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On the Derivation of Boundary Conditions for Continuum Dislocation Dynamics

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Abstract: Continuum dislocation dynamics (CDD) is a single crystal strain gradient plasticity theory based exclusively on the evolution of the dislocation state. Recently, we derived a constitutive theory for the average dislocation velocity in CDD in a phase field-type description for an infinite domain. In the current work, so-called rational thermodynamics is employed to obtain thermodynamically consistent boundary conditions for the dislocation density variables of CDD. We find that rational thermodynamics reproduces the bulk constitutive equations as obtained from irreversible thermodynamics. The boundary conditions we find display strong parallels to the microscopic traction conditions derived by Gurtin and Needleman (M.E. Gurtin and A. Needleman, J. Mech. Phys. Solids 53 (2005) 1–31) for strain gradient theories based on the Kröner–Nye tensor.

Keywords: continuum dislocation dynamics; strain gradient plasticity; boundary conditions; thermodynamic consistency; micro stresses; micro tractions

1. Introduction

Size-effects in small-scale plasticity have received much attention in continuum mechanics and materials science, starting with the work of Fleck and co-workers in the mid 1990s [1,2]. The continuum modeling of size-effects has since been divided into strain gradient approaches extending phenomenological laws from macroscopic plasticity to incorporate strain gradient effects on the one hand (influential works in this regard are due to Acharya and co-workers [3–5] and Gurtin and co-workers [6,7]) and approaches from materials science which seek continuum descriptions for the evolution of the dislocation state on the other hand (influential works are due to Groma, Zaiser, and later Hochrainer [8–11] and from Roters and co-workers and Arsenlis [12–14]). Presumably any researcher working at this cross-roads of continuum mechanics and materials science has been confronted with deep reservations of either side to acknowledge the progress of the other. The current paper tries to build a bridge between both approaches, in that the description of the dislocation state and its kinematic evolution law are taken from continuum dislocation dynamics (CDD) theory [11], while the derivation of the microscopic balance equations and the constitutive law for the average dislocation speed (substituting the flow rule from phenomenological approaches) are derived from the virtual work principle and energy imbalance in the spirit of Gurtin [6,7]. Through this combined derivation, we find on the one hand a clarification of the boundary conditions for CDD, which have not yet been achieved without abstract continuum mechanics, while the bulk constitutive laws derived for CDD provide a new perspective for phenomenological strain gradient modeling.

What we term CDD stands for a class of dislocation density-based single crystal plasticity theories which are based on conservation laws for scalar or tensorial dislocation density measures which characterize a distribution of dislocation lines (that is, oriented curves) in sufficient detail to predict at the same time the evolution of the dislocation state and the ensuing plastic slip rates [11].

A constitutive theory for CDD is given in terms of the average dislocation speeds per slip system, which govern all evolution equations including plastic slip rates. Such a constitutive theory has recently been derived [15] with methods from irreversible thermodynamics, provided that there is an energy density given in terms of the CDD density variables. A suitable energy density was recently derived from a local density approximation by Zaiser [16]. However, the constitutive model in [15] excluded the discussion of boundary conditions. The derivation of thermodynamically consistent boundary conditions for CDD is the original objective of the current paper.

CDD is uncommon from a continuum mechanical perspective, in that the material state is solely described by elastic strain and dislocation density variables, and that the plastic deformation rates (i.e., the slip rates on the individual slip systems) are exclusively due to the motion of dislocations displayed in the evolution of the density variables. On the other hand, one of the dislocation variables—namely, the dislocation density vector on each slip system—derives from the gradient of accumulated plastic shear on the slip system. Therefore, CDD theory is also related to size-dependent theories which have been derived based on the classical dislocation density tensor, and more specifically, based on the slip system-specific Burgers vector densities. For the latter types of approaches, complete theories including boundary conditions have been derived by Gurtin [6] and Gurtin and Needleman [7]. We take mostly the latter paper as a guideline for deriving boundary conditions for CDD. We also recover from this ansatz the bulk constitutive theory as earlier derived from irreversible thermodynamics in terms of a dissipation inequality.

The paper is structured as follows: after introducing notations and recalling the basics from small deformation CDD in Section 2, we postulate work-conjugates to the evolving microstructure variables and define the external and internal power expenditure of a deforming material region in Section 3. Subsequently, we introduce elastic and plastic virtual (generalized) velocities and use the principle of virtual work to derive local macroscopic and microscopic balance laws in the bulk and traction conditions at the surface. From a postulated energy density additively composed of an elastic and a dislocation density-depending part, we derive constitutive laws for the macroscopic and microscopic stresses and derive thermodynamic restrictions for the average dislocation speed in Section 4. After briefly discussing constitutive restrictions on the boundary conditions, we discuss the results in relation to those from [7] in Section 5.

2. Preliminaries

2.1. Notation

Throughout this paper, we mostly use coordinate notation for tensor calculus, but we also employ symbolic vector and tensor notation. In symbolic notation, vectors and tensors are marked by bold face letters. A central dot is used to denote contraction over one index (the last index of the left hand and the first index of the right hand tensorial argument). We refrain from introducing symbolic notations for operations involving other pairs of indices, and use coordinate notation with the Einstein summation convention instead.

In the current paper, we focus on small deformations. Let $\boldsymbol{u}$ denote the displacement field. We employ the additive decomposition of the displacement gradient in the elastic and plastic part as

$$\boldsymbol{u}_{i,j} = \beta^{\mathrm{e}}_{ji} + \beta^{\mathrm{p}}_{ji}. \tag{1}$$

Accordingly, we decompose the total strain $\varepsilon_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right)$ into its elastic $\boldsymbol{\epsilon}^{\mathrm{e}}$ and plastic part $\boldsymbol{\varepsilon}^{\mathrm{p}}$.

