \quad (2.1)$$

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<sup>1</sup>Here AFM is abbreviation for Atomic Force Microscope.

Functions (2.1) define transition to curvilinear coordinates. Transition back to Cartesian coordinates is determined by similar three functions

$$\begin{cases} x^1 = x^1(y^1, y^2, y^3), \\ x^2 = x^2(y^1, y^2, y^3), \\ x^3 = x^3(y^1, y^2, y^3). \end{cases} \quad (2.2)$$

Maps (2.1) and (2.2) are inverse to each other. Therefore if we define their Jacobi matrices  $S$  and  $T$  by partial derivatives

$$S_j^i = \frac{\partial x^i}{\partial y^j}, \quad T_j^i = \frac{\partial y^i}{\partial x^j}, \quad (2.3)$$

they are also inverse to each other:  $T = S^{-1}$ . Matrix  $S$  is called *direct transition matrix*, while  $T$  is called *inverse transition matrix*.

Let  $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$  be constant frame of Cartesian coordinates  $x^1, x^2, x^3$ , i. e. these are three base vectors directed along three coordinate axes. Then, using functions (2.1), we can define vectorial function  $\mathbf{r} = \mathbf{r}(y^1, y^2, y^3)$ :

$$\mathbf{r} = \sum_{i=1}^3 x^i(y^1, y^2, y^3) \mathbf{e}_i. \quad (2.4)$$

This is radius-vector of a point expressed through curvilinear coordinates. Differentiating (2.4) with respect to  $y^1, y^2, y^3$ , we get three vector-functions:

$$\mathbf{E}_i = \mathbf{E}_i(y^1, y^2, y^3) = \frac{\partial \mathbf{r}}{\partial y^i}, \quad i = 1, 2, 3. \quad (2.5)$$

Vectors  $\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3$  form a frame of curvilinear coordinates  $y^1, y^2, y^3$ . This is moving frame, since vectors  $\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3$  depend on coordinates of a point to which they are attached. Transition matrices (2.3) relate moving frame  $\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3$  to constant frame  $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$  of Cartesian coordinates and vice versa:

$$\mathbf{E}_i = \sum_{q=1}^3 S_i^q \mathbf{e}_q, \quad \mathbf{e}_i = \sum_{q=1}^3 T_i^q \mathbf{E}_q.$$

Mutual scalar products of frame vectors (2.5) define fundamental tensor of our space. This is metric tensor  $\mathbf{g}$  with components:

$$g_{ij} = (\mathbf{E}_i, \mathbf{E}_j). \quad (2.6)$$

Matrix (2.6) also is known as *Gram matrix* of moving frame  $\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3$ . Inverse matrix to (2.6) define another fundamental tensor. This is *dual metric tensor*; by tradition it is denoted by the same letter  $\mathbf{g}$ , but for its components upper indices are used:  $g^{ij}$ . Being mutually inverse, metric tensors are related by formula

$$\sum_{q=1}^3 g^{iq} g_{qj} = \delta_j^i.$$

Here  $\delta_j^i$  are Kronecker symbols. They determine components of unit matrix:

$$\delta_j^i = \begin{cases} 1 & \text{for } i = j, \\ 0 & \text{for } i \neq j. \end{cases}$$

### 3. TENSOR FIELDS IN CURVILINEAR COORDINATES.

All tensor fields in curvilinear coordinates  $y^1, y^2, y^3$  are referenced to moving frame  $\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3$ . This determine some features of their differentiation. Thus, if  $\varphi = \varphi(y^1, y^2, y^3)$  is a scalar field, then applying gradient operator  $\nabla$  to it we get three components defined by partial derivatives:

$$\nabla_i \varphi = \frac{\partial \varphi}{\partial y^i}, \quad i = 1, 2, 3. \quad (3.1)$$

However, unlike (3.1), applying gradient operator to tensor field  $\mathbf{X}$  is more complicated procedure. For components of resulting tensor field  $\nabla \mathbf{X}$  we have formula

$$\begin{aligned} \nabla_m X_{j_1 \dots j_s}^{i_1 \dots i_r} &= \frac{\partial X_{j_1 \dots j_s}^{i_1 \dots i_r}}{\partial y^m} + \\ &+ \sum_{k=1}^r \sum_{a_k=1}^3 \Gamma_m^{i_k a_k} X_{j_1 \dots a_k \dots j_s}^{i_1 \dots i_r} - \sum_{k=1}^s \sum_{b_k=1}^3 \Gamma_m^{b_k j_k} X_{j_1 \dots b_k \dots j_s}^{i_1 \dots i_r}. \end{aligned} \quad (3.2)$$

Here  $\Gamma_{ij}^k$  is three-dimensional array of *connection components* or *Christoffel symbols*. They are defined by metric tensor  $\mathbf{g}$  according to the following formula:

$$\Gamma_{ij}^k = \sum_{s=1}^3 \frac{g^{ks}}{2} \left( \frac{\partial g_{is}}{\partial y^j} + \frac{\partial g_{sj}}{\partial y^i} - \frac{\partial g_{ij}}{\partial y^s} \right). \quad (3.3)$$

Formulas (3.2) and (3.3) are well-known in differential geometry (see [3]).

In addition to metric tensor (2.6) and connection components (3.3) there are also *volume tensor*  $\omega$  and *dual volume tensor* denoted by the same symbol:

$$\omega_{ijk} = \sqrt{\det \mathbf{g}} \varepsilon_{ijk}, \quad \omega^{ijk} = \frac{\varepsilon^{ijk}}{\sqrt{\det \mathbf{g}}}, \quad (3.4)$$

Here  $\varepsilon_{ijk} = \varepsilon^{ijk}$  are Levi-Civita symbols. They are defined as follows:

$$\varepsilon_{ijk} = \varepsilon^{ijk} = \begin{cases} 0 & \text{if } i = j, j = k, \text{ or } k = i; \\ 1 & \text{if } (ijk) \text{ is even transposition of } (123); \\ -1 & \text{if } (ijk) \text{ is odd transposition of } (123). \end{cases} \quad (3.5)$$

Levi-Civita symbols (3.5) do not form a tensor. However, supplying scalar factors to them, we get two tensor fields (3.4).

### 4. DEFORMATION OF CONTINUOUS MEDIUM.

Suppose that our space is filled with medium of some kind. Deformation of medium is due to the displacement of its points. Suppose that the point with

coordinates  $\tilde{y}^1, \tilde{y}^2, \tilde{y}^3$  has moved to the point with coordinates  $y^1, y^2, y^3$ . This situation is expressed by the following three functions:

$$\begin{cases} y^1 = y^1(t, \tilde{y}^1, \tilde{y}^2, \tilde{y}^3), \\ y^2 = y^2(t, \tilde{y}^1, \tilde{y}^2, \tilde{y}^3), \\ y^3 = y^3(t, \tilde{y}^1, \tilde{y}^2, \tilde{y}^3). \end{cases} \quad (4.1)$$

Argument  $t$  in (4.1) is responsible for time evolution of displacement. Time derivatives of these functions determine velocity vector components:

$$v^i = \dot{y}^i = \frac{\partial y^i}{\partial t}, \quad i = 1, 2, 3. \quad (4.2)$$

