Kinematic assumptions and their consequences on the structure of field equations in continuum dislocation theory

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Abstract. Continuum Dislocation Theory (CDT) relates gradients of plastic deformation in crystals with the presence of geometrically necessary dislocations. Therefore, the dislocation tensor is introduced as an additional thermodynamic state variable which reflects tensorial properties of dislocation ensembles. Moreover, the CDT captures both the strain energy from the macroscopic deformation of the crystal and the elastic energy of the dislocation network, as well as the dissipation of energy due to dislocation motion.

The present contribution deals with the geometrically linear CDT. More precise, the focus is on the role of dislocation kinematics for single and multi-slip and its consequences on the field equations. Thereby, the number of active slip systems plays a crucial role since it restricts the degrees of freedom of plastic deformation. Special attention is put on the definition of proper, well-defined invariants of the dislocation tensor in order to avoid any spurious dependence of the resulting field equations on the coordinate system. It is shown how a slip system based approach can be in accordance with the tensor nature of the involved quantities. At first, only dislocation glide in one active slip system of the crystal is allowed. Then, the special case of two orthogonal (interacting) slip systems is considered and the governing field equations are presented. In addition, the structure and symmetry of the backstress tensor is investigated from the viewpoint of thermodynamical consistency. The results will again be used in order to facilitate the set of field equations and to prepare for a robust numerical implementation.

1. Introduction

The plastic behavior of metallic crystals strongly depends on the underlying defect structure. For a broad class of metals it is the motion of dislocations that carries plastic deformation and new macroscopic properties (e.g. hardening mechanisms) emerge from collective self-organization of dislocations. Among the resulting dislocation structures, cell patterns are often observed and seem to be of special relevance. In order to simulate the mechanical behavior of metals with dislocation cells, a model was developed which operates with scalar dislocation densities. This micro model was incorporated into a macroscopic viscoplasticity framework that allows studying the effects of complex load path changes [1]. Still, a desired validation of model assumptions as well as a reasonable estimation of introduced microstructural parameters requires a lower scale theory.

An appropriate means is the Continuum Dislocation Theory (CDT) (cf. e.g. [2-6]). In contrast to approaches such as [1], measures of dislocation density and energy are now related to gradients of
the plastic distortion. Furthermore, CDT incorporates the size effect, i.e. the material response depends on the size of the body due to some inherent length scale. Hence, a better understanding of physical phenomena may be expected. Despite the success of the CDT, some basic questions remain still open, e.g. if the theory should be based on the dislocation density tensor or on individual slip system gradients. The present study makes a contribution towards answering this question.

2. Kinematics of continuously dislocated crystals

2.1. Basic assumptions

The kinematics of continuously distributed dislocations in the geometrically linear theory is based on the additive split of the displacement gradient into elastic and plastic parts: \( \text{grad}(u) = : \beta = \beta_e + \beta_p \). They are named elastic and plastic distortion tensor, respectively. Typical for the theory, the additional primary field is considered a result of the collective motion of continuously distributed dislocations. Since crystals have a discrete lattice with different slip systems, the plastic distortion is restricted. In order to incorporate this into the continuum theory, the following expansion is used:

\[
\beta_p = \sum_{n=1}^{N} \beta_n(r) s_n \otimes m_n = \sum_{n=1}^{N} \beta_n(r) G_n ,
\]

where \( N \) is the number of slip systems and the unit vectors \( s_n \) and \( m_n \) are the slip direction and slip plane normal, respectively (figure 1). From Eq. (1) it follows that \( \beta_p \) is isochoric and thus has only 8 independent coordinates. This assumption is well supported by many experiments that demonstrate the incompressibility of plastic flow. However, in real crystals much more than 8 slip systems are present and can be active at the same time. Furthermore, the slip system tensors \( G_n \) need not be and cannot be linearly independent in case of \( N \leq 8 \) and \( N > 8 \) slip systems, respectively. At first this might seem as an unbearable ambiguity, but a remedy becomes obvious by introducing dissipation (cf. Subsection 4.3). The resulting slip (shear) with respect to a certain shear plane is then a linear combination

\[
\beta_{p1} = s_1 \cdot \beta_p \cdot m_1 = \beta_1 + \beta_2(s_1 \cdot s_2)(m_1 \cdot m_2) + \beta_3(s_1 \cdot s_3)(m_1 \cdot m_3) + \ldots ,
\]

\[
\beta_{p2} = s_2 \cdot \beta_p \cdot m_2 = \beta_2 + \beta_1(s_1 \cdot s_2)(m_1 \cdot m_2) + \beta_3(s_1 \cdot s_3)(m_1 \cdot m_3) + \ldots .
\]

Separating the individual contributions \( \beta_n \) is thus only possible for orthogonal slip systems where the scalar products on the right hand side of Eq. (2) vanish.

