

# Continuum crystal plasticity theory

Samuel Forest

MINES ParisTech, PSL Research University, MAT - Centre des matériaux,  
CNRS UMR 7633, BP 87, 91003 Evry, France  
samuel.forest@ensmp.fr

## 1 Introduction

Continuum crystal plasticity is a special class of anisotropic elastoviscoplastic behaviour of materials. It relies on the precise knowledge of the kinematics of plastic slip according to crystallographic slip systems and of the driving force for activation of plastic slip, namely the corresponding resolved shear stress. When the number of dislocations inside the material volume element is high enough, a continuum description of plastic deformation and hardening can be formulated as settled in (Mandel, 1965; Mandel, 1971; Mandel, 1973) and (Teodosiu and Sidoroff, 1976).

The objective of this contribution is to establish the continuum mechanical framework for the formulation of constitutive equations for single crystals. The considered plastic deformation mechanism is crystallographic slip but the formulation can serve as a basis for extensions to climb or twinning since thermomechanical balances and most kinematic considerations are still valid.

There exists an extreme variety of possible constitutive equations for single crystals derived in the last 40 years but the thermomechanical foundation is unique and now clearly settled. We will consider the variety of constitutive laws by introducing generic internal variables without making specific choices. Only generic examples of evolution laws for such internal variables are provided and the reader is referred to (Fivel and Forest, 2004a), and references quoted therein, for a detailed discussion of best-suited constitutive laws for metal single crystals. Also the transition from single to polycrystal behaviour is not addressed here but rather in (Fivel and Forest, 2004b; Besson et al., 2009).

The most relevant internal variables for describing the work-hardening of single crystals are undoubtedly dislocation densities,  $\rho^s$ , defined as the total length of dislocations belonging to a slip system  $s$  divided by the volume of the material volume element. Evolution equations for dislocations densities can be found in (Fivel and Forest, 2004a). In the present contribution, we introduce general isotropic and kinematic hardening variables accounting for monotonic and cyclic responses of crystals. Dislocation densities are generally related to isotropic hardening through forest hardening but recent contributions also aim at establishing dislocation based kinematic hardening dislocation rules.

Another characterisation of the dislocation distribution is the dislocation density tensor introduced by (Nye, 1953). It is defined in section 3 and contributes to many size effects observed in crystalline solids: grain size or Hall-Petch effect, precipitate size effect, etc. The dislocation density tensor cannot be handled as a usual internal variable because it is related to the gradient of the plastic deformation field. As a result, higher order partial differential equations arise when hardening laws involve the dislocation density tensor. The development of constitutive models involving the dislocation density tensor is the realm of strain gradient plasticity. Such a strain gradient plasticity theory is proposed in section 4. Even for the probably too simple constitutive equations presented here, the model shows that the dislocation density tensor is responsible for a size-dependent kinematic hardening component in the material behaviour.

## 2 Thermomechanics of single crystal behaviour

### 2.1 Balance equations

Mechanical equilibrium can be expressed in the form of the principle of virtual power

$$-\int_{\mathcal{D}} \underline{\boldsymbol{\sigma}} : \underline{\mathcal{D}}^* dv + \int_{\mathcal{D}} \rho(\underline{\mathbf{f}} - \underline{\mathbf{a}}) \cdot \underline{\mathbf{v}}^* dv + \int_{\partial\mathcal{D}} \underline{\mathbf{t}} \cdot \underline{\mathbf{v}}^* ds = 0 \quad (1)$$

for all virtual velocity fields and all subdomains,  $\mathcal{D}$ , of the current configuration  $\Omega$  of the body. The Cauchy stress tensor is  $\underline{\boldsymbol{\sigma}}$  and  $\underline{\mathcal{D}}$  is the strain rate tensor. Volume and acceleration forces are denoted by  $\underline{\mathbf{f}}$  and  $\underline{\mathbf{a}}$ , respectively, whereas  $\underline{\mathbf{t}}$  is the traction vector. The principle of virtual power implies the following balance of momentum equation

$$\operatorname{div} \underline{\boldsymbol{\sigma}} + \rho \underline{\mathbf{f}} = \rho \underline{\mathbf{a}} \quad (2)$$

The energy balance is the purpose of the first principle of thermodynamics

$$\int_{\mathcal{D}} \rho \dot{e} dv - \int_{\mathcal{D}} \rho (\underline{\mathbf{a}} - \underline{\mathbf{f}}) \cdot \underline{\mathbf{v}} dv = \int_{\partial \mathcal{D}} \underline{\mathbf{t}} \cdot \underline{\mathbf{v}} ds + \mathcal{Q} \quad (3)$$

or equivalently, after implementing the balance of momentum principle,

$$\int_{\mathcal{D}} \rho \dot{e} dv = \int_{\mathcal{D}} \underline{\boldsymbol{\sigma}} : \underline{\mathcal{D}} dv + \mathcal{Q} \quad (4)$$

where  $\rho e$  is the volume density of internal energy. The heat production rate is assumed to take the form

$$\mathcal{Q} = - \int_{\partial \mathcal{D}} \underline{\mathbf{q}} \cdot \underline{\mathbf{n}} ds \quad (5)$$

The local form of the energy principle is then

$$\rho \dot{e} = \underline{\boldsymbol{\sigma}} : \underline{\mathcal{D}} - \text{div } \underline{\mathbf{q}} \quad (6)$$

The second principle of thermodynamics stipulates that

$$\int_{\mathcal{D}} \rho \dot{\eta} dv + \int_{\partial \mathcal{D}} \frac{\underline{\mathbf{q}}}{T} \cdot \underline{\mathbf{n}} ds \geq 0 \quad (7)$$

where  $\eta$  is the mass density of entropy and  $T$  the temperature field. The validity of this principle with respect to all subdomain  $\mathcal{D}$  leads to the local form of the entropy principle

$$\rho \dot{\eta} + \text{div } \frac{\underline{\mathbf{q}}}{T} \geq 0 \quad (8)$$

Introducing the free energy density  $\Psi := e - T\eta$  and taking the balance of energy into account, we are lead to the Clausius inequality

$$\underline{\boldsymbol{\sigma}} : \underline{\mathcal{D}} - \rho \dot{\Psi} - \rho \eta \dot{T} - \underline{\mathbf{q}} \cdot \frac{\nabla T}{T} \geq 0 \quad (9)$$

## 2.2 Kinematics of single crystals

It is based on the multiplicative decomposition of the deformation gradient,  $\underline{\mathbf{F}}$ , into an elastic part,  $\underline{\mathbf{E}}$ , and a plastic part,  $\underline{\mathbf{P}}$  :

$$\underline{\mathbf{F}}(\underline{\mathbf{X}}) = \underline{\mathbf{1}} + \frac{\partial \underline{\mathbf{u}}}{\partial \underline{\mathbf{X}}} = \underline{\mathbf{1}} + \nabla_{\underline{\mathbf{X}}} \underline{\mathbf{u}}, \quad \underline{\mathbf{F}}(\underline{\mathbf{X}}) = \underline{\mathbf{E}}(\underline{\mathbf{X}}) \cdot \underline{\mathbf{P}}(\underline{\mathbf{X}}) \quad (10)$$