Velocity vector  $\mathbf{v}$  itself is calculated as a sum representing its expansion in moving frame at the point with coordinates  $y^1, y^2, y^3$ :

$$\mathbf{v} = \sum_{i=1}^3 v^i \mathbf{E}_i. \quad (4.3)$$

Functions (4.1) define time-dependent map from space to space. Let's denote it by  $\tau$ . Then inverse map  $\tau^{-1}$  is given by similar functions

$$\begin{cases} \tilde{y}^1 = \tilde{y}^1(t, y^1, y^2, y^3), \\ \tilde{y}^2 = \tilde{y}^2(t, y^1, y^2, y^3), \\ \tilde{y}^3 = \tilde{y}^3(t, y^1, y^2, y^3). \end{cases} \quad (4.4)$$

Quantities  $v^i$ , as defined in (4.2), are functions of coordinates  $\tilde{y}^1, \tilde{y}^2, \tilde{y}^3$  marking initial position of a point of medium. Using (4.4) we can convert them to the functions of coordinates  $y^1, y^2, y^3$  marking current actual position of that point:

$$v^i = v^i(t, y^1, y^2, y^3) = \frac{\partial y^i}{\partial t} \circ \tau^{-1}. \quad (4.5)$$

Time dependent maps (4.1) and (4.4) define two Jacobi matrices  $\tilde{S}$  and  $\tilde{T}$ :

$$\tilde{S}_j^i = \frac{\partial y^i}{\partial \tilde{y}^j}, \quad \tilde{T}_j^i = \frac{\partial \tilde{y}^i}{\partial y^j}. \quad (4.6)$$

Matrices (4.6) are inverse to each other and quite similar to that of (2.3). However, in contrast to matrices  $S$  and  $T$ , these two matrices depend on  $t$  and describe physical state of our continuous medium (more precisely, they describe the state of deformation). Matrix  $\tilde{T}$  has proper arguments  $t, y^1, y^2, y^3$ , while arguments of  $\tilde{S}$  should be corrected by inverse map (4.4), i. e.  $\tilde{S} \rightarrow \tilde{S} \circ \tau^{-1}$ .

Let's take vectors of moving frame  $\mathbf{E}_1, \mathbf{E}_2, \mathbf{E}_3$  at the point with coordinates  $y^1, y^2, y^3$  and send them to the point with coordinates  $\tilde{y}^1, \tilde{y}^2, \tilde{y}^3$  by means of map  $\tau^{-1}$ . As result we get another frame  $\tilde{\mathbf{E}}_1, \tilde{\mathbf{E}}_2, \tilde{\mathbf{E}}_3$ :

$$\tilde{\mathbf{E}}_i = \sum_{r=1}^3 \tilde{T}_i^r \mathbf{E}_s(\tilde{y}^1, \tilde{y}^2, \tilde{y}^3), \quad i = 1, 2, 3. \quad (4.7)$$

Mutual scalar products of frame vectors (4.7) form a matrix with components

$$G_{ij} = (\tilde{\mathbf{E}}_i, \tilde{\mathbf{E}}_j) = \sum_{r=1}^3 \sum_{s=1}^3 g_{rs}(\tilde{y}^1, \tilde{y}^2, \tilde{y}^3) \tilde{T}_i^r \tilde{T}_j^s. \quad (4.8)$$

Upon transforming all arguments in (4.8) to  $t, y^1, y^2, y^3$  we get tensor field  $\mathbf{G}$  with components  $G_{ij} = G_{ij}(t, y^1, y^2, y^3)$ . Tensor  $\mathbf{G}$  at the point with coordinates  $y^1, y^2, y^3$  is an exact quantitative measure of deformation of our medium at that point. For small deformations described in Cartesian coordinates we have

$$G_{ij}(t, x^1, x^2, x^3) = g_{ij} - 2u_{ij} + \dots \quad (4.9)$$

Tensor  $\mathbf{u}$  in (4.9) is standard *tensor of deformation* as defined in [4]:

$$u_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x^j} + \frac{\partial u_j}{\partial x^i} \right). \quad (4.10)$$

By dots in (4.9) we denote terms of higher order with respect to small displacements  $u^1 = \delta x^1, u^2 = \delta x^2, u^3 = \delta x^3$ . Relying upon above formulas (4.9) and (4.10), now we define deformation tensor  $\mathbf{u}$  as follows:

$$u_{ij} = \frac{g_{ij} - G_{ij}}{2}. \quad (4.11)$$

Using (4.11) instead of (4.10), we have not to restrict ourself to small displacements and can consider deformations of any magnitude in any curvilinear coordinates.

Let's calculate time derivative for deformation tensor  $\mathbf{u}$  defined by formula (4.11). Differentiating (4.8), by direct calculations we derive the following formula:

$$\dot{G}_{ij} = - \sum_{k=1}^3 \nabla_k G_{ij} v^k - \sum_{k=1}^3 G_{kj} \nabla_i v^k - \sum_{k=1}^3 G_{ik} \nabla_j v^k. \quad (4.12)$$

Now, combining formulas (4.11) and (4.12), we obtain ultimate expression for  $\dot{u}_{ij}$ :

$$\dot{u}_{ij} = \frac{\nabla_i v_j + \nabla_j v_i}{2} - \sum_{k=1}^3 (\nabla_k u_{ij} v^k + u_{kj} \nabla_i v^k + u_{ik} \nabla_j v^k). \quad (4.13)$$

Let's denote by  $v_{ij}$  first term in right hand side of (4.13):

$$v_{ij} = \frac{\nabla_i v_j + \nabla_j v_i}{2}. \quad (4.14)$$

Last three terms under summation in formula (4.13) are nonlinear with respect to deformation functions (4.1). They are usually omitted in the case of small deformations. In that case we would have  $\dot{u}_{ij} = v_{ij}$ .

## 5. DYNAMICS OF CONTINUOUS MEDIUM.

Dynamics of any continuous medium (either liquid, solid, or gaseous) is usually described in terms of three balance equations. These are equations for

- (1) mass balance;
- (2) momentum balance;
- (3) energy balance.

Mass balance is most simple among balance equations. It is written on the base of the following statement: change of mass enclosed in any fixed volume within continuous medium is determined by mass flow through its boundary:

$$\frac{\partial \rho}{\partial t} + \sum_{k=1}^3 \nabla_k (\rho v^k) = 0. \quad (5.1)$$

Sum in (5.1) is divergency  $\text{div } \mathbf{j}$ , where  $\mathbf{j} = \rho \mathbf{v}$  is density vector for mass flow. Components of velocity vector are determined by formula (4.5), while operator  $\nabla_k$  in (5.1) should be applied according to the formula (3.2).

Momentum balance equation is more complicated, though it has the structure similar to mass balance equation (5.1). Momentum balance is written as

$$\frac{\partial (\rho v^i)}{\partial t} + \sum_{k=1}^3 \nabla_k \Pi^{ik} = f^i. \quad (5.2)$$

Vector  $\mathbf{f}$  with components  $f^1, f^2, f^3$  in right hand side of (5.2) determines density of volume forces in continuous medium. Symmetric tensor  $\mathbf{\Pi}$  with components  $\Pi^{ik}$  determines density of momentum flow in continuous medium. Exact formulas for tensors  $\mathbf{f}$  and  $\mathbf{\Pi}$  depend on various properties of medium and on those phenomena we are going to consider.

