# A NOTE ON THE DYNAMICS AND THERMODYNAMICS OF DISLOCATED CRYSTALS.

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ABSTRACT. The dynamics and thermodynamics of dislocated crystals are studied within the framework of the nonlinear theory of elastic and plastic deformations.

#### 1. INTRODUCTION.

In the series of papers [1-4] the kinematics of crystalline media in the presence of dislocations was studied. Here we consider the dynamics and thermodynamics of a crystalline medium. This paper continues the series of papers [1-4]. Therefore, we do not provide a large introductory section in it. For more details the reader is referred to the previous papers.

### 2. Specific free energy function.

By analogy to [5], we shall construct the theory on the base of the specific free energy function f (the amount of free energy per unit mass of a medium). The deformation state of a crystalline medium in the presence of dislocations is described by the *incompatible distorsion tensor*  $\hat{\mathbf{T}}$ . This is a *double space tensor* with one upper index<sup>1</sup> associated with the *Burgers space*  $\mathbb{B}$  and with one lower index associated with the *real space*  $\mathbb{E}$ . The other physically important parameter is the tensor of the *Burgers vector density*  $\boldsymbol{\rho}$ . It is also a double space tensor with two indices. Like in the case of  $\hat{\mathbf{T}}$ , the upper index of  $\boldsymbol{\rho}$  is associated with the Burgers space, while its lower index is associated with the real space. The easiest way of choosing the specific free energy function f is to write it as

$$f = f(T, \mathbf{T}, \boldsymbol{\rho}), \tag{2.1}$$

where T is the temperature. However, we shall not write f in this simplest way (2.1). The matter is that  $\hat{\mathbf{T}}$  and  $\boldsymbol{\rho}$  contain some excessive amount of purely geometric information absolutely inessential for describing the thermodynamics of a medium. We need to make some efforts to get rid of this inessential part of information in the tensors  $\hat{\mathbf{T}}$  and  $\boldsymbol{\rho}$ .

The Burgers space  $\mathbb{B}$ , as it was defined in [1], is a copy of the real space  $\mathbb{E}$ . It is assumed to be filled with the ideal (dislocation-free and non-distorted) crystalline

<sup>&</sup>lt;sup>1</sup> It is implicitly assumed that some coordinate systems in  $\mathbb{B}$  and  $\mathbb{E}$  are chosen and  $\hat{\mathbf{T}}$  is represented by its components  $\hat{T}_i^i$  respective to those coordinate systems.

medium (see Fig. 2.2) identical to that we consider in the real space. The tensor field  $\hat{\mathbf{T}}$  determines a linear mapping at each point p of the real space:

$$\hat{\mathbf{T}}: T_p \mathbb{E} \to \mathbb{B}. \tag{2.2}$$

Here  $T_p \mathbb{E}$  is the set of vectors attached to the point  $p \in \mathbb{E}$ . In geometry, when  $\mathbb{E}$  is treated as a manifold, such a space is called a *tangent space*. Both spaces  $\mathbb{E}$  and  $\mathbb{B}$  are equipped with the Euclidean metrics  $\mathbf{g}$  and  $\overset{*}{\mathbf{g}}$  respectively. The difference is that the Burgers space  $\mathbb{B}$  in (2.2) is treated as a linear space, while  $\mathbb{E}$  is treated as



Fig. 2.1

Fig. 2.2

a point space (or a manifold). The mapping (2.2) is non-degenerate: det  $\mathbf{T} \neq 0$ . Hence, one can consider the inverse mapping

$$\hat{\mathbf{S}} \colon \mathbb{B} \to T_p \mathbb{E}. \tag{2.3}$$

The inverse mapping (2.3) is given by the *inverse incompatible distorsion tensor*  $\hat{\mathbf{S}}$ . This is also a double space tensor with two indices: its upper index is associated with  $\mathbb{E}$  and its lower index is associated with  $\mathbb{B}$ .

Suppose that the point p is fixed. The rotation of the crystalline body as a whole about the point  $p \in \mathbb{E}$  does not change its physical state (see Fig. 2.1). Such a rotation is expressed by the following transformations at the point p:

$$\hat{T}^i_k \to \sum_{\alpha=1}^3 O^{\alpha}_k \ \hat{T}^i_{\alpha}, \qquad \qquad \rho^i_k \to \sum_{\alpha=1}^3 O^{\alpha}_k \ \rho^i_{\alpha}. \tag{2.4}$$

Here  $O_k^{\alpha}$  are the components of some rotation matrix<sup>1</sup>. Since the physical state of a crystalline body is invariant under the transformations (2.4), so should be the free energy function (2.1). Let's define the following tensors  $\mathbf{\bar{G}}$  and  $\mathbf{\bar{R}}$ :

$$\overline{G}_{ij} = \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} g_{\alpha\beta} \ \hat{S}_{i}^{\alpha} \ \hat{S}_{j}^{\beta}, \qquad \qquad \overline{R}_{j}^{i} = \sum_{\alpha=1}^{3} \rho_{\alpha}^{i} \ \hat{S}_{j}^{\alpha}.$$
(2.5)

<sup>&</sup>lt;sup>1</sup> Note that the transformations (2.4) are different from those in section 2 of [3] and from those in formulas (3.19), (3.20), (3.21) in [4].

Both indices i and j in (2.5) are associated with the Burgers space  $\mathbb{B}$ . Nevertheless,  $\mathbf{\ddot{G}}$  and  $\mathbf{\ddot{R}}$  are double space tensors because their components are functions of the coordinates of a point  $p \in \mathbb{E}$  and of the time variable t:

$$\overline{G}_{ij} = \overline{G}_{ij}(t, y^1, y^2, y^3), \qquad \qquad \overline{R}_j^i = \overline{R}_j^i(t, y^1, y^2, y^3).$$
(2.6)

Note that the tensors  $\hat{\mathbf{G}}$  and  $\hat{\mathbf{R}}$  are different from the purely real space tensors  $\hat{\mathbf{G}}$  and  $\mathbf{R}$  introduced in [1] and in [3]. Their components are given by the formulas

$$\hat{G}_{\alpha\beta} = \sum_{i=1}^{3} \sum_{j=1}^{3} {}^{*}_{gij} \hat{T}^{i}_{\alpha} \hat{T}^{j}_{\beta}, \qquad \qquad R^{\alpha}_{\beta} = \sum_{i=1}^{3} \hat{S}^{\alpha}_{i} \rho^{i}_{\beta}.$$
(2.7)

The tensor  $\hat{\mathbf{G}}$  given by the first formula (2.7) is called the *elastic deformation* tensor. As for  $\mathbf{R}$ , it is the purely real space representation of the Burgers vector density tensor  $\boldsymbol{\rho}$ .

Now let's return back to the tensors  $\mathbf{\overline{G}}$  and  $\mathbf{\overline{R}}$  in (2.5) and find that they are invariant with respect to the transformations (2.4). Therefore, we can use  $\mathbf{\overline{G}}$  and  $\mathbf{\overline{R}}$  as independent variables instead of  $\mathbf{T}$  and  $\boldsymbol{\rho}$  in (2.1):

$$f = F(T, \mathbf{\bar{G}}, \mathbf{\check{g}}, \mathbf{\bar{R}}, \rho).$$
(2.8)

Note that the function F has no explicit dependence on the coordinates of a point  $p \in \mathbb{E}$ . This function represents the refined properties of a crystal in its homogeneous state (see Fig. 2.2). It should be tabulated on the base of experiments. Note also that, apart from  $\mathbf{\ddot{G}}$  and  $\mathbf{\ddot{R}}$ , we introduced the additional arguments  $\mathbf{\dot{g}}$  and  $\rho$  in (2.8), where  $\rho$  is the density of a crystal and  $\mathbf{\ddot{g}}$  is the metric tensor of the Euclidean metric in the Burgers space  $\mathbb{B}$ . The constant tensor  $\mathbf{\ddot{g}}$  does not change the time and coordinate dependence of f determined by (2.6) and by the scalar functions

$$T = T(t, y^1, y^2, y^3), \qquad \qquad \rho = \rho(t, y^1, y^2, y^3).$$

Having written (2.8) in place of (2.1), we have reached one of our goals — we have got the rotationally invariant free energy function. The experimental data should go to the theory through the function F. However, for the sake of beauty, in the formulas below we need to express f through some purely real space tensor fields. The tensor  $\mathbf{\ddot{R}}$  is expressed through  $\mathbf{R}$  as follows:

$$\overline{R}_{j}^{i} = \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \hat{T}_{\beta}^{i} \, \hat{S}_{j}^{\alpha} \, R_{\alpha}^{\beta}.$$
(2.9)