The initial coordinates of the material point in the reference configuration are denoted by  $\underline{\mathbf{X}}$  and  $\nabla_{\underline{\mathbf{X}}}$  denotes the gradient operator with respect to initial coordinates. The current position of the material point in the current configuration is  $\underline{\mathbf{x}}$ . The displacement vector is  $\underline{\mathbf{u}} = \underline{\mathbf{x}} - \underline{\mathbf{X}}$ . The multiplicative decomposition (10) is associated with the definition of an intermediate configuration for which elastic strain is unloaded, see figure 1. The intermediate released configuration is uniquely determined up to a rigid body rotation which is chosen such that the lattice orientation in the intermediate configuration is the same as the initial one. Mandel called it the *isoclinic* intermediate configuration. As a result, lattice rotation and distortion during elastoplastic deformation are contained in the elastic deformation part  $\underline{\mathbf{E}}$ , as examined at the end of this section.

The multiplicative decomposition leads to the following partition of the velocity gradient

$$\nabla \underline{\mathbf{v}} = \dot{\underline{\mathbf{F}}} \cdot \underline{\mathbf{F}}^{-1} = \dot{\underline{\mathbf{E}}} \cdot \underline{\mathbf{E}}^{-1} + \underline{\mathbf{E}} \cdot \dot{\underline{\mathbf{P}}} \cdot \underline{\mathbf{P}}^{-1} \cdot \underline{\mathbf{E}}^{-1} \quad (11)$$

We introduce the Cauchy–Green and Green–Lagrange elastic strain measures

$$\underline{\mathcal{C}}^e := \underline{\mathbf{E}}^T \cdot \underline{\mathbf{E}}, \quad \underline{\mathbf{E}}^e = \frac{1}{2}(\underline{\mathcal{C}}^e - \underline{\mathbf{1}}) \quad (12)$$

and note that

$$\begin{aligned} \dot{\underline{\mathbf{E}}}^e &= \frac{1}{2}(\dot{\underline{\mathbf{E}}}^T \cdot \underline{\mathbf{E}} + \underline{\mathbf{E}}^T \cdot \dot{\underline{\mathbf{E}}}) = \frac{1}{2}\dot{\underline{\mathcal{C}}}^e \\ &= \frac{1}{2}\underline{\mathbf{E}}^T \cdot (\underline{\mathbf{E}}^{-T} \cdot \dot{\underline{\mathbf{E}}}^T + \dot{\underline{\mathbf{E}}} \cdot \underline{\mathbf{E}}^{-1}) \cdot \underline{\mathbf{E}} = \underline{\mathbf{E}}^T \cdot \left( \dot{\underline{\mathbf{E}}} \cdot \underline{\mathbf{E}}^{-1} \right)^{sym} \cdot \underline{\mathbf{E}} \end{aligned} \quad (13)$$

where *sym* operator takes the symmetric part of the quantity in brackets. The mass density of the material point with respect to the current (resp. intermediate) configuration is denoted by  $\rho$  (resp.  $\rho_e$ ). The volume density of internal forces with respect to the intermediate configuration is

$$\begin{aligned} J_e \underline{\underline{\sigma}} : \underline{\underline{D}} &= J_e \underline{\underline{\sigma}} : (\dot{\underline{\underline{F}}} \cdot \underline{\underline{F}}^{-1}) = J_e \underline{\underline{\sigma}} : (\dot{\underline{\underline{E}}} \cdot \underline{\underline{E}}^{-1}) + J_e \underline{\underline{\sigma}} : (\underline{\underline{E}} \cdot \dot{\underline{\underline{P}}} \cdot \underline{\underline{P}}^{-1} \cdot \underline{\underline{E}}^{-1}) \\ &= J_e \underline{\underline{\sigma}} : (\dot{\underline{\underline{E}}} \cdot \underline{\underline{E}}^{-1})^{sym} + J_e \underline{\underline{\sigma}} : (\underline{\underline{E}} \cdot \dot{\underline{\underline{P}}} \cdot \underline{\underline{P}}^{-1} \cdot \underline{\underline{E}}^{-1}) \\ &= \underline{\underline{\Pi}}^e : \dot{\underline{\underline{E}}}^e + \underline{\underline{M}} : \dot{\underline{\underline{P}}} \cdot \underline{\underline{P}}^{-1} \end{aligned} \quad (14)$$

where  $J_e = \det \underline{\underline{E}}$  is the volume change from the intermediate to the current configuration,  $\underline{\underline{\Pi}}^e$  is the second Piola–Kirchhoff stress tensor with respect to the isoclinic intermediate configuration, and  $\underline{\underline{M}}$  is the Mandel stress tensor defined as :

$$\underline{\underline{\Pi}}^e = J_e \underline{\underline{E}}^{-1} \cdot \underline{\underline{\sigma}} \cdot \underline{\underline{E}}^{-T}, \quad \underline{\underline{M}} = J_e \underline{\underline{E}}^T \cdot \underline{\underline{\sigma}} \cdot \underline{\underline{E}}^{-T} = \underline{\underline{C}}^e \cdot \underline{\underline{\Pi}}^e \quad (15)$$

Plastic deformation is the result of slip processes according to  $N$  slip systems characterised by the slip direction,  $\underline{\underline{m}}^s$ , and the normal to the slip plane,  $\underline{\underline{n}}^s$ , in the intermediate configuration :

$$\dot{\underline{\underline{P}}} \cdot \underline{\underline{P}}^{-1} = \sum_{s=1}^N \dot{\gamma}^s \underline{\underline{m}}^s \otimes \underline{\underline{n}}^s \quad (16)$$

Note that plastic deformation induced by dislocation glide is isochoric so that

$$J_p = \det \underline{\underline{P}} = 1, \quad J_e = J = \det \underline{\underline{F}} \quad (17)$$