Energy per unit of volume in continuous medium is a sum of two components: *kinetic energy* and inner *thermal energy* due to chaotic motion of atoms and molecules. Therefore energy balance equation is written as follows:

$$\frac{\partial}{\partial t} \left( \frac{\rho |\mathbf{v}|^2}{2} + \rho \varepsilon \right) + \sum_{k=1}^3 \nabla_k w^k = e. \quad (5.3)$$

Vector  $\mathbf{w}$  with components  $w^1, w^2, w^3$  in (5.3) determines density of energy flow. Scalar  $e$  determines energy production/dissipation per unit volume of medium. It is due to work of force  $\mathbf{f}$  in (5.2) and from other possible sources (e. g. Joule heating due to electric current in conducting medium). Potential energy is not included into left hand side of (5.3). However, work of potential forces is taken into account among other terms as a part of scalar  $e$  in right hand side of (5.3).

Deformation state of a medium is completely determined by tensor  $\mathbf{G}$  and metric tensor  $\mathbf{g}$ . From (4.12) and (5.1) one easily derives:

$$\ln \rho - \frac{\ln \det \mathbf{G} - \ln \det \mathbf{g}}{2} = \text{const}. \quad (5.4)$$

Tensor  $\mathbf{\Pi}$  in (5.2) is usually given by the following formula:

$$\Pi^{ik} = \rho v^i v^k - \sigma^{ik}. \quad (5.5)$$

Here  $\sigma^{ik}$  is *stress tensor*. Substituting (5.5) into (5.2), we get

$$\frac{\partial(\rho v^i)}{\partial t} + \sum_{k=1}^3 \nabla_k(\rho v^i v^k) = f^i + \sum_{k=1}^3 \nabla_k \sigma^{ik}. \quad (5.6)$$

Now, taking into account (5.1), from (5.6) we derive

$$\frac{\partial v^i}{\partial t} + \sum_{k=1}^3 v^k \nabla_k v^i = \frac{f^i}{\rho} + \sum_{k=1}^3 \frac{\nabla_k \sigma^{ik}}{\rho}. \quad (5.7)$$

Using (5.4), now we can calculate time derivative for the density of kinetic energy:

$$\frac{\partial}{\partial t} \left( \frac{\rho |\mathbf{v}|^2}{2} \right) + \sum_{k=1}^3 \nabla_k \left( \frac{\rho |\mathbf{v}|^2}{2} v^k \right) = \sum_{i=1}^3 v_i f^i + \sum_{i=1}^3 \sum_{k=1}^3 v_i \nabla_k \sigma^{ik}. \quad (5.8)$$

Looking at formula (5.8), we see that right hand side of this formula is completely determined by parameters  $\sigma^{ik}$  and  $f^i$  from (5.5) and (5.2).

## 6. ELASTIC SOLIDS STATE MEDIA.

Deformation state of a medium is completely determined by tensor  $\mathbf{G}$  and metric tensor  $\mathbf{g}$ . Therefore  $\varepsilon$  in (5.3) satisfies the following equality:

$$d\varepsilon = T ds - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{\sigma}^{ij}}{2\rho} dG_{ij}. \quad (6.1)$$

Here  $s$  is an entropy per unit mass of solid state medium. Note that  $\bar{\sigma}^{ij}$  in (6.1) should not coincide with  $\sigma^{ij}$  considered above. Free energy per unit mass is determined by standard formula  $f = \varepsilon - T s$ . Therefore

$$df = -s dT - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{\sigma}^{ij}}{2\rho} dG_{ij}. \quad (6.2)$$

Free energy per unit mass  $f$  is a function of temperature  $T$  and deformation state of medium:  $f = f(T, \mathbf{G})$ . From (6.2) we derive

$$\frac{\bar{\sigma}^{ij}}{2\rho} = -\frac{\partial f(T, \mathbf{G})}{\partial G_{ij}}. \quad (6.3)$$

Solid materials can exhibit different properties in different directions. We consider only those polymer materials, which are homogeneous and isotropic (i. e. uniform

in all directions). For such materials  $f(T, \mathbf{G})$  is given by formula

$$f = f(T, \lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]}), \quad (6.4)$$

where  $\lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]}$  are three scalar invariants for linear operator  $\mathbf{G}$ :

$$\lambda_{[1]} = \frac{\text{tr}(\mathbf{G})}{3}, \quad \lambda_{[2]} = \frac{\text{tr}(\mathbf{G} \cdot \mathbf{G})}{3}, \quad \lambda_{[3]} = \frac{\text{tr}(\mathbf{G} \cdot \mathbf{G} \cdot \mathbf{G})}{3}. \quad (6.5)$$

Linear operator  $\mathbf{G}$  in (6.5) is determined by its matrix  $G_j^i$ , where

$$G_j^i = \sum_{k=1}^3 g^{ik} G_{kj}. \quad (6.6)$$

Using (6.5) and (6.6), we calculate partial derivatives

$$\frac{\partial \lambda_{[1]}}{\partial G_{ij}} = \frac{g^{ij}}{3}, \quad \frac{\partial \lambda_{[2]}}{\partial G_{ij}} = \frac{2 G^{ij}}{3}, \quad \frac{\partial \lambda_{[3]}}{\partial G_{ij}} = \sum_{k=1}^3 \sum_{q=1}^3 G^{ik} g_{kq} G^{qj}. \quad (6.7)$$

Applying (6.3) and (6.7) to (6.4), we find most general formula for  $\bar{\sigma}^{ij}$ :

$$\bar{\sigma}^{ij} = f_{[1]} g^{ij} + f_{[2]} G^{ij} + \sum_{k=1}^3 \sum_{q=1}^3 f_{[3]} G^{ik} g_{kq} G^{qj}, \quad (6.8)$$

Here  $f_{[1]}, f_{[2]}, f_{[3]}$  are coefficients depending on  $T$  and on scalar invariants (6.5):

$$f_{[i]} = -\frac{2i\rho}{3} \frac{\partial f(T, \lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]})}{\partial \lambda_{[i]}}, \quad i = 1, 2, 3. \quad (6.9)$$

Formula (6.8) is exact, but very huge. Its use in numeric simulation is impossible not because of huge computations, but since function (6.4) is not properly measured experimentally for broad range of its arguments. Formulas (6.8) and (6.9) are worth for us only because they indicate the dependence

$$\bar{\sigma}^{ij} = \bar{\sigma}^{ij}(T, \mathbf{G}). \quad (6.10)$$

Traditionally linearized version of this dependence (6.10) is used for the case of small deformations when  $u_{ij}$  are much less than  $g_{ij}$ .

Now let's consider formula (6.2) again. If function (6.4) is known, entropy per unit mass can be calculated as partial derivative:

$$s = -\frac{\partial f}{\partial T}. \quad (6.11)$$

Due to (6.11) we can treat  $s$  as a function  $s = s(T, \mathbf{G})$ . Moreover,  $s$  depends on  $\mathbf{G}$  through scalar invariants (6.5) just like function  $f$  itself:

$$s = s(T, \lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]}). \quad (6.12)$$



Then for thermal energy per unit mass we get

$$\varepsilon = f + T s = \varepsilon(T, \mathbf{G}) = \varepsilon(T, \lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]}). \quad (6.13)$$

If parameters  $w^k$  and  $e$  in (5.3) are known, then, substituting (6.13) into (5.3), we get the equation for temperature function  $T = T(t, y^1, y^2, y^3)$ .