Figure 1. Left: Single-slip with one active slip system & straight edge dislocations (symbol T). Right: Multi-slip, special case of two orthogonal slip systems with straight edge dislocations
2.2. Preliminary consideration for a single dislocation segment

For the sake of physical interpretation it is useful to first consider the dislocation density tensor of a single dislocation line segment, defined as

$$\alpha = \frac{\alpha(x)}{b} \otimes t = \rho(r) \ b \otimes t,$$  \hspace{1cm} (3)

with the crystal’s Burgers Vector \( b \), its norm \( b = |b| \), the line tangent \( t \) (unit vector) and the (signed) scalar dislocation density \( \rho(r) \) as a function of space. Since \( \alpha \) is an unsymmetric rank-one tensor, the second and third principal invariant vanish, i.e. \( I_2(\alpha) = I_3(\alpha) = 0 \). In fact, among all six independent invariants only three remain:

\[
\begin{align*}
I_1(\alpha) &= \int \alpha \cdot \alpha = \rho \ (b \cdot t), \\
I_2(\alpha) &= \frac{1}{2} \{ I_1(\alpha)^2 - \alpha \cdot \alpha^T \} = \frac{1}{2} \rho^2 \ (b \cdot t)^2 - (b \cdot b), \\
I_3(\alpha) &= \frac{1}{6} \{ I_1(\alpha)^2 - 3I_1(\alpha)\alpha \cdot \alpha^T + 2\alpha^2 \cdot \alpha^T \} = \frac{1}{6} \rho^3 \ (b \cdot t)^3 - (b \cdot b)(b \cdot t) = \frac{1}{6} I_1 I_2.
\end{align*}
\]  \hspace{1cm} (4)

Now it is very illustrative to consider both pure dislocation characters. If the dislocation line segment has edge character (denoted by \( \perp \)), \( b \) and \( t \) are parallel, hence:

$$I_1(\perp) = \rho \ b , \quad I_2(\perp) = 0 , \quad I_3(\perp) = 0 .$$  \hspace{1cm} (5)

If the dislocation line segment has edge character (denoted by \( \perp \)), \( b \) and \( t \) are perpendicular, hence:

$$I_1(\perp) = 0 , \quad I_2(\perp) = -\frac{1}{2} \rho^2 \ b^2 , \quad I_3(\perp) = 0 .$$  \hspace{1cm} (6)

A mixed dislocation segment can always be decomposed into edge and screw part. Consequently, the corresponding densities can be calculated from the invariants:

$$\bar{\rho} = \frac{1}{b} I_1(\underline{\underline{\alpha}}) , \quad \bar{\rho} = \frac{1}{b} \sqrt{-2I_2(\underline{\underline{\alpha}})} .$$  \hspace{1cm} (7)

Thus, a physical significance/interpretation of the invariants of tensor \( \alpha \) is found.

2.3. Properties and invariants of the dislocation (density) tensor

The Nye-Bilby-Kröner dislocation (density) tensor \( \underline{\underline{\alpha}} := \text{curl}(\beta_p) \) reflects tensorial dislocation properties of geometrically necessary dislocations as a result of the incompatibility of plastic (or elastic) deformation. It follows from the definition of the resultant Burgers vector using Stokes’ theorem:

$$b_r = \oint_C \beta_p \cdot dr = \int_A \text{rot} \left( \frac{\beta_p}{n} \right) \cdot n \ dA ,$$  \hspace{1cm} (8)

$$\begin{align*}
\frac{db_r}{\alpha} &= \alpha \cdot n \ dA \Rightarrow \alpha := \text{rot}(\beta_p) .
\end{align*}
$$

From Eq. (8) it follows immediately that \( \alpha \) is unsymmetric. Furthermore, the resulting Burgers vector is an integral quantity. However, multiplying the dislocation tensor \( \alpha \) with some cut plane normal \( n \), a corresponding local measure \( \alpha \) is obtained:

$$\alpha(n) = \frac{db_r}{dA} = \alpha \cdot n = \perp n + \perp_1 t_1 + \perp_2 t_2 .$$  \hspace{1cm} (9)

As shown, this vector can be decomposed into normal \((\underline{n})\) and tangential parts \((t_1, t_2)\), which may be attributed to screw and edge character dislocations, respectively [4]. Nevertheless, it
should be noted that procedure (8) is in fact a homogenization leaving only geometrically necessary dislocations over. All information about statistically stored dislocations is lost. If slip system expansion (1) is applied, the dislocation density tensor has the form:

\[ \mathbf{a} = \text{curl}(\mathbf{\beta}_p) = \sum_{n=1}^{N} \mathbf{s}_n \otimes \nabla \mathbf{\beta}_n \times \mathbf{m}_n . \]

Note that in this study, a summation over the slip systems is always indicated by a sigma sign. Else, there is no summation convention for the slip system indices.