### 2.3 Constitutive equations

Constitutive equations for elastoviscoplastic materials are based on the definition of two potential functions, namely the free energy density function and the dissipation potential. The specific energy density,  $\Psi(\underline{\underline{E}}^e, T, \alpha)$ , is a function of elastic strain, temperature and internal variables accounting for hardening properties. Writing the Clausius–Duhem inequality (9) with respect to the intermediate isoclinic configuration amounts to multiplying (9) by  $\rho_e/\rho = J_e$

$$J_e \underline{\underline{\sigma}} : \underline{\underline{D}} - \rho_e \dot{\Psi} - \rho_e \eta \dot{T} - \underline{\underline{Q}} \cdot \frac{\nabla_X T}{T} \geq 0 \quad (18)$$

where  $\underline{\underline{Q}} = J_e \underline{\underline{F}}^{-T} \cdot \underline{\underline{q}}$ . Expanding the time derivative of the free energy density, we obtain

$$\left( \underline{\underline{\Pi}}^e - \rho_e \frac{\partial \Psi}{\partial \underline{\underline{E}}^e} \right) : \dot{\underline{\underline{E}}}^e - \rho_e \left( \eta + \frac{\partial \Psi}{\partial T} \right) \dot{T} + \underline{\underline{M}} : \dot{\underline{\underline{P}}} \cdot \underline{\underline{P}}^{-1} - \rho_e \frac{\partial \Psi}{\partial \alpha} \dot{\alpha} - \underline{\underline{Q}} \cdot \frac{\nabla_X T}{T} \geq 0 \quad (19)$$

The following state laws provide the hyperelasticity relation and the entropy density :

$$\underline{\underline{\Pi}}^e = \rho_e \frac{\partial \Psi}{\partial \underline{\underline{E}}^e} = \underline{\underline{C}} : \underline{\underline{E}}^e, \quad \eta = -\frac{\partial \Psi}{\partial T}, \quad X = \rho_e \partial \Psi / \partial \alpha \quad (20)$$

where a quadratic potential for elasticity has been proposed, thus introducing the fourth rank tensor of elasticity moduli,  $\underline{\underline{C}}$ . Such an assumption is realistic for metals since elastic strain usually remains small, as discussed in the next subsection. The thermodynamic forces associated with the internal variables  $\alpha$  are called  $X$ . The residual dissipation rate is

$$\underline{\underline{M}} : \dot{\underline{\underline{P}}} \cdot \underline{\underline{P}}^{-1} - X \dot{\alpha} - \underline{\underline{Q}} \cdot \frac{\nabla_X T}{T} \geq 0 \quad (21)$$

The first term is the plastic power. Part of it is stored due to the second contribution whereas the third one denotes thermal dissipation.

At this stage, a dissipation potential  $\Omega(\underline{\underline{M}}, X)$  is introduced from which the flow rule and the evolution equation for internal variables are derived

$$\dot{\underline{\underline{P}}} \cdot \underline{\underline{P}}^{-1} = \frac{\partial \Omega}{\partial \underline{\underline{M}}}, \quad \dot{\alpha} = -\frac{\partial \Omega}{\partial X} \quad (22)$$

Positivity of dissipation rate is ensured if the dissipation potential  $\Omega(\underline{\mathbf{M}}, X)$  exhibits specific convexity properties with respect to its arguments (convex with respect to  $\underline{\mathbf{M}}$  and concave with respect to  $X$ ) and if a Fourier type of heat conduction is chosen

$$\underline{\mathbf{Q}} = -\underline{\mathbf{K}} \cdot \nabla_X (\log T) \quad (23)$$

The dissipation potential is assumed to depend on  $\underline{\mathbf{M}}$  and  $X$  via the Schmid yield function

$$f^s(\underline{\mathbf{M}}, X) = |\tau^s - x^s| - \tau_c^s, \quad \text{with} \quad \tau^s = \underline{\mathbf{M}} : \underline{\mathbf{m}}^s \otimes \underline{\mathbf{n}}^s \quad (24)$$

where  $\tau_c^s$  is the critical resolved shear stress for slip system  $s$ , which may evolve due to isotropic hardening. Kinematic hardening is accounted for by means of back-stress components  $x^s$  attached to each slip system. The resolved shear stress  $\tau^s = \underline{\mathbf{m}}^s \cdot \underline{\mathbf{M}} \cdot \underline{\mathbf{n}}^s$  on slip system  $s$  is the driving force for activation of slip. This corresponds to the specific choice of hardening variables:  $X = (\tau_c^s, x^s)$ . So we consider a function

$$\Omega(\underline{\mathbf{M}}, X) = \sum_{s=1}^N \Omega^s(f^s(\underline{\mathbf{M}}, X)) \quad (25)$$

It follows that

$$\dot{\underline{\mathbf{P}}} \cdot \underline{\mathbf{P}}^{-1} = \frac{\partial \Omega}{\partial \underline{\mathbf{M}}} = \sum_{s=1}^N \frac{\partial \Omega^s}{\partial f^s} \frac{\partial f^s}{\partial \underline{\mathbf{M}}} = \sum_{s=1}^N \dot{\gamma}^s \underline{\mathbf{m}}^s \otimes \underline{\mathbf{n}}^s \quad (26)$$

where the slip rate is computed as

$$\dot{\gamma}^s = \frac{\partial \Omega^s}{\partial f^s} \text{sign}(\tau^s - x^s) \quad (27)$$

Accordingly, the kinematics (16) is retrieved from the normality rule, showing that the crystal slip kinematics is associated with the Schmid law. Let us call  $(\rho^s, \alpha^s)$  internal variables associated with the isotropic and kinematic hardening variables  $(\tau_c^s, x^s)$ . The hardening rules in (22) become

$$\dot{\rho}^s = -\frac{\partial \Omega}{\partial \tau_c^s} = \frac{\partial \Omega^s}{\partial f^s} = |\dot{\gamma}^s|, \quad \dot{\alpha}^s = -\frac{\partial \Omega}{\partial x^s} = \frac{\partial \Omega^s}{\partial f^s} \text{sign}(\tau^s - x^s) = \dot{\gamma}^s \quad (28)$$

It is worth computing the plastic power after taking the previous relations into account

$$\underline{\mathbf{M}} : \dot{\underline{\mathbf{P}}} \cdot \underline{\mathbf{P}}^{-1} = \sum_{s=1}^N \tau^s \dot{\gamma}^s \quad (29)$$

Specific hardening laws including evolution equations for dislocation densities can be found for example in (Fivel and Forest, 2004a). As an example, we consider here a power law potential

$$\dot{\gamma}^s = \frac{\partial \Omega}{\partial \tau^s} = \left\langle \frac{|\tau^s - x^s| - \tau_c^s}{K} \right\rangle^n \text{sign}(\tau^s), \quad (30)$$

$$\Omega(\tau^s) = \sum_{s=1}^N \frac{K}{n+1} \left\langle \frac{|\tau^s - x^s| - \tau_c^s}{K} \right\rangle^{n+1} \quad (31)$$

The brackets  $\langle x \rangle$  denote the positive part of  $x$ . Viscosity parameters are  $K$  and  $n$  in (30). They can be chosen such that plastic processes are almost rate-independent in a given range of applied strain rates. As an example, we give here simple nonlinear evolution rules for the isotropic and kinematic variables that are used for practical computations

$$\tau_c^s = \tau_c + q \sum_{r=1}^N h^{sr} (1 - \exp(-bv^r)), \quad \dot{\alpha}^s = \dot{\gamma}^s - d\dot{v}^s \alpha^s \quad (32)$$

where  $q, b, d$  are material parameters. An interaction matrix  $h^{rs}$  is necessary to account for interaction between dislocations and is responsible for latent hardening (Fivel and Forest, 2004a).

