

Victor L. Berdichevsky

# Continuum theory of dislocations revisited

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**Abstract** The paper continues the discussion of continuum theory of dislocations suggested by Berdichevsky and Sedov (PMM 31(6): 981–1000, 1967). The major new points are: the choice of energy, the variational form of the governing dynamical equations, the variational principle for the final plastic state.

**Keywords** Continuum theory of dislocations · Plastic spin · Strain gradient plasticity

## 1 Introduction

Continuum theory of dislocations aims to describe the behavior of the ensembles of a huge number of dislocations by the methods of continuum mechanics. Complexity of the system makes the phenomenological approach the major tool of the theory. The number of possible phenomenological models is practically unbounded, and one needs some guiding principles to narrow down the feasible choices. Such guiding principles are the laws of thermodynamics. They govern the general structure of the basic equations. The standard thermodynamic approach applied to dislocation networks involves the three key assumptions: one has to choose the kinematic parameters of the dislocation network and specify the dependence of energy and dissipation on these parameters. The dynamic equations follow then from the usual procedure of the non-equilibrium thermodynamics. The most “rough” choice for the dislocation network kinematical parameters is just the average plastic strain tensor. The corresponding thermodynamic theory is the classical plasticity theory of crystals and polycrystals. The models of this theory may be considered as the simplest models of continuum theory of dislocations.

A natural complication of the classical plasticity is the theory which includes plastic rotations in the set of the dislocation network kinematical parameters in addition to plastic strains. An importance of such an extension may be seen from the following Gedankenexperiment. Consider a piece of a perfect two-dimensional lattice (Fig. 1a).

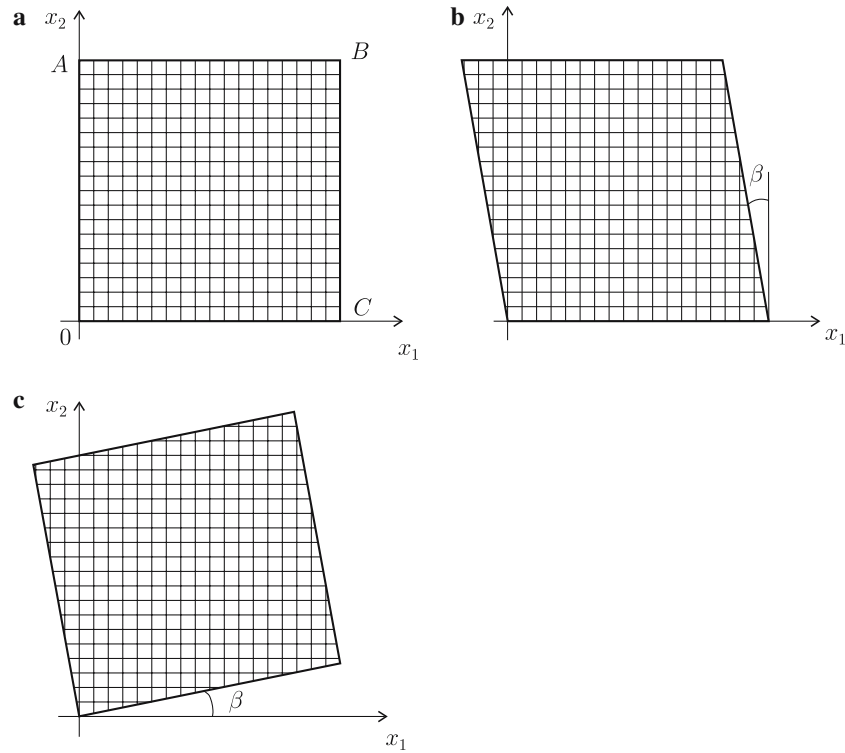
Let some edge dislocations with the Burgers vector directed along the  $x_1$ -axis pass this piece in  $x_1$ -direction and provide a homogeneous plastic deformation. Then the crystal takes the form shown in Fig. 1b. Let also an additional similar set of the edge dislocations with the Burgers vector directed along the  $x_2$ -axis goes through the crystal in the  $x_2$ -direction. The crystal gets the form shown in Fig. 1c. If the shear angle,  $\beta$ , is small, and the crystal can be modeled as an isotropic body, then the crystals in Fig. 1a, c differ by just a rigid rotation while the plastic deformation gained in the transition from the initial state, Fig. 1a, to the final state, Fig. 1c, is zero<sup>1</sup>.

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V.L. Berdichevsky (✉)  
Mechanical Engineering, Wayne State University,  
Detroit, MI 48202, USA  
E-mail: vberd@eng.wayne.edu

<sup>1</sup>To obtain a rigid plastic rotation for a finite angle  $\beta$  one can add, for example, the edge dislocation flow with the Burgers vector directed along  $OB$ .



**Fig. 1** Plastic rotation via dislocation flow

From the perspective of the classical plasticity theory which takes into account only plastic deformations, such rigid plastic rotation is unnoticeable and does not affect any relation of the theory. In reality, the initial and the final states of the crystal are different: the dislocations passing through the crystal heat the crystal, and the temperature must be higher in the final state. We see that the plastic rotation must be taken into account to obtain the adequate energy balance.

We can draw another important conclusion from this Gedankenexperiment. The dislocations passing through the crystal do not change the orientation of the crystal lattice in space. The material coordinate system rotates, however. Therefore, the tensors determining the crystal anisotropy rotate with respect to the material frame. Such rotation is caused by the plastic flow. As a result, the internal energy density becomes an explicit function of the plastic distortion. The two effects mentioned do not depend on the size of the body and should be taken into account for microscopic, mesoscopic and macroscopic bodies. It is apparent that the averaged plastic rotations should be a part of the kinematic description of the dislocation networks, and the corresponding plasticity theory must be modified accordingly (this is discussed in Sects. 2 and 5; see especially formula (93)).

To simplify the treatment in the introduction to this paper, we constraint it with geometrically linear theory (i.e. a theory with linear kinematics); the nonlinear theory will be considered further in the body of the paper. All tensors in the linear theory are referred to a Cartesian frame with the coordinates  $x_i$ , small Latin indices  $i, j, k, l$  run through the values 1, 2, 3; summation over the repeated indices is implied.

Plastic rotations appear in the kinematical description of individual dislocations, and penetrate further naturally into the macroscopic continuum description of the dislocation networks. Each dislocation may be characterized by the tensor of plastic distortion,  $A_{ij}$ . Its deviation from the identity transformation,  $\beta_{ij} \equiv A_{ij} - \delta_{ij}$ ,  $\delta_{ij}$  being the Kronecker delta, is defined as follows: let  $u_i$  be the displacement vector field from the perfect lattice to the defected one, and  $b_i = [u_i] \equiv u_i^+ - u_i^-$  the jump of the displacements on the slip surface  $\Sigma$  ( $\pm$  signs mark the limit values of the displacements on the two sides of the slip surface). Then, by definition,

$$\beta_{ij} = b_i n_j \delta(\Sigma) \quad (1)$$

where  $n_j$  are the components of the unit normal vector directed from the side  $\Sigma_-$  of the surface  $\Sigma$  to the side  $\Sigma_+$ ,  $\delta(\Sigma)$  the  $\delta$ -function of the surface  $\Sigma$

$$\delta(\Sigma) = \int_{\Sigma} \delta(x - x_{\Sigma}) dA_{\Sigma}$$

$\delta(x)$  the usual three-dimensional  $\delta$ -function,  $dA_{\Sigma}$  the area element on  $\Sigma$ . The definition (1) does not depend on the way one marks the sides of the slip surface: denoting the side  $\Sigma_-$  by  $\Sigma_+$  yields the simultaneous change of the signs of the Burgers vector and the normal vector leaving the product in (1) invariant<sup>2</sup>. For brevity, we call the tensor  $\beta_{ij}$  the tensor of plastic distortion as well.

Plastic strains,  $\varepsilon_{ij}^{(p)}$ , and plastic rotations,  $\omega_{ij}$ , are the symmetric and antisymmetric parts of the plastic distortion:

$$\varepsilon_{ij}^{(p)} = \frac{1}{2}(\beta_{ij} + \beta_{ji}) \equiv \beta_{(ij)}, \quad \omega_{ij} = \frac{1}{2}(\beta_{ij} - \beta_{ji}) \equiv \beta_{[ij]}, \quad \beta_{ij} = \varepsilon_{ij}^{(p)} + \omega_{ij}. \quad (2)$$

Round and square brackets in indices denote symmetrization and skew-symmetrization, respectively.

Nye [2] introduced an important characteristic of dislocations, the dislocation density tensor,

$$\alpha_{ij} = e_{jkl} \partial_k \beta_{il} \quad (3)$$

Here  $e_{jkl}$  the Levi-Civita symbol,  $\partial_k \equiv \partial/\partial x_k$ , partial derivatives will be also denoted by the comma in indices:  $\partial_k \beta_{il} \equiv \beta_{il,k}$ . There is an identity (see Kunin [3,4])

$$e_{jkl} \partial_k (n_l \delta(\Sigma)) = \tau_j \delta(\Gamma) \quad (4)$$

$\Gamma$  being the dislocation line, the boundary of the slip surface  $\Sigma$ ,  $\tau_j$  the tangent vector to  $\Gamma$ ,  $\delta(\Gamma)$  the delta-function of the line  $\Gamma$ ,

$$\delta(\Gamma) = \int_{\Gamma} \delta(x - x_s) ds,$$

$ds$  the arc length along  $\Gamma$ . Therefore, for an individual dislocation we have

$$\alpha_{ij} = b_i \tau_j \delta(\Gamma). \quad (5)$$

The first problem which arises here is to find the stress field for a given set of dislocations. If  $b_i = \text{const}$  along the slip surfaces, the stress field depends only on the positions of the dislocation lines; the shapes of the slip surfaces do not affect the stress field. A general solution of the problem was given by Kröner [5]. An elegant treatment in terms of the generalized functions was suggested by Kunin [3,4].

A nonlinear generalization of the theory is based on the idea by Kondo [6,7] and Bilby (see [8–10]) to consider the unloaded space as a manifold with an affine connection. The dislocation field is characterized by the metric tensor of the manifold (that is equivalent to plastic strains), the curvature tensor and the torsion tensor. Bilby argued that for crystal lattices the curvature tensor must vanish; then the only kinematic characteristics are the metric tensor and the torsion tensor, the latter being equivalent to the dislocation density tensor. This set of kinematic characteristics is equivalent to just plastic distortions: In the linear case the plastic strains and the dislocation density tensor can be found from (2) and (3); the inverse statement is also true: the plastic distortion can be found if the plastic strains and the dislocation density tensor are known (Le and Stumpf [11]). Kondo considered a more general case when the curvature tensor is not zero. Then the torsion (dislocation density tensor) cannot be expressed in terms of plastic distortion and becomes an independent field. This line of thought seems not being pursued further though it has some merits. In what follows we assume the zero curvature of the unloaded space. Thus, plasticity kinematics is characterized by the plastic distortion only, and the dislocation density tensor is determined by the plastic distortion from Eq. (3).

<sup>2</sup> Note that usually one defines the Burgers vector in a different way: on the same slip plane, for a fixed choice of the normal vector, one takes the orientation of the boundary of  $\Sigma$ , the dislocation line, to be seen in the counter clock-wise direction from the top of the normal vector; then the sign of the Burgers vector is chosen in such a way that the triad {normal vector, tangent vector to the dislocation line, Burgers vector} be right oriented. Though the signs of the Burgers vector for the definition given in the text and the usual definition can be different, the plastic distortions are the same, and this is the only what matters in our treatment.

As soon as the kinematics is fixed one can apply the methods of non-equilibrium thermodynamics to obtain the governing equations. This was done by Sedov and Berdichevsky [1]<sup>3</sup>. The equations of continuum theory of dislocations were derived in [1] using the variational approach [13]. They will be rederived here from the standard thermodynamic reasoning in a simplified setting.

In thermodynamic and variational approaches the model is specified by choosing the expressions for energy and dissipation. The example model considered in [1] has the following energy density per unit volume,  $U$ , and dissipation density,  $D$ , which we present here in their linear version and neglect, for simplicity, some interaction terms:

$$U = U_0 \left( \varepsilon_{ij}^{(e)}, S \right) + U_m, \quad (6)$$

$$U_m = \frac{1}{2} E_{ijkl} \alpha_{ij} \alpha_{kl} \quad (7)$$

$$D = \left( K_{ijkl} \dot{\varepsilon}_{ij}^{(p)} \dot{\varepsilon}_{kl}^{(p)} + M_{ijkl} \dot{\alpha}_{ij} \dot{\alpha}_{kl} \right)^{\frac{1}{2}} \quad (8)$$

Here  $\varepsilon_{ij}^{(e)}$  are the elastic strain tensor components:

$$\varepsilon_{ij}^{(e)} = \varepsilon_{ij} - \varepsilon_{ij}^{(p)}, \quad \varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}), \quad (9)$$

$S$  the entropy density,  $U_0$  the elastic energy, dot denotes the time derivative. The coefficients  $E_{ijkl}$ ,  $K_{ijkl}$ ,  $M_{ijkl}$  are some material constants.