2.2. Kinematics of Single Crystals and CDD

The evolution of the plastic distortions in single crystals is governed by plastic slip rates $\dot{\gamma}^\alpha$ on the individual slip systems (labeled with α in the sequel) through

$$\dot{\beta}^{\mathrm{P}}_{ij} = \sum_\alpha \dot{\gamma}^\alpha \; n^\alpha_i m^\alpha_j, \tag{2}$$

where $\boldsymbol{n}^\alpha$ denotes the slip plane normal and $\boldsymbol{m}^\alpha = \boldsymbol{b}^\alpha / b^\alpha$ the slip direction, which is the normalized Burgers vector $\boldsymbol{b}^\alpha$ with modulus b^α.

Given the total dislocation densities per slip system ρ^α and the average dislocation speeds v^α on the slip systems, the plastic slip rates are governed by Orowan's equation, $\dot{\gamma}^\alpha = \rho^\alpha v^\alpha b^\alpha$.

CDD includes a potential hierarchy of theories based on a tensor expansion of the local directional dislocation distribution [11]. In the current work, we focus on the most simple CDD theory for curved dislocations, which is based on the total dislocation density ρ^α, the dislocation density vector $\boldsymbol{\rho}^\alpha = \mathrm{curl}\,(\gamma^\alpha \boldsymbol{n}^\alpha)$, and the total curvature density q^α. For the conservation laws of the density variables of CDD, we employ the conservative form for q [11,17]. In the current work, we only summarize the evolution equations of the dislocation variables together with the evolution law of the plastic distortion tensor,

$$\begin{aligned}
\dot{\beta}^{\mathrm{P}}_{ij} &= \sum_\alpha \rho^\alpha v^\alpha b^\alpha \; n^\alpha_i m^\alpha_j, && (3)\\
\dot{\rho}^\alpha &= \partial_i \left(v^\alpha \rho^\alpha_j \varepsilon_{ikj} n^\alpha_k \right) + v^\alpha q^\alpha, && (4)\\
\dot{\rho}^\alpha_i &= -\varepsilon_{ikj} \partial_j \left(v^\alpha \rho^\alpha n^\alpha_k \right), && (5)\\
\dot{q}^\alpha &= \partial_i \left(v^\alpha q^\alpha_i - \rho^\alpha_{ji} \partial_j v^\alpha \right). && (6)
\end{aligned}$$

Note that these evolution equations incorporate the assumption that dislocations of every character move with the same speed v^α relative to the crystal lattice in directions perpendicular to their line-direction within the glide plane. Moreover, the curvature vectors q^α_i and the second-order dislocation density tensors ρ^α_{ij} appearing in the evolution equations of q^α (6) are in principle additional unknowns, and therefore subject to closure assumptions. Here we do not specify the closure assumptions and refer to [18] and [11] for discussions of this kinematic closure.

Given the dislocation speeds v^α on all slip systems, the plastic distortion rate and the evolution of the density variables are completely defined. These slip system-specific dislocation speeds are therefore the central quantities to be specified from a constitutive theory as developed in the sequel.

We shall now rewrite the above evolution equations in terms of flux quantities. Notably, the plastic distortion rate tensor is itself a flux-type quantity, containing the total dislocation flux $\rho^\alpha v^\alpha$. The density variables of CDD are obtained from averages over curves, and their evolution equations are accordingly conservation laws [10,11]. Each of the evolution equations hence contains first-order differential operators applied to flux-like quantities. The evolution of the total dislocation density ρ^α additionally contains a term accounting for line-length changes of curved dislocations, which acts as a source terms. Moreover, note that the evolution of the dislocation density vector is of *curl*-type. As we will be dealing with volume integrals in the sequel, it is advantageous to also write the *curl*-type evolution of the dislocation density vector as a divergence (of an antisymmetric second order tensor); that is,

$$\dot{\rho}^\alpha_i = -\partial_j \left(v^\alpha \rho^\alpha \varepsilon_{jik} n^\alpha_k \right). \tag{7}$$

With the flux variables

$$j_i^\alpha := -v^\alpha \rho_j^\alpha \varepsilon_{ikj} n_k^\alpha, \tag{8}$$
$$J_{ij}^\alpha := -v^\alpha \rho^\alpha \varepsilon_{jik} n_k^\alpha, \tag{9}$$
$$k_i^\alpha := -\left(v^\alpha q_i^\alpha - \rho_{ji}^\alpha \partial_j v^\alpha\right), \tag{10}$$

the above set of evolution equations assumes the form

$$\dot{\boldsymbol{\beta}}^{\mathrm{p}} = \sum_\alpha \gamma^\alpha \, \boldsymbol{n}^\alpha \otimes \boldsymbol{m}^\alpha, \tag{11}$$
$$\dot{\rho}^\alpha = -\mathrm{div}\boldsymbol{j}^\alpha + v^\alpha, q^\alpha \tag{12}$$
$$\dot{\boldsymbol{\rho}}^\alpha = -\mathrm{div}\boldsymbol{J}^\alpha, \tag{13}$$
$$\dot{q}^\alpha = -\mathrm{div}\boldsymbol{k}^\alpha. \tag{14}$$