The tensor  $\mathbf{\ddot{G}}$  cannot be expressed through  $\mathbf{\hat{G}}$ , but it is expressed through the metric tensor  $\mathbf{g}$  of the real space  $\mathbb{E}$  according to the first formula (2.5):

$$\vec{G}_{ij} = \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} g_{\alpha\beta} \ \hat{S}_{i}^{\alpha} \ \hat{S}_{j}^{\beta}.$$
(2.10)

Similarly, the metric tensor  $\mathbf{\dot{g}}$  in (2.8) is expressed through  $\mathbf{\ddot{G}}$  as follows:

$$\overset{*}{g}_{ij} = \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \hat{G}_{\alpha\beta} \; \hat{S}_{i}^{\alpha} \; \hat{S}_{j}^{\beta}. \tag{2.11}$$

This formula (2.11) is inverse to the first formula (2.7). Substituting (2.9), (2.10), and (2.11) into (2.8), we can write (2.8) in the following form:

$$f = f(t, p, T, \mathbf{g}, \mathbf{G}, \mathbf{R}, \rho).$$
(2.12)

We do not keep  $\hat{\mathbf{S}}$  and  $\hat{\mathbf{T}}$  in (2.12) as independent variables since they are not purely real space tensor fields. Their presence is reflected by the arguments t and p, where t is the time variable and p is a point of the real space  $\mathbb{E}$ . In a coordinate presentation of f its argument p is replaced by the variables  $y^1, y^2, y^3$ .

## 3. Specific free energy function as an extended scalar field.

The specific free energy function (2.12) is a scalar function with three tensorial arguments  $\mathbf{g}$ ,  $\hat{\mathbf{G}}$ , and  $\mathbf{R}$ . In this form it fits the definition of an extended scalar field (see definition 4.1 in [6]). The theory of extended tensor fields was especially derived in [6] for to use it in the present paper. The extended scalar field f in (2.12) is not an arbitrary extended scalar field. It is produced from the function F in (2.8). For this reason it satisfies some partial differential equations written in terms of covariant and multivariate derivatives defined in [6].

**Theorem 3.1.** The specific free energy function f of a dislocated crystalline medium is an extended scalar field satisfying the differential equation

$$\nabla_{\gamma} f = -\sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha\beta} [2] f \left( \hat{Z}_{\gamma\alpha}^{m} g_{m\beta} + \hat{Z}_{\gamma\beta}^{m} g_{\alpha m} \right) - \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha\beta} [3] f \left( \hat{Z}_{\gamma\alpha}^{m} \hat{G}_{m\beta} + \hat{Z}_{\gamma\beta}^{m} \hat{G}_{\alpha m} \right) + \sum_{n=1}^{3} \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla_{\beta}^{\alpha} [4] f \left( \hat{Z}_{\gamma m}^{\beta} R_{\alpha}^{m} - \hat{Z}_{\gamma \alpha}^{m} R_{m}^{\beta} \right), \quad (3.1)$$

where  $\hat{Z}_{ij}^k$  are the components of the tensor field  $\hat{\mathbf{Z}}$  introduced in paper [3]:

$$\hat{Z}_{ij}^{k} = \sum_{m=1}^{3} \hat{S}_{m}^{k} \nabla_{i} \hat{T}_{j}^{m} = \sum_{m=1}^{3} \hat{S}_{m}^{k} \left( \frac{\partial \hat{T}_{j}^{m}}{\partial y^{i}} - \sum_{n=1}^{3} \Gamma_{ij}^{n} \hat{T}_{n}^{m} \right).$$
(3.2)

*Proof.* First of all let's calculate the multivariate derivatives  $\nabla^{\alpha\beta}[2]f$ ,  $\nabla^{\alpha\beta}[3]f$ , and  $\nabla^{\alpha}_{\beta}[4]f$  defined due to three tensorial arguments in (2.12):

$$\nabla^{\alpha\beta}[2]f = \frac{\partial f}{\partial g_{\alpha\beta}} = \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial F}{\partial \overline{G}_{ij}} \,\hat{S}_{i}^{\alpha} \,\hat{S}_{j}^{\beta}, \qquad (3.3)$$

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$$\nabla^{\alpha\beta}[3]f = \frac{\partial f}{\partial \hat{G}_{\alpha\beta}} = \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial F}{\partial \dot{g}_{ij}} \, \hat{S}_{i}^{\alpha} \, \hat{S}_{j}^{\beta}, \qquad (3.4)$$

$$\nabla^{\alpha}_{\beta}[4]f = \frac{\partial f}{\partial R^{\beta}_{\alpha}} = \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial F}{\partial \overline{R}^{i}_{j}} \hat{S}^{\alpha}_{j} \hat{T}^{i}_{\beta}.$$
(3.5)

Then we calculate the covariant derivatives of the extended scalar field (2.12) applying the formula (13.15) from [6]:

$$\nabla_{\gamma} f = \frac{\partial f}{\partial y^{\gamma}} + \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \left( \Gamma_{\gamma\alpha}^{m} g_{m\beta} + \Gamma_{\gamma\beta}^{m} g_{\alpha m} \right) \frac{\partial f}{\partial g_{\alpha\beta}} + \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \left( \Gamma_{\gamma\alpha}^{m} \hat{G}_{m\beta} + \Gamma_{\gamma\beta}^{m} \hat{G}_{\alpha m} \right) \frac{\partial f}{\partial \hat{G}_{\alpha\beta}} + \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \left( \Gamma_{\gamma\alpha}^{m} R_{m}^{\beta} - \Gamma_{\gamma m}^{\beta} R_{\alpha}^{m} \right) \frac{\partial f}{\partial R_{\alpha}^{\beta}}.$$
(3.6)

Writing (3.6), we assume that  $y^1$ ,  $y^2$ ,  $y^3$  are some curvilinear coordinates in the real space  $\mathbb{E}$  and  $\Gamma_{ij}^k$  are the components of the metric connection for the Euclidean metric **g** in  $\mathbb{E}$ . Now let's calculate the partial derivatives  $\partial f / \partial y^{\gamma}$ :

$$\begin{split} \frac{\partial f}{\partial y^{\gamma}} &= \sum_{i=1}^{3} \sum_{j=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \frac{\partial F}{\partial \bar{G}_{ij}} \ g_{\alpha\beta} \left( \frac{\partial \hat{S}_{i}^{\alpha}}{\partial y^{\gamma}} \ \hat{S}_{j}^{\beta} + \hat{S}_{i}^{\alpha} \ \frac{\partial \hat{S}_{j}^{\beta}}{\partial y^{\gamma}} \right) + \\ &+ \sum_{i=1}^{3} \sum_{j=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \frac{\partial F}{\partial g_{ij}^{*}} \ \hat{G}_{\alpha\beta} \left( \frac{\partial \hat{S}_{i}^{\alpha}}{\partial y^{\gamma}} \ \hat{S}_{j}^{\beta} + \hat{S}_{i}^{\alpha} \ \frac{\partial \hat{S}_{j}^{\beta}}{\partial y^{\gamma}} \right) + \\ &+ \sum_{i=1}^{3} \sum_{j=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \frac{\partial F}{\partial \bar{R}_{j}^{*}} \ R_{\alpha}^{\beta} \left( \frac{\partial \hat{T}_{\beta}^{i}}{\partial y^{\gamma}} \ \hat{S}_{j}^{\alpha} + \hat{T}_{\beta}^{i} \ \frac{\partial \hat{S}_{j}^{\alpha}}{\partial y^{\gamma}} \right). \end{split}$$

