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On the Connection between Continuum Crystal Plasticity and the Mechanics of Discrete Dislocations

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Dedicated to the memory of my mentor and friend, Jürgen Olschewski

This work aims at linking the levels of the continuum crystal plasticity with that of discrete dislocations. First, some former results about the kinematics of discrete dislocations are recalled. Then the fields at the continuum level are constructed by averaging the corresponding fields at the dislocation level. Under the assumptions of small elastic strains, small lattice curvature at the dislocation level and statistical homogeneity at the scale of the representative volume element the classical forms of the balance equations for the continuous fields can be retrieved. In addition, a multiplicative decomposition the deformation gradient in an elastic part and an irreversible part is achieved. While the elastic strains are assumed to be small, the plastic strains can be arbitrarily large.

1 Introduction

This work is an attempt to bridge the gap between the description of a crystal that contains a large number of discrete dislocations and the conventional continuum crystal plasticity theory. Thereby the strains caused by plastic slip can be arbitrarily large. There already exist numerous treatments of crystals distorted by continuous distributions of dislocations, starting among others with the historical works of Nye (1953) and Kröner (1958). What is here meant is quite different: We claim that the field equations (balance + constitutive equations) in a physical treatment of crystal plasticity should be derived from the field equations of the crystal that undergoes irreversible lattice rearrangements due to discrete dislocation glide. While these irreversible processes are concentrated on discrete singular surfaces, the bulk of the crystal behaves elastically.
There exist several homogenization techniques to link two levels of descriptions. A popular and intuitive one is the use of spatial averaging at the lower level to define the fields at the higher level. However, the case of discontinuous deformations and finite strains has received little attention up to now. Due to the necessity to distinguish between the reference and the deformed state and due to the various possible measures for stress and strain in finite transformations, there is an inherent arbitrariness concerning the definition of the fields at the higher level. Moreover, because of geometric non-linearity, the various alternatives are not equivalent in the most general case. Hill (1972, 1984) and Nemat-Nasser and Hori (1999) proposed a general scheme to extend the homogenization by spatial averaging to large transformations. As a rule, the choice is guided by the desire to retrieve the familiar forms of the balance equations at the higher level. A challenging situation for the homogenization theory is given, when a perfect identification turns out to be impossible for some reason. Then the theory for the higher level has to be extended, e.g., by enriching the kinematical description. In this line of thought, Forest (1998) and Van der Sluis (1999) have recently modeled heterogeneous materials by Cosserat continua at the macroscopic level. When the central hypothesis of statistical homogeneity at the microscopic scale is not fulfilled, it turns out that the energy balance at the higher level fails to have the usual form, thus demanding an appropriate treatment.
While the present work leaves many unanswered questions, we thus believe that this approach has the potentiality to provide new insights into the mechanics of ductile crystals. The treatment relies on some recent results obtained by Fedelich (2003b) about the kinematics of dislocation glide in finite elasticity. Note that the regularization of crystals distorted by discrete dislocations through spatial averaging in the linear frame has been recently presented by Fedelich (2003a).
The paper is organized as follows:
First, some definitions and results from the above mentioned paper (Fedelich, 2003a) are briefly recalled. Then the field equations and kinematical assumptions at the dislocation level are formulated. The fields at the continuous level are first purely formally defined. We finally show that under the made assumptions, the usual

balance equations of continuum crystal plasticity are retrieved. In addition, a multiplicative decomposition of the deformation gradient in an elastic part and an irreversible part is presented.

2 Kinematics of Crystal Dislocations

2.1 Classical Deformations

The treatment of discontinuous large deformations requires some care in the language to avoid ambiguities. A very careful presentation of this matter has been given by Del Piero and Owen (1993). However, the comprehensive mathematical framework of these authors is quite cumbersome to handle with in practice. Here we adopt what we believe to be a reasonable compromise between mathematical rigor and a more intuitive presentation, in compliance with the usual standard of the mechanical engineering literature.
We throughout assume in this work a stress-free and defect-free reference configuration (natural state) of the considered body $\mathcal{B}$. In this state, the body $\mathcal{B}$ is assumed to occupy an open region $\mathcal{V}_0$ of the three-dimensional Euclidean space $\mathcal{E}$. The subset $\mathcal{V}_0$ is furthermore supposed to be regularly open, i.e., it coincides with the interior of its closure. In the following we consequently use the notations $\bar{\mathcal{D}}$ and $\partial\mathcal{D}$ to denote respectively the closure and the boundary of some subset $\mathcal{D}$ of $\mathcal{E}$.

<u>Definition 1</u>

A classical deformation is a mapping from $\mathcal{V}_0$ into $\mathcal{E}$

$$\begin{aligned} \tilde{\boldsymbol{\chi}}_0 : \quad & \mathcal{V}_0 \to \mathcal{V} := \tilde{\boldsymbol{\chi}}_0(\mathcal{V}_0) \subset \mathcal{E}, \\ & \mathbf{x}_0 \mapsto \mathbf{x} = \tilde{\boldsymbol{\chi}}_0(\mathbf{x}_0), \end{aligned} \tag{1}$$

with the properties:

1. $\tilde{\boldsymbol{\chi}}_0$ is injective, of class C^2 in $\mathcal{V}_0$ and can be extended to an injective C^2-mapping in $\mathcal{E}$. Its inverse $\tilde{\boldsymbol{\chi}}^{-1}$ is also of class C^2 in $\mathcal{E}$.
2. $\tilde{\boldsymbol{\chi}}_0$ preserves the orientation, i.e.,

$$\begin{aligned} & \det \tilde{\mathbf{F}}_0(\mathbf{x}_0) > 0, \quad \forall \mathbf{x}_0 \in \mathcal{V}_0, \\ & \text{with } \tilde{\mathbf{F}}_0 := \frac{\partial \tilde{\boldsymbol{\chi}}_0}{\partial \mathbf{x}_0} = \tilde{\boldsymbol{\chi}}_0 \otimes \tilde{\boldsymbol{\nabla}}_0. \end{aligned} \tag{2}$$

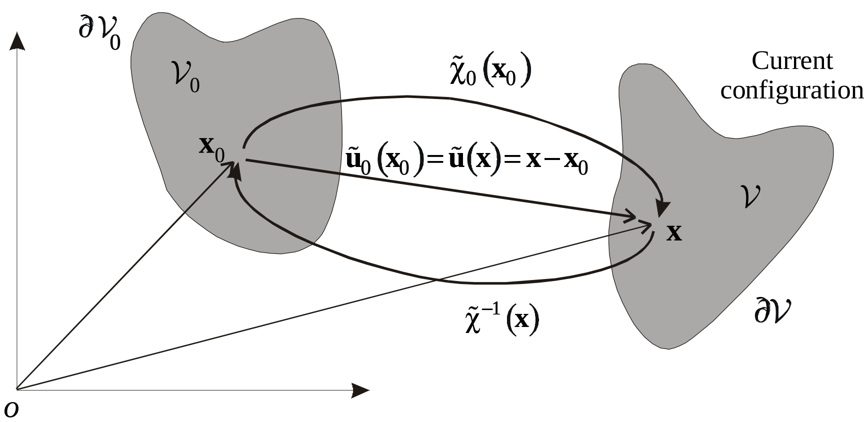

Figure 1. Reference and current configuration for a classical deformation.

In the following, it will be essential to distinguish the displacement vector expressed in terms of the positions $\mathbf{x}_0$ of material points in the reference state (see Figure 1)

$$\tilde{\mathbf{u}}_0(\mathbf{x}_0) := \tilde{\boldsymbol{\chi}}_0(\mathbf{x}_0) - \mathbf{x}_0, \tag{3}$$

from its counterpart expressed in terms of the positions $\mathbf{x}$ of material points in the deformed state

$$\tilde{\mathbf{u}}(\mathbf{x}) := \tilde{\mathbf{u}}_0\left[\tilde{\boldsymbol{\chi}}^{-1}(\mathbf{x})\right] = \mathbf{x} - \tilde{\boldsymbol{\chi}}^{-1}(\mathbf{x}). \tag{4}$$

The inverse of the deformation gradient is also the spatial gradient of the inverse mapping $\tilde{\boldsymbol{\chi}}^{-1}$

$$\tilde{\mathbf{F}}^{-1}(\mathbf{x}) := \frac{\partial \tilde{\boldsymbol{\chi}}^{-1}}{\partial \mathbf{x}}(\mathbf{x}) = \left(\tilde{\boldsymbol{\chi}}^{-1} \otimes \tilde{\boldsymbol{\nabla}}\right)(\mathbf{x}) = \tilde{\mathbf{F}}_0\left[\tilde{\boldsymbol{\chi}}^{-1}(\mathbf{x})\right]^{-1}. \tag{5}$$

In the sequel, we shall make consequent use of the subscript 0 to denote quantities relative to the reference configuration.