For the derivation of boundary conditions, we moreover introduce an auxiliary flux tensor, $\boldsymbol{K}^\alpha$, which is connected to dislocation rotations in the evolution of dislocation curvature

$$K_{ij}^\alpha = \rho_{ji}^\alpha v^\alpha. \tag{15}$$

3. Principle of Virtual Power

3.1. Internal and External Expenditure of Power

In the current section, we formulate the principle of virtual power to derive the macroscopic and microscopic force balance in order to present analogies and differences to the work of Gurtin and co-workers [6,7]. Like in the latter works, we deal with linear small deformation crystal plasticity. We also introduce the stress tensor as the power conjugate to the elastic distortions. We will not direct much attention to recovering the macroscopic force balance and the classical traction boundary condition for the stress tensor, because this remains unaltered as compared to the above named works. The important difference of CDD to phenomenological theories based on the Kröner–Nye tensor ([19,20]) is that all internal variables of CDD relate to the current dislocation state and that their evolution equations are all flux-type partial differential equations. We view the rates of these variables $(\dot{\rho}^\alpha, \dot{\boldsymbol{\rho}}^\alpha, \dot{q}^\alpha)$ as generalized velocities, and postulate the existence of according work-conjugate micro stresses $(\lambda^\alpha, \boldsymbol{\xi}^\alpha, \chi^\alpha)$. Additionally, we regard the plastic slip rates $\dot{\gamma}^\alpha$ as generalized velocities and denote their work-conjugate micro forces with π^α.

The internal power expenditure $\mathcal{I}(\Omega)$ in any part Ω of the body is hence supposed to be additively composed of the elastic power expenditure and the power expenditure due to the changing microstructure as

$$\mathcal{I}(\Omega) = \int_\Omega \left[\sigma_{ij}\dot{\epsilon}_{ij}^{\mathrm{e}} + \sum_\alpha \left(\pi^\alpha \dot{\gamma}^\alpha + \lambda^\alpha \dot{\rho}^\alpha + \xi_i^\alpha \dot{\rho}_i^\alpha + \chi^\alpha \dot{q}^\alpha\right)\right] dV. \tag{16}$$

The external power expenditure is supposed to result from body forces $\boldsymbol{b}$ within the volume and due to defect flow across the surface. To this end, we introduce chemical potential-like quantities $\left(\Lambda^\alpha, \Xi_i^\alpha, X^\alpha, X_j^\alpha\right)$ conjugate, respectively, to the normal flows $\left(j_i^\alpha n_i, J_{ij}^\alpha n_j, k_i^\alpha n_i, k_{ji} n_i\right)$ through a surface with outer normal $\boldsymbol{n}$. In line with Gurtin, we additionally introduce micro tractions $\Pi^\alpha(\boldsymbol{n})$ conjugate to the shear rates $\dot{\gamma}^\alpha$ at the surface. That is, we have the external power $\mathcal{W}(\Omega)$ expended on Ω defined as

$$\mathcal{W}(\Omega) = \int_\Omega b_i v_i dV + \int_{\partial\Omega} \left[t_i v_i + \sum_\alpha \left(\Pi^\alpha \dot{\gamma}^\alpha - \Lambda^\alpha j_i^\alpha n_i - \Xi_j^\alpha J_{ji}^\alpha n_i - X^\alpha k_i^\alpha n_i - X_j^\alpha K_{ji} n_i\right)\right] dA. \tag{17}$$

3.2. Principle of Virtual Power

In order to apply the principle of virtual power, we consider a deformation and dislocation state as given, and regard the virtual internal and external power expenditure for virtual variations of the deformation and the dislocation state. In line with [7], we postulate the principle of virtual power such that for all compatible variations of the deformation and dislocation state, the virtual external power expenditure must equal the virtual internal power expenditure. We consider a compatible variation of the deformation state to be defined by a virtual velocity field $\tilde{v}_i$, while we shall consider as compatible variations of the plastic deformation and the dislocation state $(\tilde{\rho}^\alpha, \tilde{\rho}_i^\alpha, \tilde{\boldsymbol{q}}^\alpha)$ only those which may result from a virtual dislocation speed $\tilde{v}^\alpha$ and the given state $(\rho^\alpha, \rho_i^\alpha, \boldsymbol{q}^\alpha)$ in compliance with (3)–(6), such that

$$\tilde{\beta}_{ij}^{\mathrm{p}} = \sum_\alpha \rho^\alpha \tilde{v}^\alpha b\, n_i^\alpha m_j^\alpha, \tag{18}$$

$$\tilde{\rho}^\alpha = \partial_i \left(\tilde{v}^\alpha \rho_j^\alpha \varepsilon_{ikj} n_k^\alpha \right) + \tilde{v}^\alpha q^\alpha, \tag{19}$$

$$\tilde{\rho}_i^\alpha = -\varepsilon_{ikj} \partial_j \left(\tilde{v}^\alpha \rho^\alpha n_k^\alpha \right), \tag{20}$$

$$\tilde{q}^\alpha = \partial_i \left(\tilde{v}^\alpha q_i^\alpha - \rho_{ji}^\alpha \partial_j \tilde{v}^\alpha \right). \tag{21}$$

The virtual fluxes in the interior are likewise defined in accordance with the virtual dislocation speeds.

With the virtual elastic strain variation given by $\tilde{\epsilon}_{ij}^{\mathrm{e}} = 1/2 \left(\tilde{v}_{j,i} + \tilde{v}_{i,j} \right) - 1/2 \left(\tilde{\beta}_{ij}^{\mathrm{p}} + \tilde{\beta}_{ji}^{\mathrm{p}} \right)$, we henceforth obtain the virtual internal power expenditure

$$\tilde{\mathcal{I}}(\Omega) = \int_\Omega \left[\sigma_{ij} \tilde{\epsilon}_{ij}^{\mathrm{e}} + \sum_\alpha \left(\pi^\alpha \dot{\tilde{\gamma}}^\alpha + \lambda^\alpha \tilde{\rho}^\alpha + \xi_i^\alpha \tilde{\rho}_i^\alpha + \chi^\alpha \tilde{q}^\alpha \right) \right] dV, \tag{22}$$

and likewise, the virtual external power expenditure as

$$\tilde{\mathcal{W}}(\Omega) = \int_\Omega b_i \tilde{v}_i dV + \int_{\partial\Omega} \left[t_i \tilde{v}_i + \sum_\alpha \left(\Pi^\alpha \dot{\tilde{\gamma}}^\alpha - \Lambda^\alpha \tilde{j}_i^\alpha n_i - \Xi_j^\alpha \tilde{J}_{ji}^\alpha n_i - X^\alpha \tilde{k}_i^\alpha n_i - X_j \tilde{k}_{ji} n_i \right) \right] dA. \tag{23}$$