The matrices  $\hat{\mathbf{S}}$  and  $\hat{\mathbf{T}}$  are inverse to each other. Applying this fact and the equalities (3.3), (3.4), (3.5) to the above formula, we obtain

$$\begin{split} \frac{\partial f}{\partial y^{\gamma}} &= -\sum_{n=1}^{3}\sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\frac{\partial f}{\partial g_{\alpha\beta}} \left(\hat{S}_{n}^{m}\frac{\partial \hat{T}_{\alpha}^{n}}{\partial y^{\gamma}}g_{m\beta} + \hat{S}_{n}^{m}\frac{\partial \hat{T}_{\beta}^{n}}{\partial y^{\gamma}}g_{\alpha m}\right) - \\ &-\sum_{n=1}^{3}\sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\frac{\partial f}{\partial \hat{G}_{\alpha\beta}} \left(\hat{S}_{n}^{m}\frac{\partial \hat{T}_{\alpha}^{n}}{\partial y^{\gamma}}\hat{G}_{m\beta} + \hat{S}_{n}^{m}\frac{\partial \hat{T}_{\beta}^{n}}{\partial y^{\gamma}}\hat{G}_{\alpha m}\right) + \\ &+\sum_{n=1}^{3}\sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\frac{\partial f}{\partial R_{\alpha}^{\beta}} \left(\hat{S}_{n}^{\beta}\frac{\partial \hat{T}_{m}^{n}}{\partial y^{\gamma}}R_{\alpha}^{m} - \hat{S}_{n}^{m}\frac{\partial \hat{T}_{\alpha}^{n}}{\partial y^{\gamma}}R_{m}^{\beta}\right). \end{split}$$

Now, substituting this expression for  $\partial f/\partial y^{\gamma}$  into (3.6) and taking into account (3.2), we derive the required equality (3.1). The theorem is proved.  $\Box$ 

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Note that  $\Gamma_{ij}^k$  in (3.2) and (3.6) are the components of the symmetric Euclidean connection  $\Gamma$  associated with the standard Euclidean metric **g** in the real space  $\mathbb{E}$ . These quantities are equal to zero in Cartesian coordinates and arise only if one chooses curvilinear coordinates  $y^1, y^2, y^3$ . Let's remember that there is another connection  $\hat{\Gamma}$  in the theory. Its components are given by the formula (2.3) in [4]:

$$\hat{\Gamma}^k_{ij} = \Gamma^k_{ij} + \hat{Z}^k_{ij}.$$
(3.7)

This connection (3.7) is associated with the tensor field  $\hat{\mathbf{G}}$  treated as a metric. If we replace  $\Gamma$  by  $\hat{\Gamma}$  in (3.6), then the equation (3.1) reduces to the following one:

$$\hat{\nabla}_{\gamma} f = 0. \tag{3.8}$$

**Remark.** Note that both  $\nabla_{\gamma}$  and  $\hat{\nabla}_{\gamma}$  in (3.1) and (3.8) are not standard covariant derivatives. They are so-called *spacial covariant derivatives* introduced in [6].

Now let's calculate the time derivative  $\partial f/\partial t$  considering f as an extended scalar field (2.12) and thus taking T,  $\mathbf{g}$ ,  $\hat{\mathbf{G}}$ ,  $\mathbf{R}$ , and  $\rho$  for independent variables:

$$\frac{\partial f}{\partial t} = -\sum_{n=1}^{3} \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \frac{\partial f}{\partial g_{\alpha\beta}} \left( \hat{S}_{n}^{m} \frac{\partial \hat{T}_{\alpha}^{n}}{\partial t} g_{m\beta} + \hat{S}_{n}^{m} \frac{\partial \hat{T}_{\beta}^{n}}{\partial t} g_{\alpha m} \right) - \\ -\sum_{n=1}^{3} \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \frac{\partial f}{\partial \hat{G}_{\alpha\beta}} \left( \hat{S}_{n}^{m} \frac{\partial \hat{T}_{\alpha}^{n}}{\partial t} \hat{G}_{m\beta} + \hat{S}_{n}^{m} \frac{\partial \hat{T}_{\beta}^{n}}{\partial t} \hat{G}_{\alpha m} \right) + \\ +\sum_{n=1}^{3} \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \frac{\partial f}{\partial R_{\alpha}^{\beta}} \left( \hat{S}_{n}^{\beta} \frac{\partial \hat{T}_{m}^{n}}{\partial t} R_{\alpha}^{m} - \hat{S}_{n}^{m} \frac{\partial \hat{T}_{\alpha}^{n}}{\partial t} R_{m}^{\beta} \right).$$

The components of the time derivative  $\partial \hat{\mathbf{T}} / \partial t$  are given by the formula

$$\frac{\partial \hat{T}^n_\beta}{\partial t} = -j^n_\beta - \sum_{i=1}^3 \nabla_\beta v^i \hat{T}^n_i - \sum_{i=1}^3 v^i \nabla_\beta \hat{T}^n_i.$$
(3.9)

The formula (3.9) is derived from the formulas (4.4) and (4.5) in [2]. These two formulas are valid only under the assumption that the conjecture 4.1 in [2] is valid.

**Remark.** Here we do not discuss the conjecture 4.1 from [2]. However, one should note that all results below in this paper are obtained under the assumption that this conjecture is valid.

The quantities  $j_{\beta}^{n}$  in (3.9) represent the double space tensor **j**, it is called the tensor of the *Burgers vector flow density*. The quantities  $v^{i}$  are the components of the velocity vector **v** describing the substance flow in the medium. Multiplying (3.9) by  $S_{n}^{m}$  and summing over the index n, we derive the following equality:

$$\sum_{n=1}^{3} \hat{S}_{n}^{m} \frac{\partial \hat{T}_{\beta}^{n}}{\partial t} = -J_{\beta}^{m} - \nabla_{\beta} v^{m} - \sum_{i=1}^{3} v^{i} \hat{Z}_{\beta i}^{m}.$$
(3.10)

Here  $J_{\beta}^{m}$  are the components of the tensor **J**. This tensor is the purely real space

version of the tensor  $\mathbf{j}$ . It is also called the tensor of the *Burgers vector flow density*. The components of the tensor  $\mathbf{J}$  are given by the formula (2.9) in [3]:

$$J_{\beta}^{m} = \sum_{n=1}^{3} \hat{S}_{n}^{m} j_{\beta}^{n}.$$
(3.11)

Apart from (3.11), let's recall also the formula (2.10) from [3]. It can be written as

$$\theta_{\beta}^{m} = -J_{\beta}^{m} + \sum_{i=1}^{3} v^{i} \left( \hat{Z}_{i\beta}^{m} - \hat{Z}_{\beta i}^{m} \right).$$
(3.12)

The tensor  $\theta$  with the components (3.12) is called the tensor of the rate of plastic relaxation. Applying (3.12) to (3.10), we derive the following formula:

$$\sum_{n=1}^{3} \hat{S}_{n}^{m} \frac{\partial \hat{T}_{\beta}^{n}}{\partial t} = \theta_{\beta}^{m} - \nabla_{\beta} v^{m} - \sum_{i=1}^{3} v^{i} \hat{Z}_{i\beta}^{m}.$$
(3.13)

Now let's apply (3.13) in order to transform the above expression for  $\partial f / \partial y^{\gamma}$ :

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3} v^{i} \nabla_{i} f = -\sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha\beta} [2] f \left(\theta_{\alpha}^{m} g_{m\beta} - \nabla_{\alpha} v^{m} g_{m\beta} + \theta_{\beta}^{m} g_{\alpha m} - \nabla_{\beta} v^{m} g_{\alpha m}\right) - \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha\beta} [3] f \left(\theta_{\alpha}^{m} \hat{G}_{m\beta} - \nabla_{\beta} v^{m} \hat{G}_{\alpha m} - \nabla_{\beta} v^{m} \hat{G}_{\alpha m}\right) + \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla_{\beta}^{\alpha} [4] f \times \\
\times \left(\theta_{m}^{\beta} R_{\alpha}^{m} - \nabla_{m} v^{\beta} R_{\alpha}^{m} - \theta_{\alpha}^{m} R_{m}^{\beta} + \nabla_{\alpha} v^{m} R_{m}^{\beta}\right).$$
(3.14)

The result obtained in the formula (3.14) is formulated as the following theorem.

**Theorem 3.2.** The specific free energy function f of a dislocated crystalline medium is an extended scalar field satisfying the differential equation (3.14).