In order to capture the energy of a continuously dislocated crystal (cf. Subsection 3.1), physically meaningful invariants of \( \mathbf{a} \) have to be found. As an unsymmetric second-order tensor, six independent invariants may exist. As shown in the previous subsection, the first principal invariant \( I_1(\mathbf{a}) \) is related to the dislocation density of screw segments. However, in the following only straight edge dislocations shall be considered. Since \( \mathbf{s}_n \) and \( \mathbf{m}_n \) are perpendicular, Cartesian basis systems \( \{ \mathbf{s}_n, \mathbf{m}_n, \mathbf{t}_n \} \) can be defined [4], where \( \mathbf{t}_n := \mathbf{s}_n \times \mathbf{m}_n \) is the tangent vector on the edge dislocation bundle. The assumption of straight edge dislocation lines implies zero plastic slip gradients in the tangent direction, i.e. \( \nabla \mathbf{\beta}_n \cdot \mathbf{t}_n = 0 \). This has further consequences on the properties of \( \mathbf{a} \). Calculating the first principal invariant

\[ I_1(\mathbf{a}) = \mathbf{I} : \sum_{n=1}^{N} \mathbf{s}_n \otimes \nabla \mathbf{\beta}_n \times \mathbf{m}_n = \sum_{n=1}^{N} \mathbf{s}_n \cdot (\nabla \mathbf{\beta}_n \times \mathbf{m}_n) = \sum_{n=1}^{N} \nabla \mathbf{\beta}_n \cdot (\mathbf{m}_n \times \mathbf{s}_n) = 0 , \]

it is found that the tensor is now indeed deviatoric (traceless). Hence, \( \mathbf{a} \) can have only five independent invariants. Imposing further the restriction of single slip \( (N = 1) \), it is found that \( \mathbf{a} \) is also second-order nil-potent, i.e. \( \mathbf{a}^n = 0 \forall n \geq 2 \), e.g.:

\[ \mathbf{a}^2 = \mathbf{a} \cdot \mathbf{a} = (\mathbf{s} \otimes \nabla \mathbf{\beta} \times \mathbf{m}) \cdot (\mathbf{s} \otimes \nabla \mathbf{\beta} \times \mathbf{m}) = \mathbf{s} \otimes \{(\nabla \mathbf{\beta} \times \mathbf{m}) \cdot \mathbf{s}\} \otimes \nabla \mathbf{\beta} \times \mathbf{m} = 0 . \]

Thus, all basic invariants \( J_3(\mathbf{a}) := \mathbf{I} : \mathbf{a}^3 = 0 \) for a crystal with only one active slip system and straight edge dislocation lines. Then, \( I_2(\mathbf{a}) = I_3(\mathbf{a}) = 0 \) follows immediately. Only one non-vanishing invariant remains:

\[ I_2(\mathbf{a}) = \frac{1}{2} \{ I_1(\mathbf{a}) - \mathbf{a} \cdot \mathbf{a}^T \} = \frac{1}{2} \{ 0 - \| \mathbf{a} \|^2 \} . \]

Consequently, the Frobenius norm \( \| \mathbf{a} \| \) carries all scalar information of \( \mathbf{a} \) in this special case. Thus, the (total) dislocation density may be defined as

\[ \rho = \frac{1}{b} \| \mathbf{a} \| = \frac{1}{b} \| \nabla \mathbf{\beta} \times \mathbf{m} \| = \frac{1}{b} \| \nabla \mathbf{\beta} \cdot \mathbf{s} \| . \]

However, in the general case (10) without any restrictions, the three principal invariants do not vanish. Moreover, they contain interaction terms as can be seen e.g. in the case of two slip systems with \( \mathbf{a} = \mathbf{s}_1 \otimes \nabla \mathbf{\beta}_1 \times \mathbf{m}_1 + \mathbf{s}_2 \otimes \nabla \mathbf{\beta}_2 \times \mathbf{m}_2 \) from Eq. (10):

\[ \| \mathbf{a} \|^2 = \mathbf{a} \cdot \mathbf{a}^T = \nabla \mathbf{\beta}_1 \otimes \nabla \mathbf{\beta}_1 \cdot (\mathbf{I} - \mathbf{m}_1 \otimes \mathbf{m}_1) + \nabla \mathbf{\beta}_2 \otimes \nabla \mathbf{\beta}_2 \cdot (\mathbf{I} - \mathbf{m}_2 \otimes \mathbf{m}_2) + 2 (\mathbf{s}_1 \cdot \mathbf{s}_2) \nabla \mathbf{\beta}_1 \otimes \nabla \mathbf{\beta}_2 \cdot (\mathbf{I} - \mathbf{m}_1 \otimes \mathbf{m}_2 - \mathbf{m}_1 \otimes \mathbf{m}_2) \]
\[ = (\nabla \mathbf{\beta}_1 \cdot \mathbf{s}_1)^2 + (\nabla \mathbf{\beta}_2 \cdot \mathbf{s}_2)^2 + 2 (\mathbf{s}_1 \cdot \mathbf{s}_2) (\nabla \mathbf{\beta}_1 \cdot \mathbf{s}_1) (\nabla \mathbf{\beta}_2 \cdot \mathbf{s}_2) . \]