2.2 Piecewise Classical Deformations

To describe the distortion states of bodies as those produced by dislocation glide, it becomes necessary to relax the previous requirements made to classical deformations. The following definition extends the classical deformation concept to the situation in which the mapping $\tilde{\boldsymbol{\chi}}_0$ may be discontinuous or ill defined across several internal surfaces of the body. It is similar to the definition of the "simple deformations" formulated by Del Piero and Owen (1993).

Definition 2

A piecewise classical deformation of a body $\mathcal{B}$ (see Figure 2) is a mapping $\tilde{\boldsymbol{\chi}}_0$ from $\mathcal{V}_0$ into $\mathcal{E}$ for which there exists a partition $\left\{\mathcal{V}_0^1, \mathcal{V}_0^2, ..., \mathcal{V}_0^N,\right\}$ of $\mathcal{V}_0$, i.e., N regularly open subsets of $\mathcal{V}_0$ with the following properties:

1. The regions $\mathcal{V}_0^i$ do not overlap each other, that is,
$$\mathcal{V}_0^i \cap \mathcal{V}_0^j = \varnothing \quad \text{if} \quad i \neq j. \tag{6}$$
2. The union of the closures of all subsets $\mathcal{V}_0^i$ coincides with the closure of $\mathcal{V}_0$, i.e.,
$$\bigcup_{i=1}^{N} \overline{\mathcal{V}}_0^i = \overline{\mathcal{V}}_0. \tag{7}$$
3. The restriction $\tilde{\boldsymbol{\chi}}_0^i$ of $\tilde{\boldsymbol{\chi}}_0$ to each of the regions $\mathcal{V}_0^i$ is a classical deformation.
4. The open regions defined as $\mathcal{V}^i := \tilde{\boldsymbol{\chi}}_0\left(\mathcal{V}_0^i\right)$ do not overlap: The mapping $\tilde{\boldsymbol{\chi}}_0$ is injective in $\bigcup_{i=1}^{N} \mathcal{V}_0^i$.

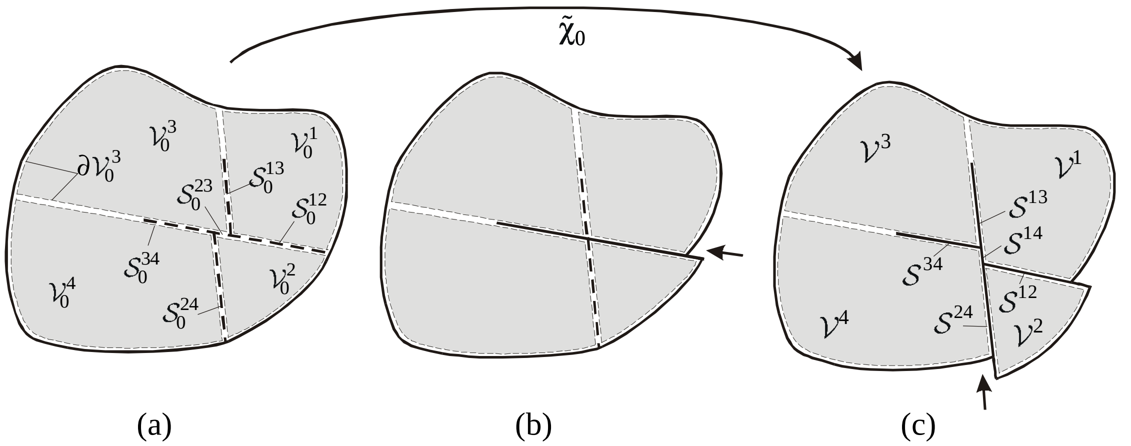

Figure 2. Example of a time dependent piece-wise classical deformation of a body induced by a sequence of two shear processes. Partition of the region occupied by the body in the reference and in the distorted state.

We also denote by $\mathcal{V}$ the interior of $\bigcup_{i=1}^{N} \overline{\mathcal{V}}^i$ or, more pictorially, the region occupied by the body in the distorted state. In the case of time-dependent mappings $\tilde{\boldsymbol{\chi}}_0(t)$, we assume that the properties (1-4) of definition 2 are satisfied at any stage with the same constant partition (see the example of Figure 2).

A consequence of the previous definitions is that the function $\tilde{\boldsymbol{\chi}}_0$ can be at most discontinuous on the internal portion $\mathcal{G}_0$ of the boundaries $\partial\mathcal{V}_0^i$ of the subsets $\mathcal{V}_0^i$. To clarify what we thereby mean, we consider a material point $\mathbf{x}_0 \in \partial\mathcal{V}_0^i$. This point is interior to $\mathcal{V}_0$ if there is another region $j \neq i$ such that $\mathbf{x}_0 \in \partial\mathcal{V}_0^i \cap \partial\mathcal{V}_0^j$. Hence, the internal portion of the boundaries $\partial\mathcal{V}_0^i$ is given by

$$\mathcal{G}_0 := \bigcup_{i,j=1}^{N} \left(\partial\mathcal{V}_0^i \cap \partial\mathcal{V}_0^j \right). \tag{8}$$

Similarly, in the distorted state, the inverse mapping $\tilde{\boldsymbol{\chi}}^{-1}$ can be at most singular across

$$\mathcal{G} := \bigcup_{i,j=1}^{N} \left(\partial\mathcal{V}^i \cap \partial\mathcal{V}^j \right). \tag{9}$$

In the following, we consequently use the superscript i to denote the extension of any function that is regular in a region of the partition to its boundary. For example, we write

$$\tilde{\boldsymbol{\chi}}_0^i(\mathbf{x}_0) := \lim_{\mathbf{y}_0 \to \mathbf{x}_0, \mathbf{y}_0 \in \mathcal{V}_0^i} \tilde{\boldsymbol{\chi}}_0^i(\mathbf{y}), \quad \mathbf{x}_0 \in \partial\mathcal{V}_0^i,$$
$$\text{and} \tag{10}$$
$$\tilde{\mathbf{F}}^{-1;i}(\mathbf{x}) := \lim_{\mathbf{y} \to \mathbf{x}, \mathbf{y} \in \mathcal{V}^i} \tilde{\mathbf{F}}^{-1}(\mathbf{y}), \quad \mathbf{x} \in \partial\mathcal{V}^i.$$

To define the possible jump of functions across $\partial\mathcal{V}_0^i \cap \partial\mathcal{V}_0^j$ (or $\partial\mathcal{V}^i \cap \partial\mathcal{V}^j$), an arbitrary choice must be made, leading to the definition of an upper and a lower side of $\partial\mathcal{V}_0^i \cap \partial\mathcal{V}_0^j$ (or $\partial\mathcal{V}^i \cap \partial\mathcal{V}^j$). The notation $i \to j$ will be consequently used to state that $\mathcal{V}_0^i$ (or $\mathcal{V}^i$) is taken as the upper side and $\mathcal{V}_0^j$ (or $\mathcal{V}^j$) as the lower side. For example, the jump of $\tilde{\boldsymbol{\chi}}_0$ across $\partial\mathcal{V}_0^i \cap \partial\mathcal{V}_0^j$ is defined as and denoted by

$$\left[\!\left[\tilde{\boldsymbol{\chi}}_0(\mathbf{x}_0) \right]\!\right]^{i \to j} := \tilde{\boldsymbol{\chi}}_0^i(\mathbf{x}_0) - \tilde{\boldsymbol{\chi}}_0^j(\mathbf{x}_0) = \left[\!\left[\tilde{\mathbf{u}}_0(\mathbf{x}_0) \right]\!\right]^{i \to j}, \quad \mathbf{x}_0 \in \partial\mathcal{V}_0^i \cap \partial\mathcal{V}_0^j. \tag{11}$$

In the same way, the jump of $\tilde{\boldsymbol{\chi}}^{-1}$ across $\partial\mathcal{V}^i \cap \partial\mathcal{V}^j$ is defined as

$$\left[\!\left[\tilde{\boldsymbol{\chi}}^{-1}(\mathbf{x}) \right]\!\right]^{i \to j} := \tilde{\boldsymbol{\chi}}^{-1;i}(\mathbf{x}) - \tilde{\boldsymbol{\chi}}^{-1;j}(\mathbf{x}) = -\left[\!\left[\tilde{\mathbf{u}}(\mathbf{x}) \right]\!\right]^{i \to j}, \quad \mathbf{x} \in \partial\mathcal{V}^i \cap \partial\mathcal{V}^j. \tag{12}$$

The part of $\partial\mathcal{V}_0^i \cap \partial\mathcal{V}_0^j$ or $\partial\mathcal{V}^i \cap \partial\mathcal{V}^j$ where the jump of $\tilde{\boldsymbol{\chi}}_0$ or $\tilde{\boldsymbol{\chi}}^{-1}$ doesn't vanish is denoted by $\mathcal{S}_0^{ij}$ or $\mathcal{S}^{ij}$, respectively. We will refer to it as a singular or jump surface in the reference state or in the distorted state, respectively.