The relevance of this model to describing the behavior of the dislocation networks was not clear. The major concern was the smallness of the second term in (6). To estimate its order denote the characteristic value of the constants  $E_{ijkl}$  by  $E$  (they have the dimension of the shear modulus,  $\mu$ , times length squared) and by  $l$  the corresponding characteristic length:  $l = (E/\mu)^{1/2}$ . The order of the dislocation density tensor,  $\alpha$ , can be obtained by noting that  $\alpha_{ij}$  can be written in terms of the elastic distortion,  $\beta_{ij}^{(e)} = u_{i,j} - \beta_{ij}$ :

$$\alpha_{ij} = -e_{jkl} \partial_k \beta_{il}^{(e)} \quad (10)$$

Assuming that the elastic distortion is of the same order as the elastic strains,  $\varepsilon^{(e)}$ , we get an estimate of the dislocation density in terms of  $\varepsilon^{(e)}$  and the characteristic length of the problem,  $L$ :  $\alpha \sim \varepsilon^{(e)}/L$ . So, the two terms in (6) are of the orders  $\mu (\varepsilon^{(e)})^2$  and  $\mu l^2 (\varepsilon^{(e)}/L)^2$ , respectively. If they are of the same order,

$$\mu (\varepsilon^{(e)})^2 \sim \mu l^2 \left( \frac{\varepsilon^{(e)}}{L} \right)^2,$$

then the characteristic lengths  $l$  and  $L$  must be also of the same order<sup>4</sup>,

$$l \sim L.$$

In a polycrystal, we have at hand a number of material characteristic lengths: the interatomic distance,  $b$ , the average distance between dislocations, the average dislocation cell size, the average grain size. If one identifies  $l$  with any of these distances, then in a macroscopic problem  $L \gg l$ , and the second term in (6) is negligible in comparison with the first one. Similar conclusion can be made with respect to the second term in (8). The problems with mesoscopic and microscopic values of  $L$  were not seen at the time, and the theory was not pursued further. Recently an interest to such type of problems has appeared motivated mostly by the experimentally observed intrinsic and extrinsic size effects on micro-level. A number of models have been suggested [14–28]<sup>5</sup>. The applicability and the meaning of continuum models on small scales are complicated issues

<sup>3</sup> The same paper was published also in the conference proceedings [12]. Only one publication will be cited further.

<sup>4</sup> Unless there is a large coefficient in  $E_{ijkl}$ . There are no reasons to assume such a coefficient.

<sup>5</sup> Gurtin [25] arrived in linear case to the same equations as given in [1]. The models proposed in [14–28] differ too much to be all physically relevant. Perhaps, the homogenization analysis of the dislocation network dynamics will determine which models from this variety are physically adequate.

(see the discussion in [29,30]); presumably, a continuum description could make sense for laminar plastic flows. Note that the question on the physical meaning of the characteristic material length still does not have a convincing answer<sup>6</sup>.

The above-mentioned difficulty seems to have been overcome, at least partially, by a proposition about the microstructure energy,  $U_m$ , made in [32]. It was shown that the microstructure energy,  $U_m$ , which includes the interaction energy between dislocations and the self-energy of dislocations is, in fact, a function of local characteristics of dislocations only, in spite of the long-range character of the dislocation interactions. The microstructure energy can be modeled in the following way. The simplest local characteristic of the dislocation network is the scalar dislocation density,  $\rho$ , the total length of the dislocation lines per unit volume. An advantage of this characteristic is that the state without dislocations corresponds to the zero value of  $\rho$ . One may assume that the microstructure energy is a function of  $\rho$ . Dislocation density cannot be bigger than some saturated value,  $\rho_s$ . A rough estimate of  $\rho_s$  is  $\rho_s \sim 1/b^2$ . It corresponds to the material completely filled with dislocations. In fact,  $\rho_s$  is considerably less: if the dislocation density becomes too high in polycrystals, then the processes set on which are not accounted for in the continuum theory of dislocations and reduce the dislocation density—the new grain boundaries develop and the average grain size drops. In energy terms, that means that, for a fixed average grain size, energy becomes very large if  $\rho \sim \rho_s$ . On the other hand, for small  $\rho$ , energy is linear in  $\rho$  at least because the energy of dislocation cores is linear in  $\rho$ . A simple model function which fits to these features of energy is [32]<sup>7</sup>

$$U_m = k\mu \ln \frac{1}{1 - \frac{\rho}{\rho_s}}. \quad (11)$$

The order of magnitude of the material constants  $k$ ,  $\rho_s$  was estimated for Al and Ni as  $k \sim 10^{-4}$ ,  $\rho_s \sim 10^{14} \text{m}^{-2}$ .

The link to the continuum theory of dislocations is provided by the following remark: the total dislocation density,  $\rho$ , is a sum of the dislocation density of the stored dislocations,  $\rho_{st}$ , and the dislocation density of moving dislocations, denote it by  $\alpha/b$ . The parameter  $\alpha$  can be modeled in the isotropic case as

$$\alpha = \sqrt{c_1 \alpha_{ij} \alpha_{ij} + c_2 \alpha_{ij} \alpha_{ji}} \quad (12)$$

$c_1, c_2$  being some phenomenological constants on the order of unity. Finally, one can put in (11)

$$\rho = \rho_{st} + \frac{\alpha}{b}. \quad (13)$$

Formulas (6),(11)–(13) determine the dependence of energy on the dislocation density tensor assuming that the material parameters  $\rho_s$  and  $\rho_{st}$  are given and do not change in the course of deformation.

Note that the ratio  $\alpha/b\rho_s \sim \varepsilon^{(e)}/b\rho_s L$  is small: even for  $L \sim 10^{-4}$  m assuming  $\varepsilon^{(e)} \sim 10^{-4}$ ,  $b \sim 10^{-10}$  m,  $\rho_s \sim 10^{14} \text{m}^{-2}$  we have  $\alpha/b\rho_s \sim 10^{-4}$ . If we linearize Eq. (11) and keep only the leading terms, we obtain

$$U_m = \frac{k\mu}{b(\rho_s - \rho_{st})} \sqrt{c_1 \alpha_{ij} \alpha_{ij} + c_2 \alpha_{ij} \alpha_{ji}} + k\mu \ln \frac{1}{1 - \frac{\rho_{st}}{\rho_s}}. \quad (14)$$

Here we assumed that  $\rho_s - \rho_{st} \sim \rho_s$ . Due to the smallness of  $\alpha/b\rho_s$ , the “square root term”<sup>8</sup> is much bigger than the quadratic term,

$$\left( \frac{\alpha}{b\rho_s} \right)^2 = \frac{1}{(b\rho_s)^2} (c_1 \alpha_{ij} \alpha_{ij} + c_2 \alpha_{ij} \alpha_{ji}).$$

<sup>6</sup> There was an interesting attempt [31] to justify formula for energy (6). It was concluded that the characteristic length has the meaning of the average distance between dislocations. Unfortunately, the derivation contains a flaw which renders an incorrect result. This will be discussed in detail elsewhere.

<sup>7</sup> Though the particular form of the microstructure energy (11) is not essential in the derivation of the governing equations, it is convenient for various estimates. Consider here the following one. An infinite value of the microstructure energy for  $\rho = \rho_s$  is, of course, an approximation which may be valid away from this point. In fact, energy is very large and finite for  $\rho = \rho_s$ . One can modify (11) as  $U_m = k\mu \ln[1/(1 + \kappa - \rho/\rho_s)]$  and seek for the corresponding value of the correction,  $\kappa$ . Let  $\rho_s \sim 1/b^2$ . If  $\rho = \rho_s$ , i.e. the dislocations occupy all the body, then the microstructure energy is on the order of the energy of a “melted body” which can be estimated as  $\lambda/b^2$ ,  $\lambda$  being the energy of the dislocation core per unit dislocation length. Hence,  $\kappa = \exp[-\lambda/k\mu b^2]$ . For the typical values  $\lambda \sim 1 - ev/b$ ,  $\mu b^3 \sim 5 - ev$  and for  $k \sim 10^{-4}$ ,  $\kappa$  is very small:  $\kappa \sim \exp[-2.5 \times 10^5]$ .

<sup>8</sup> Energy as a linear function of the square root term appeared for the first time, perhaps, in [33].

Nevertheless, linearization and neglecting the quadratic term is not always justifiable: this changes considerably the properties of the model. The model with energy (14) allows the plastic distortion to have discontinuities: the total energy remains finite for discontinuous plastic distortions. Energy (11) as well as the energy (7) prohibits the discontinuities becoming infinite for the discontinuous plastic distortions. Due to that the model with energy (11) allows one to capture such features as, for example, the structure of the dislocation pile-ups at the grain walls.

Note that the last term in (14) is quite essential. It describes the energy of the stored dislocations. This energy is huge, and, in fact, may be much bigger than the elastic energy. For example, for  $\rho_{st} = 0.1\rho_s$ , the stored dislocation energy is in the order of  $10^{-5}\mu$  while the elastic energy for  $\varepsilon^{(e)} = 10^{-4}$  is in the order of  $10^{-8}\mu$ . Therefore, even small changes in stored dislocation density has a profound effect on the energy balance, and taking into account the evolution of the stored dislocation density may be much more important than the incorporation in the theory the gradients of plastic distortion. Perhaps, the exceptions are an initial stage of plastic flow, an easy glide, when  $\rho_{st} \simeq 0$ , and the development of geometrically necessary dislocations.

In contrast to the two effects illustrated by Fig. 1, the dependence of energy density on  $\alpha_{ij}$  is essential mostly for small bodies (or small characteristic length  $L$ ). There is, however, a reason why this dependence may be of importance for macroscopic bodies as well: the leading term in energy, elastic energy, in linear approximation does not depend on plastic rotations, and the only term containing plastic rotations is  $U_m(\alpha_{ij})$ . Therefore, even being small, it becomes the leading one in determination of the plastic rotation field.

Non-equilibrium thermodynamics describes, in particular, the evolution of closed systems to their equilibrium states. According to the Gibbs variational principles, the equilibrium states are the states with the maximum value of entropy (for fixed energy) and/or the states with the minimum value of energy (for fixed entropy). The choice of energy in a theory shapes the structure of the entire non-equilibrium theory because it determines the “fixed points” of the dynamic equations. In case of plasticity this has the following implications: if one gives some displacements to the boundary points of a plastic body and keeps these displacements constant, then a plastic flow develops which drives the energy to its minimum value and stops when the energy takes this value. Our choice of energy specifies which final states will develop. If the final states are reached fast enough, one may neglect the transitional process and consider only the final states. They are determined by minimization of energy. One such problem concerning the development in the body the geometrically necessary dislocations will be considered in Sect. 3.

In what follows we give a rederivation of the equations of the paper [1] from the reasoning of non-equilibrium thermodynamics in geometrically linear case (Sect. 2) and geometrically nonlinear case (Sect. 4), consider a variational problem for determining the geometrically necessary dislocations in one constrained shear problem (Sect. 3), and suggest an energy expression for finite plastic deformation which depends explicitly on plastic distortion (Sect. 5).

## 2 Geometrically linear continuum theory of dislocations

### 2.1 System of equations

By geometrically linear continuum dislocation theory we mean the approximation of small displacements, small plastic distortions and their gradients (i.e. they all can be neglected in comparison with unity or the corresponding characteristic length or inverse length). In such theory one can disregard the differences between the Lagrangian and Eulerian coordinates. The theory to discussion of which we proceed is based on the following assumption: the energy of the crystal possesses the energy density which is a function of only local characteristics – elastic strains,  $\varepsilon_{ij}^{(e)} = \varepsilon_{ij} - \varepsilon_{ij}^{(p)}$ , plastic distortions,  $\beta_{ij}$ , dislocation density tensor,  $\alpha_{ij} = e_{jkl}\partial_k\beta_{il}$ , and entropy per unit mass,  $S$ :

$$U = U \left( S, \varepsilon_{ij}^{(e)}, \beta_{ij}, \alpha_{ij} \right). \quad (15)$$

In what follows we denote by  $U$  the energy density per unit mass. Entropy  $S$  is understood here in a usual sense as the thermodynamic entropy of thermal motion of atoms of the crystal lattice. There might be situations when energy depends also on the configurational entropy of the dislocation network (see [30,32]), but such cases are beyond the scope of this paper.

Let  $V_0$  be a subregion in the initial state of the crystal; it coincides with the corresponding actual position of this subregion in the deformed state within the framework of the linear theory. The energy of the crystal

confined in the region  $V_0$  is:

$$E = \int_{V_0} \rho_0 U \left( S, \varepsilon_{ij}^{(e)}, \beta_{ij}, \alpha_{ij} \right) dV. \quad (16)$$

Here  $\rho_0$  is the mass density in the initial state which coincides with the actual mass density in the deformed state in a linear theory.