In thermodynamics specific thermal energy  $\varepsilon$  is often treated as a function of entropy. Indeed, inverting the dependence of  $s$  on  $T$  for fixed  $\lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]}$  in (6.12) and substituting  $T = T(s, \lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]})$  into (6.13), we get

$$\varepsilon = \varepsilon(s, \mathbf{G}) = \varepsilon(s, \lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]}). \quad (6.14)$$

In the absence of heat transfer and viscosity, parameters  $w^k$  and  $e$  can be derived from entropy balance equation. In this case dynamics of solid state medium is *adiabatic*. Therefore one can write the equation

$$\frac{\partial(\rho s)}{\partial t} + \sum_{k=1}^3 \nabla_k(\rho s v^k) = 0. \quad (6.15)$$

By analogy with (6.15), now we calculate the following quantity:

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \sum_{k=1}^3 \nabla_k(\rho \varepsilon v^k) = \rho \frac{\partial \varepsilon}{\partial t} + \sum_{k=1}^3 \rho v^k \nabla_k \varepsilon. \quad (6.16)$$

Applying (6.1) and (6.14) and using  $\nabla_k g_{ij} = 0$ , which is basic property of metric tensor, we get formulas for  $\partial \varepsilon / \partial t$  and  $\nabla_k \varepsilon$  in right hand side of (6.16):

$$\begin{aligned} \frac{\partial \varepsilon}{\partial t} &= T \frac{\partial s}{\partial t} - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{\sigma}^{ij} \dot{G}_{ij}}{2\rho}, \\ \nabla_k \varepsilon &= T \nabla_k s - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{\sigma}^{ij} \nabla_k G_{ij}}{2\rho}. \end{aligned} \quad (6.17)$$

Substituting (6.17) into (6.16) and taking into account (6.15) and (5.1), we get

$$\frac{\partial(\rho \varepsilon)}{\partial t} + \sum_{k=1}^3 \nabla_k(\rho \varepsilon v^k) = - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{\sigma}^{ij}}{2} \left( \dot{G}_{ij} + \sum_{k=1}^3 v^k \nabla_k G_{ij} \right). \quad (6.18)$$

Now let's substitute (4.12) into (6.18). As a result of simple calculations we find

$$\begin{aligned} \frac{\partial(\rho \varepsilon)}{\partial t} + \sum_{k=1}^3 \nabla_k(\rho \varepsilon v^k) &= \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{\sigma}^{ij}}{2} \left( \sum_{k=1}^3 \nabla_j v^k G_{ik} + \sum_{k=1}^3 \nabla_i v^k G_{kj} \right) = \\ &= \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^3 \frac{\bar{\sigma}^{ik} G_k^j + \bar{\sigma}^{ki} G_k^j}{2} \nabla_i v_j = \sum_{i=1}^3 \sum_{k=1}^3 \nabla_k v_i \left( \sum_{j=1}^3 G_j^i \bar{\sigma}^{jk} \right). \end{aligned}$$

Note that the above formula is quite similar to formula (5.8). Adding these two formulas, we obtain the following equality:

$$\begin{aligned} & \frac{\partial}{\partial t} \left( \frac{\rho |\mathbf{v}|^2}{2} + \rho \varepsilon \right) + \sum_{k=1}^3 \nabla_k \left( \frac{\rho |\mathbf{v}|^2}{2} v^k + \rho \varepsilon v^k \right) = \\ & = \sum_{i=1}^3 v_i f^i + \sum_{i=1}^3 \sum_{k=1}^3 v_i \nabla_k \sigma^{ik} + \sum_{i=1}^3 \sum_{k=1}^3 \nabla_k v_i \left( \sum_{j=1}^3 G_j^i \bar{\sigma}^{jk} \right). \end{aligned} \quad (6.19)$$

Right hand side of the equality (6.19) simplifies substantially if stress tensor  $\sigma^{ik}$  and tensor  $\bar{\sigma}^{ij}$  introduced in (6.1) are related as follows:

$$\sigma^{ik} = \sum_{j=1}^3 G_j^i \bar{\sigma}^{jk}. \quad (6.20)$$

Due to the relationship (6.20) formula (6.19) transforms to the following one:

$$\begin{aligned} & \frac{\partial}{\partial t} \left( \frac{\rho |\mathbf{v}|^2}{2} + \rho \varepsilon \right) + \sum_{k=1}^3 \nabla_k \left( \frac{\rho |\mathbf{v}|^2}{2} v^k + \rho \varepsilon v^k \right) = \\ & = \sum_{i=1}^3 v_i f^i + \sum_{i=1}^3 \sum_{k=1}^3 \nabla_k (v_i \sigma^{ik}). \end{aligned} \quad (6.21)$$

The relationship (6.20) is self consistent. Indeed, if (6.20) is fulfilled then we have the equality (6.21) with quite transparent interpretation. First two terms in (6.21) describe energy increment and energy flow due to mass transport. Two terms in right hand side of (6.21) describe energy creation due to external forces and due to stress forces in continuous medium. Comparing (6.21) and (5.3), we get

$$w^k = \frac{\rho |\mathbf{v}|^2}{2} v^k + \rho \varepsilon v^k - \sum_{i=1}^3 v_i \sigma^{ik}, \quad e = \sum_{i=1}^3 v_i f^i. \quad (6.22)$$

Due to special form of tensor  $\bar{\sigma}$  and due to (6.20) stress tensor  $\sigma$  is symmetric:  $\sigma^{ij} = \sigma^{ji}$ . Indeed, from formula (6.8) for components of stress tensor we derive

$$\begin{aligned} \sigma^{ij} &= f_{[1]} G^{ij} + \sum_{k=1}^3 \sum_{q=1}^3 f_{[2]} G^{ik} g_{kq} G^{qj} + \\ &+ \sum_{k=1}^3 \sum_{q=1}^3 \sum_{m=1}^3 \sum_{n=1}^3 f_{[3]} G^{ik} g_{kq} G^{qm} g_{mn} G^{nj}. \end{aligned} \quad (6.23)$$

Remember that coefficients  $f_{[1]}$ ,  $f_{[2]}$ ,  $f_{[3]}$  in (6.23) are determined by formula (6.9). They depend on deformation  $\mathbf{G}$  and temperature  $T$ .

## 7. HEAT TRANSFER, VISCOSITY, AND ENTROPY PRODUCTION.

Formulas for  $\Pi^{ik}$  and  $w^k$  in balance equations (5.2) and (5.3) become more complicated if we take into account viscosity and thermal conductivity of medium.