By the standard argument of independent variations for deformations and defects, we obtain from $\tilde{\mathcal{I}}(\Omega) = \tilde{\mathcal{W}}(\Omega)$ upon varying the deformation state with fixed dislocation distribution for all suitable volumes Ω the classical (macroscopic) force balance

$$\partial_j \sigma_{ji} + b_i = 0, \tag{24}$$

and the traction boundary condition

$$t_i = \sigma_{ji} n_j. \tag{25}$$

For the microscopic force balance and tractions, we transform the microstructural part of the internal power expenditure into a volumetric part and a surface-related part via the product rule and Gauß theorem as

$$\begin{aligned} \sum_\alpha \int_\Omega \left(-\tau^\alpha \dot{\tilde{\gamma}}^\alpha + \pi^\alpha \dot{\tilde{\gamma}}^\alpha + \lambda^\alpha \tilde{\rho}^\alpha + \xi_i^\alpha \tilde{\rho}_i^\alpha + \chi^\alpha \tilde{q}^\alpha \right) dV = -\sum_\alpha \int_{\partial\Omega} \left(\lambda^\alpha \tilde{j}_i^\alpha + \xi_j^\alpha \tilde{J}_{ij}^\alpha + \chi^\alpha \tilde{k}_i^\alpha \right) n_i dA + \\ \sum_\alpha \int_\Omega \left(-\tau^\alpha \tilde{\gamma}^\alpha + \pi^\alpha \tilde{j}^\alpha + \tilde{j}_i^\alpha \partial_i \lambda^\alpha + \right. \\ \left. \tilde{v}^\alpha q^\alpha \lambda^\alpha + \tilde{J}_{ij}^\alpha \partial_i \xi_i^\alpha + \tilde{k}_i^\alpha \partial_i \chi^\alpha \right) dV, \end{aligned} \tag{26}$$

where $\tau^\alpha = \sigma_{ij} n_i^\alpha m_j^\alpha$ are the resolved shear stresses in the direction of slip on the individual slip systems.

A standard argument requires that for the microscopic force balance in the bulk, the volume integral vanishes for all virtual dislocation velocities $\tilde{v}^\alpha$. Note, however, that the curvature density flux k_i^α contains spatial derivatives of the virtual dislocation velocities—compare (10). In order to formulate the microscopic force balance in the bulk independent of these derivatives, we apply Gauß theorem once more to the according portion of the power expenditure to find

$$\begin{aligned}\int_\Omega \tilde{k}_i^\alpha \partial_j \chi^\alpha dV &= \int_\Omega \left(\tilde{v}^\alpha q_i^\alpha \partial_i \chi^\alpha + \tilde{v}^\alpha \partial_j \rho_{ji}^\alpha \partial_i \chi^\alpha + \tilde{v}^\alpha \rho_{ji}^\alpha \partial_j \partial_i \chi^\alpha\right) dV - \int_{\partial\Omega} \tilde{v}^\alpha \rho_{ji}^\alpha \partial_i \chi^\alpha n_j dA \\ &= \int_\Omega \left(2\tilde{v}^\alpha q_i^\alpha \partial_i \chi^\alpha + \tilde{v}^\alpha \rho_{ji}^\alpha \partial_j \partial_i \chi^\alpha\right) dV - \int_{\partial\Omega} \tilde{k}_{ij} \partial_i \chi^\alpha n_j . dA \end{aligned} \tag{27}$$

In the second step, we used the fact that the curvature vector derives as the divergence of the second order alignment tensor; i.e., $q_i^\alpha = \partial_j \rho_{ji}^\alpha$, cf. [11].

As already noted, we require that the volume integrals in (26) vanish identically. In this we assume the dislocation velocities on the individual slip systems to be independent of each other such that the summands are presumed to vanish independently. Inserting (27) into (26) yields a pointwise equation which we divide by $\rho^\alpha b^\alpha$ such that we obtain the microscopic force balance in the form

$$\pi^\alpha - \tau^\alpha + \frac{\rho_j^\alpha}{\rho^\alpha b^\alpha} \varepsilon_{ikj} n_k^\alpha \partial_i \lambda^\alpha + \frac{q^\alpha}{\rho^\alpha b^\alpha} \lambda^\alpha + \frac{1}{b^\alpha} \varepsilon_{ijk} n_k^\alpha \partial_i \xi_j^\alpha + 2 \frac{q_i^\alpha}{\rho^\alpha b^\alpha} \partial_i \chi^\alpha + \frac{\rho_{ji}^\alpha}{\rho^\alpha b^\alpha} \partial_j \partial_i \chi^\alpha = 0. \tag{28}$$

For the microtraction condition, we likewise require that the remaining surface integrals vanish. These surface integrals contain the surface terms from the external power expenditure (23) and the boundary terms obtained from applying Gauß integration theorem to the internal work rate (26). The resulting micro traction condition reads

$$\int_{\partial\Omega} \sum_\alpha \left[\Pi^\alpha \dot{\gamma}^\alpha - \left(\Lambda^\alpha - \lambda^\alpha\right) \tilde{j}_i^\alpha n_i - \left(\Xi_j^\alpha - \xi_j^\alpha\right) \tilde{J}_{ij}^\alpha n_i - \left(X^\alpha - \chi^\alpha\right) \tilde{k}_i^\alpha n_i - \left(X_j^\alpha - \partial_j \chi^\alpha\right) \tilde{k}_{ij}^\alpha n_i\right] dA = 0. \tag{29}$$