Let the crystal be adiabatically isolated. Besides, we assume for simplicity that the heat conductivity is negligible, i.e. for any region  $V_0$  there are no heat flux through the boundary  $\partial V_0$  of the region  $V_0$ . Then the first law of thermodynamics states that the energy rate is equal to the power of the external forces:

$$\frac{d}{dt} \int_{V_0} \rho_0 U \left( S, \varepsilon_{ij}^{(e)}, \beta_{ij}, \alpha_{ij} \right) dV = P. \quad (17)$$

The structure of the power is controlled by the form of the energy. For example, if  $U$  depended only on  $S$  and  $\varepsilon_{ij}^{(e)} = u_{(i,j)} - \beta_{(ij)}$ , and, thus, only the space derivatives of displacements entered the energy density, then

$$P = \int_{\partial V_0} \sigma_{ij} n_j \dot{u}_i dA,$$

where dot denotes the time derivative,  $n_j$  the components of unit normal vector at  $\partial V_0$ , and  $\sigma_{ij}$ , the components of the stress tensor, are some functions of space coordinates and time. In general, if  $U$  were dependent on the gradients of some parameter,  $\varphi$ , then there are some "generalized stresses",  $\sigma_i$ , such that

$$P = \int_{\partial V_0} \sigma_j n_j \dot{\varphi} dA.$$

The origin of such a special structure of the power has the deep roots in the Gibbs variational principles; it is explained also by Sedov's variational equation [13].

In our case, due to the assumed form of the internal energy, the power should have the form

$$P = \int_{\partial V_0} (\sigma_{ij} n_j \dot{u}_i + \sigma_{ijk} n_k \dot{\beta}_{ij}) dA. \quad (18)$$

We see that some stresses of higher order,  $\sigma_{ijk}$ , enter into the theory as a result of the dependence of energy density on the gradients of plastic distortion.

Transforming the surface integral in (18) into the volume integral by means of the divergence theorem, we obtain from (16)–(18) the equation:

$$\int_{V_0} \left[ \rho_0 \frac{\partial U}{\partial S} \dot{S} + \rho_0 \frac{\partial U}{\partial \varepsilon_{ij}^{(e)}} (\dot{u}_{(i,j)} - \dot{\beta}_{(ij)}) + \rho_0 \frac{\partial U}{\partial \beta_{ij}} \dot{\beta}_{ij} + \rho_0 \frac{\partial U}{\partial \alpha_{ij}} e_{jkl} \partial_k \dot{\beta}_{il} - \sigma_{ij} \dot{u}_{i,j} - \sigma_{ij,j} \dot{u}_i - \sigma_{ijk} \dot{\beta}_{ij,k} - \sigma_{ijk,k} \dot{\beta}_{ij} \right] dV = 0 \quad (19)$$

Since the region  $V_0$  is arbitrary, this equation may be satisfied only if the integrand is zero identically. Employing the standard notation,  $T$ , for the derivative,  $\partial U / \partial S$ , which is the absolute temperature,

$$\frac{\partial U}{\partial S} = T \quad (20)$$

we have

$$\begin{aligned} \rho_0 T \dot{S} + \left( \rho_0 \frac{\partial U}{\partial \varepsilon_{ij}^{(e)}} - \sigma_{ij} \right) \dot{u}_{i,j} + \left( \rho_0 \frac{\partial U}{\partial \beta_{ij}} - \rho_0 \frac{\partial U}{\partial \varepsilon_{ij}^{(e)}} - \sigma_{ijk,k} \right) \dot{\beta}_{ij} \\ + \left( \rho_0 \frac{\partial U}{\partial \alpha_{im}} e_{mkj} - \sigma_{ijk} \right) \dot{\beta}_{ij,k} - \sigma_{ij,j} \dot{u}_i = 0 \end{aligned} \quad (21)$$

Here we used that, due to the symmetry of the derivatives,  $\partial U / \partial \varepsilon_{ij}^{(e)}$ ,

$$\rho_0 \frac{\partial U}{\partial \varepsilon_{ij}^{(e)}} \dot{u}_{(i,j)} = \rho_0 \frac{\partial U}{\partial \varepsilon_{ij}^{(e)}} \dot{u}_{i,j}, \quad \rho_0 \frac{\partial U}{\partial \varepsilon_{ij}^{(e)}} \dot{\beta}_{(i,j)} = \rho_0 \frac{\partial U}{\partial \varepsilon_{ij}^{(e)}} \dot{\beta}_{i,j}.$$

For rigid translational motion, entropy,  $S$ , and stresses,  $\sigma_{ij}$ , do not change while  $\dot{u}_{i,j}$  and  $\dot{\beta}_{ij}$  are zero. Therefore, in order the first law of thermodynamics to be fulfilled, the stresses must obey to the equilibrium equations:

$$\sigma_{ij,j} = 0. \quad (22)$$

For rigid rotations, i.e. for arbitrary  $\dot{u}_{[i,j]}$ , entropy and stresses do not change as well, while  $\dot{u}_{(i,j)}$  and  $\dot{\beta}_{ij}$  are zero. The first law of thermodynamics can be satisfied only for symmetric stress tensor,

$$\sigma_{ij} = \sigma_{ji} \quad (23)$$

Let us introduce the following notation:

$$\tau_{ij} = \sigma_{ij} - \rho_0 \frac{\partial U}{\partial \varepsilon_{ij}^{(e)}}, \quad \tau_{ijk} = \sigma_{ijk} - \rho_0 \frac{\partial U}{\partial \alpha_{im}} e_{mkj}, \quad (24)$$

$$\varkappa_{ij} = \rho_0 \frac{\partial U}{\partial \varepsilon_{ij}^{(e)}} - \rho_0 \frac{\partial U}{\partial \beta_{ij}} + \sigma_{ijk,k}. \quad (25)$$

Then, the first law of thermodynamics takes the form:

$$\rho_0 T \dot{S} = \tau_{ij} \dot{u}_{i,j} + \varkappa_{ij} \dot{\beta}_{ij} + \tau_{ijk} \dot{\beta}_{ij,k} \quad (26)$$

Equations (24), (26) show that the tensors  $\tau_{ij}$ ,  $\tau_{ijk}$  are the parts of the stresses  $\sigma_{ij}$  and the higher order stresses  $\sigma_{ijk}$  which cause heating of the crystal. To emphasize that the stresses contain two parts, the one related to energy and irrelevant to heating and the another one which causes heating, we rewrite the Eqs. (24) in the form:

$$\sigma_{ij} = \rho_0 \frac{\partial U}{\partial \varepsilon_{ij}^{(e)}} + \tau_{ij}, \quad \sigma_{ijk} = \rho_0 \frac{\partial U}{\partial \alpha_{im}} e_{mkj} + \tau_{ijk}. \quad (27)$$

Tensor  $\tau_{ij}$  describes heating in a non-uniform flow, and, thus, has the meaning of viscous stresses. It is symmetric due to symmetry of  $\sigma_{ij}$  and  $\partial U / \partial \varepsilon_{ij}^{(e)}$ . Tensors  $\varkappa_{ij}$  and  $\tau_{ijk}$  describe heating which is caused by homogeneous and inhomogeneous plastic deformation, respectively.

A widely used closure of non-equilibrium thermodynamics, which satisfies the Onsager reciprocal relations in linear case, assumes that the right hand side of Eq. (26), the dissipation,  $D$ , is a given function of  $\dot{u}_{i,j}$ ,  $\dot{\beta}_{ij}$ ,  $\dot{\beta}_{ij,k}$ ,<sup>9</sup>:

$$\rho_0 T \dot{S} = D (\dot{u}_{i,j}, \dot{\beta}_{ij}, \dot{\beta}_{ij,k}) \quad (28)$$

and that the the tensors  $\tau_{ij}$ ,  $\varkappa_{ij}$ ,  $\tau_{ijk}$  controlling the irreversible processes in the crystal are linked to  $\dot{u}_{i,j}$ ,  $\dot{\beta}_{ij}$ ,  $\dot{\beta}_{ij,k}$  by the relations:

$$\tau_{ij} = \lambda \frac{\partial D}{\partial \dot{u}_{i,j}}, \quad \varkappa_{ij} = \lambda \frac{\partial D}{\partial \dot{\beta}_{ij}}, \quad \tau_{ijk} = \lambda \frac{\partial D}{\partial \dot{\beta}_{ij,k}} \quad (29)$$

Then the parameter  $\lambda$  is determined from (26), (29):

$$\lambda = D \left/ \left( \frac{\partial D}{\partial \dot{u}_{i,j}} \dot{u}_{i,j} + \frac{\partial D}{\partial \dot{\beta}_{ij}} \dot{\beta}_{ij} + \frac{\partial D}{\partial \dot{\beta}_{ij,k}} \dot{\beta}_{ij,k} \right) \right. \quad (30)$$

<sup>9</sup> and, possibly, the arguments of the energy density; the latter are not mentioned explicitly among the arguments of the dissipation function.



Some relaxed versions of the potential relations (29) are also possible [1].

It is worthy to emphasize that, in contrast to the Onsager reciprocal relations, the potential law (29) is not a “law of Nature” (see [34]). However, the potential law seems to cover most of the currently employed models of plasticity.

For a given internal energy,  $U(S, \varepsilon_{ij}^{(e)}, \beta_{ij}, \alpha_{ij})$ , and dissipation,  $D(\dot{u}_{i,j}, \dot{\beta}_{ij}, \dot{\beta}_{ij,k})$ , the Eqs. (22), (23), (25), (26), (20) along with the constitutive equations (27)–(30) and the kinematic formulas (2), (3), (9), form a closed system of equations.

In what follows we ignore the viscous effects; accordingly, dissipation does not depend on the velocity gradients, and viscous stresses vanish

$$\tau_{ij} = 0.$$

## 2.2 Dissipation potential

The major physical motivation to use the potential form of the constitutive equations (29) is the Onsager reciprocal relations of linear thermodynamics. In the nonlinear region one may use other nonlinear equations which yield the Onsager reciprocal relations in the linear case. As such we will use the assumption on the existence of the dissipation potential,  $\mathcal{D}$ , such that

$$\kappa_{ij} = \frac{\partial \mathcal{D}}{\partial \dot{\beta}_{ij}}, \quad \tau_{ijk} = \frac{\partial \mathcal{D}}{\partial \dot{\beta}_{ij,k}}. \quad (31)$$

The dissipation potential is linked to the dissipation by the formula

$$\frac{\partial \mathcal{D}}{\partial \dot{\beta}_{ij}} \dot{\beta}_{ij} + \frac{\partial \mathcal{D}}{\partial \dot{\beta}_{ij,k}} \dot{\beta}_{ij,k} = D.$$

For homogeneous dissipation of the order  $m$ , i.e. for the function  $D(\dot{\beta}_{ij}, \dot{\beta}_{ij,k})$  possessing the property: for any positive number,  $\mu$ ,

$$D(\mu \dot{\beta}_{ij}, \mu \dot{\beta}_{ij,k}) = \mu^m D(\dot{\beta}_{ij}, \dot{\beta}_{ij,k}),$$

the equality holds

$$\frac{\partial D}{\partial \dot{\beta}_{ij}} \dot{\beta}_{ij} + \frac{\partial D}{\partial \dot{\beta}_{ij,k}} \dot{\beta}_{ij,k} = mD,$$

thus, the constant  $\lambda$  (30) is equal to  $1/m$ . Hence, the Eqs. (31) and (29) coincide for

$$\mathcal{D} = \frac{D}{m}. \quad (32)$$

In general, the Eqs. (31) and (29) are different. There are no physical reasons at the moment to prefer (31) or (29). Equations (31) possess, however, one advantage: the constitutive equations can be written in a very compact and beautiful “variational” form:

$$\frac{\delta \mathcal{D}}{\delta \dot{\beta}_{ij}} = \sigma_{ij} - \rho_0 \frac{\delta U}{\delta \beta_{ij}}, \quad \sigma_{ij} = \rho_0 \frac{\partial U}{\partial \varepsilon_{ij}^{(e)}}. \quad (33)$$

Here the notation for the variational derivative is used: for any function  $\varphi(u, \dot{u}, u_{,i})$ ,

$$\frac{\delta \varphi}{\delta u} \equiv \frac{\partial \varphi}{\partial u} - \frac{\partial}{\partial t} \frac{\partial \varphi}{\partial \dot{u}} - \frac{\partial}{\partial x_i} \frac{\partial \varphi}{\partial u_{,i}}.$$

In particular,

$$\frac{\delta \mathcal{D}}{\delta \dot{\beta}_{ij}} = \frac{\delta \mathcal{D}}{\delta \dot{\beta}_{ij}} - \frac{\partial}{\partial x_k} \frac{\delta \mathcal{D}}{\delta \dot{\beta}_{ij,k}}, \quad \frac{\delta U}{\delta \beta_{ij}} \equiv \frac{\partial U}{\partial \beta_{ij}} - \frac{\partial}{\partial x_k} \frac{\partial U}{\partial \beta_{ij,k}} = \frac{\partial U}{\partial \beta_{ij}} - \frac{\partial}{\partial x_k} \frac{\partial U}{\partial \alpha_{im}} e_{mkj}$$

Equations (33) can be checked by inspection. According to these equations, the inclusion of gradients of  $\beta_{ij}$  in  $U$  and gradients of  $\dot{\beta}_{ij}$  in  $\mathcal{D}$  yields only one change in the equations: the usual partial derivatives must be changed by the variational derivatives.