In the case when  $\nabla \mathbf{v} \neq 0$  different parts of medium immediately adjacent to each other move with different velocities. This gives rise to forces of viscous friction. These forces are described by additional term in (5.5):

$$\Pi^{ik} = \rho v^i v^k - \sigma^{ik} - \tilde{\sigma}^{ik}. \quad (7.1)$$

Here  $\tilde{\sigma}^{ik}$  are components of *viscous stress tensor*  $\tilde{\boldsymbol{\sigma}}$ . In linear approximation they are linear with respect to velocity gradients:

$$\tilde{\sigma}^{ik} = \sum_{j=1}^3 \sum_{q=1}^3 \eta^{ikjq} v_{jq}. \quad (7.2)$$

Here  $v_{jq}$  are components of symmetric tensor introduced in (4.14), while  $\eta^{ikjq}$  in (7.2) are components of *viscosity tensor*. They possess the following symmetry:

$$\eta^{ikjq} = \eta^{jqik} = \eta^{kijq} = \eta^{ikqj}. \quad (7.3)$$

Components of viscosity tensor (7.3) are kinetic coefficients. In near equilibrium deformations they are functions of temperature and deformation tensor:

$$\eta^{ikjq} = \eta^{ikjq}(T, \mathbf{G}). \quad (7.4)$$

If continuous medium is non-uniformly heated, i. e.  $\nabla T \neq 0$ , this may cause direct heat transfer without mass transport in it. This phenomenon is due to *thermal conductivity* of medium. Thermal conductivity of medium is described by additional term in formula for density of energy flow  $\mathbf{w}$ :

$$\mathbf{w}^k = \frac{\rho |\mathbf{v}|^2}{2} v^k + \rho \varepsilon v^k - \sum_{i=1}^3 v_i \sigma^{ik} - \sum_{i=1}^3 v_i \tilde{\sigma}^{ik} - \sum_{i=1}^3 \nabla_i T \varkappa^{ik}. \quad (7.5)$$

As compared to (6.22), in (7.5) we have two extra terms. First is due to viscous stress tensor  $\tilde{\boldsymbol{\sigma}}$ , second term contains components of *heat conductivity tensor*  $\varkappa^{ik}$ . Like  $\eta^{ikjq}$  in (7.4), components of heat conductivity tensor are kinetic coefficients, they depend on temperature  $T$  and deformation  $\mathbf{G}$ :

$$\varkappa^{ik} = \varkappa^{ik}(T, \mathbf{G}). \quad (7.6)$$

Heat conductivity tensor (7.6) is symmetric, i. e.  $\varkappa^{ik} = \varkappa^{ki}$ .

Let's recalculate entropy balance equation (6.15), taking into account additional terms in (7.1) and (7.5). Instead of (6.21) now we have

$$\begin{aligned} & \frac{\partial}{\partial t} \left( \frac{\rho |\mathbf{v}|^2}{2} + \rho \varepsilon \right) + \sum_{k=1}^3 \nabla_k \left( \frac{\rho |\mathbf{v}|^2}{2} v^k + \rho \varepsilon v^k \right) = \\ & = \sum_{i=1}^3 v_i f^i + \sum_{i=1}^3 \sum_{k=1}^3 \nabla_k (v_i \sigma^{ik} + v_i \tilde{\sigma}^{ik}) + \sum_{i=1}^3 \sum_{k=1}^3 \nabla_k (\nabla_i T \varkappa^{ik}). \end{aligned} \quad (7.7)$$

Equations (5.7) and (5.8) are replaced by the following two equalities respectively:

$$\begin{aligned} \frac{\partial v^i}{\partial t} + \sum_{k=1}^3 v^k \nabla_k v^i &= \frac{f^i}{\rho} + \sum_{k=1}^3 \frac{\nabla_k \sigma^{ik}}{\rho} + \sum_{k=1}^3 \frac{\nabla_k \tilde{\sigma}^{ik}}{\rho}, \\ \frac{\partial}{\partial t} \left( \frac{\rho |\mathbf{v}|^2}{2} \right) + \sum_{k=1}^3 \nabla_k \left( \frac{\rho |\mathbf{v}|^2}{2} v^k \right) &= \\ &= \sum_{i=1}^3 v_i f^i + \sum_{i=1}^3 \sum_{k=1}^3 v_i \nabla_k \sigma^{ik} + \sum_{i=1}^3 \sum_{k=1}^3 v_i \nabla_k \tilde{\sigma}^{ik}. \end{aligned} \quad (7.8)$$

Subtracting (7.8) from (7.7) and taking into account (5.1), we obtain

$$\rho \frac{\partial \varepsilon}{\partial t} + \sum_{k=1}^3 \rho v^k \nabla_k \varepsilon = \sum_{i=1}^3 \sum_{k=1}^3 (\nabla_k v_i (\sigma^{ik} + \tilde{\sigma}^{ik}) + \nabla_k (\nabla_i T \chi^{ik})). \quad (7.9)$$

For derivatives  $\partial \varepsilon / \partial t$  and  $\nabla_k \varepsilon$  in left hand side of (7.9) we can apply (6.17). Then

$$\begin{aligned} T \frac{\partial(\rho s)}{\partial t} + \sum_{k=1}^3 T \nabla_k (\rho s v^k) - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{\sigma}^{ij}}{2} \left( \dot{G}_{ij} + \sum_{k=1}^3 v^k \nabla_k G_{ij} \right) &= \\ = \sum_{i=1}^3 \sum_{k=1}^3 (\nabla_k v_i (\sigma^{ik} + \tilde{\sigma}^{ik}) + \nabla_k (\nabla_i T \chi^{ik})). \end{aligned} \quad (7.10)$$

Now let's substitute (4.12) into (7.10) and take into account formula (6.20):

$$\begin{aligned} \frac{\partial(\rho s)}{\partial t} + \sum_{k=1}^3 \nabla_k (\rho s v^k) &= \sum_{i=1}^3 \sum_{k=1}^3 \frac{\nabla_k v_i \tilde{\sigma}^{ik} + \nabla_k (\nabla_i T \chi^{ik})}{T} = \\ = \sum_{i=1}^3 \sum_{k=1}^3 \nabla_k \left( \frac{\nabla_i T \chi^{ik}}{T} \right) + \sum_{i=1}^3 \sum_{k=1}^3 \sum_{j=1}^3 \sum_{q=1}^3 \frac{v_{ik} \eta^{ikjq} v_{jq}}{T} + \sum_{i=1}^3 \sum_{k=1}^3 \frac{\nabla_i T \chi^{ik} \nabla_k T}{T^2}. \end{aligned}$$

In ultimate form this is entropy balance equation generalizing equation (6.15):

$$\begin{aligned} \frac{\partial(\rho s)}{\partial t} + \sum_{k=1}^3 \nabla_k \left( \rho s v^k - \sum_{i=1}^3 \frac{\nabla_i T \chi^{ik}}{T} \right) &= \\ = \sum_{i=1}^3 \sum_{k=1}^3 \sum_{j=1}^3 \sum_{q=1}^3 \frac{v_{ik} \eta^{ikjq} v_{jq}}{T} + \sum_{i=1}^3 \sum_{k=1}^3 \frac{\nabla_i T \chi^{ik} \nabla_k T}{T^2}. \end{aligned} \quad (7.11)$$

Last two terms in (7.11) are positive. This means that total entropy is ever growing, when medium is evolving toward thermodynamic equilibrium.