For this purpose, the Identity tensor was represented by \( \mathbf{I} = \mathbf{m}_n \otimes \mathbf{m}_n + \mathbf{s}_n \otimes \mathbf{s}_n + \mathbf{t}_n \otimes \mathbf{t}_n \) and \( \nabla \mathbf{\beta}_n \cdot \mathbf{t}_n = 0 \) was exploited according to the assumptions above. Since the physical significance of
these interactions is not clear, a definition of scalar dislocation densities from principal invariants or from the norm $||\alpha||$ is not favorable. Instead, another slip-system-based set of invariants is preferred. First, the corresponding local dislocation vector of all dislocations piercing a plane with $\mathbf{n} = t_n$ is calculated, i.e. the dislocation tangents $t_n$ are cut perpendicularly. Now the resulting vector is decomposed according to Eq. (9). This is demonstrated on the example of two slip systems again:

$$\alpha_1 = s_1 \cdot \alpha \cdot t_1 = (\nabla \beta_1 \cdot s_1) + (\nabla \beta_2 \cdot s_2)(s_1 \cdot s_2),$$
$$\alpha_2 = s_2 \cdot \alpha \cdot t_2 = (\nabla \beta_2 \cdot s_2) + (\nabla \beta_1 \cdot s_1)(s_1 \cdot s_2).$$

Recalling Eq. (3) it becomes clear that these invariants measure the (signed) dislocation density multiplied by $b$ from all segments with Burgers vector $b = b_s \alpha_n$ at some position $\mathbf{r}$. Consequently, unsigned dislocation densities can be defined as $\rho_n = |\alpha_n|/b$. In case of orthogonal slip systems (here: $m_1 \cdot m_2 = s_1 \cdot s_2 = 0$), there are no contributions from one slip system to the other. Hence, the dislocation densities are proportional to the gradients of plastic slip in the slip direction only:

$$\rho_1 = \frac{1}{b}|\alpha_1| = \frac{1}{b}|\nabla \beta_1 \cdot s_1|, \quad \rho_2 = \frac{1}{b}|\alpha_2| = \frac{1}{b}|\nabla \beta_2 \cdot s_2|.$$

The total dislocation density is then simply a sum: $\rho_{tot} = \rho_1 + \rho_2$. However, in the general case of non-orthogonal slip systems (as in most real crystals), the mere gradients $\nabla \beta_n \cdot s_n$ are no invariants of $\alpha$. In other words, it is not possible to only extract them from $\alpha$ in a way that does not depend on the chosen coordinate system. Instead, additional terms result from the tensor nature of the involved quantities (as can be seen in Eq. (16)). Taking them into account, the resultant field equations for $\beta_1, \beta_2, \ldots, \beta_N$ will be in fact coupled, but invariant with respect to a change of the coordinate system.

From the physical point of view the CDT can neither determine the dislocation configuration which has led to the plastic distortion, nor can the CDT uniquely determine the character of the dislocations that are geometrically necessary at the moment. Rather, the only information which is accessible is the resultant Burgers vector with respect to any cut plane as a measure of the crystal’s closure failure.

3. Thermodynamics of continuously dislocated crystals

3.1. State variables, stored energy and external power

The free energy density of the dislocated crystal depends on the thermodynamical state variables $\xi_\varepsilon, \xi_v = \text{sym}(\beta_v)$. An additive decomposition $\varphi = \varphi_v(\xi_v) + \varphi_p(\alpha)$ is assumed. The (macroscopic) elastic strain energy is given by Hooke’s law:

$$\varphi_v(\xi_v) = \mu ||\xi_v||^2 + \frac{1}{2} \lambda \xi_1^2(\xi_v),$$

where $\mu$ and $\lambda$ denote Lam’s constants. The dislocation energy $\varphi_p$ depends on the number of active slip systems as well as the slip mechanisms (e.g. glide or cross slip). However, in this study only two special cases are considered. For single slip conditions, motivated by statistical mechanics [2], the dislocation energy can be specified as

$$\varphi_p(\alpha) = k \mu \ln[(1 - \rho/\rho_s)^{-1}],$$

with a scaling parameter $k > 0$ and the dislocation density $\rho$ according to definition (14). This ansatz features both the linear dependence of the dislocation energy for small densities and the steep upturn when $\rho$ approaches the saturation density $\rho_s$. In case of two active slip systems many forms are possible depending on the choice of invariants of the dislocation tensor. For the
reasons discussed in Subsection 2.2, invariants \( \rho_n = |\alpha_n|/b \) from Eq. (16) should be preferred. Consider an example from [3]:

\[
\phi_p(\alpha) = k\mu \left( \ln \left( 1 - \frac{\rho_1}{\rho_s} \right)^{-1} \right) + \ln \left( 1 - \frac{\rho_2}{\rho_s} \right)^{-1} + \chi \frac{\rho_1 \rho_2}{\rho_s^2} \right) .
\] (20)

Here, the interaction between the two slip systems is modeled by the quadratic term with some interaction parameter \( \chi > 0 \) (figure 2). For two orthogonal slip systems \( (m_1 \cdot m_2 = s_1 \cdot s_2 = 0, \text{cf. Eq. (17)}) \) this is the only interaction. In the general case \( (m_1 \cdot m_2 \neq 0) \), the first two summands of Eq. (20) include some inherent interaction as well. Consequently, the numerical simulations for \( m_1 \cdot m_2 = 0 \) and \( m_1 \cdot m_2 \neq 0 \) are expected to give insights into the effects of these differences.