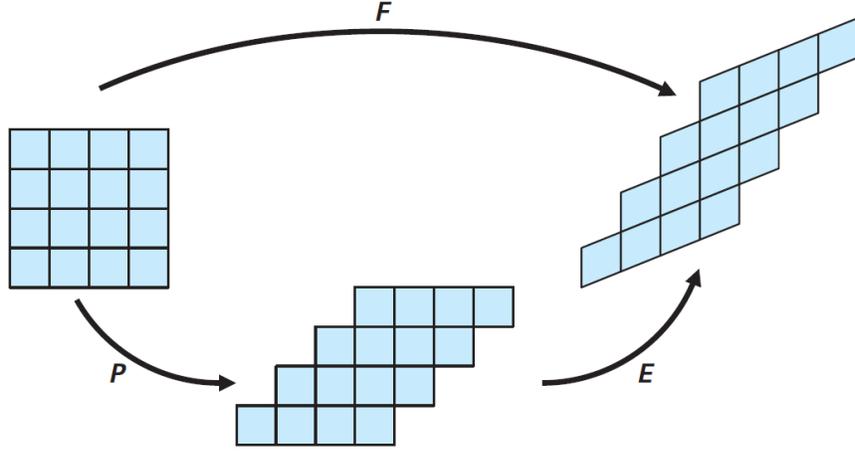


Figure 1: Multiplicative decomposition of the deformation gradient into elastic and plastic parts.

## 2.4 Lattice rotation

The previous continuum mechanical approach makes it possible to distinguish between the transformation of material and lattice directions. Material lines are made of material points that are subjected to the motion  $\underline{u}(\underline{X})$ . The tangent to a material line at  $\underline{X}$  is a material direction  $\underline{d}$  in the reference configuration that transforms into the material direction  $\underline{d}'$  in the current configuration by means of the deformation gradient:

$$\underline{d}'(\underline{X}) = \underline{F}(\underline{X}) \cdot \underline{d}(\underline{X}) \quad (33)$$

In contrast, lattice directions are not material insofar as they are not necessarily made of the same material points (atoms) in the initial and current configurations due to the passing of dislocations, but keep the same crystallographic meaning. According to the concept of isoclinic configuration, lattice directions are unchanged from the initial to the intermediate configuration of figure 1. Glide of dislocations through, and thus leaving, the material volume element do not distort nor rotate the lattice, although material lines are sheared. According to the continuum theory of dislocations, statistically stored dislocations accumulating in the material volume element affect material hardening but do not change the element shape. Accordingly, an initial lattice direction  $\underline{d}^\sharp$  is transformed into  $\underline{d}^{\sharp'}$  by means of the elastic deformation:

$$\underline{d}^{\sharp'}(\underline{X}) = \underline{E}(\underline{X}) \cdot \underline{d}^\sharp(\underline{X}) \quad (34)$$

The kinematics of elastoplastic deformation recalled in section 2.2 can be expanded in the case of small strains and small rotations, based on the polar decompositions of total, elastic and plastic deformations:

$$\underline{E} = \underline{R}^e \cdot \underline{U}^e \simeq (\underline{1} + \underline{\omega}^e) \cdot (\underline{1} + \underline{\varepsilon}^e) \simeq \underline{1} + \underline{\varepsilon}^e + \underline{\omega}^e \quad (35)$$

$$\underline{P} = \underline{R}^p \cdot \underline{U}^p \simeq (\underline{1} + \underline{\omega}^p) \cdot (\underline{1} + \underline{\varepsilon}^p) \simeq \underline{1} + \underline{\varepsilon}^p + \underline{\omega}^p \quad (36)$$

where  $\underline{R}^e, \underline{R}^p$  and  $\underline{U}^e, \underline{U}^p$  are rotations and symmetric stretch tensors, respectively. Accordingly,  $\underline{\varepsilon}^e, \underline{\omega}^e$  (resp.  $\underline{\varepsilon}^p, \underline{\omega}^p$ ) represent small elastic (resp. plastic) strain and rotation. The elastic rotation accounts for lattice rotation, as follows from the proposed kinematics of plastic slip. Similarly, the following holds for the total deformation:

$$\underline{F} = \underline{R} \cdot \underline{U} = (\underline{1} + \underline{\omega}) \cdot (\underline{1} + \underline{\varepsilon}) \simeq \underline{1} + \underline{\varepsilon} + \underline{\omega} \quad (37)$$

so that

$$\underline{\varepsilon} = \underline{\varepsilon}^e + \underline{\varepsilon}^p, \quad \underline{\omega} = \underline{\omega}^e + \underline{\omega}^p \quad (38)$$

where all strain tensors are symmetric whereas all  $\omega$  tensors are skew-symmetric.

In metals, elastic strain remains small whereas lattice rotations can become very large. That is why the kinematics of crystallographic slip is very often approximated as

$$\underline{F} \simeq \underline{R}^e \cdot \underline{P} \quad (39)$$

especially for the simulation of metal forming processes. Lattice rotation is then directly given by  $\underline{\mathbf{R}}^e$ .

Let us consider also rotation rates by introducing the material spin tensor  $\underline{\mathbf{W}}$  which is the skew-symmetric part of the velocity gradient

$$\dot{\underline{\mathbf{F}}} \cdot \underline{\mathbf{F}}^{-1} = \underline{\mathbf{D}} + \underline{\mathbf{W}} = \dot{\underline{\mathbf{E}}} \cdot \underline{\mathbf{E}}^{-1} + \underline{\mathbf{E}} \cdot \dot{\underline{\mathbf{P}}} \cdot \underline{\mathbf{P}}^{-1} \cdot \underline{\mathbf{E}}^{-1} = \underline{\mathbf{D}}^e + \underline{\mathbf{W}}^e + \underline{\mathbf{D}}^p + \underline{\mathbf{W}}^p \quad (40)$$

where the elastic and plastic contributions have been split into their symmetric and skew-symmetric parts. The elastic spin tensor is therefore defined as

$$\underline{\mathbf{W}}^e = \left( \dot{\underline{\mathbf{E}}} \cdot \underline{\mathbf{E}}^{-1} \right)^{skew} = \left( \dot{\underline{\mathbf{R}}}^e \cdot \underline{\mathbf{R}}^{e-1} + \underline{\mathbf{R}}^e \cdot \dot{\underline{\mathbf{U}}}^e \cdot \underline{\mathbf{U}}^e \cdot \underline{\mathbf{R}}^{e-1} \right)^{skew} \quad (41)$$