## 8. LIQUID STATE MEDIA.

Balance equations in liquids are quite similar to those in elastic solid materials. The only difference is that liquids are always isotropic. Deformation state of liquid

material is completely determined by its density  $\rho$ . Therefore, instead of (6.13), for specific thermal energy per unit mass we have

$$\varepsilon = \varepsilon(T, \rho). \quad (8.1)$$

Like  $\varepsilon$  in (8.1), specific free energy per unit mass is given by formula

$$f = f(T, \rho). \quad (8.2)$$

Density  $\rho$  is related to deformation  $\mathbf{G}$  by means of formula (5.4). Hence

$$\frac{d\rho}{\rho} = \frac{d(\ln \det \mathbf{G})}{2} = \frac{\text{tr}(\mathbf{G}^{-1} d\mathbf{G})}{2} = \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{G}^{ij} dG_{ij}}{2}, \quad (8.3)$$

where  $\bar{G}^{ij}$  are components of inverse matrix  $\mathbf{G}^{-1}$ . Differentiating (8.2) and taking into account (8.3), due to the equality (6.2) we have

$$\bar{\sigma}^{ij} = -\rho^2 \frac{\partial f}{\partial \rho} \bar{G}^{ij}. \quad (8.4)$$

Substituting (8.4) into (6.20), we obtain formula for stress tensor in liquid medium:

$$\sigma^{ij} = -\rho^2 \frac{\partial f}{\partial \rho} g^{ij}. \quad (8.5)$$

Scalar factor in (8.5) is interpreted as *pressure*. Indeed, we have

$$p = \rho^2 \frac{\partial f}{\partial \rho}, \quad \sigma^{ij} = -p g^{ij}. \quad (8.6)$$

Viscosity tensor in liquids simplifies and takes the following form:

$$\eta^{ikjq} = \eta (g^{ij} g^{kq} + g^{iq} g^{jk}) + \left( \zeta - \frac{2}{3} \eta \right) g^{ik} g^{jq}. \quad (8.7)$$

Heat conductivity tensor in liquid medium is also simpler than in solid media:

$$\varkappa^{ik} = \varkappa g^{ik}. \quad (8.8)$$

Pressure  $p$  in (8.6) and scalar parameters  $\eta$ ,  $\zeta$ , and  $\varkappa$  in (8.7) and (8.8) all are functions of temperature  $T$  and density  $\rho$  of continuous medium:

$$\begin{aligned} p &= p(T, \rho), & \eta &= \eta(T, \rho), \\ \zeta &= \zeta(T, \rho), & \varkappa &= \varkappa(T, \rho). \end{aligned}$$

Other parameters in balance equations (5.1), (5.2), (5.3) for liquids are same as for solid state media.

## 9. PLASTIC MATERIALS.

Saying plastic materials we mean pitch-like very dense sticky liquids and many solid materials with no crystalline grid, e.g. glass and polymer materials. They resist to deformations like solids and can flow like liquids, though sometimes very slowly. In order to describe such materials mathematically we need to divide deformation  $\mathbf{G}$  into two parts: elastic deformation  $\hat{\mathbf{G}}$  and plastic deformation  $\check{\mathbf{G}}$ :

$$G_{ij} = \sum_{k=1}^3 \sum_{q=1}^3 \check{G}_i^k \hat{G}_{kq} \check{G}_j^q. \quad (9.1)$$

Like  $G_{ij}$ , elastic deformation tensor  $\hat{G}_{ik}$  in (9.1) is symmetric:  $\hat{G}_{ik} = \hat{G}_{ki}$ . Plastic deformation tensor  $\check{G}_{kj}$  is not necessarily symmetric.

Plastic deformation arises as a response to stress tending to relax this stress. Elastic deformation tensor  $\hat{\mathbf{G}}$  is thermodynamic parameter of plastic medium, while plastic deformation tensor  $\check{\mathbf{G}}$  is kinetic parameter. Therefore all thermodynamic quantities and kinetic coefficients for near thermodynamic equilibrium deformations of plastic medium depend on elastic deformation tensor  $\hat{\mathbf{G}}$  and on temperature:

$$\begin{aligned} \varepsilon &= \varepsilon(T, \hat{\mathbf{G}}), & f &= f(T, \hat{\mathbf{G}}), \\ \bar{\sigma}^{ij} &= \bar{\sigma}^{ij}(T, \hat{\mathbf{G}}), & \sigma^{ij} &= \sigma^{ij}(T, \hat{\mathbf{G}}), \\ \eta^{ikjq} &= \eta^{ikjq}(T, \hat{\mathbf{G}}), & \varkappa^{ik} &= \varkappa^{ik}(T, \hat{\mathbf{G}}). \end{aligned} \quad (9.2)$$

Components of total deformation tensor  $G_{ij}$  in (9.1) satisfy differential equations (4.12). These equations can be written as follows:

$$\frac{\partial G_{ij}}{\partial t} + \sum_{r=1}^3 v^r \nabla_r G_{ij} = - \sum_{r=1}^3 \nabla_i v^r G_{rj} - \sum_{r=1}^3 G_{ir} \nabla_j v^r. \quad (9.3)$$

For components of elastic deformation tensor  $\hat{G}_{ij}$  we write analogous equation:

$$\frac{\partial \hat{G}_{kq}}{\partial t} + \sum_{r=1}^3 v^r \nabla_r \hat{G}_{kq} = - \sum_{r=1}^3 \nabla_k v^r \hat{G}_{rq} - \sum_{r=1}^3 \hat{G}_{kr} \nabla_q v^r + 2 \Theta_{kq}. \quad (9.4)$$

Components of symmetric tensor  $\Theta$  in (9.4) are kinetic coefficients. Therefore

$$\Theta_{kq} = \Theta_{kq}(T, \hat{\mathbf{G}}). \quad (9.5)$$

Now we need some special facts concerning all three deformation tensors in (9.1). Symmetric matrix  $G_{ij}$  determined by formula (4.8) is non-degenerate and positive. Due to (9.1) we have the equality  $\det \mathbf{G} = \det \hat{\mathbf{G}} \cdot (\det \check{\mathbf{G}})^2$ . Hence

$$\det \hat{\mathbf{G}} \neq 0, \quad \det \check{\mathbf{G}} \neq 0. \quad (9.6)$$

Moreover, due to (9.1) and (9.6) matrix  $\hat{G}_{kq}$  is also positive. Now let's use formula

analogous to (6.6) and define linear operator  $\hat{\mathbf{G}}$  with components

$$\hat{G}_j^i = \sum_{k=1}^3 g^{ik} \hat{G}_{kj}. \quad (9.7)$$

**Theorem 9.1.** *For any symmetric matrix  $\Theta_{kq}$  and for linear operator  $\hat{\mathbf{G}}$  determined by formula (9.7) there is unique symmetric matrix  $\theta_{kq}$  such that*

$$2\Theta_{kq} = \sum_{r=1}^3 \theta_{kr} \hat{G}_q^r + \sum_{r=1}^3 \hat{G}_k^r \theta_{rq}. \quad (9.8)$$