Figure 2. Surface plot of the dislocation energy according to Eq. (20). As indicated by the dashed lines, the dislocation densities cannot exceed the saturation value (here \( \rho_s = 4 \cdot 10^2 \mu m^{-2} \)). In addition, a minor effect of parameter \( \chi \) is visible.

Next, the internal power (external power minus the rate of kinetic energy) has to be defined in a suitable way. Postulating the existence of a hyper stress tensor conjugate to the plastic distortion field, the internal power density is finally obtained as

\[
p_{in} = \text{div}(\dot{\sigma} \cdot \hat{u}) + \dot{\rho}_m(f - \ddot{\hat{u}}) + \text{div}(\dot{\beta}_p \cdot \Sigma) ,
\] (21)

with \( \rho_m \) denoting the mass density, \( \sigma \) the Cauchy stress tensor and \( f \) the body forces. The first two terms in Eq. (21) are classical while the third one arises from the incorporation of higher gradients in the CDT.

3.2. Evaluation of the Clausius-Duhem inequality

The field equations of the CDT are obtained exploiting the laws of thermodynamics in the form of the Clausius-Duhem inequality. In the isothermal case it reads \( p_{in} - \dot{\phi} \geq 0 \). With the previous assumptions the dissipation (dissipated power \( p_{in} - \dot{\phi} \)) follows as:

\[
\left( \text{div}(\dot{\sigma}) + \rho_m(f - \ddot{\hat{u}}) \right) \cdot \dot{u} + \left( \sigma \cdot \frac{\partial \phi}{\partial \beta} \right) \frac{\partial \beta}{\partial \beta} T + \left( \text{div}(\Sigma) - \frac{\partial \phi}{\partial \beta} \right) \frac{\partial \beta}{\partial \beta} T + \left( \Sigma + \frac{\partial \phi}{\partial \alpha} \cdot \epsilon \right) \text{grad}(\dot{\beta} \Sigma) \geq 0 .
\]

where \( \epsilon \) denotes the Ricci tensor and \( \beta \) stands for the displacement gradient. Now, Galilean invariance of the dissipation implies \( \text{div}(\dot{\sigma}) + \rho_m(f - \ddot{\hat{u}}) = 0 \) (local balance of forces). In this
contribution, a special form of the theory is considered employing the following potential relations for the stress tensors:

$$\sigma = \frac{\partial \phi(\varepsilon_e, \alpha)}{\partial \beta_e}, \quad \Sigma = -\frac{\partial \phi}{\partial \alpha} \cdot \varepsilon.$$

(22)

Consequently, the only remaining part of the dissipation inequality to be fulfilled is

$$\text{div} \left( \Sigma - \frac{\partial \phi}{\partial \beta_p} \right) \cdot \dot{\beta}_p^T = -\text{curl} \left( \frac{\partial \phi}{\partial \alpha} \right) - \frac{\partial \phi}{\partial \beta_p} \cdot \dot{\beta}_p^T \geq 0.$$

(23)

It can either be set zero (zero dissipation case, cf. also [6]) or equal to some corresponding partial derivative of a so-called dissipation potential $D$:

i) $-\text{curl} \left( \frac{\partial \phi}{\partial \alpha} \right) - \frac{\partial \phi}{\partial \beta_p} = 0$ or ii) $-\text{curl} \left( \frac{\partial \phi}{\partial \alpha} \right) - \frac{\partial \phi}{\partial \beta_p} = \frac{\partial D}{\partial \beta_p}.$

(24)

Choosing the dissipation potential as a positive, homogeneous function the dissipation inequality is fulfilled a priori without further specifications. In addition, the introduction of the dissipation potential facilitates the modeling of different dissipative phenomena in a thermodynamically consistent way: It is experimentally confirmed that dislocation motion requires exceeding a critical resolved shear stress $\tau_{cr}$. This can be taken into account by $D(\dot{\beta}_p) = \tau_{cr} \parallel \dot{\beta}_p \parallel$. The quadratic form $D(\dot{\beta}_p) = \frac{1}{2} \eta_p \| \dot{\beta}_p \|^2$ captures viscous interaction of moving dislocations and crystal lattice. For the same reasons as discussed in Subsection 2.2 for tensor $\alpha$, slip system based invariants of the rate of plastic distortion should be preferred. Recalling Eq. (2), it is possible to define an invariant dissipation potential in the following way:

$$D(\dot{\beta}_p) = \tau_{cr} \left( |\dot{\beta}_{p2}| + |\dot{\beta}_{p1}| \right) + \frac{1}{2} \eta_p \left( \dot{\beta}_{p2}^2 + \dot{\beta}_{p1}^2 \right).$$

(25)

Note that taking merely the slip rates $\dot{\beta}_n$ would, in general, imply that the dissipation is not invariant with respect to a change of coordinate system anymore.