#### 4. BALANCE EQUATIONS. THE DYNAMICS AND THERMODYNAMICS.

Like in [5], here we shall develop the theory on the base of the balance equations. The first balance equation is very simple. This is the mass balance equation:

$$\partial_t \rho + \sum_{k=1}^3 \nabla_k (\rho v^k) = 0.$$
(4.1)

The momentum balance equation looks not much more complicated than (4.1):

$$\partial_t (\rho v^i) + \sum_{k=1}^3 \nabla_k \Pi^{ik} = f^i.$$
(4.2)

However, the whole complexity of this equation is hidden in the tensor  $\Pi$ . As for the quantities  $f^i$  in the right hand side of (4.2), they are the components of the vector **f**. They define the density of volume forces acting upon the medium. The components of the tensor  $\Pi$  are given by the following formula:

$$\Pi^{ik} = \rho \, v^i \, v^k - \sigma^{ik} - \tilde{\sigma}^{ik}. \tag{4.3}$$

Here  $\sigma^{ik}$  and  $\tilde{\sigma}^{ik}$  are the components of two stress tensors  $\sigma$  and  $\tilde{\sigma}$  respectively. The first of them  $\sigma$  is the *regular stress tensor*, we shall study it in more details a little bit later below. The second tensor  $\tilde{\sigma}$  in the formula (4.3) is the *viscosity stress tensor*. Its components are given by the formula

$$\tilde{\sigma}^{ik} = \frac{1}{2} \sum_{j=1}^{3} \sum_{q=1}^{3} \eta^{ikjq} \left( \nabla_{j} v_{q} + \nabla_{q} v_{j} \right), \tag{4.4}$$

where  $\eta^{ikjq}$  are the components of the viscosity tensor  $\eta$ .

The third balance equation expresses the *energy balance* in a medium. This equation is written in the following form:

$$\partial_t \left( \frac{\rho \, |\mathbf{v}|^2}{2} + \rho \, \varepsilon \right) + \sum_{k=1}^3 \nabla_k w^k = e. \tag{4.5}$$

Here  $\varepsilon$  is the *specific inner thermal energy*. We shall discuss it a little bit later below along with the regular stress tensor  $\sigma$ . The quantities  $w^k$  in (4.5) are the components of the vector **w**. They are given by the formula

$$w^{k} = \frac{\rho |\mathbf{v}|^{2}}{2} v^{k} + \rho \varepsilon v^{k} - \sum_{i=1}^{3} v_{i} \sigma^{ik} - \sum_{i=1}^{3} v_{i} \tilde{\sigma}^{ik} - \sum_{i=1}^{3} \nabla_{i} T \varkappa^{ik}.$$
 (4.6)

The vector **w** with the components (4.6) is responsible for the energy transport in a medium. It is called the *energy flow density vector*. The first two terms in the right hand side of (4.6) correspond to the energy transported with the mass flow. The next two terms represent the work performed by the stress forces. And the last term describes the *heat conductivity phenomenon*. The quantities  $\varkappa^{ik}$  are the components of the heat conductivity tensor.

The quantity e in the right hand side of (4.5) describes the energy sources within the bulk of a medium. In the simplest case the energy is produced by the work of the volume force **f**. In this case we can write

$$e = \sum_{i=1}^{3} v_i f^i, \tag{4.7}$$

where  $f^i$  are the same as in (4.2). They are the components of the vector **f**.

Our further goal is to specify the above three balance equations (4.1), (4.2), and (4.5) for the case of a crystalline medium with dislocations. The specific inner thermal energy  $\varepsilon$  is related to the specific free energy f as follows:

$$\varepsilon = T \, s + f. \tag{4.8}$$

Here s is the specific entropy. It is derived from f by means of the formula

$$s = -\frac{\partial f}{\partial T}.\tag{4.9}$$

In this form the formula (4.9) is applicable to (2.8) and to (2.12) as well. However, applying it to (2.12), we can use the notations introduced in [6]:

$$s = -\nabla[1]f = s(t, p, T, \mathbf{g}, \hat{\mathbf{G}}, \mathbf{R}, \rho).$$

$$(4.10)$$

Applying (4.9) to the function (2.8), we obtain the following equality:

$$s = -\frac{\partial F}{\partial T} = S(T, \mathbf{\bar{G}}, \mathbf{\dot{g}}, \mathbf{\bar{R}}, \rho).$$
(4.11)

The functions S and s in the right hand sides of (4.11) and (4.10) are related to each other in the same way as the functions F and f in (2.8) and (2.12). For this reason we can write the differential equations

$$\nabla_{\gamma}s = -\sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\nabla^{\alpha\beta}[2]s\left(\hat{Z}_{\gamma\alpha}^{m} g_{m\beta} + \hat{Z}_{\gamma\beta}^{m} g_{\alpha m}\right) - \\ -\sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\nabla^{\alpha\beta}[3]s\left(\hat{Z}_{\gamma\alpha}^{m} \hat{G}_{m\beta} + \hat{Z}_{\gamma\beta}^{m} \hat{G}_{\alpha m}\right) + \\ +\sum_{n=1}^{3}\sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\nabla^{\alpha\beta}[4]s\left(\hat{Z}_{\gamma m}^{\beta} R_{\alpha}^{m} - \hat{Z}_{\gamma\alpha}^{m} R_{m}^{\beta}\right), \\ \frac{\partial s}{\partial t} + \sum_{i=1}^{3}v^{i}\nabla_{i}s = -\sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\nabla^{\alpha\beta}[2]s\left(\theta_{\alpha}^{m} g_{m\beta} - \nabla_{\alpha}v^{m} g_{m\beta} + \\ +\theta_{\beta}^{m} g_{\alpha m} - \nabla_{\beta}v^{m} g_{\alpha m}\right) - \sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\nabla^{\alpha\beta}[3]s\left(\theta_{\alpha}^{m} \hat{G}_{m\beta} - \\ -\nabla_{\alpha}v^{m} \hat{G}_{m\beta} + \theta_{\beta}^{m} \hat{G}_{\alpha m} - \nabla_{\beta}v^{m} \hat{G}_{\alpha m}\right) + \sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\nabla^{\alpha}_{\beta}[4]s\times$$

$$(4.13)$$

$$\times \left(\theta_m^\beta \ R_\alpha^m - \nabla_m v^\beta \ R_\alpha^m - \theta_\alpha^m \ R_m^\beta + \nabla_\alpha v^m \ R_m^\beta\right)$$

**Theorem 4.1.** The specific entropy of a dislocated crystalline medium s is an extended scalar field satisfying the differential equations (4.12) and (4.13).

It is known that S is a monotonic function of T in (4.11). The same is true for s in (4.10). Moreover, we have the thermodynamical inequalities (see [7]):

$$\frac{\partial S}{\partial T} > 0, \qquad \qquad \frac{\partial s}{\partial T} > 0. \tag{4.14}$$

This means that we can introduce the inverse functions

$$T = T(s, \mathbf{\bar{G}}, \mathbf{\check{g}}, \mathbf{\bar{R}}, \rho), \qquad T = T(t, p, s, \mathbf{g}, \mathbf{\hat{G}}, \mathbf{R}, \rho).$$
(4.15)

Applying the inequalities (4.14) to the functions (4.10) and (4.11), we derive

$$c = T \frac{\partial s}{\partial T} > 0.$$

Here c is the specific heat capacity of a medium for the case where the density  $\rho$  and the other arguments t, p, g,  $\hat{\mathbf{G}}$ ,  $\mathbf{R}$ ,  $\mathbf{G}$ ,  $\mathbf{g}$ ,  $\mathbf{R}$  in (4.10) and (4.11) are constants.

Let's substitute the temperature expressed in the form of the function (4.15) into (4.8). As a result we get two functions

$$\varepsilon = E(s, \mathbf{\bar{G}}, \mathbf{\dot{g}}, \mathbf{\bar{R}}, \rho), \qquad \varepsilon = \varepsilon(t, p, s, \mathbf{g}, \mathbf{\bar{G}}, \mathbf{R}, \rho). \tag{4.16}$$

Passing from (2.8) and (2.12) to the functions (4.16), we perform the so-called *Legendre transformations*. The functions (4.15) are related to each other through (2.9), (2.10), and (2.11). The same is true for the functions (4.16). The second function in (4.16) is an extended scalar field, though with the slightly different set of arguments than in (2.12). From (2.9), (2.10), (2.11), and (4.16) we derive

$$\nabla^{\alpha\beta}[2]\varepsilon = \frac{\partial\varepsilon}{\partial g_{\alpha\beta}} = \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial E}{\partial \overline{G}_{ij}} \, \hat{S}_{i}^{\alpha} \, \hat{S}_{j}^{\beta}, \qquad (4.17)$$

$$\nabla^{\alpha\beta}[3]\varepsilon = \frac{\partial\varepsilon}{\partial\hat{G}_{\alpha\beta}} = \sum_{i=1}^{3}\sum_{j=1}^{3}\frac{\partial E}{\partial\hat{g}_{ij}}\,\hat{S}_{i}^{\alpha}\,\hat{S}_{j}^{\beta},\tag{4.18}$$

$$\nabla^{\alpha}_{\beta}[4]\varepsilon = \frac{\partial\varepsilon}{\partial R^{\beta}_{\alpha}} = \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\partial E}{\partial \overline{R}^{i}_{j}} \hat{S}^{\alpha}_{j} \hat{T}^{i}_{\beta}.$$
(4.19)