This is purely mathematical fact with rather simple proof. Applying theorem 9.1 to matrix (9.5) we get tensor  $\boldsymbol{\theta}$  with components

$$\theta_{kq} = \theta_{kq}(T, \hat{\mathbf{G}}). \quad (9.9)$$

Raising index in (9.9) we get symmetric linear operator  $\boldsymbol{\theta}$  with components

$$\theta_j^i = \sum_{k=1}^3 g^{ik} \theta_{kj}. \quad (9.10)$$

Due to (9.8), (9.9), and (9.10) we can write equation (9.4) in the following form:

$$\begin{aligned} \frac{\partial \hat{G}_{kq}}{\partial t} + \sum_{r=1}^3 v^r \nabla_r \hat{G}_{kq} &= - \sum_{r=1}^3 \nabla_k v^r \hat{G}_{rq} - \\ &- \sum_{r=1}^3 \hat{G}_{kr} \nabla_q v^r + \sum_{r=1}^3 \theta_k^r \hat{G}_{rq} + \sum_{r=1}^3 \hat{G}_{kr} \theta_q^r. \end{aligned} \quad (9.11)$$

Now we are able to write differential equations for plastic deformation tensor:

$$\frac{\partial \check{G}_i^k}{\partial t} + \sum_{r=1}^3 v^r \nabla_r \check{G}_i^k = \sum_{r=1}^3 (\check{G}_i^r \nabla_r v^k - \nabla_i v^r \check{G}_r^k) - \sum_{r=1}^3 \theta_r^k \check{G}_i^r. \quad (9.12)$$

**Forgetting principle.** This is basic principle characterizing plastic deformations that we consider in present paper. Suppose that plastic medium evolves from initial state with no deformation at time instant  $t = 0$  to some intermediate state at  $t = t_0$ , then it continues its evolution for  $t > t_0$ . Forgetting principle states that if in intermediate state total deformation of medium is purely plastic, then further evolution of medium will be so as if in intermediate state it had no deformation at all. Equation (9.12) is written on the base of this principle. It is compatible with (9.1) and with equations (9.3) and (9.11).

## 10. THERMODYNAMICS OF PLASTIC MEDIUM.

Balance equations (5.1), (5.2), and (5.3) remain unchanged for plastic medium. We also keep unchanged formulas (7.1), (7.2), (7.5), and second formula in (6.22). However, due to (9.2) and (9.11) we should revise formulas (6.2), (6.3), (6.4), (6.5), and (6.6). Formulas (6.2) and (6.3) are replaced by the following ones:

$$df = -s dT - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{\sigma}^{ij} d\hat{G}_{ij}}{2\rho}, \quad \frac{\bar{\sigma}^{ij}}{2\rho} = -\frac{\partial f(T, \hat{\mathbf{G}})}{\partial \hat{G}_{ij}}. \quad (10.1)$$

For homogeneous and isotropic plastic material function  $f(T, \hat{\mathbf{G}})$  is more special:

$$f = f(T, \lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]}). \quad (10.2)$$

Though  $\lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]}$  in (10.2) are different from that of (6.4), they are scalar invariants of linear operator  $\hat{\mathbf{G}}$  that was defined above by formula (9.7):

$$\lambda_{[1]} = \frac{\text{tr}(\hat{\mathbf{G}})}{3}, \quad \lambda_{[2]} = \frac{\text{tr}(\hat{\mathbf{G}} \cdot \hat{\mathbf{G}})}{3}, \quad \lambda_{[3]} = \frac{\text{tr}(\hat{\mathbf{G}} \cdot \hat{\mathbf{G}} \cdot \hat{\mathbf{G}})}{3}. \quad (10.3)$$

Next two formulas are analogous to (6.8) and (6.9):

$$\bar{\sigma}^{ij} = f_{[1]} g^{ij} + f_{[2]} \hat{G}^{ij} + \sum_{k=1}^3 \sum_{q=1}^3 f_{[3]} \hat{G}^{ik} g_{kq} \hat{G}^{qj}, \quad (10.4)$$

$$f_{[i]} = -\frac{2i\rho}{3} \frac{\partial f(T, \lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]})}{\partial \lambda_{[i]}}, \quad i = 1, 2, 3. \quad (10.5)$$

As we said above, we keep unchanged energy balance equation (5.3) with  $w^k$  given by formula (7.5) and  $e$  given by second formula (6.22). This means that we keep unchanged formula (7.7). However, thermal energy  $\varepsilon$  now depends only on elastic part of deformation tensor. Therefore, we should recalculate relation of  $\bar{\sigma}^{ij}$  and stress tensor  $\sigma^{ij}$ . Due to (10.1) and consequent formulas (10.2), (10.3), (10.4), and (10.5) instead of (6.14) now we should write

$$\varepsilon = \varepsilon(s, \hat{\mathbf{G}}) = \varepsilon(s, \lambda_{[1]}, \lambda_{[2]}, \lambda_{[3]}). \quad (10.6)$$

By the same reason instead of formulas (6.17) we should write

$$\begin{aligned} \frac{\partial \varepsilon}{\partial t} &= T \frac{\partial s}{\partial t} - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{\sigma}^{ij}}{2\rho} \frac{\partial \hat{G}_{ij}}{\partial t}, \\ \nabla_k \varepsilon &= T \nabla_k s - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{\sigma}^{ij} \nabla_k \hat{G}_{ij}}{2\rho}. \end{aligned} \quad (10.7)$$

Applying (5.1) and (7.8) to (7.7), we derive the following equation:

$$\rho \frac{\partial \varepsilon}{\partial t} + \sum_{k=1}^3 \rho v^k \nabla_k \varepsilon = \sum_{i=1}^3 \sum_{k=1}^3 (\nabla_k v_i (\sigma^{ik} + \bar{\sigma}^{ik}) + \nabla_k (\nabla_i T \varkappa^{ik})). \quad (10.8)$$



Note that (10.8) is just the same as the equation (7.9). Now we should substitute (10.7) into this equation. As a result we obtain

$$\begin{aligned} \rho T \frac{\partial s}{\partial t} + \sum_{k=1}^3 \rho T v^k \nabla_k s - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\bar{\sigma}^{ij}}{2} \left( \frac{\partial \hat{G}_{ij}}{\partial t} + \sum_{k=1}^3 v^k \nabla_k \hat{G}_{ij} \right) = \\ = \sum_{i=1}^3 \sum_{k=1}^3 (\nabla_k v_i (\sigma^{ik} + \tilde{\sigma}^{ik}) + \nabla_k (\nabla_i T \varkappa^{ik})). \end{aligned} \quad (10.9)$$

Applying (9.4) to the equation (10.9), we transform it to the following one:

$$\begin{aligned} \rho T \frac{\partial s}{\partial t} + \sum_{k=1}^3 \rho T v^k \nabla_k s + \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^3 \frac{\bar{\sigma}^{ij}}{2} (\nabla_i v^k \hat{G}_{kj} + \hat{G}_{ik} \nabla_j v^k - \\ - 2 \Theta_{ij}) = \sum_{i=1}^3 \sum_{k=1}^3 (\nabla_k v_i (\sigma^{ik} + \tilde{\sigma}^{ik}) + \nabla_k (\nabla_i T \varkappa^{ik})). \end{aligned} \quad (10.10)$$

Now let's recall formula (6.20) and write analogous formula in present case

$$\sigma^{ik} = \sum_{j=1}^3 \hat{G}_j^i \bar{\sigma}^{jk}. \quad (10.11)$$

Applying (10.11) to (10.10), we simplify it substantially. Here is resulting equation

$$\begin{aligned} T \frac{\partial(\rho s)}{\partial t} + \sum_{k=1}^3 T \nabla_k (\rho s v^k) = \sum_{i=1}^3 \sum_{j=1}^3 \sigma^{ij} \theta_{ij} + \\ + \sum_{i=1}^3 \sum_{k=1}^3 (\nabla_k v_i (\sigma^{ik} + \tilde{\sigma}^{ik}) + \nabla_k (\nabla_i T \varkappa^{ik})). \end{aligned} \quad (10.12)$$