The microtraction condition may be fulfilled by setting the microtraction to zero, $\Pi^\alpha = 0$, and the "chemical potentials" of the density variables equal to the limiting values of the micro forces from the bulk. This yields open boundary conditions, where all flux terms may, for example, be obtained as the limiting values of the according bulk quantities. Note, however, that this also allows for any other prescribed fluxes at the boundary. An alternative trivial option is to set all fluxes to zero. In that , we distinguish two cases: (*i*) if the micro tractions are not zero, $\Pi^\alpha(\boldsymbol{n}) \neq 0$, setting the flux quantities to zero would include all plastic slip rates, $\dot{\gamma}^\alpha = 0$, which is the hard-slip condition of [6]. (*ii*) if the micro tractions are set to zero, $\Pi^\alpha(\boldsymbol{n}) = 0$, the no-flux condition will only restrict normal fluxes and therefore this reproduces the micro-hard boundary condition as developed by [7], because the slip rates on slip systems which are *parallel to the boundary* will not be affected. As a further condition, we may allow for chemical potentials at the boundary which are not equal to the micro forces in the bulk. This is the general case which we expect to be necessary for modeling non-trivial surface behavior where dislocations may neither freely pass the surface nor are fully blocked by it. This is of interest when targeting grain boundaries as internal surfaces or free surfaces as sources of dislocations in future work. Similar to the case of the bulk, all boundary fluxes appearing in (29) are linear in the dislocation velocities, except for a term in the curvature fluxes $\tilde{k}_i^\alpha$ which involves derivatives of the velocities. This term reads

$$\int_{\partial\Omega} -\left(X^\alpha - \chi^\alpha\right) \rho_{ji}^\alpha \partial_j v^\alpha n_i dA. \tag{30}$$

Note that in the above form this term will involve derivatives of the velocity in tangential direction (i.e., along the intersecting line of slip plane and outer boundary) which may not be prescribed independently of the velocity at the boundary. This conflict would be circumvented if we succeed in reducing the term such that it only involves derivatives of the velocity normal to the boundary. (This may be paralleled to the boundary values for the Kirchhoff–Love plate theory,

where torques derive from the tangential derivative of the out-of-plane displacement and are hence not considered independent boundary conditions; meanwhile, bending moments—deriving as normal derivatives—may be prescribed independently). In order to see that in fact only normal derivatives contribute to the integral in (30), we make use of the following theorem on the integrals of the divergence of a vector field over a surface.

Theorem 1. *Let S be a surface patch in $\mathbb{R}^3$ with normal vector field $\boldsymbol{n}$. Furthermore, ∂S denotes the boundary curve with normal vector field $\boldsymbol{\nu}$ (which is tangential to the surface). Moreover, let $\boldsymbol{X}$ be a vector field $\boldsymbol{X}:\mathbb{R}^3\to\mathbb{R}^3$ which is defined in a surrounding of S. The normal vector field $\boldsymbol{n}$ is likewise supposed to be extended to a unit vector field in a neighborhood of S. Moreover, let κ be the mean curvature function on the surface S. With these notations, the following equality holds:*

$$\int_S \operatorname{div}\boldsymbol{X}dS=\int_{\partial S}\boldsymbol{X}\cdot\boldsymbol{\nu}ds+\int_S\left(\nabla_{\boldsymbol{n}}\boldsymbol{X}\cdot\boldsymbol{n}-2\boldsymbol{X}\cdot\boldsymbol{n}\kappa\right)dS \tag{31}$$

Proof. This is a simple corollary to the surface divergence theorem found in [21], upon realizing that the divergence relates to the surface divergence div^S through

$$\operatorname{div}\boldsymbol{X}=\operatorname{div}^S\boldsymbol{X}+\nabla_{\boldsymbol{n}}\boldsymbol{X}\cdot\boldsymbol{n}. \tag{32}$$

The above-cited surface divergence theorem states that

$$\int_S\operatorname{div}^S\boldsymbol{X}dS=\int_{\partial S}\boldsymbol{X}\cdot\boldsymbol{\nu}ds-\int_S 2\boldsymbol{X}\cdot\boldsymbol{n}\kappa dS, \tag{33}$$

which finishes the proof. □

In order to employ Theorem 1, we first transform the integrand of (30) in divergence form by the product rule,

$$-\left(X^\alpha-\chi^\alpha\right)\rho^\alpha_{ji}\partial_j v^\alpha n_i=-\partial_j\left[\left(X^\alpha-\chi^\alpha\right)\rho^\alpha_{ji}v^\alpha n_i\right]+v^\alpha\partial_j\left[\left(X^\alpha-\chi^\alpha\right)\rho^\alpha_{ji}n_i\right]. \tag{34}$$

The first term on the right side of the last equation is a divergence, and we may thus apply Theorem 1. Note here that the integral in (30) is performed over the boundary $\partial\Omega$, which is a closed surface without boundary. Therefore, the first term on the right side of (33) vanishes in this case. We thence find

$$\int_{\partial\Omega}-\partial_j\left[\left(X^\alpha-\chi^\alpha\right)\rho^\alpha_{ji}v^\alpha n_i\right]dA=\int_{\partial\Omega}\left\{-n_k\partial_k\left[\left(X^\alpha-\chi^\alpha\right)\rho^\alpha_{ji}v^\alpha n_i\right]n_j-2n_j\left[\left(X^\alpha-\chi^\alpha\right)\rho^\alpha_{ji}v^\alpha n_i\right]\kappa\right\}dA. \tag{35}$$