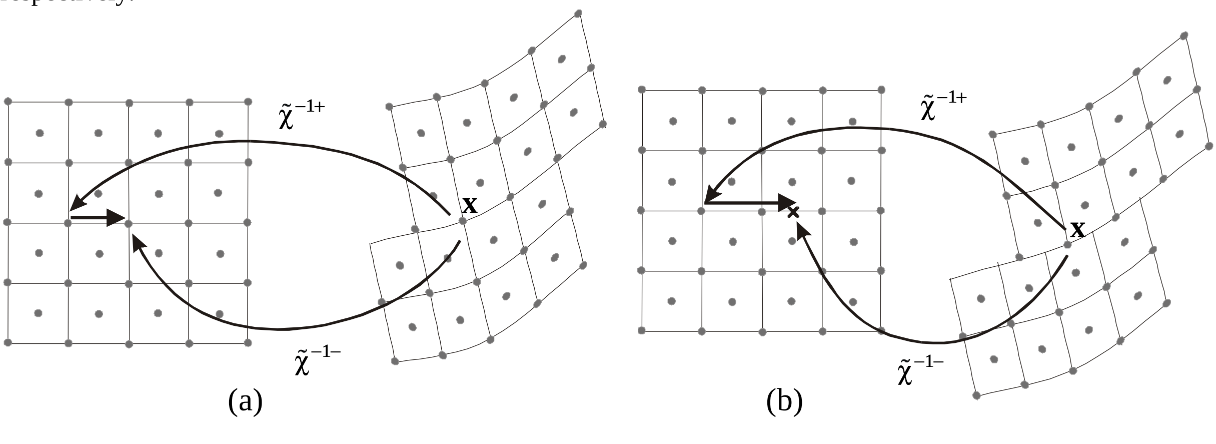

Figure 3. Illustration of the coherency condition: In (a) the coherency condition is satisfied while it is violated in (b).

2.3 Coherency Hypothesis

If $\tilde{\boldsymbol{\chi}}_0$ is a piecewise classical deformation of a crystal and if the reference configuration is a natural state:

1. There is a constant lattice vector $\mathbf{b}_0^{i \to j}$ of the defect-free crystal characterizing each singular surface $\mathcal{S}^{ij}$, such that the displacement jump across $\mathcal{S}^{ij}$ is given by

$$[\![\tilde{\mathbf{u}}(\mathbf{x})]\!]^{i\to j} = \mathbf{b}_0^{i\to j}. \tag{13}$$

2. The inverse of the deformation gradient $\tilde{\mathbf{F}}^{-1}$ is continuous across $\mathcal{S}^{ij}$.

The physical meaning of the coherency hypothesis is that jump surfaces are indiscernible in the distorted state (see Figure 3). By using the theorem of Stokes, one can easily show that a coherent singular surface cannot end inside a simply connected region $\mathcal{V}$. To describe a crystal dislocation, which is nothing else than the curve $\mathcal{L}^{ij}$ bounding a singular surface $\mathcal{S}^{ij}$, one can relax the coherency hypothesis in a narrow strip $\mathcal{Z}^{ij}$ along $\mathcal{L}^{ij}$. This procedure is supported by the fact that the crystal is highly distorted in the dislocation core region. In the region $\mathcal{Z}^{ij}$, the displacement jump is suitably tapered off toward the boundary line $\mathcal{L}^{ij}$ (see Figure 4). The equilibrium of elastic solids containing singular surfaces where an arbitrary displacement jump is prescribed was first analyzed by Somigliana (1914, 1915), following the pioneering works of Weingarten (1901) and Volterra (1907). An introduction to the various dislocation models available in continuum elasticity can be also found in the textbook of Teodosiu (1982). A model of Somigliana-type dislocations following this line is presented in next section. The reasons motivating this choice and some properties resulting from this definition can be found in (Fedelich, 2003b).

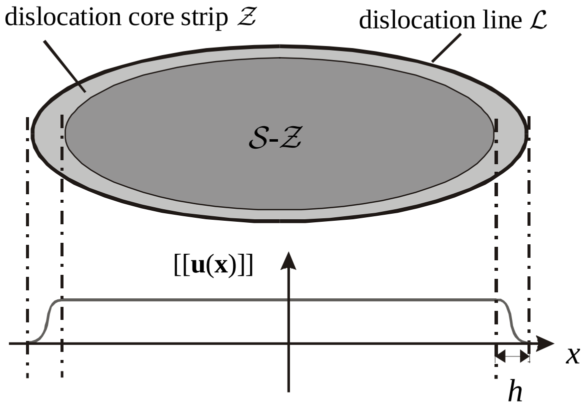

Figure 4. Schematic of a dislocation core model.

2.4 Distortion of a Crystal by Somigliana-type Dislocations

We first recall the definition of the distance between a point $\mathbf{x}_0$ and a smooth curve $\mathcal{L}_0$:

$$\delta(\mathcal{L}_0, \mathbf{x}_0) := \min_{\mathbf{y}_0 \in \mathcal{L}_0} \|\mathbf{y}_0 - \mathbf{x}_0\|. \tag{14}$$

Definition 3

We call distortion of a crystal by Somigliana-type dislocations, in short distortion, any piecewise classical deformation $\tilde{\boldsymbol{\chi}}_0$ with the following properties for each singular surface $\mathcal{S}_0^{ij}$:

1. $\mathcal{S}_0^{ij}$ is plane and the internal part $\mathcal{L}_0^{ij}$ of its boundary curve, i.e., the part of $\mathcal{S}_0^{ij}$ that doesn't intercept $\partial\mathcal{V}$, is smooth and connected.
2. The mapping $\tilde{\boldsymbol{\chi}}_0$ is continuous at $\mathcal{L}_0^{ij}$. In particular, the image of $\mathcal{L}_0^{ij}$ is the same when it is mapped from either above or below, that is $\tilde{\boldsymbol{\chi}}_0^i\left(\mathcal{L}_0^{ij}\right) = \tilde{\boldsymbol{\chi}}_0^j\left(\mathcal{L}_0^{ij}\right) = \mathcal{L}^{ij}$.
3. The dislocation core in the reference configuration is represented by a strip $\mathcal{Z}_0^{ij} \subset \mathcal{S}_0^{ij}$ of constant width h_0, i.e.,
$$\mathcal{Z}_0^{ij} = \left\{\mathbf{y}_0 \in \mathcal{S}_0^{ij},\quad \delta\left(\mathbf{y}_0, \mathcal{L}_0^{ij}\right) \le h_0\right\} \tag{15}$$
and its counterpart in the distorted state is defined as
$$\mathcal{Z}^{ij} := \tilde{\boldsymbol{\chi}}_0^i\left(\mathcal{Z}_0^{ij}\right). \tag{16}$$
4. The displacement jump referred to the distorted state is given by

$$[\![\tilde{\mathbf{u}}(\mathbf{x})]\!]^{i\to j} = \varphi\left[\overline{r}_0(\mathbf{x})\right] \mathbf{b}_0^{i\to j} \quad \text{in } \mathcal{S}^{ij}, \tag{17}$$

where $\mathbf{b}_0^{i\to j}$ is a constant lattice vector of the defect-free crystal contained in the plane of $\mathcal{S}_0^{ij}$, $\varphi(r)$ is a suitably smooth increasing function such that

$$\varphi(0)=0, \quad \varphi(r)=1 \quad \text{if } r \geq h_0, \quad \varphi'(r)>0 \,\text{if } r \in \left]0,h_0\right[, \tag{18}$$

and $\overline{r}_0(\mathbf{x})$ is the distance between the curve $\mathcal{L}_0^{ij}$ and the place initially occupied by the material point on the upper side i of the jump surface that moves to $\mathbf{x}$, i.e.,

$$\overline{r}_0(\mathbf{x}) = \delta\left[\mathcal{L}_0^{ij}, \tilde{\boldsymbol{\chi}}^{-1;i}(\mathbf{x})\right]. \tag{19}$$

5. The inverse of the deformation gradient $\tilde{\mathbf{F}}^{-1}$ is continuous across $\mathcal{S}^{ij} - \mathcal{Z}^{ij}$ and the stress vector $\tilde{\boldsymbol{\sigma}}\cdot\mathbf{n}^{i\to j}$ is continuous across $\mathcal{S}^{ij}$, where $\tilde{\boldsymbol{\sigma}}$ is the Cauchy stress tensor and $\mathbf{n}^{i\to j}$ the unit normal vector to $\mathcal{S}^{ij}$ that points outward from $\mathcal{V}^i$.