$$\simeq \dot{\underline{\mathbf{R}}}^e \cdot \underline{\mathbf{R}}^{e-1} = \dot{\underline{\mathbf{R}}}^e \cdot \underline{\mathbf{R}}^{eT} \quad (42)$$

where the exponent *skew* denotes the skew-symmetric part of the tensor in brackets. The latter approximation is valid when elastic strain rates can be neglected compared to rotation rates, which is generally the case for metals at sufficiently high total strains. Note that for any rotation  $\underline{\mathbf{Q}}$ , the rotation rate  $\dot{\underline{\mathbf{Q}}} \cdot \underline{\mathbf{Q}}^{-1} = \dot{\underline{\mathbf{Q}}} \cdot \underline{\mathbf{Q}}^T$  is a skew-symmetric tensor due to the fact that a rotation is an orthogonal tensor<sup>1</sup>. The plastic spin rate is

$$\underline{\mathbf{W}}^p = \left( \underline{\mathbf{E}} \cdot \left( \sum_{s=1}^N \dot{\gamma}^s \underline{\mathbf{m}}^s \otimes \underline{\mathbf{n}}^s \right) \cdot \underline{\mathbf{E}}^{-1} \right)^{skew} \quad (43)$$

$$\simeq \left( \underline{\mathbf{R}}^e \cdot \left( \sum_{s=1}^N \dot{\gamma}^s \underline{\mathbf{m}}^s \otimes \underline{\mathbf{n}}^s \right) \cdot \underline{\mathbf{R}}^{eT} \right)^{skew}$$

$$\simeq \underline{\mathbf{R}}^e \cdot \left( \sum_{s=1}^N \dot{\gamma}^s (\underline{\mathbf{m}}^s \otimes \underline{\mathbf{n}}^s)^{skew} \right) \cdot \underline{\mathbf{R}}^{eT} \quad (44)$$

In the case of small elastic strain and rotations, the expressions simplify and we obtain

$$\underline{\mathbf{D}}^p \simeq \dot{\underline{\boldsymbol{\varepsilon}}}^p = \sum_{s=1}^N \dot{\gamma}^s (\underline{\mathbf{m}}^s \otimes \underline{\mathbf{n}}^s)^{sym} \quad (45)$$

$$\underline{\mathbf{W}}^p \simeq \dot{\underline{\boldsymbol{\omega}}}^p = \sum_{s=1}^N \dot{\gamma}^s (\underline{\mathbf{m}}^s \otimes \underline{\mathbf{n}}^s)^{skew} \quad (46)$$

$$\underline{\mathbf{D}}^e \simeq \dot{\underline{\boldsymbol{\varepsilon}}}^e = \dot{\underline{\boldsymbol{\varepsilon}}} - \dot{\underline{\boldsymbol{\varepsilon}}}^p, \quad \underline{\mathbf{W}}^e \simeq \dot{\underline{\boldsymbol{\omega}}}^e = \dot{\underline{\boldsymbol{\omega}}} - \dot{\underline{\boldsymbol{\omega}}}^p \quad (47)$$

### 3 The dislocation density tensor

#### 3.1 Elements of tensor analysis

The Euclidean space is endowed with an arbitrary coordinate system characterizing the points  $M(q^i)$ . The basis vectors are defined as

$$\underline{\mathbf{e}}_i = \frac{\partial M}{\partial q^i} \quad (48)$$

The reciprocal basis  $(\underline{\mathbf{e}}^i)_{i=1,3}$  of  $(\underline{\mathbf{e}}_i)_{i=1,3}$  is the unique triad of vectors such that

$$\underline{\mathbf{e}}^i \cdot \underline{\mathbf{e}}_j = \delta_j^i \quad (49)$$

If a Cartesian orthonormal coordinate system is chosen, then both bases coincide.

The gradient operator for a tensor field  $T(\underline{\mathbf{X}})$  of arbitrary rank is then defined as

$$\text{grad } T = T \otimes \nabla := \frac{\partial T}{\partial q^i} \otimes \underline{\mathbf{e}}^i \quad (50)$$

The gradient operation therefore increases the tensor rank by one.

<sup>1</sup>meaning that  $\underline{\mathbf{Q}} \cdot \underline{\mathbf{Q}}^T = \underline{\mathbf{Q}}^T \cdot \underline{\mathbf{Q}} = \underline{\mathbf{1}}$

The divergence operator for a tensor field  $T(\underline{\mathbf{X}})$  of arbitrary rank is then defined as

$$\operatorname{div} T = T \cdot \nabla := \frac{\partial T}{\partial q^i} \cdot \underline{\mathbf{e}}^i \quad (51)$$

The divergence operation therefore decreases the tensor rank by one.

The curl operator<sup>2</sup> for a tensor field  $T(\underline{\mathbf{X}})$  of arbitrary rank is then defined as

$$\operatorname{curl} T = T \wedge \nabla := \frac{\partial T}{\partial q^i} \wedge \underline{\mathbf{e}}^i \quad (52)$$

where the vector product is  $\wedge$ . The curl operation therefore leaves the tensor rank unchanged. The vector product on an oriented Euclidean space is

$$\underline{\mathbf{a}} \wedge \underline{\mathbf{b}} = \epsilon_{ijk} a_j b_k \underline{\mathbf{e}}_i = \underline{\boldsymbol{\epsilon}} : (\underline{\mathbf{a}} \otimes \underline{\mathbf{b}}) \quad (53)$$

The component  $\epsilon_{ijk}$  of the third rank permutation tensor is the signature of the permutation of (1, 2, 3).

With respect to a Cartesian orthonormal basis, the previous formula simplify. We give the expressions for a second rank tensor  $\underline{\mathbf{T}}$

$$\operatorname{grad} \underline{\mathbf{T}} = T_{ij,k} \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \otimes \underline{\mathbf{e}}_k \quad (54)$$

$$\operatorname{div} \underline{\mathbf{T}} = T_{ij,j} \underline{\mathbf{e}}_i \quad (55)$$

We consider then successively the curl of a vector field and of a second rank vector field, in a Cartesian orthonormal coordinate frame

$$\operatorname{curl} \underline{\mathbf{u}} = \frac{\partial \underline{\mathbf{u}}}{\partial X_j} \wedge \underline{\mathbf{e}}_j = u_{i,j} \underline{\mathbf{e}}_i \wedge \underline{\mathbf{e}}_j = \epsilon_{kij} u_{i,j} \underline{\mathbf{e}}_k \quad (56)$$

$$\operatorname{curl} \underline{\mathbf{A}} = \frac{\partial \underline{\mathbf{A}}}{\partial x_k} \wedge \underline{\mathbf{e}}_k = A_{ij,k} \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \wedge \underline{\mathbf{e}}_k = \epsilon_{mjk} A_{ij,k} \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_m \quad (57)$$

These definitions are the same as in (Teodosiu, 1982). Other conventions are used in the literature involving transpose and opposites of the considered tensors.