By employing the product rule once more to the first term in the integral on the right side, we isolate the normal derivative of the velocity. Moreover, we introduce the short-hand notations $\Delta\Lambda^\alpha=\Lambda^\alpha-\lambda^\alpha$, $\Delta\Xi^\alpha_j=\Xi^\alpha_j-\xi^\alpha_j$, $\Delta X^\alpha=X^\alpha-\chi^\alpha$, and $\Delta X^\alpha_j=X^\alpha_j-\partial_j\chi^\alpha$. Using this notation, we summarize the just-derived reformulation of (30) through

$$\begin{aligned}-\int_{\partial\Omega}\Delta X^\alpha\rho^\alpha_{ji}\partial_j v^\alpha n_i dA=\int_{\partial\Omega}\Big\{&\tilde{v}^\alpha\left[\partial_j\left(\Delta X^\alpha\rho^\alpha_{ji}n_i\right)-n_k\partial_k\left(\Delta X^\alpha\rho^\alpha_{ji}n_i\right)n_j-2\kappa\Delta X^\alpha\rho^\alpha_{ji}n_jn_i\right]-\\&n_k\partial_k\tilde{v}^\alpha\Delta X^\alpha\rho^\alpha_{ji}n_jn_i\Big\}dA\end{aligned} \tag{36}$$

Collecting terms for the integral (30), we arrive at the following micro traction condition as a reformulation of (29)

$$\begin{aligned}0=\int_{\partial\Omega}\sum_\alpha\Big\{v^\alpha\Big[&\Pi^\alpha\rho^\alpha b^\alpha-\Delta\Lambda^\alpha\rho^\alpha_j\varepsilon_{ikj}n^\alpha_k n_i-\Delta\Xi^\alpha_j\rho^\alpha\varepsilon_{ijk}n^\alpha_k n_i-\Delta X^\alpha q^\alpha_i n_i+\partial_j\left(\Delta X^\alpha\rho^\alpha_{ji}n_i\right)-\\&n_k\partial_k\left(\Delta X^\alpha\rho^\alpha_{ji}n_i\right)n_j-2\kappa\Delta X^\alpha\rho^\alpha_{ji}n_jn_i-\Delta X^\alpha_j\rho^\alpha_{ji}n_i\Big]-n_k\partial_k\tilde{v}^\alpha\Delta X^\alpha\rho^\alpha_{ji}n_jn_i\Big\}dA.\end{aligned} \tag{37}$$

For these integrals to vanish identically for any variational velocity $\tilde{v}^\alpha$, we obtain the following two microtraction conditions:

$$\begin{aligned} 0 = \Pi^\alpha - \Delta\Lambda^\alpha \frac{\rho^\alpha_j}{\rho^\alpha b^\alpha} \varepsilon_{ikj} n^\alpha_k n_i - \Delta\Xi^\alpha_j \frac{1}{b^\alpha} \varepsilon_{ijk} n^\alpha_k n_i - \Delta X^\alpha \frac{q^\alpha_i}{\rho^\alpha b^\alpha} n_i + \frac{1}{\rho^\alpha b^\alpha} \partial_j \left(\Delta X^\alpha \rho^\alpha_{ji} n_i \right) - \\ \frac{1}{\rho^\alpha b^\alpha} n_k \partial_k \left(\Delta X^\alpha \rho^\alpha_{ji} n_i \right) n_j - 2\kappa \Delta X^\alpha \frac{\rho^\alpha_{ji}}{\rho^\alpha b^\alpha} n_j n_i - \Delta X^\alpha_j \frac{\rho^\alpha_{ji}}{\rho^\alpha b^\alpha} n_i \end{aligned} \tag{38}$$

$$0 = \Delta X^\alpha \rho^\alpha_{ji} n_j n_i. \tag{39}$$

If $\Delta X^\alpha \neq 0$, the second equation demands that there be no total dislocation density perpendicular to the surface, as $\rho^\alpha_{ji} n_j n_i$ is interpreted as the total dislocation density in the direction of $\boldsymbol{n}$ (cf. [11]) on slip system α. This seems to be an unreasonable requirement, and we conclude that $\Delta X^\alpha = 0$ should be enforced. Alternatively, one might restrict variations to dislocation speeds with vanishing normal derivative $n_k \partial_k \tilde{v}^\alpha = 0$. We note that when transferred to a boundary condition for the actual dislocation velocity, setting the normal derivative of the velocity to zero becomes another way to model open boundary conditions. This has been employed for CDD in that the computational domain contains a layer around the actual crystal where the dislocation flux quantities are duplicated from the last layer of the bulk [22].

In order to reduce complexity, we assume in the following that the effective chemical potential for dislocation curvature vanishes; i.e., $\Delta X^\alpha = 0$ such that the normal derivative does not need to be specified. Then, the microtraction condition reduces to

$$0 = \Pi^\alpha - \Delta\Lambda^\alpha \frac{\rho^\alpha_j}{\rho^\alpha b^\alpha} \varepsilon_{ikj} n^\alpha_k n_i - \Delta\Xi^\alpha_j \frac{1}{b^\alpha} \varepsilon_{ijk} n^\alpha_k n_i - \Delta X^\alpha_j \frac{\rho^\alpha_{ji}}{\rho^\alpha b^\alpha} n_i. \tag{40}$$

4. Constitutive Theory

4.1. Energy Imbalance

In a purely mechanical theory, the second law of thermodynamics requires that the temporal increase of energy in any part Ω is less than or equal to the power expended on Ω. If ψ denotes the free energy density per unit volume, this is expressed by the inequality

$$\int_\Omega \dot{\psi} dV \leq \mathcal{W}(\Omega) = \mathcal{I}(\Omega) = \int_\Omega \left[\sigma_{ij} \dot{\epsilon}^{\mathrm{e}}_{ij} + \sum_\alpha \left(\pi^\alpha \dot{\gamma}^\alpha + \lambda^\alpha \dot{\rho}^\alpha + \xi^\alpha_i \dot{\rho}^\alpha_i + \chi^\alpha \dot{q}^\alpha \right) \right] dV. \tag{41}$$