3.3. Thermodynamic consistency of the case with zero dissipation

If decomposition (1) is applied, i.e. the crystal nature is taken into account using slip systems, further considerations are necessary. This stems from the fact that the plastic distortion is then not arbitrary anymore. Let us introduce some abbreviations:

$$\text{curl} \left( \frac{\partial \phi}{\partial \alpha} \right) = X, \quad \frac{\partial \phi}{\partial \beta_p} = \frac{\partial \phi_e(\varepsilon - \varepsilon_p)}{\partial \beta_p} = -\frac{\partial \phi_e}{\partial \varepsilon} = -\sigma.$$

(26)

The second-order tensor $X$ is the well-known backstress tensor, which is obviously unsymmetric in general. The Cauchy stress tensor however is symmetric for the chosen strain energy (18). Rewriting Eq. (24) for zero dissipation in the form of an effective stress $\sigma = X$ reveals a contradiction: the difference of a symmetric and an unsymmetric tensor can never vanish. However, this discrepancy can be solved realizing that the problem originates going from Eq. (23) to (24). Implicitly, it was assumed that inequality (23) must hold for arbitrary plastic distortions, which is now not the case anymore. Instead, expansion (1) must be introduced into inequality (23). In case of zero dissipation this yields

$$(\sigma - X) \cdot \sum_{n=1}^{N} \dot{\beta}_n \cdot s_n \otimes m_n = \sum_{n=1}^{N} s_n \cdot (\sigma - X) \cdot m_n \cdot \dot{\beta}_n = 0.$$

(27)
Now demanding this equation to be fulfilled for arbitrary plastic slip rates $\dot{\beta}_n$ yields a much weaker condition.

Let us first consider single slip ($N = 1$). In order to obtain zero dissipation, only one coefficient $s \cdot (\sigma \cdot X) \cdot m$ must vanish. In other words, only this coefficient is physically significant. All other components are simply undefined. The next interesting scenario is $1 < N < 8$. Now $N$ coefficients of $\sigma \cdot X$ (or linear combinations of them) have to vanish. However, the backstress tensor $X$ may still be unsymmetric. Nevertheless, special cases can occur where $X$ is symmetric, e.g. for two orthogonal slip systems (see Subsection 4.2). In the case of $N > 8$ independent slip systems the plastic distortion tensor has a sufficient degree of freedom such that it can take arbitrary values (though it still is a sum of slip system contributions). As a consequence, $X$ now must be and will be symmetric in order to fulfill the partial differential equation (24), in short $\sigma \cdot X = 0$ (cf. [5]). This is in accordance with symmetric backstress tensors known from purely phenomenological models (cf. e.g. [7]). The results are summarized below.

Table 1. Restrictions imposed on the effective stress $\sigma \cdot X$ for zero dissipation

| Case | Number of active slip systems | Restrictions | Symmetry of $X$ |
|------|-------------------------------|--------------|-----------------|
| a)   | $N = 1$                       | $s \cdot (\sigma \cdot X) \cdot m = 0$ | unsymmetric    |
| b)   | $1 < N < 8$                   | $s_n \cdot (\sigma \cdot X) \cdot m_n = 0 \ \forall \ n \in [1, N]$ | unsymmetric    |
| c)   | $N \geq 8$                    | $\sigma \cdot X = 0$ | symmetric       |

There is another important consequence: Obviously, for $N < 8$ slip systems some components of $X$ are neither defined nor physically significant. This also holds for non-zero dissipation. Hence, the field equations cannot be formulated for the entire plastic distortion tensor in this case. Instead, scalar field equations operating on the slip system level have to be used. Still, for $N \geq 8$ independent slip systems, this approach is depleted and a tensor field equation has to be solved.

4. Field equations for special slip conditions

4.1. One active slip system with straight dislocation lines

In this case (cf. figure 1, left), the plastic distortion tensor has the simple form $\beta_p = \beta \cdot s \otimes m$.

It is interesting to note that thus plastic slip results both in plastic strain and plastic spin, as it can be seen from:

$$\varepsilon_p = \text{sym}(\beta_p) = \frac{\beta}{\gamma} (s \otimes m + m \otimes s), \quad w_p = \text{skw}(\beta_p) = \frac{\beta}{\gamma} (s \otimes m - m \otimes s).$$

(28)

Hence, it is not possible to obtain an irrotational plastic distortion field. Furthermore, case a) from table 1 applies. Consequently, the field equations for the plastic distortion tensor are simplified to a scalar field equation for the plastic slip $\beta(x)$:

$$-s \cdot \left( \frac{\partial \phi}{\partial \beta_p} + \text{curl} \left( \frac{\partial \phi}{\partial \alpha} \right) \right) \cdot m = s \cdot \frac{\partial D}{\partial \beta_p} \cdot m \quad \Rightarrow \quad -\frac{\partial \phi}{\partial \beta} + \text{div} \left( \frac{\partial \phi}{\partial \nabla \beta} \right) = \frac{\partial D}{\partial \beta}.$$  