For  $\Theta_{ij}$  in (10.10) we used formula (9.8). By further transformations similar to that of section 7 we can bring the equation (10.12) to the form analogous to (7.11):

$$\begin{aligned} \frac{\partial(\rho s)}{\partial t} + \sum_{k=1}^3 \nabla_k \left( \rho s v^k - \sum_{i=1}^3 \frac{\nabla_i T \varkappa^{ik}}{T} \right) = \sum_{i=1}^3 \sum_{j=1}^3 \frac{\sigma^{ij} \theta_{ij}}{T} + \\ + \sum_{i=1}^3 \sum_{k=1}^3 \sum_{j=1}^3 \sum_{q=1}^3 \frac{v_{ik} \eta^{ikjq} v_{jq}}{T} + \sum_{i=1}^3 \sum_{k=1}^3 \frac{\nabla_i T \varkappa^{ik} \nabla_k T}{T^2}. \end{aligned} \quad (10.13)$$

As compared to (7.11) in (10.13) we have one extra term in right hand side. It should be positive like other two terms in right hand side of (10.13):

$$\sum_{i=1}^3 \sum_{j=1}^3 \frac{\sigma^{ij} \theta_{ij}}{T} \geq 0. \quad (10.14)$$

Formulas (10.13) and (10.14) yield physical interpretation of tensor (9.9). This tensor determines entropy production due to plastic deformation of medium.

Formula (10.11) relates tensor  $\bar{\sigma}$  and stress tensor  $\sigma$ . Applying (10.11) to (10.4), we derive formula for stress tensor of isotropic plastic medium:

$$\begin{aligned} \sigma^{ij} = & f_{[1]} \hat{G}^{ij} + \sum_{k=1}^3 \sum_{q=1}^3 f_{[2]} \hat{G}^{ik} g_{kq} \hat{G}^{qj} + \\ & + \sum_{k=1}^3 \sum_{q=1}^3 \sum_{m=1}^3 \sum_{n=1}^3 f_{[3]} \hat{G}^{ik} g_{kq} \hat{G}^{qm} g_{mn} \hat{G}^{nj}. \end{aligned} \quad (10.15)$$

Formula (10.15) is analogous to (6.23). Like formula (6.23), this formula means that stress tensor  $\sigma$  is symmetric:  $\sigma^{ij} = \sigma^{ji}$ . In general case for non-isotropic media symmetry of tensor  $\mathbf{\Pi}$  in (7.1) and hence symmetry of  $\sigma$  is derived from conservation law for angular momentum (see [4]).

Note that in (9.2) we declared that tensors  $\sigma$  and  $\bar{\sigma}$  depend only on elastic part of deformation tensor (9.1). However, for coefficients  $f_{[1]}$ ,  $f_{[2]}$ ,  $f_{[3]}$  in formulas (10.4) and (10.15) we have explicit expression (10.5) containing entry of density  $\rho$ . Due to (5.4) density of medium depends on total deformation tensor  $\mathbf{G}$ , but not on its elastic part  $\hat{\mathbf{G}}$  only. In order to avoid this discrepancy we need to introduce additional restriction for plastic part of deformation tensor

$$\det \check{\mathbf{G}} = 1. \quad (10.16)$$

Then due to (9.1) and (10.16) we get  $\det \hat{\mathbf{G}} = \det \mathbf{G}$  and (5.4) is replaced by analogous relationship binding density  $\rho$  to elastic deformation tensor  $\hat{\mathbf{G}}$ :

$$\ln \rho - \frac{\ln \det \hat{\mathbf{G}} - \ln \det \mathbf{g}}{2} = \text{const}. \quad (10.17)$$

Restriction (10.16) and the equality (10.17) following from it are reasonable from physical point of view. Indeed, according to forgetting principle (see above), plastic deformations are those which can be forgotten. However deformations changing density of medium cannot be forgotten. Hence they cannot be purely plastic.

Restriction (10.16) leads to the restriction for tensor  $\theta$  in (9.12). Indeed, differentiating (10.16) and applying equation (9.12), we derive

$$\text{tr } \theta = \sum_{k=1}^3 \theta_k^k = 0. \quad (10.18)$$

Thus, formula (10.18) means that tensor  $\theta$  determines symmetric linear operator with zero trace. It is symmetric due to (9.10) and symmetry  $\theta_{kq} = \theta_{qk}$ .

Plastic deformation is a way for draining stress. Tensor  $\theta$  determines the rate of such draining. In elastic solid materials total deformation is purely elastic. Therefore  $\check{G}_j^i = \delta_j^i$ . Substituting  $\check{G}_j^i = \delta_j^i$  into the equations (9.12), we find

$$\theta_j^i = 0. \quad (10.19)$$

Thus, elastic solid medium can be treated as limiting case of plastic medium with vanishing tensor  $\theta_j^i \rightarrow 0$ .

In liquids tensor  $\boldsymbol{\theta}$  is undetermined. Indeed, above in section 8 we treated liquid state media in the same way as purely elastic solid state media, but with special form of free energy function (see formula (8.2)). Then  $\boldsymbol{\theta}$  is equal to zero like in (10.19). However, we could treat liquids as plastic media by introducing some arbitrary tensor  $\boldsymbol{\theta}$ . In any case stress tensor in liquids is determined by formula

$$\sigma^{ij} = -p g^{ij}, \quad (10.20)$$

see (8.6) above. Substituting (10.20) into left hand side of (10.14), then taking into account (9.10) and trace condition (10.18), we derive

$$\sum_{i=1}^3 \sum_{j=1}^3 \frac{\sigma^{ij} \theta_{ij}}{T} = - \sum_{i=1}^3 \sum_{j=1}^3 \frac{p}{T} g^{ij} \theta_{ij} = - \sum_{i=1}^3 \frac{p}{T} \theta_i^i = 0.$$

This means that tensor  $\boldsymbol{\theta}$  for liquid media is not thermodynamically fixed. Therefore asymptotical behavior of functions  $\theta_{kq} = \theta_{kq}(T, \hat{\mathbf{G}})$  near phase transition point from plastic solid state to liquid state  $T \rightarrow T_{\text{ph.tr.}}$  requires separate investigation. This will be done in separate paper.

#### REFERENCES

1. Juhl S., Lyuksyutov S. F., Paramonov P. B., Sigalov G., Vaia R. A., *Peculiarities of electrostatic resistless AFM nanolithography in polymers*, MRS Meeting, December 2-6, 2002, Boston MA.
2. Juhl S., Lyuksyutov S. F., Paramonov P. B., Ralich R. M., Sancaktar E., Sigalov G., Vaia R. A., Waterhouse L., *AFM-assisted electrostatic nanolithography in polymers* (to appear).
3. Sharipov R. A., *Course of differential geometry*, Baskir State University, Ufa, Russia, 1996.
4. Landau L. D., Lifshits E. M., *Theory of elasticity. Theoretical physics, Vol. VII*, Nauka publishers, Moscow, 1987.

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