In (33), the derivatives of  $U$  with respect to  $\beta_{ij}$  are computed when the elastic strains are fixed. If the derivatives of  $U$  with respect to  $\beta_{ij}$  for fixed total strains,  $\varepsilon_{ij}$ , are used,  $\delta_\varepsilon U / \delta \beta_{ij}$ , then the equations serving to determine  $\beta_{ij}$  take especially simple form:

$$\frac{\delta \mathcal{D}}{\delta \dot{\beta}_{ij}} = -\rho_0 \frac{\delta_\varepsilon U}{\delta \beta_{ij}}. \quad (34)$$

Note also that Eqs. (33) retain their form if energy density depends on all the gradients of plastic distortion, not only on their anti-symmetric part,  $\alpha_{ij}$ , as we assumed in the derivation.

### 2.3 Plastic incompressibility

If the plastic distortion obeys some kinematic constraints, the equations change accordingly. The case of plastic incompressibility,

$$\beta_{ii} = 0 \quad (35)$$

is especially interesting.

We are going to show that the equations serving to determine  $\beta_{ij}$  for plastic incompressible flows can be written in the form:

$$\frac{\delta \mathcal{D}}{\delta \dot{\beta}'_{ij}} = \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{ij}} \quad (36)$$

where prime denotes the deviatoric part of the tensor, e.g.  $\sigma'_{ij} = \sigma_{ij} - 1/3 \sigma_{kk} \delta_{ij}$ .

There are two key points in the derivation of equations (36). The first one is the meaning of the derivatives  $\partial U / \partial \varepsilon_{ij}^{(e)}$ ,  $\partial U / \partial \beta_{ij}$  in case when  $\varepsilon_{ij}^{(e)}$  and  $\beta_{ij}$  obey to some constraints. Consider first the symmetry constraint for the strain tensor,  $\varepsilon_{ij}^{(e)}$ , and take an example:  $U$  is a quadratic form of a two-dimensional symmetric tensor  $\varepsilon_{ij}^{(e)}$ ,

$$U = \frac{1}{2} \varepsilon_{ij}^{(e)} \varepsilon_{ij}^{(e)} = \frac{1}{2} \left( \varepsilon_{11}^{(e)} \varepsilon_{11}^{(e)} + 2\varepsilon_{12}^{(e)} \varepsilon_{12}^{(e)} + \varepsilon_{22}^{(e)} \varepsilon_{22}^{(e)} \right).$$

If we take the derivatives of this function in the usual sense,

$$\frac{\partial U}{\partial \varepsilon_{11}^{(e)}} = \varepsilon_{11}^{(e)}, \quad \frac{\partial U}{\partial \varepsilon_{12}^{(e)}} = 2\varepsilon_{12}^{(e)}, \quad \frac{\partial U}{\partial \varepsilon_{22}^{(e)}} = \varepsilon_{22}^{(e)}$$

they do not form the components of a tensor. To get a tensor, we must take derivatives of function  $U$  with respect to  $\varepsilon_{ij}^{(e)}$  as if this tensor is not symmetric; such derivatives,

$$\frac{\partial U}{\partial \varepsilon_{11}^{(e)}} = \varepsilon_{11}^{(e)}, \quad \frac{\partial U}{\partial \varepsilon_{12}^{(e)}} = \varepsilon_{12}^{(e)}, \quad \frac{\partial U}{\partial \varepsilon_{21}^{(e)}} = \varepsilon_{21}^{(e)}, \quad \frac{\partial U}{\partial \varepsilon_{22}^{(e)}} = \varepsilon_{22}^{(e)}$$

do form a tensor. The similar remark pertains to the other constraints as well, in particular, to the incompressibility constraint (35). Energy and dissipation in this case must be defined not only for the incompressible plastic fields, but for all fields as if these fields could be compressible. Incompressibility implies that  $\beta_{ij}$  enters in  $U$  only through the combination,

$$\beta'_{ij} = \beta_{ij} - \frac{1}{3} \beta_{kk} \delta_{ij},$$

and in  $D$  through the combinations,

$$\dot{\beta}'_{ij} = \dot{\beta}_{ij} - \frac{1}{3}\dot{\beta}_{kk}\delta_{ij}, \quad \dot{\beta}'_{ij,k} = \dot{\beta}_{ij,k} - \frac{1}{3}\dot{\beta}_{mm,k}\delta_{ij}.$$

Computing the derivatives of  $U$  and  $D$  we admit all fields, not only the incompressible ones. Thus,

$$\frac{\partial U}{\partial \beta'_{ij}} = \frac{\partial U}{\partial \beta'_{ij}} - \frac{1}{3} \frac{\partial U}{\partial \beta'_{kl}} \delta_{kl} \delta_{ij} = \left( \frac{\partial U}{\partial \beta'_{ij}} \right)' \quad (37)$$

and, similarly,

$$\frac{\partial D}{\partial \dot{\beta}'_{ij}} = \frac{\partial D}{\partial \dot{\beta}'_{ij}} - \frac{1}{3} \frac{\partial D}{\partial \dot{\beta}'_{kl}} \delta_{kl} \delta_{ij} = \left( \frac{\partial D}{\partial \dot{\beta}'_{ij}} \right)', \quad \frac{\partial D}{\partial \dot{\beta}'_{ij,k}} = \frac{\partial D}{\partial \dot{\beta}'_{ij,k}} - \frac{1}{3} \frac{\partial D}{\partial \dot{\beta}'_{ml,k}} \delta_{ml} \delta_{ij} = \left( \frac{\partial D}{\partial \dot{\beta}'_{ij,k}} \right)'$$

The equations for  $\beta_{ij}$  (31) are replaced by the equations:

$$\varkappa_{ij} = \left( \frac{\partial \mathcal{D}}{\partial \dot{\beta}'_{ij}} \right)', \quad \tau_{ijk} = \left( \frac{\partial \mathcal{D}}{\partial \dot{\beta}'_{ij,k}} \right)' \quad (38)$$

Therefore, the tensors  $\varkappa_{ij}$  and  $\tau_{ijk}$  automatically have zero traces:

$$\varkappa_{ii} = 0, \quad \tau_{iik} = 0 \quad (39)$$

According to Eq. (27), the scalar,  $\varkappa_{ii}/3$ , has the meaning of ‘‘plastic pressure’’, and the assumptions made yield zero plastic pressure.

Equations (37) and (38) can be further simplified if we accept that energy and dissipation possess the property: for any constants  $\lambda$  and  $\lambda_k$

$$\begin{aligned} U(\beta'_{ij} + \lambda \delta_{ij}, \beta'_{ij,k} + \lambda_k \delta_{ij}) &= U(\beta'_{ij}, \beta'_{ij,k}), \\ \mathcal{D}(\dot{\beta}'_{ij} + \lambda \delta_{ij}, \dot{\beta}'_{ij,k} + \lambda_k \delta_{ij}) &= \mathcal{D}(\dot{\beta}'_{ij}, \dot{\beta}'_{ij,k}) \end{aligned} \quad (40)$$

Such a property is not fulfilled automatically (it is enough to consider a linear function,  $a_{ij}\beta'_{ij}$ , were tensor  $a_{ij}$  has a non-zero trace), but it is not physically constraining since it can be achieved by the corresponding redefinition of the arguments of energy and dissipation (in the above example of a linear function, we replace the tensor  $a_{ij}$  by  $a'_{ij}$ ; then energy satisfies to the condition (40) and has the same values as before). Differentiating (40) with respect to  $\lambda$  and  $\lambda_k$  we obtain the identities

$$\frac{\partial U}{\partial \beta'_{ij}} \delta_{ij} = 0, \quad \frac{\partial U}{\partial \beta'_{ij,k}} \delta_{ij} = 0, \quad \frac{\partial \mathcal{D}}{\partial \dot{\beta}'_{ij}} \delta_{ij} = 0, \quad \frac{\partial \mathcal{D}}{\partial \dot{\beta}'_{ij,k}} \delta_{ij} = 0$$

and, hence,

$$\varkappa_{ij} = \frac{\partial \mathcal{D}}{\partial \dot{\beta}'_{ij}}, \quad \tau_{ijk} = \frac{\partial \mathcal{D}}{\partial \dot{\beta}'_{ij,k}} \quad (41)$$

One can check that the Eqs. (36) follow from (33) and (41).

The second point concerning the derivation of (36) is that the rule of computation the derivatives described above is not a pure mathematical issue: it has a physical origin. Usually, the constraints have a physical nature: the unconstrained deformation is possible but yields either very large energy or very large dissipation, and, therefore, is not realized. Accepting the plastic incompressibility constraint we ignore the dislocation climb. In order to justify Eqs. (36) one should consider a more complete theory which allows the dislocation climb to occur. Such theory should include also the additional required fields, concentrations of vacancies and interstitial atoms which are responsible for the volume change and accompany the dislocation climb. An asymptotic analysis of this more complete theory will presumably yield the equations formulated<sup>10</sup>. Such a derivation seems not have been attempted though<sup>11</sup>.

<sup>10</sup> In particular, in such asymptotic analysis one should presumably obtain that plastic pressure is negligible compared with elastic pressure.

<sup>11</sup> A similar problem, the transition from slightly compressible fluid to incompressible fluid, was considered in [35].

## 2.4 Dissipation in rate independent plasticity

For a wide range of plastic flows, the plastic deformation may be viewed as rate independent. That means the following. Consider homogeneous plastic deformation,  $\beta_{ij}(t)$  ( $\beta_{ij,k} = 0$ ). Let  $\beta_{ij} = B_{ij}(t)$  be a closed deformation loop in the space of  $\beta_{ij}$ -variables,  $t_0 \leq t \leq t_1$ ,  $B_{ij}(t_0) = B_{ij}(t_1)$ . The total dissipation (the total amount of heat generated in the course of deformation along this loop) is equal to

$$\int_{t_0}^{t_1} D(\dot{B}_{ij}(t)) dt. \quad (42)$$

For rate independent flow, the total dissipation is the same for all flows  $\beta_{ij} = B_{ij}(\theta(t))$  with any function  $\theta(t)$ ,  $\theta(t_0) = t_0$ ,  $\theta(t_1) = t_1$ . We accept additionally that dissipation does not change if the direction of flow is reversed,  $D(-\dot{\beta}_{ij}) = D(\dot{\beta}_{ij})$ . It is easy to see that dissipation must be a first-order homogeneous function of  $\dot{\beta}_{ij}$  for the rate independent flows. The dissipation potential,  $\mathcal{D}$ , and dissipation,  $D$ , coincide for the rate independent flows.

Dislocation motion is governed by usual rate dependent (primary) thermodynamics. Macroscopic crystal plasticity is an averaged description of dislocation networks, and, thus, is a subject of the next level thermodynamics called secondary in [34]. The mechanism of the development the rate independence in the transition from the primary to the secondary thermodynamics was explained by Puglisi and Truskinovsky [36].

Independence of the integral (42) on the strain rate for any deformation path is a far going three-dimensional generalization of a quite restricted set of one-dimensional experiments. In any case, it is the base of classical plasticity. Von Mises plasticity theory corresponds to the dissipation

$$D = \mathcal{D} = K \sqrt{\dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)}} \quad (43)$$

and the internal energy,

$$U = U(S, \varepsilon_{ij}^{(e)}). \quad (44)$$

In the case of the von Mises dissipation (43) and the internal energy (44) the equations to determine plastic deformations, (36), take the form:

$$\frac{K \dot{\beta}'_{(ij)}}{\sqrt{\dot{\beta}'_{(kl)} \dot{\beta}'_{(kl)}}} = \sigma'_{ij}$$

The anti-symmetric part of (36) is satisfied automatically.

For the general energy density (15) and dissipation (43), Eqs. (36) form a system of nine equations,

$$\frac{K \dot{\beta}'_{(ij)}}{\sqrt{\dot{\beta}'_{(kl)} \dot{\beta}'_{(kl)}}} = \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{ij}} \quad (45)$$

the six symmetric ones<sup>12</sup>,

$$\frac{K \dot{\beta}'_{(ij)}}{\sqrt{\dot{\beta}'_{(kl)} \dot{\beta}'_{(kl)}}} = \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \quad (46)$$

<sup>12</sup> One can check that

$$\frac{1}{2} \rho_0 \left( \frac{\delta U}{\delta \beta'_{ij}} + \frac{\delta U}{\delta \beta'_{ji}} \right) = \frac{\delta U}{\delta \beta'_{(ij)}}$$

and the tree equations which are anti-symmetric with respect to  $i, j$

$$\frac{\delta U}{\delta \beta'_{ij}} - \frac{\delta U}{\delta \beta'_{ji}} = 0. \quad (47)$$

Equations (47) may be considered as equations serving to determine the plastic rotations,  $\beta_{ij} - \beta_{ji}$ . Plastic rotations remain undetermined in von Mises theory and similar theories of classical plasticity. In continuum theory of dislocations with energy (6), (7), plastic rotations are determined uniquely. It is worthy to emphasize that including into the theory the microstructure energy,  $U_m$ , even (7) which is small compared to the elastic energy, is essential for determining the plastic rotations: according to the general rules of asymptotic analysis of functionals depending on small parameters [35,37], only those small terms can be neglected for which the bigger ones depending on the same variables can be found. Since the plastic rotations enter only in  $U_m$ , the microstructure energy is the leading term depending on plastic rotations and, therefore, cannot be neglected. In terms of equations (47), this means that, though only small terms contribute to these equations, they cannot be neglected because they all are of the same order.