To define the distance of a material point to the dislocation curve in the reference configuration, when this material point is identified by its place in the distorted state, an arbitrary choice must be made between the upper and the lower mappings $\tilde{\boldsymbol{\chi}}_0^i$ and $\tilde{\boldsymbol{\chi}}_0^j$. Clearly, the symmetric choice can be made, leading to an equivalent model.

In (Fedelich, 2003b) the displacement jump in the reference configuration corresponding to the relation (17) is derived

$$[\![\tilde{\boldsymbol{\chi}}_0(\mathbf{x}_0)]\!]^{i\to j} = [\![\tilde{\mathbf{u}}_0(\mathbf{x}_0)]\!]^{i\to j} = \int_{\mathbf{x}_0}^{\mathbf{x}_0+\varphi(r_0)\mathbf{b}_0^{i\to j}} \tilde{\mathbf{F}}_0^j \cdot d\mathbf{y}_0 \quad \text{on } \mathcal{S}_0^{ij}. \tag{20}$$

The definition 3, which can be regarded as a particular model of a dislocation core, is mainly motivated by the following result: The velocity field is denoted by $\tilde{\mathbf{v}}(\mathbf{x})$. Let l_0 be a curvilinear coordinate along the dislocation line $\mathcal{L}_0^{ij}$ in the reference state. If $\mathcal{L}_0^{ij}$ glides in its plane with a normal velocity $\mathrm{v}_0^{ij} = \mathrm{v}_0^{ij}(l_0)$, the jump of the velocity referred to the distorted state is found to be

$$\begin{aligned} &[\![\tilde{\mathbf{v}}(\mathbf{x})]\!]^{i\to j} = \varphi'\left[\overline{r}_0(\mathbf{x})\right] \mathrm{v}_0^{ij}\left[\overline{l}_0(\mathbf{x})\right] \tilde{\mathbf{F}}_0^j\left[\boldsymbol{\chi}^{-1;j}(\mathbf{x})\right]\cdot\mathbf{b}_0^{i\to j}, \quad \mathbf{x}\in\mathcal{Z}^{ij}, \\ &[\![\tilde{\mathbf{v}}(\mathbf{x})]\!]^{i\to j} = \mathbf{0}, \quad \mathbf{x}\in\mathcal{S}^{ij}-\mathcal{Z}^{ij}, \end{aligned} \tag{21}$$

where $\overline{l}_0(\mathbf{x})$ is the curvilinear coordinate of the point of $\mathcal{L}_0^{ij}$ nearest to $\boldsymbol{\chi}^{-1;i}(\mathbf{x})$. This means that the velocity jump only depends on the gliding movement of the dislocation. It is in particular independent of the elastic strain variations. Hence, dissipation can only occur when the dislocation is gliding.

3 Transition between the Dislocation and the Continuous Level

3.1 Field Equations at the Dislocation Level

In the following, the level with discrete dislocations, at which the deformation is discontinuous, will be referred to as the dislocation level. All fields defined at this level are denoted by a tilde. The higher level, at which the transformations are described by continuous fields, will be referred to as the continuous level. The strain at the dislocation level is purely elastic. It is defined at any regular material point $\mathbf{x}_0 \in \mathcal{V}_0^i$ as

$$\tilde{\boldsymbol{\varepsilon}}(\mathbf{x}) = \tilde{\boldsymbol{\varepsilon}}_0(\mathbf{x}_0) := \frac{1}{2}\left[\tilde{\mathbf{F}}_0^T(\mathbf{x}_0)\cdot\tilde{\mathbf{F}}_0(\mathbf{x}_0) - \mathbf{1}\right], \quad \mathbf{x} = \tilde{\boldsymbol{\chi}}_0(\mathbf{x}_0). \tag{22}$$

We now make the assumption of small strains $\|\tilde{\boldsymbol{\varepsilon}}\| \ll 1$. Notwithstanding the smallness of the strains at the dislocation level, the magnitude of the lattice rearrangements due to dislocation glide can be arbitrarily large. Thus, the resulting strains at the continuous level will be considered as being large.

We denote the mass density in the reference configuration by $\tilde{\rho}_0$. Due to the small strains approximation, the mass density in the distorted state $\tilde{\rho}$ is approximately unchanged, i.e., $\tilde{\rho} \simeq \tilde{\rho}_0$. The internal energy is denoted by $\tilde{e}$ and the heat flux by $\tilde{\mathbf{q}}$. The balance equations at the dislocation level are assumed to hold in their usual form, that is,

$$
\begin{aligned}
&\tilde{\boldsymbol{\sigma}} \cdot \tilde{\boldsymbol{\nabla}} = \mathbf{0}, \\
&\tilde{\boldsymbol{\sigma}} = \tilde{\boldsymbol{\sigma}}^{T}, \\
&\tilde{\rho}\dot{\tilde{e}} = \tilde{\boldsymbol{\sigma}} : \left(\tilde{\mathbf{v}} \otimes \tilde{\boldsymbol{\nabla}}\right) - \tilde{\mathbf{q}} \cdot \tilde{\boldsymbol{\nabla}},
\end{aligned}
\tag{23}
$$

where we assume no bulk forces and static equilibrium to simplify the presentation. The jump conditions at any singular surface $\mathcal{S}^{ij}$ are given by

$$
\begin{aligned}
&\tilde{\boldsymbol{\sigma}}^{\,i\to j} \cdot \mathbf{n}^{i\to j} = \mathbf{0}, \\
&[\![\tilde{\mathbf{v}}^{\,i\to j} \cdot \tilde{\boldsymbol{\sigma}} \cdot \mathbf{n}^{i\to j} = [\![\tilde{\mathbf{q}}^{\,i\to j} \cdot \mathbf{n}^{i\to j}.
\end{aligned}
\tag{24}
$$

At this level, the linear elastic law takes the form

$$
\tilde{\boldsymbol{\sigma}} = \mathbf{C} : \tilde{\boldsymbol{\varepsilon}}, \quad \text{or } \tilde{\boldsymbol{\varepsilon}} = \mathbf{S} : \tilde{\boldsymbol{\sigma}}. \tag{25}
$$

The elastic stiffness tensor $\mathbf{C}$ and the compliance tensor $\mathbf{S}$ are supposed to be spatially homogeneous, which means that we consider pure crystals without second phase or precipitates.

3.2 General Methodology for Formally Constructing the Fields at the Continuous Level

The corresponding fields at the continuous level are defined by a weighted spatial averaging procedure over a representative volume element $RVE(\mathbf{x}_0)$, $\mathbf{x}_0 \in \mathcal{V}_0$. More details on spatial averaging methods can be found in the textbook of Nemat-Nasser and Hori (1993). The representative volume element (RVE) is a region of $\mathcal{E}$ translating with its centroid $\mathbf{x}_0$ and having a piece-wise smooth boundary (see Figure 5). Since in this work we focus on the bulk behavior of the crystal, we assume that $\mathbf{x}_0$ is far enough from $\partial\mathcal{V}_0$ so that $RVE(\mathbf{x}_0) \subset \mathcal{V}_0$. First, we introduce a suitably smooth weighting function $J_0(\mathbf{y}_0 - \mathbf{x}_0)$ with the properties

$$
\begin{aligned}
&J_0(\mathbf{y}_0 - \mathbf{x}_0) \geq 0 \quad \text{for } \mathbf{y}_0 \text{ in } RVE(\mathbf{x}_0), \\
&J_0(\mathbf{y}_0 - \mathbf{x}_0) = 0 \quad \text{otherwise},
\end{aligned}
\tag{26}
$$

and

$$
\int_{\mathcal{V}_0} J_0(\mathbf{y}_0 - \mathbf{x}_0)\, dV_{\mathbf{y}_0} = 1.
$$

Typically, $J_0(\mathbf{y}_0 - \mathbf{x}_0)$ is nearly constant in the largest part of $RVE(\mathbf{x}_0)$ and smoothly vanishes toward $\partial RVE(\mathbf{x}_0)$. A limiting case for $J_0(\mathbf{y}_0 - \mathbf{x}_0)$ is the characteristic function $J_c(\mathbf{y}_0 - \mathbf{x}_0)$ of the representative volume element $RVE(\mathbf{x}_0)$, having the value $1/V_0$ in $RVE(\mathbf{x}_0)$ and zero otherwise. Here, V_0 denotes the volume of $RVE(\mathbf{x}_0)$.

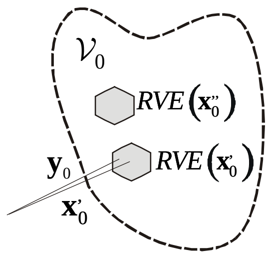

Figure 5. Body $\mathcal{V}_0$ with translating RVE.