(29)

Together with the other field equation, which reduces to $\text{div}(\sigma) = 0$ in absence of body and inertia forces, the set of field equations is complete. Defining proper initial and boundary conditions, the evolution of the fields $u(x)$ and $\beta(x)$ can be predicted. Numerical solutions of the corresponding initial boundary value problems were obtained for the case of plane deformations using an in-house finite difference simulation code. The results will be presented in a forthcoming article.
4.2 Two orthogonal slip systems with straight dislocation lines

In this case (cf. figure 1, right) \( \beta_p = \beta_1 \xi_1 \otimes m_1 + \beta_2 \xi_2 \otimes m_2 \). Consider an example:

\[
\xi_1 = \xi_x, \quad m_1 = \xi_y, \quad \xi_2 = \xi_y, \quad m_2 = -\xi_x, \quad (30)
\]

for the basis \( \xi_a = \{ \xi_x, \xi_y, \xi_z \} \). The plastic distortion has then the following coefficient matrix:

\[
[\xi_a \cdot x \cdot \xi_b] = \begin{bmatrix}
0 & \beta_1 \\
-\beta_2 & 0
\end{bmatrix}. \quad (31)
\]

In contrast to the previous subsection, \( \beta_p \) may be symmetric or skew-symmetric now. The dislocation density tensor \( \alpha = \text{curl}(\beta_p) = \xi_1 \otimes \nabla \beta_1 \times m_1 + \xi_2 \otimes \nabla \beta_2 \times m_2 \) follows straightforward. Without loss of generality, let us for now assume a quadratic form of the dislocation energy \( \phi_p(\alpha) = C/2 ||\alpha||^2 \) [4] such that the backstress tensor follows as

\[
X = \text{curl} \left( \frac{\partial \phi}{\partial \alpha} \right) = C \left( \xi_1 \otimes m_1 \cdot (\Delta \beta_1 I - \nabla \otimes \nabla \beta_1) + \xi_2 \otimes m_2 \cdot (\Delta \beta_2 I - \nabla \otimes \nabla \beta_2) \right), \quad (32)
\]

with the Laplace operator defined as \( \Delta = \nabla \cdot \nabla \). Introducing the relations (30) yields

\[
[\xi_a \cdot x \cdot \xi_b] = C \left[ \begin{array}{cc}
\nabla_y \nabla_x \beta_1 & -\Delta \beta_1 + \nabla_y \nabla \beta_1 \\
\nabla_x \nabla_y \beta_2 & -\Delta \beta_2 + \nabla_x \nabla \beta_2
\end{array} \right] = C \left[ \begin{array}{cc}
\nabla_y \nabla_x \beta_1 & -\nabla_x \nabla_y \beta_1 \\
\nabla_y \nabla_x \beta_2 & -\nabla_x \nabla_y \beta_2
\end{array} \right]. \quad (33)
\]

As this corresponds to case b) from table 1, the following restrictions must hold for zero dissipation:

\[
\xi_1 \cdot (\sigma - X) \cdot m_1 = 0, \quad \xi_2 \cdot (\sigma - X) \cdot m_2 = 0. \quad (34)
\]

Inserting relations (30) again yields \( \sigma_{xy} = X_{xy} \) and \( \sigma_{yx} = X_{yx} \). Considering the symmetry of the Cauchy stress tensor, it is inferred that \( X_{yx} = X_{xy} \). Hence, the backstress tensor must be symmetric, which implies

\[
-\nabla_x \nabla_x \beta_1 = -\nabla_y \nabla_y \beta_2 \iff -\xi_1 \cdot \nabla \otimes \nabla \beta_1 \cdot \xi_1 = \xi_2 \cdot \nabla \otimes \nabla \beta_2 \cdot \xi_2. \quad (35)
\]

This theoretical statement is of high importance for the numerical solution of the field equations in this case. They are obtained employing now the dislocation energy in the form (20) and the dissipation according to Eq. (25) (with \( \tau_{ex} = \chi = 0 \) for simplicity):

\[
(\lambda + \mu) \nabla \otimes \nabla \cdot u + \mu \nabla \cdot \nabla \otimes \cdot u - \mu \text{sym}(G) \cdot (\nabla \beta_1 - \nabla \beta_2) = 0, \\
2\mu \text{sym}(G) \cdot \nabla \otimes \cdot u + \mu(\beta_2 - \beta_1) + C \xi_1 \cdot \nabla \otimes \nabla \beta_1 \cdot \xi_1 \left( 1 - \frac{|\nabla \beta_1 \cdot \xi_1|^2}{b \rho_1} \right)^2 = \eta_p \beta_1, \\
-2\mu \text{sym}(G) \cdot \nabla \otimes \cdot u - \mu(\beta_2 - \beta_1) + C \xi_2 \cdot \nabla \otimes \nabla \beta_2 \cdot \xi_2 \left( 1 - \frac{|\nabla \beta_2 \cdot \xi_2|^2}{b \rho_2} \right)^2 = \eta_p \beta_2. \quad (36)
\]