Applying (4.17), (4.18), (4.19), and the formula (13.15) from [6], we get

$$\nabla_{\gamma}\varepsilon = -\sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\nabla^{\alpha\beta}[2]\varepsilon \left(\hat{Z}_{\gamma\alpha}^{m} g_{m\beta} + \hat{Z}_{\gamma\beta}^{m} g_{\alpha m}\right) - \sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\nabla^{\alpha\beta}[3]\varepsilon \left(\hat{Z}_{\gamma\alpha}^{m} \hat{G}_{m\beta} + \hat{Z}_{\gamma\beta}^{m} \hat{G}_{\alpha m}\right) + \sum_{n=1}^{3}\sum_{m=1}^{3}\sum_{\alpha=1}^{3}\sum_{\beta=1}^{3}\nabla_{\beta}^{\alpha}[4]\varepsilon \left(\hat{Z}_{\gamma m}^{\beta} R_{\alpha}^{m} - \hat{Z}_{\gamma\alpha}^{m} R_{m}^{\beta}\right),$$
(4.20)

Like the equation (3.1), the equation (4.20) can be simplified by means of (3.7):

$$\hat{\nabla}_{\gamma}\varepsilon = 0. \tag{4.21}$$

Note that the remark following the formula (3.8) is valid for the covariant derivatives  $\nabla_{\gamma}$  and  $\hat{\nabla}_{\gamma}$  in the above formulas (4.20) and (4.21) as well.

**Theorem 4.2.** The specific inner thermal energy  $\varepsilon$  of a dislocated crystalline medium is an extended scalar field satisfying the differential equation (4.20), or the differential equation (4.21) equivalent to it.

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From (4.16), (4.17), (4.18), (4.19), and from (4.20), applying (3.13), we obtain

$$\frac{\partial \varepsilon}{\partial t} + \sum_{i=1}^{3} v^{i} \nabla_{i} \varepsilon = -\sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha\beta} [2] \varepsilon \left( \theta^{m}_{\alpha} g_{m\beta} - \nabla_{\alpha} v^{m} g_{m\beta} + \right. \\ \left. + \theta^{m}_{\beta} g_{\alpha m} - \nabla_{\beta} v^{m} g_{\alpha m} \right) - \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha\beta} [3] \varepsilon \left( \theta^{m}_{\alpha} \hat{G}_{m\beta} - \right. \\ \left. - \nabla_{\alpha} v^{m} \hat{G}_{m\beta} + \theta^{m}_{\beta} \hat{G}_{\alpha m} - \nabla_{\beta} v^{m} \hat{G}_{\alpha m} \right) + \sum_{m=1}^{3} \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha}_{\beta} [4] \varepsilon \times \\ \left. \times \left( \theta^{\beta}_{m} R^{m}_{\alpha} - \nabla_{m} v^{\beta} R^{m}_{\alpha} - \theta^{m}_{\alpha} R^{\beta}_{m} + \nabla_{\alpha} v^{m} R^{\beta}_{m} \right). \end{aligned}$$

$$(4.22)$$

**Theorem 4.3.** The specific inner thermal energy  $\varepsilon$  of a dislocated crystalline medium is an extended scalar field satisfying the differential equation (4.22).

The equalities (4.17), (4.18), and (4.19) should be completed with the following one being analogous to the equality (4.9):

$$T = \frac{\partial \varepsilon}{\partial s}.$$
(4.23)

The equality (4.23) applies to both functions (4.16) and to both functions (4.15):

$$T(s, \mathbf{\bar{G}}, \mathbf{g}, \mathbf{\bar{R}}, \rho) = \frac{\partial \varepsilon(s, \mathbf{\bar{G}}, \mathbf{g}, \mathbf{\bar{R}}, \rho)}{\partial s},$$
$$T(t, p, s, \mathbf{g}, \mathbf{\hat{G}}, \mathbf{R}, \rho) = \frac{\partial \varepsilon(t, p, s, \mathbf{g}, \mathbf{\hat{G}}, \mathbf{R}, \rho)}{\partial s} = \nabla[1]\varepsilon.$$
(4.24)

Now let's return to the balance equation (4.5). Substituting (4.6) and (4.7) into (4.5), then taking into account other two balance equations (4.1), (4.2) and the formula (4.3), for the function  $\varepsilon$  we derive

$$\rho \,\partial_t \varepsilon + \sum_{k=1}^3 \rho \, v^k \,\partial_k \varepsilon = \sum_{i=1}^3 \sum_{k=1}^3 \left( \nabla_k v_i \left( \sigma^{ik} + \tilde{\sigma}^{ik} \right) + \nabla_k \left( \nabla_i T \,\varkappa^{ik} \right) \right). \tag{4.25}$$

(see more details in [5]). All tensor fields in the balance equations (4.1), (4.2), (4.5) and in the formulas (4.3), (4.4), (4.6), (4.7), (4.25) are treated as regular (not extended) tensor fields and covariant derivatives  $\nabla_k$  and  $\nabla_i$  are understood as regular covariant derivatives different from those in left hand sides of (4.20) and (4.22). The partial derivative  $\partial_t \varepsilon$  is expressed through  $\partial \varepsilon / \partial t$  in (4.22) as follows:

$$\partial_t \varepsilon = \frac{\partial \varepsilon}{\partial t} + \nabla [1] \varepsilon \ \partial_t s + \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \nabla^{\alpha\beta} [2] \varepsilon \ \partial_t g_{\alpha\beta} + \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \nabla^{\alpha\beta} [3] \varepsilon \ \partial_t \hat{G}_{\alpha\beta} + \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \nabla^{\alpha}_{\beta} [4] \varepsilon \ \partial_t R^{\beta}_{\alpha} + \nabla [5] \varepsilon \ \partial_t \rho.$$

$$(4.26)$$

Similarly, for the partial derivative  $\partial_k \varepsilon$  in (4.25) we can derive the formula expressing it through the covariant derivative (4.20):

$$\partial_k \varepsilon = \nabla_k \varepsilon + \overline{\nabla}[1] \varepsilon \ \partial_k s + \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \overline{\nabla}^{\alpha\beta}[2] \varepsilon \ \nabla_k g_{\alpha\beta} + \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \overline{\nabla}^{\alpha\beta}[3] \varepsilon \ \nabla_k \hat{G}_{\alpha\beta} + \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \overline{\nabla}^{\alpha}_{\beta}[4] \varepsilon \ \nabla_k R^{\beta}_{\alpha} + \overline{\nabla}[5] \varepsilon \ \partial_k \rho.$$

$$(4.27)$$

In deriving (4.27) we used the formula (17.9) from [6]. Now let's use (4.24), (4.26), and (4.27) in order to calculate the following expression:

$$\partial_{t}\varepsilon + \sum_{k=1}^{3} v^{k} \partial_{k}\varepsilon = \left(\frac{\partial\varepsilon}{\partial t} + \sum_{k=1}^{3} v^{k} \nabla_{k}\varepsilon\right) + T\left(\partial_{t}s + \sum_{k=1}^{3} v^{k} \partial_{k}s\right) + \\ + \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha\beta}[3]\varepsilon \left(\partial_{t}\hat{G}_{\alpha\beta} + \sum_{k=1}^{3} v^{k} \nabla_{k}\hat{G}_{\alpha\beta}\right) + \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha}_{\beta}[4]\varepsilon \times \\ \times \left(\partial_{t}R^{\beta}_{\alpha} + \sum_{k=1}^{3} v^{k} \nabla_{k}R^{\beta}_{\alpha}\right) + \nabla[5]\varepsilon \left(\partial_{t}\rho + \sum_{k=1}^{3} v^{k} \partial_{k}\rho\right).$$
(4.28)

The terms containing  $\partial_t g_{\alpha\beta}$  and  $\nabla_k g_{\alpha\beta}$  do vanish due to the following equalities:

$$\partial_t g_{\alpha\beta} = 0, \qquad \nabla_k g_{\alpha\beta} = 0.$$

$$(4.29)$$

The first equality (4.29) is obvious: the metric tensor **g** is a geometric equipment of the real space  $\mathbb{E}$ , its components are constants. The second equality (4.29) expresses the concordance condition for the metric and connection (see [8] and [9]).