3.3 Definition of the Deformation at the Continuous Level

We start by defining the deformation at the continuous level as

$$
\boldsymbol{\chi}_0(\mathbf{x}_0) := \int_{\mathcal{V}_0} \tilde{\boldsymbol{\chi}}_0(\mathbf{y}_0)\, J(\mathbf{y}_0 - \mathbf{x}_0)\, dV_{\mathbf{y}_0} = \sum_i \int_{\mathcal{V}_0^i} \tilde{\boldsymbol{\chi}}_0(\mathbf{y}_0)\, J(\mathbf{y}_0 - \mathbf{x}_0)\, dV_{\mathbf{y}_0}. \tag{27}
$$

This averaging procedure has a regularizing effect: If the weighting function $J_0(\mathbf{y}_0 - \mathbf{x}_0)$ is indefinitely differentiable, the deformation at the continuous level $\boldsymbol{\chi}_0$ is also indefinitely differentiable (Schwartz, 1961). The deformation gradient at the continuous level is then

$$\mathbf{F}_0\left(\mathbf{x}_0\right) := \frac{\partial \boldsymbol{\chi}_0}{\partial \mathbf{x}_0}\left(\mathbf{x}_0\right) = \sum_i \int_{\mathcal{V}_0^i} \tilde{\boldsymbol{\chi}}_0\left(\mathbf{y}_0\right) \frac{\partial J_0}{\partial \mathbf{x}_0}\left(\mathbf{y}_0 - \mathbf{x}_0\right) dV_{\mathbf{y}_0} = -\sum_i \int_{\mathcal{V}_0^i} \tilde{\boldsymbol{\chi}}_0\left(\mathbf{y}_0\right) \frac{\partial J_0}{\partial \mathbf{y}_0}\left(\mathbf{y}_0 - \mathbf{x}_0\right) dV_{\mathbf{y}_0}\,. \tag{28}$$

By applying the theorem of Gauss to each subset $\mathcal{V}_0^i$ we obtain

$$\mathbf{F}_0\left(\mathbf{x}_0\right) = -\sum_i \int_{\partial\mathcal{V}_0^i} \tilde{\boldsymbol{\chi}}_0\left(\mathbf{y}_0\right) \otimes \mathbf{n}_0\, J_0\left(\mathbf{y}_0 - \mathbf{x}_0\right) dS_{\mathbf{y}_0} + \sum_i \int_{\mathcal{V}_0^i} \frac{\partial \tilde{\boldsymbol{\chi}}_0}{\partial \mathbf{y}_0}\left(\mathbf{y}_0\right) J_0\left(\mathbf{y}_0 - \mathbf{x}_0\right) dV_{\mathbf{y}_0}\,. \tag{29}$$

Since $RVE\left(\mathbf{x}_0\right) \subset \mathcal{V}_0$, the portions of the boundaries $\partial\mathcal{V}_0^i$ contained in $RVE\left(\mathbf{x}_0\right)$ are all strictly contained in $\mathcal{V}_0$. This means that each surface element $dS_{\mathbf{y}_0} \subset \partial\mathcal{V}_0^i$ is also common to the boundary $\partial\mathcal{V}_0^j$ of some other element $j \neq i$ of the partition of $\mathcal{V}_0$. The first term of the right hand side of equation (29) can thus be rearranged in a sum of surface integrals over the singular surfaces $\mathcal{S}_0^{ij}$. We can rewrite it as

$$\mathbf{F}_0\left(\mathbf{x}_0\right) = \sum_i \int_{\mathcal{V}_0^i} \tilde{\mathbf{F}}_0\left(\mathbf{y}_0\right) J_0\left(\mathbf{y}_0 - \mathbf{x}_0\right) dV_{\mathbf{y}_0} - \sum_i \int_{\mathcal{S}_0^{ij}} \left[\!\left[\tilde{\boldsymbol{\chi}}_0\left(\mathbf{y}_0\right) \right]\!\right]^{i\to j} \otimes \mathbf{n}_0^{i\to j}\, J_0\left(\mathbf{y}_0 - \mathbf{x}_0\right) dS_{\mathbf{y}_0}\,. \tag{30}$$

In particular, the deformation gradient at the continuous level is not the average of the deformation gradient at the dislocation level. There is an additional term that arises from irreversible lattice rearrangements. Note, that as can be seen in equation (20), the jump $\left[\!\left[\tilde{\boldsymbol{\chi}}_0\left(\mathbf{y}_0\right) \right]\!\right]^{i\to j}$ depends in general on elastic strains.

3.4 Hypothesis of Slowly Varying Rotations

We now make the additional assumption of slowly varying rotations or of small lattice curvature at the dislocation level. First, we recall the polar decomposition of the deformation gradient

$$\tilde{\mathbf{F}}_0\left(\mathbf{x}_0\right) = \tilde{\mathbf{R}}_0\left(\mathbf{x}_0\right) \cdot \tilde{\mathbf{W}}_0\left(\mathbf{x}_0\right), \tag{31}$$

where $\tilde{\mathbf{R}}_0$ is a field of orthogonal tensors and $\tilde{\mathbf{W}}_0$ of symmetric tensors. The hypothesis of slowly varying rotations can be mathematically formulated by introducing the wryness tensor (Kadafar and Eringen, 1971),

$$\tilde{\boldsymbol{\Gamma}}_0 := -\frac{1}{2} \boldsymbol{\in} : \left[\tilde{\mathbf{R}}_0^T \cdot \left(\tilde{\mathbf{R}}_0 \otimes \tilde{\boldsymbol{\nabla}}_0 \right) \right], \tag{32}$$

where $\boldsymbol{\in}$ is the permutation tensor. It is a measure of the relative orientation of two neighboring triads and remains invariant under rigid motion. Specifically, if L_{RVE} is a characteristic dimension of the RVE, we suppose that

$$L_{RVE} \left\| \tilde{\boldsymbol{\Gamma}}_0 \right\| \ll 1\,. \tag{33}$$

Physically, the low curvature assumption is related to a low density of geometrically necessary dislocations as shown by Nye (1953). The hypothesis (33) means that the rotation is approximately homogeneous at the scale of the RVE.

Within this assumption, the deformation gradient at the continuous level may be approximated by

$$\mathbf{F}_0\left(\mathbf{x}_0\right) \simeq \tilde{\mathbf{R}}_0\left(\mathbf{x}_0\right) \cdot \sum_i \int_{\mathcal{V}_0^i} \tilde{\mathbf{W}}_0\left(\mathbf{y}_0\right) J_0\left(\mathbf{y}_0 - \mathbf{x}_0\right) dV_{\mathbf{y}_0} - \sum_i \int_{\mathcal{S}_0^{ij}} \left[\!\left[\tilde{\boldsymbol{\chi}}_0\left(\mathbf{y}_0\right) \right]\!\right]^{i\to j} \otimes \mathbf{n}_0^{i\to j}\, J_0\left(\mathbf{y}_0 - \mathbf{x}_0\right) dS_{\mathbf{y}_0}\,. \tag{34}$$

There remains the open question of the injectivity of the continuous deformation $\boldsymbol{\chi}_0$, which is difficult to infer from the previous definitions without additional assumptions. In the following, we will throughout suppose that $\boldsymbol{\chi}_0$ is injective in $\mathcal{V}_0$ and denote its inverse by $\boldsymbol{\chi}^{-1}$. As a partial justification, we note that the small elastic strain hypothesis implies that $\tilde{\mathbf{W}}_0 \simeq \mathbf{1}$. Hence, when the slip intensity, which is represented by the second term of the right hand side of (34), vanishes, then $\det\left[\mathbf{F}_0\left(\mathbf{x}_0\right)\right] \to 1$ and $\boldsymbol{\chi}_0$ is locally one-to-one. From this reasoning follows that the local injectivity of $\boldsymbol{\chi}_0$ is at least guaranteed for moderate slip activity.