Because the subvolume Ω is arbitrary, we obtain the pointwise inequality

$$\dot{\psi} - \left[\sigma_{ij} \dot{\epsilon}^{\mathrm{e}}_{ij} + \sum_\alpha \left(\pi^\alpha \dot{\gamma}^\alpha + \lambda^\alpha \dot{\rho}^\alpha + \xi^\alpha_i \dot{\rho}^\alpha_i + \chi^\alpha \dot{q}^\alpha \right) \right] \leq 0. \tag{42}$$

4.2. Dissipation Inequality

We assume the free energy density to be of the form

$$\psi = \frac{1}{2} \epsilon^{\mathrm{e}}_{ij} C_{ijkl} \epsilon^{\mathrm{e}}_{kl} + \sum_\alpha \psi^\alpha \left(\rho^\alpha, \boldsymbol{\rho}^\alpha, q^\alpha \right), \tag{43}$$

which is also obtained from the local density approximation by Zaiser [16]. The time evolution of the free energy consequently reads

$$\dot{\psi} = \epsilon^{\mathrm{e}}_{ij} C_{ijkl} \dot{\epsilon}^{\mathrm{e}}_{kl} + \sum_\alpha \left(\frac{\partial \psi^\alpha}{\partial \rho^\alpha} \dot{\rho}^\alpha + \frac{\partial \psi^\alpha}{\partial \rho^\alpha_j} \dot{\rho}^\alpha_j + \frac{\partial \psi^\alpha}{\partial q^\alpha} \dot{q}^\alpha \right). \tag{44}$$

Employing this, we reformulate the free-energy inequality in terms of dissipation as

$$\left(\sigma_{ij} - C_{ijkl}\epsilon^{\mathrm{e}}_{kl}\right)\dot{\epsilon}^{\mathrm{e}}_{ij} + \sum_{\alpha}\left[\left(\lambda^{\alpha} - \frac{\partial\psi^{\alpha}}{\partial\rho^{\alpha}}\right)\dot{\rho}^{\alpha} + \left(\xi^{\alpha}_{j} - \frac{\partial\psi^{\alpha}}{\partial\rho^{\alpha}_{j}}\right)\dot{\rho}^{\alpha}_{j} + \left(\chi^{\alpha} - \frac{\partial\psi^{\alpha}}{\partial q^{\alpha}}\right)\dot{q}^{\alpha}\right] + \pi^{\alpha}\dot{\gamma}^{\alpha} \geq 0. \quad (45)$$

This inequality must hold for all deformation and dislocation states and all choices of $\dot{\epsilon}^{\mathrm{e}}_{ij}, \dot{\rho}^{\alpha}, \dot{\rho}^{\alpha}_{j}, \dot{q}^{\alpha}$, and $\dot{\gamma}^{\alpha}$. Consequently, one obtains the constitutive relations

$$\sigma_{ij} = C_{ijkl}\epsilon^{\mathrm{e}}_{kl}, \quad (46)$$

$$\lambda^{\alpha} = \frac{\partial\psi^{\alpha}}{\partial\rho^{\alpha}}, \quad (47)$$

$$\xi^{\alpha}_{j} = \frac{\partial\psi^{\alpha}}{\partial\rho^{\alpha}_{j}}, \quad (48)$$

$$\chi^{\alpha} = \frac{\partial\psi^{\alpha}}{\partial q^{\alpha}}. \quad (49)$$

The dissipation inequality consequently reduces to the familiar form

$$\pi^{\alpha}\dot{\gamma}^{\alpha} \geq 0. \quad (50)$$

The dislocation densities ρ^{α} and the length of the Burgers vectors b^{α} are positive, such that due to the Orowan equation the dissipation inequality is tantamount to

$$\pi^{\alpha}v^{\alpha} \geq 0. \quad (51)$$

Assuming the dislocation velocity v^{α} to be a function of the microscopic force π^{α}, this may for example be fulfilled in the form

$$v^{\alpha} = M\left(\pi^{\alpha}, \rho^{\alpha}\right)\pi^{\alpha}, \quad (52)$$

with a non-negative mobility function $M\left(\pi^{\alpha}, \rho^{\alpha}\right)$ as introduced in [15]. With the above constitutive relations, we find that the microscopic force balance yields

$$\pi^{\alpha} = \tau_{\mathrm{net}}, \quad (53)$$

with the net shear stress defined in the just-named paper from a phase-field type derivation,

$$\tau_{\mathrm{net}} = \tau^{\alpha} - \frac{\rho^{\alpha}_{j}}{\rho^{\alpha}b}\varepsilon_{ikj}n^{\alpha}_{k}\partial_{i}\frac{\partial\psi^{\alpha}}{\partial\rho^{\alpha}} - \frac{q^{\alpha}}{\rho^{\alpha}b}\frac{\partial\psi^{\alpha}}{\partial\rho^{\alpha}} - \frac{1}{b}\varepsilon_{ijk}n^{\alpha}_{k}\partial_{i}\frac{\partial\psi^{\alpha}}{\partial\rho^{\alpha}_{j}} - 2\frac{q^{\alpha}_{i}}{\rho^{\alpha}b}\partial_{i}\frac{\partial\psi^{\alpha}}{\partial q^{\alpha}} - \frac{\rho^{\alpha}_{ji}}{\rho^{\alpha}b}\partial_{j}\partial_{i}\frac{\partial\psi^{\alpha}}{\partial q^{\alpha}}. \quad (54)$$