For  $\dot{\beta}'_{(ij)} \neq 0$ , as follows from (45), the stresses must obey the condition:

$$\left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) = K^2. \quad (48)$$

This is a cylindrical "yield surface" in the stress space. The term  $\rho_0 \delta U / \delta \beta'_{(ij)}$  describes translational work hardening.

If

$$\dot{\beta}'_{(ij)} = 0 \quad (49)$$

then the left hand side of (45) contains an uncertainty of the type 0/0. In this case, the equation (45) are replaced by (49).

As was mentioned in Introduction, dissipation must depend on the plastic spin<sup>13</sup>,  $\dot{\beta}'_{[kl]}$ . In the case of rate independent isotropic plasticity we have

$$D = \sqrt{K_1^2 \dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} + K_2^2 \dot{\beta}'_{[ij]} \dot{\beta}'_{[ij]}}. \quad (50)$$

The Eqs. (46) and (47) are replaced by the equations:

$$\frac{K_1^2 \dot{\beta}'_{(ij)}}{\sqrt{K_1^2 \dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} + K_2^2 \dot{\beta}'_{[ij]} \dot{\beta}'_{[ij]}}} = \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \quad (51)$$

$$\frac{K_2^2 \dot{\beta}'_{[ij]}}{\sqrt{K_1^2 \dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} + K_2^2 \dot{\beta}'_{[ij]} \dot{\beta}'_{[ij]}}} = -\rho_0 \frac{\delta U}{\delta \beta'_{[ij]}} \quad (52)$$

Similarly to the previous case, for  $\dot{\beta}'_{ij} \neq 0$ , the stresses must lie on the yield surface

$$\frac{1}{K_1^2} \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) + \frac{1}{K_2^2} \rho_0 \frac{\delta U}{\delta \beta'_{[ij]}} \rho_0 \frac{\delta U}{\delta \beta'_{[ij]}} = 1. \quad (53)$$

The second term in the left hand side indicates that the dependence of energy on plastic rotations results in some decrease of the yield stress.

The experimental values of the constants,  $K_1$  and  $K_2$ , seem not known. The Gedankenexperiment described in Sect. 1 suggests that these constants must be of the same order. If this is indeed the case, then for the plastic flows satisfying the condition

$$\left| \rho_0 \frac{\delta U}{\delta \beta_{ij}} \rho_0 \frac{\delta U}{\delta \beta_{ij}} \right| \ll \left| \sigma'_{ij} \sigma'_{ij} \right|, \quad (54)$$

<sup>13</sup> It was called in [1] the plastic whirl. The term "plastic spin" is commonly accepted nowadays.

the rate of plastic rotations is much smaller than that of plastic strains. If initially  $\beta_{[ij]} = 0$ , then  $\beta_{[ij]} \approx 0$  in the course of deformation<sup>14</sup>. The inequality (54) is plausible for the macro-samples with energy (7) or (11), (12), but it does not hold for micro-samples. This inequality may be also violated if the Bauschinger effect is taken into account.

If the dissipation is a function like (8) then, for  $M_{ijkl} \neq 0$ , the yield surface becomes a surface in the space of variables  $\sigma'_{ij}$ ,  $\tau_{ijk}$ . The scope of physical mechanisms which are covered by such models has not been revealed yet.

## 2.5 Dissipation in rate dependent plasticity

According to the rate independent plasticity the plastic deformation do not develop until stresses reach the yield surface; besides, stresses cannot exceed the yield stress. Both features do not correspond to reality: plastic deformations may develop at any value of stresses, and, due to the external forces, stresses in the body can be made much higher then the yield stress. This discrepancy is caused by the approximate nature of the rate independence hypothesis. In fact, there is a rate dependence which is weak for small stresses but becomes quite pronounced for high stresses. A way to take the rate dependence into account is to modify the dissipation. In the case of von Mises dissipation (43) we put

$$D = K \left( \dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} \right)^{\frac{1}{2}(1+\frac{1}{m})}. \quad (55)$$

Here  $m$  is a big number. In the limit  $m \rightarrow \infty$ , dissipation (55) tends to von Mises dissipation (43). Function (55) is a homogeneous function of  $1 + (1/m)$  order; according to (32), the dissipative potential is

$$\mathcal{D} = \frac{D}{1 + \frac{1}{m}} = \frac{K}{1 + \frac{1}{m}} \left( \dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} \right)^{\frac{1}{2}(1+\frac{1}{m})}.$$

The flow rule, (36) becomes:

$$\frac{K \dot{\beta}'_{(ij)}}{\left( \dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} \right)^{\frac{1}{2}(1-\frac{1}{m})}} = \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{ij}}. \quad (56)$$

The antisymmetric part of equations (56) is again (47) while the symmetric one is

$$\frac{K \dot{\beta}'_{(ij)}}{\left( \dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} \right)^{\frac{1}{2}(1-\frac{1}{m})}} = \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}}. \quad (57)$$

To determine an analogue of the yield surface in this model it is worthy to resolve equations (57) with respect to the strain rate. First, we have from (57):

$$K^2 \left( \dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} \right)^{1/m} = \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right).$$

Hence,

$$\dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} = \left[ \frac{1}{K^2} \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) \right]^m$$

and

$$\dot{\beta}'_{(ij)} = \frac{1}{K} \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) \left[ \frac{1}{K^2} \left( \sigma'_{kl} - \rho_0 \frac{\delta U}{\delta \beta'_{(kl)}} \right) \left( \sigma'_{kl} - \rho_0 \frac{\delta U}{\delta \beta'_{(kl)}} \right) \right]^{\frac{1}{2}(m-1)}.$$

<sup>14</sup> From other reasoning this conclusion was made by Dafalias [38]. It was used by Bassani [22] in constructing a model of strain gradient plasticity. Similar point was made also by Gurtin [25].

For very large  $m$ ,  $\dot{\beta}'_{(ij)} \approx 0$  if

$$\frac{1}{K^2} \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) < 1$$

$\dot{\beta}'_{(ij)}$  becomes finite for

$$\frac{1}{K^2} \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) = 1$$

and  $\dot{\beta}'_{(ij)}$  are huge if

$$\frac{1}{K^2} \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) > 1.$$

The similar modification of the dissipation (50) is

$$D = \left( K_1^{\frac{2}{1+\frac{1}{m}}} \dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} + K_2^{\frac{2}{1+\frac{1}{m}}} \dot{\beta}'_{[ij]} \dot{\beta}'_{[ij]} \right)^{\frac{1}{2}(1+\frac{1}{m})}.$$

Then again  $\mathcal{D} = D/(1 + \frac{1}{m})$ , and

$$\frac{K_1^{\frac{2}{1+\frac{1}{m}}} \dot{\beta}'_{(ij)}}{\left( K_1^{\frac{2}{1+\frac{1}{m}}} \dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} + K_2^{\frac{2}{1+\frac{1}{m}}} \dot{\beta}'_{[ij]} \dot{\beta}'_{[ij]} \right)^{\frac{1}{2}(1-\frac{1}{m})}} = \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}}$$

$$\frac{K_2^{\frac{2}{1+\frac{1}{m}}} \dot{\beta}'_{[ij]}}{\left( K_1^{\frac{2}{1+\frac{1}{m}}} \dot{\beta}'_{(ij)} \dot{\beta}'_{(ij)} + K_2^{\frac{2}{1+\frac{1}{m}}} \dot{\beta}'_{[ij]} \dot{\beta}'_{[ij]} \right)^{\frac{1}{2}(1-\frac{1}{m})}} = \rho_0 \frac{\delta U}{\delta \beta'_{[ij]}}.$$

The magnitude of plastic rate is determined by the value of the function

$$\frac{1}{K_2^{\frac{2}{1+\frac{1}{m}}}} \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) \left( \sigma'_{ij} - \rho_0 \frac{\delta U}{\delta \beta'_{(ij)}} \right) + \frac{1}{K_2^{\frac{2}{1+\frac{1}{m}}}} \left( \rho_0 \frac{\delta U}{\delta \beta'_{[ij]}} \right) \left( \rho_0 \frac{\delta U}{\delta \beta'_{[ij]}} \right).$$

The plastic rate becomes finite if this function is equal to unity, and huge if it exceeds unity. Now we proceed to the discussion of the issues which do not depend on the character of dissipation.

### 3 Plastic deformation and energy minimization

Consider a crystal the boundary displacements of which,  $u_i^{(b)}$ , are prescribed,

$$u_i = u_i^{(b)} \quad \text{at } \partial V_0 \quad (58)$$

Functions  $u_i^{(b)}$  are assumed to be continuous, therefore no dislocations enter into the crystal in the course of deformation. Accordingly, at the boundary<sup>15</sup>

$$\beta_{ij} = 0. \quad (59)$$

Equation (59) models, e.g., a situation at a high angle grain boundary when stresses are not large enough to push the dislocations through the boundary.

If we wait long enough, the crystal will arrive at the state with the minimum value of energy,  $\check{E}$ . In crystals with negligible resistance to dislocation motion, like pure copper, such state can be reached very fast.

The minimum value of energy is determined from the variational problem:

$$\check{E} = \min_{\substack{u_i \in (58) \\ \beta_{ij} \in (59) V_0}} \int \rho_0 U(S, \varepsilon_{ij}^{(e)}, \beta_{ij}, \alpha_{ij}) dV \quad (60)$$

where minimum is sought with respect to all displacement fields obeying to the boundary conditions (58) and all plastic distortions which are zero at the boundary<sup>16</sup>. We assume also that energy density does not depend on plastic distortion explicitly,

$$U = U(S, \varepsilon_{ij}^{(e)}, \alpha_{ij}),$$

besides, it is a strictly convex function of  $\varepsilon_{ij}^{(e)}$  and  $\alpha_{ij}$ , and the minimum value of  $U(S, \varepsilon_{ij}^{(e)}, \alpha_{ij})$  is achieved when  $\varepsilon_{ij}^{(e)}$  and  $\alpha_{ij}$  are zero.

The functional to be minimized is convex but not strictly convex functional of displacements and plastic distortion: its value does not change if one make a ‘‘compatible plastic shift’’,

$$u_i \rightarrow u_i + u_i^{(p)}, \quad \beta_{ij} \rightarrow \beta_{ij} + \frac{\partial u_i^{(p)}}{\partial x_j} \quad (61)$$

where  $u_i^{(p)}(x_i)$  are arbitrary functions. The minimizing functions in the variational problem (60) are determined up to an arbitrary compatible plastic shift,  $u_i^{(p)}(x_i)$ , which satisfies the boundary conditions:

$$u_i^{(p)} = 0, \quad \frac{\partial u_i^{(p)}}{\partial x_j} = 0 \quad \text{at } \partial V_0.$$

The dynamics of the plastic flow determines the plastic shift uniquely. Usually, it depends on the history of deformation. There are situations, however, when the final state is determined uniquely and independently on the deformation history due to the additional constraints for the plastic distortion caused by a special orientation of the slip planes. Here we consider one such example.