3.5 A Hypothesis of Statistical Homogeneity

Another hypothesis, which is related to the statistical homogeneity of the fields at the scale of the RVE, will turn out to be useful in the sequel. To formulate it in the most general way, we now consider an arbitrary piece-wise regular function, $\tilde{g}_0\left(\mathbf{x}_0\right)$, defined in the reference configuration at the dislocation level and its counterpart $\tilde{g}(\mathbf{x}) = \tilde{g}_0\left[\tilde{\boldsymbol{\chi}}^{-1}(\mathbf{x})\right]$ referred to the deformed configuration. The corresponding field at the continuous level can be defined as

$$g_0(\mathbf{x}_0) := \int_{\mathcal{V}_0} \tilde{g}_0(\mathbf{y}_0)\, J_0(\mathbf{y}_0 - \mathbf{x}_0)\, dV_0 \,, \tag{35}$$

in line with the definition of the continuous deformation (27). Obviously, a similar definition can be formulated with respect to the current state, that is,

$$g(\mathbf{x}) := \int_{\mathcal{V}} \tilde{g}(\mathbf{y})\, J(\mathbf{y} - \mathbf{x})\, dV \,, \tag{36}$$

with a suitably chosen weighting function J in the deformed configuration. In the following, we consequently make the hypothesis that for the choice $J = J_0$ the relation

$$g\left[\boldsymbol{\chi}_0(\mathbf{x}_0)\right] = g_0(\mathbf{x}_0) \tag{37}$$

holds for any field $\tilde{g}_0(\mathbf{x}_0)$. To better grasp the meaning of the statement (37), we resort to the extreme case of J being the characteristic function of the RVE J_c. In this case, by applying the variable change $\boldsymbol{\chi}_0^i(\mathbf{y}_0) = \mathbf{y}$ in each subset $\mathcal{V}_0^i$ under the hypothesis of small elastic strains, we have

$$\begin{aligned} g_0(\mathbf{x}_0) &= \frac{1}{V_0} \iiint_{RVE(\mathbf{x}_0)} \tilde{g}_0(\mathbf{y}_0)\, dV_0 = \frac{1}{V_0} \sum_i \iiint_{RVE(\mathbf{x}_0) \cap \mathcal{V}_0^i} \tilde{g}_0(\mathbf{y}_0)\, dV_0 \\ &= \frac{1}{V_0} \sum_i \iiint_{\tilde{\boldsymbol{\chi}}_0\left[RVE(\mathbf{x}_0) \cap \mathcal{V}_0^i\right]} \tilde{g}(\mathbf{y}) \left(\det \tilde{\mathbf{F}}_0\right)^{-1} dV \simeq \frac{1}{V_0} \sum_i \iiint_{\tilde{\boldsymbol{\chi}}_0\left[RVE(\mathbf{x}_0) \cap \mathcal{V}_0^i\right]} \tilde{g}(\mathbf{y})\, dV \\ &=: \frac{1}{V_0} \iiint_{\tilde{\boldsymbol{\chi}}_0\left[RVE(\mathbf{x}_0)\right]} \tilde{g}(\mathbf{y})\, dV, \end{aligned} \tag{38}$$

since $\det\left(\tilde{\mathbf{F}}_0\right) \simeq 1$. The hypothesis (37) is therefore equivalent to

$$\frac{1}{V_0} \int_{\tilde{\boldsymbol{\chi}}_0\left[RVE(\mathbf{x}_0)\right]} \tilde{g}(\mathbf{y})\, dV = \frac{1}{V_0} \int_{RVE\left[\boldsymbol{\chi}_0(\mathbf{x}_0)\right]} \tilde{g}(\mathbf{y})\, dV \,. \tag{39}$$

The underlying physical assumption is that if the RVE is large enough with respect to the typical distance between dislocations L_D and small enough with respect to the macro structural characteristic dimension L_S, i.e., if

$$L_S \gg L_{RVE} \gg L_D \,, \tag{40}$$

the fields at the continuous level should not critically depend on the particular choice of the averaging domain (RVE). Since $\tilde{\boldsymbol{\chi}}_0\left\{RVE\left[\boldsymbol{\chi}^{-1}(\mathbf{x})\right]\right\}$ and $RVE(\mathbf{x})$ can be regarded as two particular choices of the RVE at the material point $\mathbf{x}$ (see Figure 6) the relation (39) also follows from this assumption. This hypothesis completes the duality between descriptions referring to the initial and the current state at the continuous level. Because of the one-to-one correspondence between these two states, the subscript 0 may be dropped and we write when there is no ambiguity, e.g., $g(\mathbf{x}) = g(\mathbf{x}_0) = g_0(\mathbf{x}_0)$ if $\mathbf{x} = \boldsymbol{\chi}(\mathbf{x}_0) \equiv \boldsymbol{\chi}_0(\mathbf{x}_0)$.

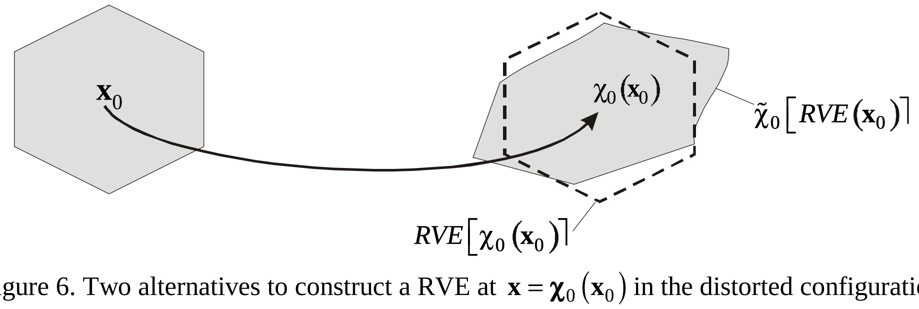

Figure 6. Two alternatives to construct a RVE at $\mathbf{x} = \boldsymbol{\chi}_0(\mathbf{x}_0)$ in the distorted configuration.

3.6 Formal Definition of the Remaining Fields at the Continuous Level

First, the velocity at the continuous level is defined as

$$\mathbf{v}(\mathbf{x}) := \int_{\mathcal{V}} \tilde{\mathbf{v}}(\mathbf{y})\, J(\mathbf{y}-\mathbf{x})\, dV_{\mathbf{y}} \; . \tag{41}$$

The spatial gradient of the velocity can be evaluated by the same procedure as the deformation gradient (30). After performing the same transformations we obtain

$$\mathbf{v}\otimes\nabla(\mathbf{x}) = \sum_i \int_{\mathcal{V}^i} \tilde{\mathbf{v}}\otimes\tilde{\nabla}(\mathbf{y})\, J(\mathbf{y}-\mathbf{x})\, dV_{\mathbf{y}} - \sum_i \int_{\mathcal{S}^{ij}} \llbracket \tilde{\mathbf{v}}(\mathbf{y}) \rrbracket^{i\to j} \otimes \mathbf{n}^{i\to j}\, J(\mathbf{y}-\mathbf{x})\, dS_{\mathbf{y}} \; . \tag{42}$$

Eventually, the Cauchy stress tensor, the mass density, the heat flux and the internal energy are defined at the continuous level as follows

$$\begin{aligned}
\boldsymbol{\sigma}(\mathbf{x}) &:= \int_{\mathcal{V}} \tilde{\boldsymbol{\sigma}}(\mathbf{y})\, J(\mathbf{y}-\mathbf{x})\, dV_{\mathbf{y}},\\
\rho(\mathbf{x}) &:= \int_{\mathcal{V}} \tilde{\rho}(\mathbf{y})\, J(\mathbf{y}-\mathbf{x})\, dV_{\mathbf{y}},\\
\mathbf{q}(\mathbf{x}) &:= \int_{\mathcal{V}} \tilde{\mathbf{q}}(\mathbf{y})\, J(\mathbf{y}-\mathbf{x})\, dV_{\mathbf{y}},\\
e(\mathbf{x}) &:= \int_{\mathcal{V}} \tilde{e}(\mathbf{y})\, J(\mathbf{y}-\mathbf{x})\, dV_{\mathbf{y}}.
\end{aligned} \tag{43}$$

3.7 Balance Equations for the Linear and the Angular Momentum at the Continuous Level

First, note that because $\tilde{\rho} = \tilde{\rho}_0$ the mass density at the continuous level is $\rho(\mathbf{x}) = \tilde{\rho}_0 =: \rho_0$. The spatial divergence of the Cauchy stress tensor is obtained by the same procedure as for the deformation gradient (30). We have

$$\boldsymbol{\sigma}\cdot\nabla(\mathbf{x}) = \sum_i \int_{\mathcal{V}^i} \tilde{\boldsymbol{\sigma}}\cdot\tilde{\nabla}(\mathbf{y})\, J(\mathbf{y}-\mathbf{x})\, dV_{\mathbf{y}} - \sum_i \int_{\mathcal{S}^{ij}} \llbracket \tilde{\boldsymbol{\sigma}}(\mathbf{y}) \rrbracket^{i\to j} \cdot \mathbf{n}^{i\to j}\, J(\mathbf{y}-\mathbf{x})\, dS_{\mathbf{y}} \; . \tag{44}$$