4.3. Surface Constitutive Theory

The free energy inequality fixes the constitutive theory for the stress tensor and the micro stresses. We note that the micro stresses have the appearance of chemical potentials in that they are the change of energy associated with a change in the according density variable. The micro-free boundary condition

is hence fulfilled if what has been called chemical potentials at the surface are actually the (bulk) chemical potentials of the density variables; i.e., if

$$\Lambda^\alpha = \frac{\partial \psi^\alpha}{\partial \rho^\alpha}, \tag{55}$$

$$\Xi_j^\alpha = \frac{\partial \psi^\alpha}{\partial \rho_j^\alpha}, \tag{56}$$

$$X^\alpha = \frac{\partial \psi^\alpha}{\partial q^\alpha}, \tag{57}$$

$$X_j^\alpha = \partial_j \frac{\partial \psi^\alpha}{\partial q^\alpha}, \tag{58}$$

and additionally $\Pi^\alpha = 0$. If the surface is impenetrable for dislocations (e.g., due to surface treatment or because the crystal is tied to a plastically non-deformable body), it seems appropriate to assume that no dislocation may move through the surface, enforcing the micro hard boundary condition. The microtraction condition provides freedom to chose the surface chemical potential which yields the definition of the micro tractions. This case yields no guidance on choosing the surface chemical potentials. This is reasonable because these quantities are dependent on details of the surface structure, which are largely independent of the bulk constitutive theory. In order to evoke parallels to the micro traction conditions presented by [6,7], we will from now on set all the surface chemical potentials to zero, such that only the bulk chemical potentials remain in (40); that is,

$$0 = \Pi^\alpha - \lambda^\alpha \frac{\rho_j^\alpha}{\rho^\alpha b^\alpha} \varepsilon_{ikj} n_k^\alpha n_i + \xi_j^\alpha \frac{1}{b^\alpha} \varepsilon_{ijk} n_k^\alpha n_i + \partial_j \chi^\alpha \frac{\rho_{ji}^\alpha}{\rho^\alpha b^\alpha} n_i. \tag{59}$$

5. Discussion

In this discussion, we focus on parallels and differences of the current theory to the phenomenological theories presented in [6,7]. In order to reveal the parallels, we realize that the strain gradient theory of Gurtin and co-workers involves the slip rates and—implicitly—the dislocation density vector, which contributes to the Kröner–Nye tensor which is considered as the microstructural variable by Gurtin. Because the total dislocation density and the curvature density are absent, we may only expect to find direct parallels regarding the terms which involve the micro stress $\boldsymbol{\xi}^\alpha$, which is work conjugate to the rate of the dislocation density vector $\dot{\boldsymbol{\rho}}^\alpha$ and which was found to be given as a chemical potential through (48). We deliberately denoted the micro stress conjugate to the dislocation density vector as $\boldsymbol{\xi}^\alpha$, which is the same symbol used by Gurtin and Needleman for the micro stress conjugate to the gradient of the plastic shear rate on the slip system. In [6,7], the authors assume that the energy is given terms of the dislocation density tensor. From the work of Zaiser [16], we rather assume the energetic dependency to be given additively from terms formulated on the slip system level in terms of the slip gradients, where only the gradient within the slip plane actually matters. With this energetic assumption, the micro stress of Gurtin and co-workers is a vector, tangent to the slip plane, given by

$$\xi_i^{\alpha,\mathrm{GN}} = \frac{\partial \psi}{\partial \left(\partial_i \gamma^\alpha\right)}. \tag{60}$$

Between the dislocation density vector and the slip gradient, there is the following relation:

$$\rho_i^\alpha = -\frac{1}{b} \partial_j \gamma^\alpha \varepsilon_{ikj} n_k^\alpha, \tag{61}$$

which easily yields that

$$\xi_i^{\alpha,\mathrm{GN}} = \frac{\partial \psi}{\partial \rho_j^\alpha} \frac{\partial \rho_j^\alpha}{\partial \left(\partial_i \gamma^\alpha\right)} = -\frac{1}{b} \varepsilon_{ikj} n_k^\alpha \xi_j^\alpha. \tag{62}$$

With this stipulation, we see that for the case that the energy would be independent of the total dislocation density and the curvature density, we reproduce both the bulk microscopic stress balance of Gurtin,

$$\pi^{\alpha} = \tau^{\alpha} + \operatorname{div}\boldsymbol{\xi}^{\alpha,\mathrm{GN}} \tag{63}$$

and the micro traction boundary condition of Gurtin and Needleman, which reads in the current notation

$$\Pi^{\alpha} = \boldsymbol{\xi}^{\alpha,\mathrm{GN}} \cdot \boldsymbol{n} \tag{64}$$

Recent numerical investigations [23] revealed unconventional and apparently as-of-yet unresolved behavior of phenomenological gradient theories employing the micro-free ($\Pi^{\alpha} = 0$) boundary condition in simulations of micro bending. It will be an interesting question for future research to investigate how the additional terms, due to the further density variables in the micro traction condition of CDD (59), will modify the behavior at micro traction-free boundaries.

In the current work, we achieved two things. What is actually new is the consequent treatment of boundary conditions for CDD, which leads to different types of admissible boundary conditions, including entirely open boundary conditions, hard and micro-hard boundary conditions, as well as a generalization of the micro traction boundary conditions derived by Gurtin and Needleman for phenomenological theories accounting for the dislocation density tensor. Besides the boundary conditions, we also regard the derivation of the constitutive law in analogy to the work of Gurtin and Needleman as a new result of this paper. We very much hope that the incorporation of CDD theory into the framework of rational thermodynamics helps lower the barrier to understanding between researchers educated in materials science and those rooted in modern continuum mechanics—for the better of common research on a dislocation-based continuum theory of crystal plasticity.

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Abbreviations

The following abbreviations are used in this manuscript:

CDD Continuum dislocation dynamics

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