Let's apply the formula (4.22) and the first balance equation (4.1) in order to transform the equality (4.28). As a result we write it as follows:

$$\partial_{t}\varepsilon + \sum_{k=1}^{3} v^{k} \partial_{k}\varepsilon = T\left(\partial_{t}s + \sum_{k=1}^{3} v^{k} \partial_{k}s\right) + \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha\beta}[2]\varepsilon \times \\ \times \left(\nabla_{\alpha}v_{\beta} + \nabla_{\beta}v_{\alpha} - \sum_{m=1}^{3} \left(\theta_{\alpha}^{m} g_{m\beta} + \theta_{\beta}^{m} g_{\alpha m}\right)\right) + \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha\beta}[3]\varepsilon \times \\ \times \left(\partial_{t}\hat{G}_{\alpha\beta} + \sum_{k=1}^{3} v^{k} \nabla_{k}\hat{G}_{\alpha\beta} + \sum_{m=1}^{3} \nabla_{\alpha}v^{m} \hat{G}_{m\beta} + \sum_{m=1}^{3} \nabla_{\beta}v^{m} \hat{G}_{\alpha m} - \\ - \sum_{m=1}^{3} \theta_{\alpha}^{m} \hat{G}_{m\beta} - \sum_{m=1}^{3} \theta_{\beta}^{m} \hat{G}_{\alpha m}\right) + \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla_{\beta}^{\alpha}[4]\varepsilon \left(\partial_{t}R_{\alpha}^{\beta} + \\ + \sum_{k=1}^{3} v^{k} \nabla_{k}R_{\alpha}^{\beta} - \sum_{m=1}^{3} \nabla_{m}v^{\beta} R_{\alpha}^{m} + \sum_{m=1}^{3} \nabla_{\alpha}v^{m} R_{m}^{\beta} + \sum_{m=1}^{3} \theta_{m}^{\beta} R_{\alpha}^{m} - \\ - \sum_{m=1}^{3} \theta_{\alpha}^{m} R_{m}^{\beta}\right) + \sum_{k=1}^{3} \nabla[5]\varepsilon \rho \nabla_{k}v^{k}.$$

Now it is worth to remember the differential equation for the elastic deformation tensor  $\hat{\mathbf{G}}$ . It was suggested empirically for plastic media in [5]. Later it was derived for dislocated crystalline media in [1] (see formula (3.8) over there):

$$\frac{\partial \hat{G}_{kq}}{\partial t} + \sum_{r=1}^{3} v^{r} \nabla_{r} \hat{G}_{kq} = -\sum_{r=1}^{3} \nabla_{k} v^{r} \hat{G}_{rq} - \sum_{r=1}^{3} \hat{G}_{kr} \nabla_{q} v^{r} + \sum_{r=1}^{3} \theta_{k}^{r} \hat{G}_{rq} + \sum_{r=1}^{3} \hat{G}_{kr} \theta_{q}^{r}.$$
(4.31)

Comparing (4.31) and (4.30), we find that the term with  $\nabla^{\alpha\beta}[3]\varepsilon$  in (4.30) vanishes due to the equation (4.31). As a result we get

$$\partial_{t}\varepsilon + \sum_{k=1}^{3} v^{k} \partial_{k}\varepsilon = T\left(\partial_{t}s + \sum_{k=1}^{3} v^{k} \partial_{k}s\right) + \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla^{\alpha\beta}[2]\varepsilon \times \left(\nabla_{\alpha}v_{\beta} + \nabla_{\beta}v_{\alpha} - \sum_{m=1}^{3} \left(\theta_{\alpha}^{m} g_{m\beta} + \theta_{\beta}^{m} g_{\alpha m}\right)\right) + \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla_{\beta}^{\alpha}[4]\varepsilon \times \left(\partial_{t}R_{\alpha}^{\beta} + \sum_{k=1}^{3} v^{k} \nabla_{k}R_{\alpha}^{\beta} - \sum_{m=1}^{3} \nabla_{m}v^{\beta} R_{\alpha}^{m} + \sum_{m=1}^{3} \nabla_{\alpha}v^{m} R_{m}^{\beta} + \sum_{m=1}^{3} \theta_{m}^{\beta} R_{\alpha}^{m} - \sum_{m=1}^{3} \theta_{\alpha}^{m} R_{m}^{\beta}\right) + \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla[5]\varepsilon \rho g^{\alpha\beta} \nabla_{\alpha}v_{\beta}.$$

$$(4.32)$$

In the next step we should recall the differential equation that determines the time evolution of the tensor  $\mathbf{R}$  (see (4.11) in [3] or (4.1) in [4]):

$$\frac{\partial R_{\alpha}^{\beta}}{\partial t} = \sum_{m=1}^{3} J_{m}^{\beta} R_{\alpha}^{m} + \sum_{m=1}^{3} \nabla_{m} v^{\beta} R_{\alpha}^{m} + \sum_{m=1}^{3} \sum_{p=1}^{3} v^{p} \hat{Z}_{mp}^{\beta} R_{\alpha}^{m} - \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{s=1}^{3} g_{\alpha m} \, \omega^{mrs} \, \nabla_{r} J_{s}^{\beta} - \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{p=1}^{3} g_{\alpha m} \, \omega^{mrs} \, \hat{Z}_{rp}^{\beta} J_{s}^{p}.$$

$$(4.33)$$

Let's apply the relationship (3.12) to the term  $J_m^{\beta}$  in the first sum of (4.33):

$$\frac{\partial R_{\alpha}^{\beta}}{\partial t} = -\sum_{m=1}^{3} \theta_{m}^{\beta} R_{\alpha}^{m} + \sum_{m=1}^{3} \nabla_{m} v^{\beta} R_{\alpha}^{m} + \sum_{m=1}^{3} \sum_{p=1}^{3} v^{p} \hat{Z}_{pm}^{\beta} R_{\alpha}^{m} - \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} g_{\alpha m} \, \omega^{mrs} \, \nabla_{r} J_{s}^{\beta} - \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{p=1}^{3} g_{\alpha m} \, \omega^{mrs} \, \hat{Z}_{rp}^{\beta} J_{s}^{p}.$$

$$(4.34)$$

Then let's recall that the formula (3.12) can be written in a different form:

$$J_{s}^{p} = -\theta_{s}^{p} + \sum_{\tau=1}^{3} \sum_{\gamma=1}^{3} \sum_{n=1}^{3} \omega_{\tau\gamma s} v^{\gamma} g^{\tau n} R_{n}^{p}$$
(4.35)

(see formula (2.13) in [3]). Before substituting (4.35) into the equation (4.34) let's recall the following purely algebraic identity (it was already used in [2] and [3]):

$$\sum_{s=1}^{3} \omega_{\tau\gamma s} \,\omega^{mrs} = \delta_{\tau}^{m} \,\delta_{\gamma}^{r} - \delta_{\gamma}^{m} \,\delta_{\tau}^{r}. \tag{4.36}$$

Here  $\delta_{\tau}^{m}$ ,  $\delta_{\gamma}^{r}$ ,  $\delta_{\gamma}^{m}$ , and  $\delta_{\tau}^{r}$  are Kronecker  $\delta$ -symbols. Now substituting (4.35) into the last term of (4.34) and taking into account (4.36), we derive

$$\begin{split} \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{p=1}^{3} g_{\alpha m} \, \omega^{mrs} \, \hat{Z}_{rp}^{\beta} \, J_{s}^{p} = -\sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{p=1}^{3} g_{\alpha m} \, \omega^{mrs} \, \hat{Z}_{rp}^{\beta} \, \theta_{s}^{p} \, + \\ & + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{p=1}^{3} \sum_{\tau=1}^{3} \sum_{\gamma=1}^{3} \sum_{n=1}^{3} \sum_{n=1}^{3} g_{\alpha m} \, \omega^{mrs} \, \hat{Z}_{rp}^{\beta} \, \omega_{\tau\gamma s} \, v^{\gamma} \, g^{\tau n} \, R_{n}^{p} = \\ & = -\sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{p=1}^{3} g_{\alpha m} \, \omega^{mrs} \, \hat{Z}_{rp}^{\beta} \, \theta_{s}^{p} \, + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{p=1}^{3} \sum_{\tau=1}^{3} \sum_{\gamma=1}^{3} \sum_{n=1}^{3} g_{\alpha m} \, \omega^{mrs} \, \hat{Z}_{rp}^{\beta} \, \theta_{s}^{p} \, + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{p=1}^{3} \sum_{n=1}^{3} \sum_{r=1}^{3} \sum_{p=1}^{3} \sum_{r=1}^{3} \sum_{p=1}^{3} \sum_{n=1}^{3} \sum_{r=1}^{3} \sum_{p=1}^{3} \sum_{r=1}^{3} \sum_{r=1}^{3} \sum_{p=1}^{3} \sum_{r=1}^{3} \sum_{r=1}^{3} \sum_{p=1}^{3} \sum$$