Due to the jump condition $(24)_1$ for the stress vector across a singular surface, the second term of the right hand side of equation (44) vanishes and the balance equations for the linear and the angular momentum at the continuous level are readily established by spatially averaging the corresponding equations $(23)_1$ and $(23)_2$

$$\begin{aligned}
\boldsymbol{\sigma}\cdot\nabla &= \mathbf{0},\\
\boldsymbol{\sigma}^T &= \boldsymbol{\sigma}.
\end{aligned} \tag{45}$$

Remark:
Hill (1972, 1984), Nemat-Nasser and Hori (1999) chose to define the non-symmetric first Piola-Kirchhoff stress tensor $\mathbf{S}_0$ at the macroscopic level by averaging its counterpart at the microscopic level $\tilde{\mathbf{S}}_0$ in the reference configuration. In this line of thought, $\mathbf{S}_0$ is regarded as the prime stress measure and the Cauchy stress is defined from $\mathbf{S}_0$ by

$$\boldsymbol{\sigma} := \frac{1}{\det \mathbf{F}_0}\mathbf{S}_0\cdot\mathbf{F}_0^T \tag{46}$$

instead of $(43)_1$. The advantage of this choice is that the hypothesis (37) is no longer necessary. However, these authors only considered regular processes at the microscopic level. To demonstrate the difficulties occasioned by singular surfaces at the microscopic level with this choice, we tentatively define $\mathbf{S}_0$ by spatially averaging $\tilde{\mathbf{S}}_0$ in the reference configuration. In this eventuality the gradient of $\mathbf{S}_0$ is given by

$$\mathbf{S}_0\cdot\nabla_0(\mathbf{x}_0) = \sum_i \int_{\mathcal{V}_0^i} \tilde{\mathbf{S}}_0\cdot\tilde{\nabla}_0(\mathbf{y}_0)\, J_0(\mathbf{y}_0-\mathbf{x}_0)\, dV_{\mathbf{y}_0} - \sum_i \int_{\mathcal{S}_0^{ij}} \llbracket \tilde{\mathbf{S}}_0(\mathbf{y}_0) \rrbracket^{i\to j} \cdot \mathbf{n}_0^{i\to j}\, J_0(\mathbf{y}_0-\mathbf{x}_0)\, dS_{\mathbf{y}_0} \; . \tag{47}$$

But in general the jump $\llbracket \tilde{\mathbf{S}}_0(\mathbf{y}_0) \rrbracket^{i\to j}\cdot\mathbf{n}_0^{i\to j}$ is not zero for the singular surfaces caused by dislocation glide because the material points $\tilde{\boldsymbol{\chi}}_0^i(\mathbf{y}_0)$ and $\tilde{\boldsymbol{\chi}}_0^j(\mathbf{y}_0)$ lie apart in the distorted state when $\mathbf{y}_0 \in \mathcal{S}_0^{ij}$. Due to these additional terms in the right hand side of the expression (47), this alternative doesn't yield the desired form of the equilibrium equations, i.e., $\mathbf{S}_0 \cdot \boldsymbol{\nabla}_0 \neq \mathbf{0}$. Furthermore, the Cauchy stress defined by the formula (46) is not necessarily symmetric in the most general case.

3.8 Balance Equation for the Energy at the Continuous Level

First, the divergence of the heat flux is given by

$$\mathbf{q}\cdot\boldsymbol{\nabla}(\mathbf{x}) = \sum_i \iiint_{\mathcal{V}^i} \tilde{\mathbf{q}}\cdot\tilde{\boldsymbol{\nabla}}(\mathbf{y})\, J(\mathbf{y}-\mathbf{x})\, dV_{\mathbf{y}} - \sum_i \iint_{\mathcal{S}^{ij}} [\![\tilde{\mathbf{q}}(\mathbf{y})]\!]^{i\to j}\cdot\mathbf{n}^{i\to j}\, J(\mathbf{y}-\mathbf{x})\, dS_{\mathbf{y}}. \tag{48}$$

We will need the auxiliary quantity $H(\mathbf{x})$ defined as

$$H(\mathbf{x}) := \iiint_{\mathcal{V}} \left\{\tilde{\mathbf{v}}(\mathbf{y}) - \left[\mathbf{v}\otimes\boldsymbol{\nabla}(\mathbf{x})\right]\cdot\mathbf{y}\right\}\cdot\left[\tilde{\boldsymbol{\sigma}}(\mathbf{y}) - \boldsymbol{\sigma}(\mathbf{x})\right]\cdot\frac{\partial J}{\partial \mathbf{y}}\, dV_{\mathbf{y}}\ . \tag{49}$$

By decomposing the volume integral (49), using the theorem of Gauss and the continuity of the stress vector we obtain the following alternative expression for $H(\mathbf{x})$

$$\begin{aligned} H(\mathbf{x}) = {} & \sum_i \iint_{\partial\mathcal{V}^i} \tilde{\mathbf{v}}(\mathbf{y})\cdot\tilde{\boldsymbol{\sigma}}(\mathbf{y})\cdot\mathbf{n}\, J(\mathbf{y}-\mathbf{x})\, dS_{\mathbf{y}} - \sum_i \iiint_{\mathcal{V}^i} \left[\tilde{\mathbf{v}}\otimes\tilde{\boldsymbol{\nabla}}(\mathbf{y})\right] : \tilde{\boldsymbol{\sigma}}(\mathbf{y})\, J(\mathbf{y}-\mathbf{x})\, dV_{\mathbf{y}} \\ & -\boldsymbol{\sigma}(\mathbf{x}) : \sum_i \iint_{\partial\mathcal{V}^i} \left[\tilde{\mathbf{v}}(\mathbf{y})\otimes\mathbf{n}\right] J(\mathbf{y}-\mathbf{x})\, dS_{\mathbf{y}} + \boldsymbol{\sigma}(\mathbf{x}) : \sum_i \iiint_{\mathcal{V}^i} \left[\tilde{\mathbf{v}}\otimes\tilde{\boldsymbol{\nabla}}(\mathbf{y})\right] J(\mathbf{y}-\mathbf{x})\, dV_{\mathbf{y}}. \end{aligned} \tag{50}$$

Following the same argumentation that permitted the derivation of the result (30), the surface integrals in (50) can be rearranged in surface integrals on the singular surfaces $\mathcal{S}^{ij}$. Invoking the form (42) of the velocity gradient, we obtain the following identity

$$\begin{aligned} H(\mathbf{x}) = {} & \sum_i \iint_{\mathcal{S}^{ij}} [\![\tilde{\mathbf{v}}(\mathbf{y})]\!]^{i\to j}\cdot\tilde{\boldsymbol{\sigma}}(\mathbf{y})\cdot\mathbf{n}^{i\to j}\, J(\mathbf{y}-\mathbf{x})\, dS_{\mathbf{y}} - \sum_i \iiint_{\mathcal{V}^i} \left[\tilde{\mathbf{v}}\otimes\tilde{\boldsymbol{\nabla}}(\mathbf{y})\right] : \tilde{\boldsymbol{\sigma}}(\mathbf{y})\, J(\mathbf{y}-\mathbf{x})\, dV_{\mathbf{y}} \\ & +\boldsymbol{\sigma}(\mathbf{x}) : \left[\mathbf{v}(\mathbf{x})\otimes\boldsymbol{\nabla}\right]. \end{aligned} \tag{51}$$

By averaging the energy balance equation $(23)_3$ we obtain with this last result

$$\rho_0\dot{e} = \boldsymbol{\sigma} : (\mathbf{v}\otimes\boldsymbol{\nabla}) + \sum_i \iint_{\mathcal{S}^{ij}} [\![\tilde{\mathbf{v}}]\!]^{i\to j}\cdot\tilde{\boldsymbol{\sigma}}\cdot\mathbf{n}^{i\to j}\, J\, dS_{\mathbf{y}} - \mathbf{q}\cdot\boldsymbol{\nabla} - \sum_i \iint_{\mathcal{S}^{ij}} [\![\tilde{\mathbf{q}}]\!]^{i\to j}\cdot\mathbf{n}^{i\to j}\, J\, dS_{\mathbf{y}} - H. \tag{52}$$

Eventually, taking into account the energy balance at a singular surface $(24)_2$ we get the local form of the balance energy at the continuous level

$$\rho_0\dot{e} = \boldsymbol{\sigma} : (\mathbf{v}\otimes\boldsymbol{\nabla}) - \mathbf{q}\cdot\boldsymbol{\nabla} - H\ . \tag{53}$$

With exception of the last term H, we have recovered the usual form for the balance energy. To better understand the meaning of the quantity H we again resort to the limiting case for J of the characteristic function J_c of the RVE. By performing the limiting procedure $J \to J_c$ in equation (49) we obtain a surface integral on the boundary of the RVE

$$H(\mathbf{x}) \to H_c(\mathbf{x}) = \frac{1}{V_0} \iint_{\partial RVE(\mathbf{x})} \left\{\tilde{\mathbf{v}}(\mathbf{y}) - \left[\mathbf{v}\otimes\boldsymbol{\nabla}(\mathbf{x})\right]\cdot\mathbf{y}\right\}\cdot\left[\tilde{\boldsymbol{\sigma}}(\mathbf{y}) - \boldsymbol{\sigma}(\mathbf{x})\right]\cdot\mathbf{n}\, dS_{\mathbf{y}}\ . \tag{54}$$

The surface integral $H_c(\mathbf{x})$ vanishes for homogeneous or periodic boundary conditions on $\partial RVE(\mathbf{x})$. As noted by Fedelich (2003a), such conditions are approximately satisfied if the scale of the macroscopic structure and the dislocation scale can be separated, as stated by the double requirement (40).