Let the deformation does not depend on the coordinate  $x_3$ , and the cross-sections of the body by the planes  $x_3 = \text{const}$  is a rectangle,  $0 \leq x_1 \leq l$ ,  $0 \leq x_2 \leq h$ . We clamp the bottom side of the rectangle,

$$u_1 = u_2 = 0 \quad \text{at } x_2 = 0 \quad (62)$$

and shift the top side:

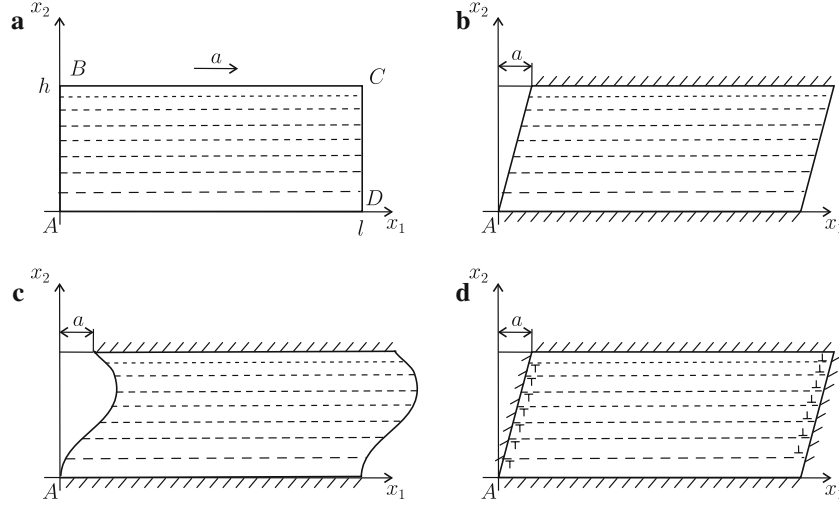
$$u_1 = a, \quad u_2 = 0 \quad \text{at } x_2 = h \quad (63)$$

(see Fig. 2a). Let the plastic deformation is possible only along the planes  $x_2 = \text{const}$  (they are shown in Fig. 2 by dash lines); at these planes the edge dislocations may appear. So, only one component of the plastic

<sup>15</sup> More precisely, the boundary displacements are assumed to be the same both on micro- and macro-levels. The boundary condition (59) is a consequence of continuity of the microscopic displacement field: due to (1), if a slip plane crosses the boundary there is a jump of displacements at the boundary, and  $\beta_{ij} \neq 0$  at the boundary. In principle, in a macroscopic theory, the macroscopic displacement field may be continuous even for non-zero  $\beta_{ij}$  at the boundary.

<sup>16</sup> Not all boundary conditions (59) may be essential in the minimization problem, i.e. removing some of the constraints (59) may not alter the minimum value. We do not pay attention to this issue here because the functional determines itself which boundary conditions it must respect.





**Fig. 2** Constrained shear problem: geometry

distortion,  $\beta_{12} \equiv \beta$ , may be non-zero. The dislocation density tensor has also only one non-zero component,  $\alpha_{13} \equiv \alpha = \beta_{,1}$ . For simplicity we assume that the body is isotropic and take <sup>17</sup>

$$\begin{aligned} \rho_0 U = & \frac{1}{2} (\lambda(u_{1,1} + u_{2,2})^2 + 2\mu(u_{1,1})^2 + 2\mu(u_{2,2})^2 \\ & + \mu(u_{1,2} + u_{2,1} - \beta)^2) + k\mu \ln \frac{1}{1 - \frac{\rho_{st} + |\beta_{,1}|/b}{\rho_s}} \end{aligned}$$

where  $\lambda$ ,  $\mu$  are the Lamé constants.

Let first the edges of the rectangle, AB and CD, are traction free, and, hence, the dislocations may enter the body through these edges. The final state of deformation gives minimum to the functional

$$\begin{aligned} & \int_0^l \int_0^h \left[ \frac{1}{2} (\lambda(u_{1,1} + u_{2,2})^2 + 2\mu(u_{1,1})^2 + 2\mu(u_{2,2})^2 \right. \\ & \left. + \mu(u_{1,2} + u_{2,1} - \beta)^2) + k\mu \ln \frac{1}{1 - \frac{\rho_{st} + |\beta_{,1}|/b}{\rho_s}} \right] dx_1 dx_2. \end{aligned} \quad (64)$$

Minimum is sought with respect to all functions  $u_1$ ,  $u_2$  and  $\beta$  which satisfy the boundary conditions (62), (63). Obviously, the minimum value of energy is zero and achieved at the fields

$$u_1 = \frac{a}{h}x_2, \quad u_2 = 0, \quad \beta = \frac{a}{2h}.$$

All dislocations passed through the body, and there are no dislocations in the final state ( $\alpha = 0$ ). The compatible plastic shift is possible in this problem: the functions,

$$u_1 = \frac{a}{h}x_2 + u_1^{(p)}(x_2), \quad u_2 = 0, \quad \beta = \frac{a}{2h} + \frac{\partial u_1^{(p)}(x_2)}{\partial x_2}$$

also give zero value to energy for arbitrary plastic displacement  $u_1^{(p)}(x_2)$  (Fig. 2c).

The situation changes if we prescribe the displacements also at the edges, AB and CD,

$$u_1 = \frac{a}{h}x_2, \quad u_2 = 0 \quad \text{at } x_1 = 0 \text{ and } x_1 = l \quad (65)$$

<sup>17</sup> The constant  $c_1$  in (12) is set to be equal unity.

Dislocations cannot enter the body through the boundary. We have to set

$$\beta = 0 \quad \text{at } x_1 = 0 \text{ and } x_1 = l \quad (66)$$

Dislocations may be nucleated only inside the body (in neutral pairs) so that the total Burgers vector at each slip plane is zero due to the boundary conditions (66):

$$\int_0^l \alpha dx_1 = \int_0^l \frac{\partial \beta}{\partial x_1} dx_1 = 0$$

Now the minimum of the functional (64) must be sought under the additional constraints, (65) and (66). The constraints (65) and (66) eliminate the kernel of energy: if  $U = 0$ , and, hence,  $\varepsilon_{11}^{(e)} = \varepsilon_{12}^{(e)} = \varepsilon_{22}^{(e)} = \alpha = 0$ , then the required functions,  $u_1$ ,  $u_2$ , and  $\beta$  are also zero. It follows from the equations

$$u_{1,1} = 0, \quad u_{2,2} = 0, \quad u_{1,2} + u_{2,1} - \beta = 0, \quad \beta_{,1} = 0$$

and the boundary conditions (62), (63), (65), (66). Therefore, the minimizing functions are unique.

The problem formulated does not seem to admit an analytical solution. However, qualitatively one may expect the following behavior: for sufficiently small shear,  $\gamma \equiv a/h$ , the body deforms purely elastically, and  $\beta \equiv 0$ . If the shear exceeds some critical value,  $\gamma^*$ , then the dislocations nucleate to reduce the energy, and  $\beta$  becomes non-zero. Dislocations will accumulate near the boundaries (Fig. 2d). Such expectations are supported by the following approximate solution. Since  $u_1 - ax_2/h$  and  $u_2$  vanish at the boundary, we may assume that, approximately, they are equal to zero everywhere in the strip

$$u_1 \equiv \frac{ax_2}{h}, \quad u_2 \equiv 0 \quad (67)$$

while  $\beta$  is a function of only longitudinal coordinate,  $x_1$ . On such fields the functional (64) becomes a functional of  $\beta(x_1)$  only:

$$\check{E} = \min_{\beta(x_1) \in (66)} h\mu \int_0^l \left[ \frac{1}{2}(\gamma - \beta)^2 + k \ln \frac{1}{1 - \frac{\rho_{st} + |\beta_{,x_1}|/b}{\rho_s}} \right] dx_1. \quad (68)$$

It is convenient to make a change of the variables,

$$\beta = \gamma u(x), \quad x_1 = ax, \quad a \equiv \frac{\gamma}{b(\rho_s - \rho_{st})}.$$

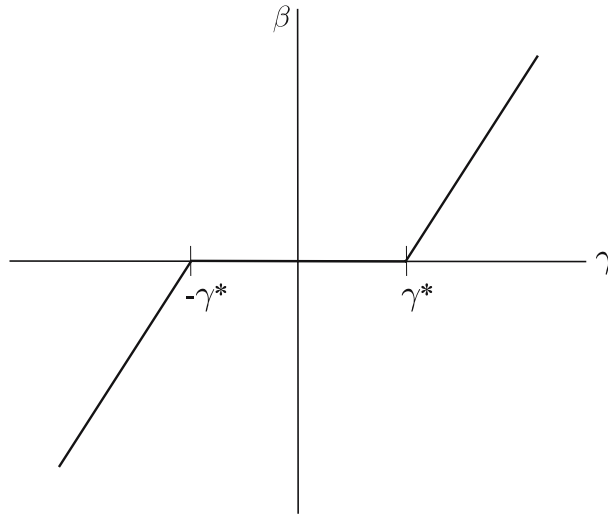
The new independent dimensionless variable,  $x$ , changes on the segment  $[0, L]$ ,  $L = l/a$ . The variational problem takes the form:

$$\begin{aligned} \check{E} &= h\mu l k \ln \frac{1}{1 - \frac{\rho_{st}}{\rho_s}} + h\mu a \gamma^2 \Phi(m), \quad m \equiv \frac{k}{\gamma^2} \\ \Phi(m) &= \min_{\substack{u(x): \\ u(0)=u(L)=0}} I(u), \\ I(u) &= \int_0^L \left[ \frac{1}{2}(1 - u(x))^2 + m \ln \frac{1}{1 - |u_{,x}|} \right] dx. \end{aligned} \quad (69)$$

Consider first the linearized version of the microstructure energy:

$$I(u) = \int_0^L \left[ \frac{1}{2}(1 - u(x))^2 + m |u_{,x}| \right] dx \quad (70)$$

The major difference between (69) and (70) is that the minimizing function of the functional (69) must be smooth (derivatives,  $u_{,x}$ , cannot exceed unity) while the minimizing function of the functional (70) may



**Fig. 3** Dependence of the plastic strain on the total shear strain

have discontinuities, and each discontinuity,  $[u]$ , gives a contribution to the functional equal to  $m |[u]|$ . The minimizing functions of the functional (70) are piece-wise constant functions. Indeed, if  $u_{,x} \neq 0$  in a vicinity of some point, then the integrand in (70) is differentiable, and one can write the Euler equation for (70) which gives  $u = \text{const}$ : we come to contradiction. Hence,  $u_{,x} = 0$ . The functional (70) is strictly convex, therefore it has the only minimizing function. This function cannot have jumps inside the segment  $[0, L]$ : if it does and has at some point  $x^*$  a jump, then moving  $x^*$  in the direction where  $(1 - u)^2$  is bigger, we decrease the functional, and such a function cannot provide the minimum value. So, the jumps may be only at the end points. Denote by  $u$  the constant value of  $u(x)$  inside the segment. The functional is a function of one variable,  $u$ :

$$I(u) = \frac{1}{2}(1 - u)^2 L + 2m |u|.$$

Its minimum value is

$$\Phi(m) = \begin{cases} 2m \left(1 - \frac{m}{L}\right) & \text{if } \frac{2m}{L} \leq 1 \\ \frac{L}{2} & \text{if } \frac{2m}{L} \geq 1 \end{cases}.$$

It is achieved for

$$u = \begin{cases} 1 - \frac{2m}{L} & \text{if } \frac{2m}{L} \leq 1 \\ 0 & \text{if } \frac{2m}{L} \geq 1 \end{cases}.$$

This justifies the statement made: the dislocations do not appear ( $u = 0$ ) until shear exceeds some critical value. For the critical value we have

$$\frac{2m}{L} = \frac{2ka}{\gamma^* 2l} = \frac{2k}{\gamma^* bl(\rho_s - \rho_{st})} = 1$$

thus,

$$\gamma^* = \frac{2k}{bl(\rho_s - \rho_{st})}.$$

The dependence of plastic deformation,  $\beta$ , on the external shear,  $\gamma$ , is shown in Fig. 3.

This simple model describes geometrical hardening, kind of Hall–Petch effect: the shorter the strip the larger shear must be to initiate the plastic deformation. After overcoming the threshold there is no work hardening in the course of deformation: the growth of the plastic shear strain,

$$\varepsilon^{(p)} = \beta/2 = \gamma u/2 = \gamma \frac{\left(1 - \frac{2k}{\gamma bl(\rho_s - \rho_{st})}\right)}{2}$$

occurs for a constant shear stress,  $\sigma = \mu(\gamma - \beta)$

$$\sigma = \mu(\gamma - \beta) = \mu\gamma(1 - u) = \mu \frac{2k}{bl(\rho_s - \rho_{st})}.$$

Such a behavior is caused by linearization of the problem. In case of the original functional (69) one would observe the work hardening as well.

The role of the logarithmic term in (69) is that it prohibits the jumps, and transforms the jumps into the boundary layers. We consider here the boundary layer near  $x = 0$ . To this end it is enough to put in (69)  $L = \infty$  and drop the boundary condition  $u(L) = 0$ . We obtain the variational problem,

$$\min_{\substack{u(x): \\ u(0)=0}} \int_0^\infty \left[ \frac{1}{2}(1 - u(x))^2 + m \ln \frac{1}{1 - |u_{,x}|} \right] dx \quad (71)$$

The minimizing function increases from zero to unity, therefore  $u_{,x} > 0$ , and the sign of the absolute value in (71) can be dropped. Denote by  $p(x)$  the function

$$p(x) = \frac{d}{du_{,x}} m \ln \frac{1}{1 - u_{,x}} = \frac{m}{1 - u_{,x}}.$$

The minimizing function satisfies the boundary value problem:

$$\frac{dp}{dx} = u - 1, \quad \frac{du}{dx} = 1 - \frac{m}{p}, \quad u(0) = 0, \quad u(\infty) = 1. \quad (72)$$

Function  $p(x)$  is a decreasing function of  $x$ . Since  $du/dx \rightarrow 0$  at infinity,  $p(\infty) = m$ .