We also recall the Stokes formula for a vector field for a surface  $\mathcal{S}$  with unit normal vector  $\underline{\mathbf{n}}$  and oriented closed border line  $\mathcal{L}$ :

$$\oint_{\mathcal{L}} \underline{\mathbf{u}} \cdot \underline{\mathbf{dl}} = - \int_{\mathcal{S}} (\operatorname{curl} \underline{\mathbf{u}}) \cdot \underline{\mathbf{n}} \, ds, \quad \oint_{\mathcal{L}} u_i \, dl_i = - \epsilon_{mij} \int_{\mathcal{S}} u_{i,j} n_m \, ds \quad (58)$$

Applying the previous formula to  $u_i = A_{ki}$  at fixed  $k$  leads to the Stokes formula for a tensor field of rank 2:

$$\oint_{\mathcal{L}} \underline{\mathbf{T}} \cdot \underline{\mathbf{dl}} = - \int_{\mathcal{S}} (\operatorname{curl} \underline{\mathbf{T}}) \cdot \underline{\mathbf{n}} \, ds, \quad \oint_{\mathcal{L}} A_{ki} \, dl_i = - \epsilon_{mij} \int_{\mathcal{S}} A_{ki,j} n_m \, ds \quad (59)$$

### 3.2 Dislocation density tensor

In continuum mechanics, the previous differential operators are used with respect to the initial coordinates  $\underline{\mathbf{X}}$  or with respect to the current coordinates  $\underline{\mathbf{x}}$  of the material points. In the latter case, the notation  $\nabla$ , grad, div and curl are used but in the former case we adopt  $\nabla_X$ , Grad, Div and Curl. For instance,

$$\underline{\mathbf{F}} = \underline{\mathbf{1}} + \operatorname{Grad} \underline{\mathbf{u}} \implies \operatorname{Curl} \underline{\mathbf{F}} = 0 \quad (60)$$

This result expresses the fact that the deformation gradient is a compatible field which derives from the displacement vector field. This is generally not the case for elastic and plastic deformation:

$$\operatorname{Curl} \underline{\mathbf{E}} \neq 0, \quad \operatorname{Curl} \underline{\mathbf{P}} \neq 0 \quad (61)$$

Elastic and plastic deformations are generally incompatible tensor fields, even though the product  $\underline{\mathbf{F}} = \underline{\mathbf{E}} \cdot \underline{\mathbf{P}}$  is compatible. It may happen incidentally that elastic deformation be compatible for instance when plastic or elastic deformation is homogeneous.

---

<sup>2</sup>or rotational operator.

A consequence of the incompatibility of the elastic deformation is that, for an oriented surface  $\mathcal{S} \subset \Omega$  of the body, with border  $\mathcal{L}$ , the vector  $\underline{\mathbf{B}}$  belonging to the intermediate isoclinic configuration

$$\underline{\mathbf{B}} = \oint_{\mathcal{L}} \underline{\tilde{\mathbf{E}}}^{-1} \cdot d\underline{\mathbf{l}} = - \int_{\mathcal{S}} (\text{curl } \underline{\tilde{\mathbf{E}}}^{-1}) \cdot \underline{\mathbf{n}} ds \quad (62)$$

does not vanish in general. It can be interpreted as the continuum Burgers vector for the circuit  $\mathcal{L}$ . It represents a generalization of the concept of Burgers vector for dislocations. This geometric definition was introduced by (Bilby et al., 1957; Teodosiu, 1970; Kröner and Teodosiu, 1972) within the context of the continuum theory of dislocations. The previous calculation leads to the definition of the dislocation density tensor

$$\underline{\boldsymbol{\alpha}} := -\text{curl } \underline{\tilde{\mathbf{E}}}^{-1} = -\epsilon_{jkl} E_{ik,l}^{-1} \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \quad (63)$$

which is used to compute the resulting Burgers vector for dislocations crossing the surface  $\mathcal{S}$ :

$$\underline{\mathbf{B}} = \int_{\mathcal{S}} \underline{\boldsymbol{\alpha}} \cdot \underline{\mathbf{n}} ds \quad (64)$$

The Burgers vector can also be computed by means of a closed circuit  $\mathcal{L}_0 \subset \Omega_0$  connected from  $\mathcal{L} \subset \Omega$ :

$$\underline{\mathbf{B}} = \oint_{\mathcal{L}} \underline{\tilde{\mathbf{E}}}^{-1} \cdot d\underline{\mathbf{x}} = \oint_{\mathcal{L}_0} \underline{\tilde{\mathbf{E}}}^{-1} \cdot \underline{\tilde{\mathbf{F}}} \cdot d\underline{\mathbf{X}} = \oint_{\mathcal{L}_0} \underline{\tilde{\mathbf{P}}} \cdot d\underline{\mathbf{X}} \quad (65)$$

$$= \int_{\mathcal{S}_0} (\text{Curl } \underline{\tilde{\mathbf{P}}}) \cdot d\underline{\mathbf{S}} = - \int_{\mathcal{S}} (\text{Curl } \underline{\tilde{\mathbf{P}}}) \cdot \underline{\tilde{\mathbf{F}}}^T \cdot \frac{d\underline{\mathbf{s}}}{J} \quad (66)$$

Nanson's formula<sup>3</sup> has been used. We obtain the alternative definition of the dislocation density tensor

$$\underline{\boldsymbol{\alpha}} = -\text{curl } \underline{\tilde{\mathbf{E}}}^{-1} = -\frac{1}{J} (\text{Curl } \underline{\tilde{\mathbf{P}}}) \cdot \underline{\tilde{\mathbf{F}}}^T \quad (67)$$

The present modern treatment of the dislocation density tensor was settled by (Cermelli and Gurtin, 2001; Svendsen, 2002). A statistical mechanics perspective of the dislocation density tensor can be found in (Kröner, 1969).

It can be noticed that the relation (67) implies

$$J(\text{curl } \underline{\tilde{\mathbf{E}}}^{-1}) \cdot \underline{\tilde{\mathbf{E}}}^{-T} = (\text{Curl } \underline{\tilde{\mathbf{P}}}) \cdot \underline{\tilde{\mathbf{P}}}^T \quad (68)$$

which is a consequence of (60),  $\text{curl } \underline{\tilde{\mathbf{F}}} = \text{curl } (\underline{\tilde{\mathbf{E}}} \cdot \underline{\tilde{\mathbf{P}}}) = 0$ .