Here, the abbreviations \( G = \xi_1 \otimes m_1 = -m_2 \otimes \xi_2 \) and \( C = k \mu/(b \rho_1) \) were used. System (36) constitutes a set of coupled partial differential equations. Let us first consider its stationary points. To this end, suppose a constant displacement gradient such that the total shear \( \gamma = 2 \text{sym}(G) \cdot \nabla \otimes u \) is constant as well. Further, assume homogeneous plastic slip fields. In equilibrium the temporal change of the plastic slip in system 1 and 2 comes to an end. Hence, the left hand side of system (36) becomes zero, i.e.:

\[
\text{sym}(G) \cdot (\nabla \beta_1 - \nabla \beta_2) = 0, \\
\mu \gamma + \mu(\beta_2 - \beta_1) = 0, \\
-\mu(\beta_2 - \beta_1) = 0. \quad (37)
\]
The solution is a fixed line \( \beta_2^0 = \beta_1^0 - \gamma \). Consider some small perturbations \( \dot{\beta} \ll 1 \) around these stationary points:

\[
\begin{bmatrix}
\beta_1 \\
\beta_2
\end{bmatrix} = \begin{bmatrix}
\beta_1^0 \\
\beta_2^0
\end{bmatrix} + \dot{\beta} \begin{bmatrix}
v_1 \\
v_2
\end{bmatrix} \exp(S t \mu/\eta_p) = \begin{bmatrix}
\beta_1^0 \\
\beta_2^0 - \gamma
\end{bmatrix} + \dot{\beta} \begin{bmatrix}
v_1 \\
v_2
\end{bmatrix} \exp(S t \mu/\eta_p).
\]

(38)

Inserting the perturbations into system (36) yields an eigenvalue problem in the form

\[
([S] - S_K[I]) [v_K] = [0] \quad \rightarrow \quad S_I = 0, [v_I] = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad S_H = -2, [v_H] = \begin{bmatrix} 1 \\ -1 \end{bmatrix},
\]

(39)

with the matrix \([S] = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}\) and the identity matrix \([I] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\). Looking at the eigenvectors \([v_K]\) and at the eigenvalues \(S_K\) as growth rates of the perturbations, the following conclusion is drawn: Perturbations with \(\beta_2 = -\beta_1\) will decay very quickly \((S_H < 0)\), other than perturbations with \(\beta_2 = \beta_1\) that persist \((S_I = 0)\). Numerical simulations showed this type of behavior which is considered unphysical. Fortunately, a remedy is already given by condition (35). Inserting it into system (36) reveals that the evolution of both plastic slips is identical. Hence, only one such equation must be solved. This is also evident from the physical point of view: as the conditions in both slip systems are exactly the same considering (critical) resolved shear stress and viscosity, there is no reason why the evolution should be different. The consequence is a symmetric plastic distortion (no plastic spin) and a symmetric backstress tensor. As shown in [5], the symmetry of \(X\) can also contribute to the well-posedness of the numerical problem.

4.3. Multiple slip systems with straight dislocation lines – an outlook

The extension towards multi-slip is a non-trivial task due to the proper definition of the scalar dislocation densities and the corresponding free energy of the dislocation network. If merely the plastic slips \(\beta_p\) and their gradients are used without any further considerations, a major problem arises: the field equations could depend on the chosen coordinate system. This is in contradiction to general principles of physics and should therefore be avoided. Instead, invariants of the tensor quantities need to be used. However, this might yield strongly coupled field equations with respect to the plastic slips (only for linearly independent slip systems a weaker coupling seems feasible, cf. Subsection 4.2). From the physical point of view, this stems from the multitude of active slip system combinations that result in the same overall plastic distortion. Considering the critical resolved shear stress as threshold for dislocation motion in a slip system offers a first possibility to reduce this ambiguity: Depending on the corresponding resolved shear stress only a subset of all slip systems is activated. Moreover, in real crystals other involved defects will always lead to a preference of some slip system, even though it is crystallographically equivalent to others. If this happens, the symmetry of the setting is broken and there should be no ambiguity anymore. The major task seems to consistently incorporate this behavior into the CDT.

5. Conclusions

For a single dislocation segment, the physical significance of the invariants of the dislocation tensor was shown. However, in case of continuously distributed dislocations it is more difficult to interpret the (principal) invariants due to interaction terms of different slip systems. Hence, slip system based invariants were suggested that facilitate the definition of invariant energies and dissipation potentials. Further, it was demonstrated that the structure of the plastic distortion field equation depends on the number of slip systems. For less than eight independent slip systems, only scalar field equations (flow rules) for a subset of coefficients need to be solved. Else, a tensor field equation has to be solved. This entails further consequences on the symmetry of the backstress tensor. The results of this study promote the idea that a physically meaningful backstress tensor ought to be symmetric in general.
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