The system (72) admits the first integral,

$$\frac{1}{2}(1 - u(x))^2 + m \ln p - p = \text{const.}$$

The value of the constant can be found from the conditions at infinity:

$$\frac{1}{2}(1 - u(x))^2 + m \ln p - p = m \ln m - m.$$

Hence,

$$1 - u(x) = \sqrt{2m \left( \frac{p(x)}{m} - 1 - \ln \frac{p(x)}{m} \right)}. \quad (73)$$

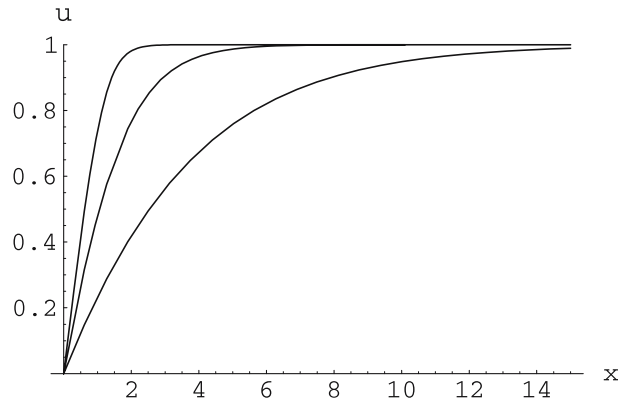
The expression under the square root is positive because  $p(x) \geq m$  and  $x \geq \ln x + 1$  for  $x \geq 1$ . Finally, for the function  $q(x) = p(x)/m - 1$ , we have the initial value problem

$$\frac{dq}{dx} = -\sqrt{\frac{2}{m}(q - \ln(1 + q))}, \quad q(0) = q_0$$

where, according to (73),  $q_0$  is the solution of the equation

$$q_0 - \ln(1 + q_0) = \frac{1}{2m}.$$

The dependence of the normalized plastic distortion,  $u(x) = \beta/\gamma$ , is shown in Fig. 4 for the three values of  $m = k/\gamma^2$ .



**Fig. 4** Distribution of the normalized plastic strain,  $u = \beta/\gamma$ , in the boundary layer for the three values of the parameter  $m$ ,  $m = k/\gamma^2$  :  $m = 0.1$  (the top curve),  $m = 1$  (the middle curve) and  $m = 10$  (the bottom curve)

## 4 Nonlinear continuum theory of dislocations

### 4.1 Kinematics

Denote by  $x^i$  and  $X^a$  the Eulerian and Lagrangian coordinates of the body, Latin indices  $i, j, k, l$  correspond to projections on the Eulerian coordinates while  $a, b, c, d$  to Lagrangian coordinates. Eulerian observer's frame is assumed Cartesian with the basic vectors,  $\mathbf{e}_i$ . The metric tensor in the observer's frame,  $g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$ , coincides with the Kronecker delta,  $\delta_{ij}$ , however, this is not used to maintain the tensor's nature of all relations.

The deformed state of the body is determined by the functions,

$$x^i = x^i(t, X^a). \quad (74)$$

Initially the particles of the body occupy the positions,

$$x^i = \hat{x}^i(X^a) = x^i(t_0, X^a).$$

The functions (74) can be inverted:

$$X^a = X^a(t, x^i).$$

The distortion is denoted by

$$x_a^i \equiv \frac{\partial x^i(t, X^a)}{\partial X^a}$$

while  $X_i^a$  is the inverse distortion:

$$X_i^a = \frac{\partial X^a(t, x^i)}{\partial x^i}, \quad X_i^a x_b^i = \delta_b^a, \quad X_i^a x_a^j = \delta_i^j.$$

Similarly, in the initial state,

$$\hat{x}_a^i \equiv \frac{\partial \hat{x}^i(X^a)}{\partial X^a}, \quad \hat{X}_i^a = \frac{\partial \hat{X}^a(x^i)}{\partial x^i}, \quad \hat{X}_i^a \hat{x}_b^i = \delta_b^a, \quad \hat{X}_i^a \hat{x}_a^j = \delta_i^j.$$

There are two sets of Lagrangian basic vectors with low indices,

$$\mathbf{e}_a = x_a^i \mathbf{e}_i, \quad \hat{\mathbf{e}}_a = \hat{x}_a^i \mathbf{e}_i$$

and the corresponding basic vectors with upper indices

$$\mathbf{e}^a = X_i^a \mathbf{e}^i, \quad \hat{\mathbf{e}}^a = \hat{X}_i^a \mathbf{e}^i.$$

For a plastically deformed body, one introduces one more set of vectors,  $\mathbf{e}_a^*(t, X^a)$ , which is the result of the following thought procedure: one cuts off a small piece of material in the vicinity of the point  $X^a$  and unload it; then vectors  $\mathbf{e}_a(t, X^a)$  transform into vectors  $\mathbf{e}_a^*(t, X^a)$ . The components of the vectors  $\mathbf{e}_a^*(t, X^a)$  are denoted by  $A_a^i$ ,

$$\mathbf{e}_a^* = A_a^i(t, X^a)\mathbf{e}_i$$

These nine fields,  $A_a^i(t, X^a)$ , describe the kinematics of plastic deformation. The inverse tensor is denoted by  $B_i^a$ ,

$$\mathbf{e}_i = B_i^a \mathbf{e}_a^*, \quad \mathbf{e}^{*a} = B_i^a \mathbf{e}^i, \quad A_a^i B_j^a = \delta_j^i, \quad A_a^i B_i^b = \delta_a^b$$

The Eulerian indices are moved by means of the metric tensor  $g_{ij}$ .

There are three metric tensors in the Lagrangian frame,

$$g_{ab} = g_{ij}x_a^i x_b^j, \quad g_{ab}^* = g_{ij}A_a^i A_b^j, \quad \mathring{g}_{ab} = g_{ij}\mathring{x}_a^i \mathring{x}_b^j$$

and, accordingly, the three measures of strains: total strains,

$$\varepsilon_{ab} = \frac{1}{2} (g_{ab} - \mathring{g}_{ab}) \quad (75)$$

elastic strains,

$$\varepsilon_{ab}^{(e)} = \frac{1}{2} (g_{ab} - g_{ab}^*) \quad (76)$$

and plastic strains,

$$\varepsilon_{ab}^{(p)} = \frac{1}{2} (g_{ab}^* - \mathring{g}_{ab}). \quad (77)$$

Total strain is the sum of elastic and plastic strains,

$$\varepsilon_{ab} = \varepsilon_{ab}^{(e)} + \varepsilon_{ab}^{(p)}. \quad (78)$$

To measure strains as the differences, (75)–(77), is feasible if the strains are small, otherwise metric tensors are the adequate measures of deformations themselves. In crystal plasticity, the elastic strains are small while the plastic strains can be large. This corresponds to smallness of the difference,  $\mathbf{e}_a - \mathbf{e}_a^* = (x_a^i - A_a^i)\mathbf{e}_i$ .

Incompatibility of the plastic deformation is measured by the tensor,  $A_{[a,b]}^i$ . To have all its components in one coordinate system, we put

$$\alpha^{ab} = B_i^a \varepsilon^{bcd} A_{d,c}^i. \quad (79)$$

Here  $\varepsilon^{bcd}$  are the contravariant components of the Levi–Civita tensor in the Lagrangian frame:  $\varepsilon^{bcd} = e^{bcd}/\sqrt{g}$ ,  $e^{bcd}$  the Levi–Civita symbols,  $g$  being the determinant of the matrix  $||g_{ab}||$ .

Three comments concerning the motivation for the notation chosen are in order to conclude this subsection.

1. The continuum mechanics equations are invariant with respect to the two groups of transformations: transformations of the observer's frames,

$$x'^i = x'^i(x^j) \quad (80)$$

and transformations of the Lagrangian frames,

$$X'^a = X'^a(X^b). \quad (81)$$

The group (80) causes the transformation of Eulerian indices,  $i, j, k, l$ , while the objects with the Lagrangian indices,  $a, b, c, d$ , are not affected by this group and behave as scalars. Similarly, the group (81) yields the transformations of the objects with the Lagrangian indices leaving the objects with the Eulerian indices unchanged. This is why one needs to distinguish these two types of indices in the notation.

2. An alternative would be to use the direct tensor notation when, for example, for a vector, one writes  $\mathbf{v}$ , implying that  $\mathbf{v} = v^i \mathbf{e}_i$ . Unfortunately, the attractive simplicity of the direct notation is accompanied by some shortcomings. Dealing with the components of a vector we do not know the vector. This is emphasized by the formula  $\mathbf{v} = v^i \mathbf{e}_i$  : to prescribe a vector one needs to specify both the components,  $v^i$ , and the frame,  $\mathbf{e}_i$ . For the same components of, say, the elastic strain tensor (75), one can define three different tensors

$$\varepsilon_1 = \varepsilon_{ab}^{(e)} \mathbf{e}^a \mathbf{e}^b, \quad \varepsilon_2 = \varepsilon_{ab}^{(e)} \hat{\mathbf{e}}^a \hat{\mathbf{e}}^b, \quad \varepsilon_3 = \varepsilon_{ab}^{(e)} \mathbf{e}^{*a} \mathbf{e}^{*b}.$$

We are interested in the dependence of energy on the components of the strain tensor, not on the entire tensor itself: it does not matter whether the strain tensor is the tensor  $\varepsilon_1$ ,  $\varepsilon_2$  or  $\varepsilon_3$ . If we, nevertheless, write  $U = U(\varepsilon_1)$ , we introduce into energy the extra arguments, the basic vectors, on which energy, in fact, does not depend. Mathematically, nothing is wrong: function may be independent on some of the arguments, but physically, this complication does not seem reasonable. Another shortcoming with the formula  $U = U(\varepsilon_1)$  is that one has to list all other arguments of energy, and the form of the arguments not mentioned may affect the function  $U(\varepsilon_1)$ . For example, in the case of an isotropic media the additional argument is just a tensor of the second order formed from the metric tensor. We have, however, a number of possibilities:

$$\mathbf{g}_1 = g^{ab} \mathbf{e}_a \mathbf{e}_b, \quad \mathbf{g}_2 = \hat{g}^{ab} \hat{\mathbf{e}}_a \hat{\mathbf{e}}_b, \quad \mathbf{g}_3 = g^{*ab} \mathbf{e}_a \mathbf{e}_b, \quad \mathbf{g}_4 = g^{ab} \hat{\mathbf{e}}_a \hat{\mathbf{e}}_b$$

not to mention a few more. The models with energies, say,  $U = U(\varepsilon_1, \mathbf{g}_1)$  and  $U = U(\varepsilon_1, \mathbf{g}_2)$  are different. For example, in the case of the linear dependence of energy on the elastic strains,

$$U(\varepsilon_1, \mathbf{g}_1) = \text{const } g^{ab} \varepsilon_{ab}^{(e)}, \quad U(\varepsilon_1, \mathbf{g}_2) = \text{const } \hat{g}^{ab} \varepsilon_{ab}^{(e)}$$

These are two different functions. Without specifying the additional arguments in energy the model remains undetermined. These issues are not essential in a linear theory but becomes important in nonlinear ones. Of course, after all necessary specializations, the direct notation makes sense; however, such specializations are needed only because we introduced the artificial argument into energy, the basic vectors. This is why the author prefers the index notation which avoids any ambiguities.

3. One can introduce the elastic distortion, the transition from the vectors  $\mathbf{e}_a^*$  to the vectors  $\mathbf{e}_a$ , and the plastic distortion, the transition from vectors  $\hat{\mathbf{e}}_a$  to vectors  $\mathbf{e}_a^*$ , by the formulas

$$\mathbf{e}_a = F_a^{(e)b} \mathbf{e}_b^*, \quad \mathbf{e}_a^* = F_a^{(p)b} \hat{\mathbf{e}}_b.$$

These distortions are linked to the distortions used,  $x_a^i$  and  $A_a^i$ , by the relations:

$$x_a^i = F_a^{(e)b} A_b^i, \quad A_a^i = F_a^{(p)b} \hat{x}_b^i.$$

The elastic and plastic distortions,  $F_a^{(e)b}$  and  $F_a^{(p)b}$ , can be expressed in terms of distortions  $x_a^i$  and  $A_a^i$  :

$$F_a^{(e)b} = B_i^b x_a^i, \quad F_a^{(p)b} = \hat{X}_i^b A_a^i.$$

The total distortion is a multiplication of elastic and plastic distortions,

$$x_a^i = F_a^{(e)b} F_b^{(p)c} \hat{x}_c^i. \quad (82)$$

The measure of elastic strains,  $\varepsilon_{ab}^{(e)}$ , can be expressed in terms of elastic distortions as:

$$\varepsilon_{ab}^{(e)} = \frac{1}{2} \left( g_{ij} F_a^{(e)c} A_c^i F_b^{(e)d} A_d^j - g_{ab}^* \right) = \frac{1}{2} g_{cd}^* \left( F_a^{(e)c} F_b^{(e)d} - \delta_a^c \delta_b^d \right) \quad (83)$$

The decomposition of the total distortion,  $x_a^i$ , into the product of elastic and plastic distortions was first introduced by Bilby, et al. [39] and further discussed by Kröner [40] and Lee [41]. The distortions used here,  $x_a^i$  and  $A_a^i$ , seem more convenient in the development of the general relationships.