Within the small perturbation framework, we introduce the notations

$$\underline{\mathbf{H}} = \text{Grad } \underline{\mathbf{u}} = \underline{\mathbf{H}}^e + \underline{\mathbf{H}}^p, \quad \text{with } \underline{\mathbf{H}}^e = \underline{\boldsymbol{\xi}}^e + \underline{\boldsymbol{\omega}}^e, \quad \underline{\mathbf{H}}^p = \underline{\boldsymbol{\xi}}^p + \underline{\boldsymbol{\omega}}^p \quad (69)$$

We have

$$\underline{\tilde{\mathbf{E}}}^{-1} \simeq \underline{\mathbf{1}} - \underline{\mathbf{H}}^e \quad (70)$$

so that the dislocation density tensor can be computed as

$$\underline{\boldsymbol{\alpha}} \simeq \text{Curl } \underline{\mathbf{H}}^e = -\text{Curl } \underline{\mathbf{H}}^p \quad (71)$$

since  $\text{Curl } \underline{\mathbf{H}} = 0$  due to the compatibility of the deformation gradient.

### 3.3 Lattice curvature

Experimental techniques like EBSD provide the field of lattice orientation and, consequently, of lattice rotation  $\underline{\mathbf{R}}^e$  during deformation. Since

$$\underline{\boldsymbol{\alpha}} = -\text{curl } \underline{\tilde{\mathbf{E}}}^{-1} = -\text{curl } (\underline{\mathbf{U}}^{e-1} \cdot \underline{\mathbf{R}}^{eT}) \quad (72)$$

the hypothesis of small elastic strain implies

$$\underline{\boldsymbol{\alpha}} \simeq -\text{curl } \underline{\mathbf{R}}^{eT} \quad (73)$$

---

<sup>3</sup> $d\underline{\mathbf{s}} = J\underline{\tilde{\mathbf{F}}}^{-T} \cdot d\underline{\mathbf{S}}$

If, in addition, elastic rotations are small, we have

$$\underline{\alpha} \simeq -\text{curl}(\underline{\mathbf{1}} - \underline{\omega}^e) = \text{curl} \underline{\omega}^e \quad (74)$$

The small rotation axial vector is defined as

$$\underline{\omega}^e = -\frac{1}{2}\underline{\epsilon} : \underline{\omega}^e, \quad \underline{\omega}^e = -\underline{\epsilon} \cdot \underline{\omega}^e \quad (75)$$

or, in matrix notations,

$$[\underline{\omega}^e] = \begin{bmatrix} 0 & \omega_{12}^e & -\omega_{31}^e \\ -\omega_{12}^e & 0 & \omega_{23}^e \\ \omega_{31}^e & -\omega_{23}^e & 0 \end{bmatrix} = \begin{bmatrix} 0 & -\dot{\omega}_3^e & \dot{\omega}_2^e \\ \dot{\omega}_3^e & 0 & -\dot{\omega}_1^e \\ -\dot{\omega}_2^e & \dot{\omega}_1^e & 0 \end{bmatrix} \quad (76)$$

The gradient of the lattice rotation field delivers the lattice curvature tensor. In the small deformation context, the gradient of the rotation tensor is represented by the gradient of the axial vector:

$$\underline{\kappa} := \text{grad} \underline{\omega}^e \quad (77)$$

One can establish a direct link between  $\text{curl} \underline{\omega}^e$  and the gradient of the axial vector associated with  $\underline{\omega}$ . For that purpose, the matrix form of  $\text{curl} \underline{\omega}^e$  is derived according to (57):

$$[\text{curl} \underline{\omega}^e] = \begin{bmatrix} \omega_{12,3}^e + \omega_{31,2}^e & -\omega_{31,1}^e & -\omega_{12,1}^e \\ -\omega_{23,2}^e & \omega_{12,3}^e + \omega_{23,1}^e & -\omega_{12,2}^e \\ -\omega_{23,3}^e & -\omega_{31,3}^e & \omega_{23,1}^e + \omega_{31,2}^e \end{bmatrix} \quad (78)$$

or equivalently

$$[\text{curl} \underline{\omega}^e] = \begin{bmatrix} -\dot{\omega}_{3,3}^e - \dot{\omega}_{2,2}^e & \dot{\omega}_{2,1}^e & \dot{\omega}_{3,1}^e \\ \dot{\omega}_{1,2}^e & -\dot{\omega}_{3,3}^e - \dot{\omega}_{1,1}^e & \dot{\omega}_{3,2}^e \\ \dot{\omega}_{1,3}^e & \dot{\omega}_{2,3}^e & -\dot{\omega}_{1,1}^e - \dot{\omega}_{2,2}^e \end{bmatrix} \quad (79)$$

from which it becomes apparent that

$$\underline{\alpha} = \underline{\kappa}^T - (\text{trace} \underline{\kappa})\underline{\mathbf{1}}, \quad \underline{\kappa} = \underline{\alpha}^T - \frac{1}{2}(\text{trace} \underline{\alpha})\underline{\mathbf{1}} \quad (80)$$

This is a remarkable relation linking, with the context of small elastic strains<sup>4</sup> and rotations, the dislocation density tensor to lattice curvature. It is known as Nye's formula (Nye, 1953).

Exact relations follow from the previous derivations and involve the curl of elastic strain tensor:

$$\underline{\alpha} = \text{curl} \underline{\epsilon}^e + \underline{\kappa}^T - (\text{trace} \underline{\kappa})\underline{\mathbf{1}}, \quad \underline{\kappa} = \underline{\alpha}^T - \frac{1}{2}(\text{trace} \underline{\alpha})\underline{\mathbf{1}} - (\text{curl} \underline{\omega}^e)^T + \frac{1}{2}(\text{trace} \text{curl} \underline{\omega}^e)\underline{\mathbf{1}} \quad (81)$$

as discussed in (Arsenlis and Parks, 1999).

## 4 Strain gradient plasticity: The “*curlH<sup>p</sup>*” model

We consider now a strain gradient plasticity theory which includes the full curl of the plastic deformation tensor,  $\underline{H}^p$ , into constitutive modelling. This approach, therefrom to be referred to as the “*curlH<sup>p</sup>*” model, was proposed by (Gurtin, 2002) and applied to a constrained layer and a composite problem in (Bittencourt et al., 2003; Cordero et al., 2010). The balance and constitutive equations are introduced in the context of small perturbations. Then the model is applied to a crystal undergoing single slip. It will be shown that a specific form of the back stress arises from this application.

<sup>4</sup> and in fact of small gradient of elastic strain.