Applying this result to the equation (4.34), we can write this equation as follows:

$$\frac{\partial R_{\alpha}^{\beta}}{\partial t} = -\sum_{m=1}^{3} \theta_{m}^{\beta} R_{\alpha}^{m} + \sum_{m=1}^{3} \nabla_{m} v^{\beta} R_{\alpha}^{m} + \sum_{r=1}^{3} \sum_{p=1}^{3} \sum_{n=1}^{3} v_{\alpha} \hat{Z}_{rp}^{\beta} g^{rn} R_{n}^{p} - \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} g_{\alpha m} \omega^{mrs} \nabla_{r} J_{s}^{\beta} + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{p=1}^{3} g_{\alpha m} \omega^{mrs} \hat{Z}_{rp}^{\beta} \theta_{s}^{p}.$$

$$(4.37)$$

Now let's apply the operator  $\nabla_r$  to the equality (4.35). As a result we obtain

$$\nabla_{r} J_{s}^{\beta} = -\nabla_{r} \theta_{s}^{\beta} + \sum_{\tau=1}^{3} \sum_{\gamma=1}^{3} \sum_{n=1}^{3} \omega_{\tau\gamma s} \nabla_{r} v^{\gamma} g^{\tau n} R_{n}^{\beta} + \sum_{\tau=1}^{3} \sum_{\gamma=1}^{3} \sum_{n=1}^{3} \omega_{\tau\gamma s} v^{\gamma} g^{\tau n} \nabla_{r} R_{n}^{\beta}.$$

$$(4.38)$$

Taking into account (4.38) and (4.36), we can perform the following calculations:

$$\sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} g_{\alpha m} \,\omega^{mrs} \,\nabla_{r} J_{s}^{\beta} = -\sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} g_{\alpha m} \,\omega^{mrs} \,\nabla_{r} \theta_{s}^{\beta} + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{\tau=1}^{3} \sum_{r=1}^{3} \sum_{n=1}^{3} g_{\alpha m} \,\omega^{mrs} \,\omega_{\tau\gamma s} \,\nabla_{r} v^{\gamma} \,g^{\tau n} \,R_{n}^{\beta} +$$

$$\begin{split} &+ \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{\tau=1}^{3} \sum_{\gamma=1}^{3} \sum_{n=1}^{3} g_{\alpha m} \ \omega^{mrs} \ \omega_{\tau\gamma s} \ v^{\gamma} \ g^{\tau n} \ \nabla_{r} R_{n}^{\beta} = - \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} g_{\alpha m} \times \\ &\times \omega^{mrs} \ \nabla_{r} \theta_{s}^{\beta} + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{\tau=1}^{3} \sum_{\gamma=1}^{3} \sum_{n=1}^{3} g_{\alpha m} \left( \delta_{\tau}^{m} \ \delta_{\gamma}^{r} - \delta_{\gamma}^{m} \ \delta_{\tau}^{r} \right) \nabla_{r} v^{\gamma} \ g^{\tau n} \ R_{n}^{\beta} + \\ &+ \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{\gamma=1}^{3} \sum_{n=1}^{3} \sum_{n=1}^{3} g_{\alpha m} \left( \delta_{\tau}^{m} \ \delta_{\gamma}^{r} - \delta_{\gamma}^{m} \ \delta_{\tau}^{r} \right) v^{\gamma} \ g^{\tau n} \ \nabla_{r} R_{n}^{\beta} = \\ &= - \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} g_{\alpha m} \ \omega^{mrs} \ \nabla_{r} \theta_{s}^{\beta} + \sum_{r=1}^{3} \nabla_{r} v^{r} \ R_{\alpha}^{\beta} - \sum_{r=1}^{3} \sum_{n=1}^{3} \nabla_{r} v_{\alpha} \ g^{rn} \ R_{n}^{\beta} + \\ &+ \sum_{r=1}^{3} v^{r} \ \nabla_{r} R_{\alpha}^{\beta} - \sum_{r=1}^{3} \sum_{n=1}^{3} v_{\alpha} \ g^{rn} \ \nabla_{r} R_{n}^{\beta}. \end{split}$$

The result of these calculations is used in order to transform the equation (4.37):

$$\frac{\partial R_{\alpha}^{\beta}}{\partial t} = -\sum_{m=1}^{3} \theta_{m}^{\beta} R_{\alpha}^{m} + \sum_{m=1}^{3} \nabla_{m} v^{\beta} R_{\alpha}^{m} + \sum_{r=1}^{3} \sum_{p=1}^{3} \sum_{n=1}^{3} v_{\alpha} \hat{Z}_{rp}^{\beta} g^{rn} R_{n}^{p} - \sum_{r=1}^{3} \left( \nabla_{r} v^{r} R_{\alpha}^{\beta} + v^{r} \nabla_{r} R_{\alpha}^{\beta} \right) + \sum_{r=1}^{3} \sum_{n=1}^{3} g^{rn} \left( \nabla_{r} v_{\alpha} R_{n}^{\beta} + v_{\alpha} \nabla_{r} R_{n}^{\beta} \right) + \left( 4.39 \right) + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} g_{\alpha m} \omega^{mrs} \nabla_{r} \theta_{s}^{\beta} + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} g_{\alpha m} \omega^{mrs} \hat{Z}_{rp}^{\beta} \theta_{s}^{p}.$$

The following identity is known as the zero divergency condition (see (4.8) in [3]):

$$\sum_{r=1}^{3} \sum_{r=1}^{3} g^{rn} \nabla_{r} R_{n}^{\beta} + \sum_{p=1}^{3} \sum_{r=1}^{3} \sum_{n=1}^{3} \hat{Z}_{rp}^{\beta} g^{rn} R_{n}^{p} = 0.$$
(4.40)

Applying (4.40) to (4.39), we find that two terms in (4.39) are canceled:

$$\frac{\partial R_{\alpha}^{\beta}}{\partial t} = \sum_{m=1}^{3} \nabla_{m} v^{\beta} R_{\alpha}^{m} - \sum_{r=1}^{3} \nabla_{r} v^{r} R_{\alpha}^{\beta} - \sum_{r=1}^{3} v^{r} \nabla_{r} R_{\alpha}^{\beta} + \sum_{r=1}^{3} \sum_{n=1}^{3} g^{rn} \nabla_{r} v_{\alpha} R_{n}^{\beta} + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} g_{\alpha m} \omega^{mrs} \nabla_{r} \theta_{s}^{\beta} + (4.41) + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{p=1}^{3} g_{\alpha m} \omega^{mrs} \hat{Z}_{rp}^{\beta} \theta_{s}^{p} - \sum_{m=1}^{3} \theta_{m}^{\beta} R_{\alpha}^{m}.$$

Having completed the transformations of the differential equation (4.33), now we return to the formula (4.32). Substituting (4.41) into (4.32), we obtain

$$\partial_t \varepsilon + \sum_{k=1}^3 v^k \,\partial_k \varepsilon = T\left(\partial_t s + \sum_{k=1}^3 v^k \,\partial_k s\right) + \sum_{\alpha=1}^3 \sum_{\beta=1}^3 \nabla^{\alpha\beta} [2]\varepsilon \times$$

$$\times \left( \nabla_{\alpha} v_{\beta} + \nabla_{\beta} v_{\alpha} - \sum_{m=1}^{3} \left( \theta_{\alpha}^{m} g_{m\beta} + \theta_{\beta}^{m} g_{\alpha m} \right) \right) + \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla_{\beta}^{\alpha} [4] \varepsilon \times \\ \times \left( \sum_{m=1}^{3} \nabla_{\alpha} v^{m} R_{m}^{\beta} - \sum_{r=1}^{3} \nabla_{r} v^{r} R_{\alpha}^{\beta} + \sum_{r=1}^{3} \sum_{n=1}^{3} g^{rn} \nabla_{r} v_{\alpha} R_{n}^{\beta} + \\ + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} g_{\alpha m} \omega^{mrs} \nabla_{r} \theta_{s}^{\beta} + \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{s=1}^{3} \sum_{p=1}^{3} g_{\alpha m} \omega^{mrs} \hat{Z}_{rp}^{\beta} \theta_{s}^{p} - \\ - \sum_{m=1}^{3} \theta_{\alpha}^{m} R_{m}^{\beta} \right) + \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \nabla [5] \varepsilon \rho g^{\alpha \beta} \nabla_{\alpha} v_{\beta}.$$