## 4.2 Thermodynamics

Now we repeat the derivation of the basic equations of the Sect. 2 in the nonlinear setting. The energy density is assumed to be a function of entropy density, total and plastic distortions and the dislocation density tensor:

$$U = U \left( S, x_a^i, A_a^i, \alpha^{ab} \right). \quad (84)$$

There are additional arguments of energy which do not depend on time and, thus, are not listed among the arguments. These are the components of some tensors  $L_1^{a_1 a_2 \dots a_s}$ , ..., which describe the physical properties of the media. It is essential that the components of all tensors are taken in Lagrangian coordinates. One can use the Eulerian components of the tensors as well, but in this case, the physical characteristics of the body,  $L_1^{i_1 i_2 \dots i_s} = x_{a_1}^{i_1} x_{a_2}^{i_2} \dots x_{a_s}^{i_s} L_1^{a_1 a_2 \dots a_s}$ , ..., are dependent on the deformation, and the form of the equations becomes unnecessary complicated. Energy may depend on the initial distortion,  $\hat{x}_a^i$ , which also does not change in time.

So, for total energy of body we have

$$E = \int_{V_0} \rho_0 U \left( S, x_a^i, A_a^i, \alpha^{ab} \right) dV$$

where  $dV = \sqrt{\hat{g}} dX^1 dX^2 dX^3$ ,  $\hat{g}$  being the determinant of the initial metric,  $\hat{g} = \det \|\hat{g}_{ab}\|$ . The power of the external forces acting at the boundary of the body is

$$P = \int_{\partial V_0} (\sigma_i^j n_j v^i + \sigma_i^{aj} n_j \hat{A}_a^i) dA.$$

Here  $v^i$  is the particle velocity,

$$v^i \equiv \frac{\partial x^i(t, X^a)}{\partial t}$$

In the same way as in Sect. 2 one obtains the equilibrium equations (22), the symmetry of the stress tensor (23), the constitutive equations (further equations are given under the assumption that the viscous stresses are zero),

$$\sigma_i^j = \rho_0 \frac{\partial U}{\partial x_a^i} x_b^j - \frac{\partial U}{\partial \alpha^{cd}} \alpha^{cd} \delta_i^j \quad (85)$$

$$\kappa_i^a = -\rho_0 \frac{\partial U}{\partial A_a^i} + \rho_0 \frac{\partial U}{\partial \alpha^{cd}} \alpha^{ad} B_i^c + \sigma_{i,j}^{aj} \quad (86)$$

$$\sigma_i^{aj} = \rho_0 \frac{\partial U}{\partial \alpha^{cd}} B_i^c \varepsilon^{dba} x_b^j + \tau_i^{aj} \quad (87)$$

and the equation for entropy,

$$\rho_0 T \dot{S} = \kappa_i^a \dot{A}_a^i + \tau_i^{aj} \dot{A}_{a,j}^i. \quad (88)$$

The derivation proceeds as follows. First, note the kinematical relations for the time derivatives:

$$\begin{aligned} \dot{x}_a^i &= \frac{\partial v^i(t, X^a)}{\partial X^a}, & \dot{B}_j^a &= -B_j^b B_i^a \dot{A}_b^i, & \dot{g} &= g \frac{\partial v^i}{\partial x^i} \\ \dot{\varepsilon}^{bcd} &= -\varepsilon^{bcd} \frac{\partial v^i}{\partial x^i}, & \dot{\alpha}^{ab} &= B_i^a \varepsilon^{bcd} \dot{A}_{d,c}^i - B_i^a \dot{A}_c^i \alpha^{cb} - \alpha^{ab} \frac{\partial v^i}{\partial x^i} \end{aligned}$$

From the first law of thermodynamics,

$$\frac{d}{dt} \int_{V_0} \rho_0 U \left( S, x_a^i, A_a^i, \alpha^{ab} \right) dV = \int_{\partial V_0} (\sigma_i^j n_j v^i + \sigma_i^{aj} n_j \hat{A}_a^i) dA$$



we obtain the local equation

$$\begin{aligned} \rho_0 T \dot{S} + \left( \rho_0 \frac{\partial U}{\partial x_a^i} x_b^j - \frac{\partial U}{\partial \alpha^{cd}} \alpha^{cd} \delta_i^j - \sigma_i^j \right) v_{,j}^i + \left( \rho_0 \frac{\partial U}{\partial A_a^i} - \rho_0 \frac{\partial U}{\partial \alpha^{cd}} \alpha^{cd} B_i^c - \sigma_{i,j}^{aj} \right) \dot{A}_a^i \\ + \left( \rho_0 \frac{\partial U}{\partial \alpha^{cd}} B_i^c \varepsilon^{dba} x_b^j - \sigma_i^{aj} \right) \dot{A}_{a,j}^i - \sigma_{,j}^{ij} v_i = 0. \end{aligned} \quad (89)$$

As before, from the condition of the invariance of energy, stresses and entropy with respect to translations and rigid motions, we obtain the equilibrium equations (22) and the symmetry of the stress tensor (23). Denoting by  $\chi_i^a$  and  $\tau_i^{aj}$  the tensors (86) and (87), we arrive at the Eq. (88).

If the dissipation potential exists such that

$$\chi_i^a = \frac{\partial \mathcal{D}(\dot{A}_a^i, \dot{A}_{a,j}^i)}{\partial \dot{A}_a^i}, \quad \tau_i^{aj} = \frac{\partial \mathcal{D}(\dot{A}_a^i, \dot{A}_{a,j}^i)}{\partial \dot{A}_{a,j}^i} \quad (90)$$

then equations (86) and (87) reduce to the equations determining the plastic distortion:

$$\frac{\delta \mathcal{D}(\dot{A}_a^i, \dot{A}_{a,j}^i)}{\delta \dot{A}_a^i} = -\rho_0 \frac{\delta U}{\delta A_a^i} \quad (91)$$

where the variational derivatives are

$$\begin{aligned} \frac{\partial \mathcal{D}(\dot{A}_a^i, \dot{A}_{a,j}^i)}{\partial \dot{A}_a^i} &= \frac{\partial \mathcal{D}(\dot{A}_a^i, \dot{A}_{a,j}^i)}{\partial \dot{A}_a^i} - \left( \frac{\partial \mathcal{D}(\dot{A}_a^i, \dot{A}_{a,j}^i)}{\partial \dot{A}_{a,j}^i} \right)_{,j} \\ \frac{\delta U}{\delta A_a^i} &= \frac{\partial U}{\partial A_a^i} - \left( \frac{\partial U}{\partial A_{a,j}^i} \right)_{,j} = \frac{\partial U}{\partial A_a^i} - \rho \frac{\partial U}{\partial \alpha^{cd}} \alpha^{cd} B_i^c - \left( \rho_0 \frac{\partial U}{\partial \alpha^{cd}} B_i^c \varepsilon^{dba} x_b^j \right)_{,j}. \end{aligned}$$

Note that the dissipation potential may depend on all arguments of energy as well, but we do not mention this in the notation explicitly.

Equations (91) are a nonlinear version of the Eqs. (34). The equations presented are equivalent to that of [1] where they were written in a slightly different form using only the Lagrangian components of the tensors. Here is the notation correspondence:

$$\begin{aligned} \text{Latin indices } i, j, k, l &\longleftrightarrow \text{Greek indices } \alpha, \beta, \gamma, \delta \\ \text{Latin indices } a, b, c, d &\longleftrightarrow \text{Greek indices } \mu, \nu, \lambda, \kappa \\ \chi_i^a B^{bi} &\longleftrightarrow Q^{\mu\nu}, \quad \tau_i^{aj} A_b^i X_j^c \longleftrightarrow Q^{\mu\nu\lambda}, \quad X^a \longleftrightarrow \xi^\mu, \quad \alpha_{ij} \longleftrightarrow 2S_{ij} \end{aligned}$$

## 5 Energy and dissipation for finite crystal plasticity

### 5.1 Energy

As was mentioned in Sect. 1, the crystal lattice orientation is not changed by a compatible plastic deformation. This feature results in a special dependence of energy on the elastic strains: there are three fixed directions in the body such that energy is a universal function of the strains computed for these directions. Without loss of generality, we may take as such directions the vectors  $\hat{\mathbf{e}}_a = \hat{x}_a^i \mathbf{e}_i$ . For simplicity we assume that  $\hat{x}_a^i$  are some constants. Consider in the actual state a point  $x^i$  and an infinitesimally small material fiber directed along the vector  $\hat{\mathbf{e}}_a$ ,  $\hat{\mathbf{e}}_a d\xi$ . It corresponds to the increment of Lagrangian coordinates,  $dX_{(a)}^b$ , determined by the equation

$$x_b^i dX_{(a)}^b = \hat{x}_a^i d\xi$$

or

$$dX_{(a)}^b = X_i^b \hat{x}_a^i d\xi.$$

For each fiber,  $dX^b$ , the change of its length,  $ds$ , from the initial value,  $d\hat{s}$ , to the final value is

$$ds^2 - d\hat{s}^2 = \frac{1}{2}\varepsilon_{ab}dX^a dX^b$$

while the pure elastic change of length is

$$ds^2 - ds^{*2} = \frac{1}{2}\varepsilon_{ab}^{(e)}dX^a dX^b.$$

The elastic deformation along the direction  $\hat{\mathbf{e}}_a$ , can be written as

$$ds_{(a)}^2 - ds_{(a)}^{*2} = \frac{1}{2}\varepsilon_{a'b'}^{(e)}dX_{(a)}^{a'}dX_{(a)}^{b'} \equiv \frac{1}{2}\mathcal{E}_{aa}d\xi^2.$$

This suggests to characterize the deformations of the fibers directed along  $\hat{\mathbf{e}}_a$  by the tensor

$$\mathcal{E}_{ab} = \varepsilon_{a'b'}^{(e)}X_i^{a'}\hat{x}_a^i X_j^{b'}\hat{x}_b^j.$$

Elastic energy is a universal function of  $\mathcal{E}_{ab}$ . In particular, for small elastic strains the elastic energy is

$$U = \frac{1}{2}\hat{C}^{abcd}\mathcal{E}_{ab}\mathcal{E}_{cd}$$

where the elastic moduli,  $\hat{C}^{abcd}$ , are some constants. In terms of the usual elastic strain tensor,  $\varepsilon_{ab}^{(e)}$ , this function has the form<sup>18</sup>,

$$\begin{aligned} U &= \frac{1}{2}C^{abcd}\varepsilon_{ab}^{(e)}\varepsilon_{cd}^{(e)}, \quad C^{abcd} \equiv \hat{C}^{ijkl}X_i^a X_j^b X_k^c X_l^d \\ \hat{C}^{ijkl} &= \hat{C}^{a'b'c'd'}\hat{x}_a^i \hat{x}_b^j \hat{x}_c^k \hat{x}_d^l. \end{aligned} \quad (92)$$

We see that energy is a complex function of the distortion,  $x_a^i$ . Function (92) can be simplified if we take into account that elastic distortions are small, and, hence,  $x_a^i - A_a^i$  are small as well. Therefore, the inverse distortion,  $X_i^a$ , in the first approximation is equal to  $B_i^a$ . If we substitute  $X_i^a$  in (92) by  $B_i^a$ , all small corrections to  $X_i^a$  can be dropped because only quadratic terms are kept in (92). The tensor  $C^{abcd}$  takes the form

$$C^{abcd} = \hat{C}^{ijkl}B_i^a B_j^b B_k^c B_l^d. \quad (93)$$

The factors,  $B_i^a$ , are essential even in the isotropic case, when

$$\hat{C}^{ijkl} = \lambda g^{ij}g^{kl} + \mu (g^{ik}g^{jl} + g^{il}g^{jk}).$$

We have

$$C^{abcd} = \lambda g^{*ab}g^{*cd} + \mu (g^{*ac}g^{*bd} + g^{*ad}g^{*bc}).$$

The derivatives of this tensor with respect to  $A_a^i$  contribute to the constitutive equations, however energy does not depend on the plastic rotations. In anisotropic cases, as is seen from (93), energy does depend on plastic rotations.

<sup>18</sup> The necessity to introduce into plasticity theory the unchanged directions was recognized first, perhaps, by Mandel [42].

## 5.2 Dissipation

Similarly, for the dissipation one can write in the case of the power law flow rule:

$$D = \left( K^{abcd} \pi_{ab} \pi_{ab} \right)^{\frac{1}{2} \left( 1 + \frac{1}{m} \right)}$$

where

$$\pi_{ab} = A_{ia} \dot{A}_b^i, \quad K^{abcd} = \hat{K}^{ijkl} X_i^a X_j^b X_k^c X_l^d,$$

and  $\hat{K}^{ijkl}$  is some tensor which does not depend on deformations.

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