4 Multiplicative Decomposition of the Deformation Gradient at the Continuous Level

4.1 Formal Decomposition of F

We start by formally defining the two following tensor fields

$$\mathbf{E}(\mathbf{x}_0) := \sum_i \int_{\mathcal{V}_0^i} \tilde{\mathbf{F}}_0(\mathbf{y}_0)\, J_0(\mathbf{y}_0 - \mathbf{x}_0)\, dV_{\mathbf{y}_0} \tag{55}$$

and

$$\mathbf{P}(\mathbf{x}_0) := \mathbf{E}^{-1}(\mathbf{x}_0)\cdot\mathbf{F}(\mathbf{x}_0) = \mathbf{1} - \mathbf{E}^{-1}(\mathbf{x}_0)\cdot\left(\sum_i \iint_{\mathcal{S}_0^{ij}} [\![\tilde{\boldsymbol{\chi}}_0(\mathbf{y}_0)]\!]^{i\to j} \otimes \mathbf{n}_0^{i\to j}\, J_0(\mathbf{y}_0 - \mathbf{x}_0)\, dS_{\mathbf{y}_0}\right). \tag{56}$$

We also define the strain tensor associated to **E** by

$$\boldsymbol{\varepsilon} := \frac{1}{2}\left(\mathbf{E}^T \cdot \mathbf{E} - \mathbf{1}\right). \tag{57}$$

4.2 Interpretation of E

Invoking the hypothesis of slowly varying rotations (33) we can approximate the tensor **E** by

$$\mathbf{E}(\mathbf{x}_0) \simeq \tilde{\mathbf{R}}_0(\mathbf{x}_0)\cdot \sum_i \int_{\mathcal{V}_0^i} \tilde{\mathbf{W}}_0(\mathbf{y}_0)\, J_0(\mathbf{y}_0 - \mathbf{x}_0)\, dV_{\mathbf{y}_0}. \tag{58}$$

Under the assumption of small strains at the dislocation level $\|\tilde{\boldsymbol{\varepsilon}}\| \ll 1$ we have

$$\boldsymbol{\varepsilon}(\mathbf{x}_0) \simeq \sum_i \int_{\mathcal{V}_0^i} \left[\tilde{\mathbf{W}}_0(\mathbf{y}_0) - \mathbf{1}\right] J_0(\mathbf{y}_0 - \mathbf{x}_0)\, dV_{\mathbf{y}_0} = \sum_i \int_{\mathcal{V}_0^i} \tilde{\boldsymbol{\varepsilon}}_0(\mathbf{y}_0)\, J_0(\mathbf{y}_0 - \mathbf{x}_0)\, dV_{\mathbf{y}_0}. \tag{59}$$

Finally, taking into account the hypothesis (37), it follows from this last result for pure crystals

$$\boldsymbol{\varepsilon}(\mathbf{x}_0) = \boldsymbol{\varepsilon}(\mathbf{x}) = \sum_i \int_{\mathcal{V}^i} \tilde{\boldsymbol{\varepsilon}}(\mathbf{y})\, J(\mathbf{y} - \mathbf{x})\, dV_{\mathbf{y}} = \sum_i \int_{\mathcal{V}^i} \mathbf{S} : \tilde{\boldsymbol{\sigma}}(\mathbf{y})\, J(\mathbf{y} - \mathbf{x})\, dV_{\mathbf{y}} = \mathbf{S} : \boldsymbol{\sigma}(\mathbf{x}), \tag{60}$$

for $\mathbf{x} = \boldsymbol{\chi}(\mathbf{x}_0)$. Hence, the nature of the strains associated to **E** is purely elastic. These strains can be removed by macroscopically unloading the material element.

4.3 Interpretation of P

Again, by using the hypothesis of slowly varying rotations (33), the expression (20) of the deformation jump and the approximation $\tilde{\mathbf{W}}_0 \simeq \mathbf{1}$ we can derive a simplified expression for the tensor **P**. We have

$$\begin{aligned}\mathbf{P}(\mathbf{x}_0) &\simeq \mathbf{1} - \tilde{\mathbf{R}}_0(\mathbf{x}_0)^{-1}\cdot \sum_i \iint_{\mathcal{S}_0^{ij}} \varphi(r_0)\, \tilde{\mathbf{R}}_0(\mathbf{y}_0)^{-1}\cdot \mathbf{b}_0^{i\to j} \otimes \mathbf{n}_0^{i\to j}\, J_0(\mathbf{y}_0 - \mathbf{x}_0)\, dS_{\mathbf{y}_0} \\ &\simeq \mathbf{1} - \sum_i \iint_{\mathcal{S}_0^{ij}} \varphi(r_0)\, \mathbf{b}_0^{i\to j} \otimes \mathbf{n}_0^{i\to j}\, J_0(\mathbf{y}_0 - \mathbf{x}_0)\, dS_{\mathbf{y}_0}.\end{aligned} \tag{61}$$

According to this last expression, the tensor **P** only depends on the irreversible lattice rearrangements due to dislocation glide. It is independent of the elastic strains. The apparent simplicity of the last form in (61) is somewhat deceiving: The deformation jumps and the topology of the singular surfaces $\mathcal{S}_0^{ij}$ depend on the history of the glide process, as shown by Figure 7. When a dislocation crosses an already existing jump surface, the deformation jump across the former singular surface changes.

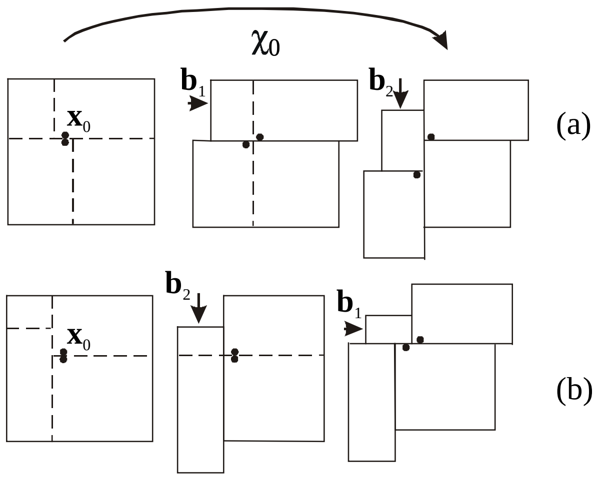

Figure 7. Illustration of the history dependence by a sequence of two shear processes on perpendicular planes. In case (a), the final value of the displacement jump of the point $\mathbf{x}_0$ is $[\![\mathbf{u}_0(\mathbf{x}_0)]\!] = \mathbf{b}_1 + \mathbf{b}_2$. In case (b) the displacement jump of the same point is $[\![\mathbf{u}_0(\mathbf{x}_0)]\!] = \mathbf{b}_1$.

5 Conclusions

Under the hypotheses of small (elastic) strains (i), small lattice curvature at the dislocation scale (ii) and of statistical homogeneity at the scale of the representative volume element (iii), we have constructed the continuum model for ductile crystals by suitably averaging the fields at the (discontinuous) dislocation level. Thereby we have retrieved the usual balance equations at the continuous level. We have also proposed a multiplicative decomposition of the continuous deformation gradient that is reminiscent of the usually postulated decomposition in an elastic and a plastic part. While the strains are small at the dislocation level, the strains resulting from plastic slip at the continuous level may be arbitrarily large.
Without being exhaustive, let us mention the following remaining open questions:

- Are all assumptions (i-iii) necessary to retrieve the classical balance equations and the multiplicative decomposition of **F**?
- What happens if the stress tensor at the continuous level is primary defined by averaging the nominal stress tensor instead of the Cauchy stress?
- To complete the identification of the present theory with the classical crystal plasticity theory, the time variation of the tensor **P** must be evaluated. This task is quite intricate because of the random character of the crossing events between moving dislocations and existing singular surfaces. This will be the object of a future work.
- The paper focuses on the field equations in the bulk of the material. There remains to derive the appropriate boundary conditions and the jump conditions at singular surfaces at the continuous level.

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