Let's perform some rearrangement of terms in the above equality. We write it as

$$\partial_t \varepsilon + \sum_{k=1}^3 v^k \,\partial_k \varepsilon = T\left(\partial_t s + \sum_{k=1}^3 v^k \,\partial_k s\right) + \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^3 T \times \frac{\nabla_k \left(P^{kij} \,\theta_{ij}\right)}{\rho} + \sum_{i=1}^3 \sum_{j=1}^3 \frac{\sigma^{ij} \,\nabla_i v_j}{\rho} - \sum_{i=1}^3 \sum_{j=1}^3 \frac{\mathfrak{S}^{ij} \,\theta_{ij}}{\rho}.$$

$$(4.42)$$

For this purpose we introduce some auxiliary notations. We denote

$$\theta_{ij} = \sum_{k=1}^{3} g_{ik} \; \theta_j^{\;k}. \tag{4.43}$$

It is easy to see that the formula (4.42) expresses the standard index lowering procedure. The other notations are less trivial. We denote

$$P^{kij} = \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \sum_{m=1}^{3} \frac{\rho \ g^{\beta i} \ g_{\alpha m} \ \omega^{mkj}}{T} \ \nabla_{\beta}^{\alpha}[4]\varepsilon.$$

$$(4.44)$$

The quantities (4.43) define a tensor field of the type (3,0). Then we introduce the symmetric tensor field  $\sigma$  of the type (2,0):

$$\sigma^{ij} = \rho \left( \nabla^{ij}_{\beta}[2]\varepsilon + \nabla^{ji}[2]\varepsilon \right) +$$

$$+ \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \rho \left( \nabla^{j}_{\beta}[4]\varepsilon R^{\beta}_{\alpha} g^{\alpha i} + \nabla^{i}_{\beta}[4]\varepsilon R^{\beta}_{\alpha} g^{\alpha j} \right) -$$

$$- \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \rho \nabla^{\alpha}_{\beta}[4]\varepsilon R^{\beta}_{\alpha} g^{ij} + \rho^{2} \nabla[5]\varepsilon g^{ij}.$$

$$(4.45)$$

And finally, we introduce another tensor field of the type (2,0) with the components

$$\mathfrak{S}^{ij} = \rho \left( \nabla^{ij}[2]\varepsilon + \nabla^{ji}[2]\varepsilon \right) + \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \rho \nabla_{\beta}^{j}[4]\varepsilon R_{\alpha}^{\beta} g^{\alpha i} - \sum_{\alpha=1}^{3} \sum_{\beta=1}^{3} \sum_{m=1}^{3} \sum_{r=1}^{3} \sum_{p=1}^{3} \rho \nabla_{\beta}^{\alpha}[4]\varepsilon g_{\alpha m} \omega^{mrj} \hat{Z}_{rp}^{\beta} g^{pi} + \sum_{k=1}^{3} T \nabla_{k} P^{kij}.$$

$$(4.46)$$

Note that (4.45) is not simply a notation. The same symbol  $\sigma$  is used in (4.25) and in (4.3), where it represents the components of the regular stress tensor.

**Theorem 4.4.** In the case of frozen dislocations the components of the regular stress tensor  $\sigma$  are given by the formula (4.45).

*Proof.* Let's remember that the case of frozen dislocations is that very case where the dislocation lines move together with the medium like water-plants frozen into the ice (see [2]). In this case we have purely elastic response of the medium:

$$\theta_j^k = 0 \tag{4.47}$$

(see theorem 2.2 in [3]). From (4.43) and (4.47) we derive

$$\theta_{ij} = 0. \tag{4.48}$$

Let's substitute (4.48) into (4.42) and replace  $\sigma^{ij}$  by  $\hat{\sigma}^{ij}$  in this formula:

$$\partial_t \varepsilon + \sum_{k=1}^3 v^k \,\partial_k \varepsilon = T\left(\partial_t s + \sum_{k=1}^3 v^k \,\partial_k s\right) + \sum_{i=1}^3 \sum_{j=1}^3 \frac{\hat{\sigma}^{ij} \,\nabla_i v_j}{\rho}.\tag{4.49}$$

Then we substitute (4.49) into (4.25). Taking into account (4.3), (4.4), and the first balance equation (4.1), from we (4.25) derive

$$\frac{\partial(\rho s)}{\partial t} + \sum_{k=1}^{3} \nabla_{k} \left( \rho s v^{k} - \sum_{i=1}^{3} \frac{\nabla_{i} T \varkappa^{ik}}{T} \right) = \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{(\sigma^{ij} - \hat{\sigma}^{ij}) v_{ij}}{T} + \sum_{i=1}^{3} \sum_{k=1}^{3} \sum_{j=1}^{3} \sum_{q=1}^{3} \frac{v_{ik} \eta^{ikjq} v_{jq}}{T} + \sum_{i=1}^{3} \sum_{k=1}^{3} \frac{\nabla_{i} T \varkappa^{ik} \nabla_{k} T}{T^{2}},$$

$$(4.50)$$

where  $v_{ij}$  are determined by the following formula:

$$v_{ij} = \frac{\nabla_i v_j + \nabla_j v_i}{2}.$$
(4.51)

The equation (4.50) has a quite transparent interpretation. This is the entropy balance equation. Each term in its right hand side corresponds to some definite mechanism of entropy production. Last two terms correspond to viscosity and heat conductivity phenomena respectively. In the case of frozen dislocations, i. e. in the case of purely elastic medium response, we have no additional entropy production mechanisms. Hence, the first term in the right hand side of (4.50) should vanish:

$$\sigma^{ij} - \hat{\sigma}^{ij} = 0. \tag{4.52}$$

The equality (4.52) means that  $\hat{\sigma}^{ij}$  coincides with  $\sigma^{ij}$ , i. e. (4.45) is a true expression for the components of the regular stress tensor in the case of frozen dislocations. The theorem is proved.  $\Box$ 

**Conjecture 4.1.** The components of the regular stress tensor  $\sigma$  for a dislocated crystalline medium are always given by the formula (4.45).

Assuming that the conjecture 4.1 is valid, we substitute (4.42) into the equality (4.25). As a result from (4.25) we derive the entropy balance equation

$$\frac{\partial(\rho s)}{\partial t} + \sum_{k=1}^{3} \nabla_{k} \left( \rho s v^{k} - \sum_{i=1}^{3} \frac{\nabla_{i} T \varkappa^{ik}}{T} + \sum_{i=1}^{3} \sum_{j=1}^{3} P^{kij} \theta_{ij} \right) =$$

$$= \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\mathfrak{S}^{ij} \theta_{ij}}{T} + \sum_{i=1}^{3} \sum_{k=1}^{3} \sum_{j=1}^{3} \sum_{q=1}^{3} \frac{v_{ik} \eta^{ikjq} v_{jq}}{T} + \sum_{i=1}^{3} \sum_{k=1}^{3} \frac{\nabla_{i} T \varkappa^{ik} \nabla_{k} T}{T^{2}},$$
(4.53)

where  $v_{ik}$  and  $v_{jq}$  are determined by the formula (4.51).

#### 5. Some conclusions.

The equation (4.53) is a basic equation for understanding the thermodynamics of plasticity in crystals. It is similar to the equation (10.13) in [5]. However, there are some visible differences. In the left hand side of (4.53) we have the additional term produced by the tensor **P** with the components (4.44). It describes the entropy carried by moving dislocations. As for the first term in the right hand side of (4.53), it is also different from such a term in [5] since  $\sigma^{ij} \neq \mathfrak{S}^{ij}$  (compare (4.45) and (4.46) above). The entropy growth condition leads to the inequality

$$\sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\mathfrak{S}^{ij} \,\theta_{ij}}{T} \ge 0.$$

It is similar to (10.14) in [5]. Note that in the present theory we have no restrictions like det  $\hat{\mathbf{G}} = \det \mathbf{G}$  and det  $\check{\mathbf{G}} = 1$ . We got rid of them by including the density  $\rho$ as an explicit argument in (2.8) and (2.12). As a result we have no restriction for the trace of the matrix  $\theta_i^i$ . The symmetry condition for  $\theta_{ij}$  is also absent.

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