## 4.1 Balance equations

Following (Gurtin, 2002), we consider a continuum whose power density of internal forces takes the form:

$$p^{(i)} = \underline{\boldsymbol{\sigma}} : \underline{\dot{\mathbf{H}}} + \underline{\boldsymbol{s}} : \underline{\dot{\mathbf{H}}}^p + \underline{\boldsymbol{M}} : \text{curl } \underline{\dot{\mathbf{H}}}^p. \quad (82)$$

For objectivity reasons, the stress tensor  $\underline{\boldsymbol{\sigma}}$  is symmetric whereas the micro-stress tensor  $\underline{\boldsymbol{s}}$  and the double-stress tensor  $\underline{\boldsymbol{M}}$  are generally asymmetric. The total power of internal forces in a domain  $V$ , with boundary  $\partial V$ , is

$$\begin{aligned} \mathcal{P}^{(i)} &= \int_V \left( \underline{\boldsymbol{\sigma}} : \underline{\dot{\mathbf{H}}} + \underline{\boldsymbol{s}} : \underline{\dot{\mathbf{H}}}^p + \underline{\boldsymbol{M}} : \text{curl } \underline{\dot{\mathbf{H}}}^p \right) dV, \\ &= \int_V \left( (\sigma_{ij} \dot{u}_i)_{,j} + (M_{ij} \epsilon_{jkl} \dot{H}_{ik}^p)_{,l} \right) dV \\ &+ \int_V \left( -\sigma_{ij,j} \dot{u}_i + s_{ij} \dot{H}_{ij}^p - \epsilon_{jkl} M_{ij,l} \dot{H}_{ik}^p \right) dV, \\ &= - \int_V \left( \sigma_{ij,j} \dot{u}_i - (\epsilon_{kjl} M_{ik,l} + s_{ij}) \dot{H}_{ij}^p \right) dV \\ &+ \int_{\partial V} \left( \sigma_{ij} n_j \dot{u}_i + \epsilon_{jkl} M_{ij} n_l \dot{H}_{ik}^p \right) dS. \end{aligned}$$

The power density of contact forces is taken as

$$p^{(c)} = \underline{\boldsymbol{t}} \cdot \underline{\dot{\mathbf{u}}} + \underline{\boldsymbol{m}} : \underline{\dot{\mathbf{H}}}^p, \quad (83)$$

where  $\underline{\boldsymbol{t}}$ ,  $\underline{\boldsymbol{m}}$  are, respectively, the surface simple and double tractions. Volume forces are not written for simplicity. The method of virtual power can be used to derive the field equations governing the continuum, based on the virtual motions  $\underline{\dot{\mathbf{u}}}$  and  $\underline{\dot{\mathbf{H}}}^p$ :

$$\text{div } \underline{\boldsymbol{\sigma}} = 0, \quad \sigma_{ij,j} = 0, \quad (84)$$

$$\text{curl } \underline{\boldsymbol{M}} + \underline{\boldsymbol{s}} = 0, \quad \epsilon_{jkl} M_{ik,l} + s_{ij} = 0, \quad (85)$$

for all regular points of the domain  $V$ . Furthermore, the following boundary conditions on  $\partial V$  can be derived:

$$\underline{\boldsymbol{t}} = \underline{\boldsymbol{\sigma}} \cdot \underline{\boldsymbol{n}}, \quad t_i = \sigma_{ij} n_j, \quad (86)$$

$$\underline{\boldsymbol{m}} = \underline{\boldsymbol{M}} \cdot \underline{\boldsymbol{\epsilon}} \cdot \underline{\boldsymbol{n}}, \quad m_{ij} = M_{ik} \epsilon_{kjl} n_l. \quad (87)$$

## 4.2 Energy and entropy principles, constitutive equations

Under isothermal conditions, the energy balance in its local form states that:

$$\rho \dot{e} = p^{(i)}, \quad (88)$$

where  $e$  is the internal energy density function and,  $\rho$ , the mass density. The entropy principle is formulated as

$$\rho(\dot{e} - \dot{\psi}) \geq 0 \quad (89)$$

where  $\psi$  is the Helmholtz free energy function. The free energy is taken as a function of the elastic strain,  $\underline{\boldsymbol{\xi}}^e$ , the dislocation density tensor, or  $\text{curl } \underline{\boldsymbol{H}}^p$ , and a generic internal hardening variable,  $q$ , viz.  $\psi(\underline{\boldsymbol{\xi}}^e, \text{curl } \underline{\boldsymbol{H}}^p, q)$ . As a result, the Clausius–Duhem inequality becomes

$$\left( \underline{\boldsymbol{\sigma}} - \rho \frac{\partial \psi}{\partial \underline{\boldsymbol{\xi}}^e} \right) : \dot{\underline{\boldsymbol{\xi}}^e} + \left( \underline{\boldsymbol{M}} - \rho \frac{\partial \psi}{\partial \text{curl } \underline{\boldsymbol{H}}^p} \right) : \text{curl } \underline{\dot{\mathbf{H}}}^p + (\underline{\boldsymbol{\sigma}} + \underline{\boldsymbol{s}}) : \underline{\dot{\mathbf{H}}}^p - \rho \frac{\partial \psi}{\partial q} \dot{q} \geq 0. \quad (90)$$

Here, the constitutive assumption is made that the two first terms in the previous inequality are non dissipative and therefore should vanish. Then,

$$\underline{\boldsymbol{\sigma}} = \rho \frac{\partial \psi}{\partial \underline{\boldsymbol{\xi}}^e}, \quad \underline{\boldsymbol{M}} = \rho \frac{\partial \psi}{\partial \text{curl } \underline{\boldsymbol{H}}^p}. \quad (91)$$

It follows that the residual dissipation rate is

$$D = (\underline{\boldsymbol{\sigma}} + \underline{\boldsymbol{s}}) : \underline{\dot{\mathbf{H}}}^p - R\dot{q} \geq 0, \quad (92)$$

where  $R = \rho\partial\psi/\partial q$  is the thermodynamic force associated with the internal variable,  $q$ . The existence of a dissipation potential, namely  $\Omega(\underline{\boldsymbol{\sigma}} + \underline{\boldsymbol{s}}, R)$ , is postulated so that

$$\underline{\dot{\mathbf{H}}}^p = \frac{\partial\Omega}{\partial(\underline{\boldsymbol{\sigma}} + \underline{\boldsymbol{s}})}, \quad \dot{q} = -\frac{\partial\Omega}{\partial R}. \quad (93)$$

### 4.3 Application of the “*curlH<sup>p</sup>*” model to a single slip problem

For a crystal deforming under single slip conditions, the plastic deformation rate is given by:

$$\underline{\dot{\mathbf{H}}}^p = \dot{\gamma}\underline{\mathbf{P}} = \dot{\gamma}\underline{\mathbf{l}} \otimes \underline{\mathbf{n}}, \quad (94)$$

where  $\underline{\mathbf{P}} = \underline{\mathbf{l}} \otimes \underline{\mathbf{n}}$  is the orientation tensor,  $\underline{\mathbf{l}}$  is the slip direction and  $\underline{\mathbf{n}}$  the normal to the slip plane. The dissipation rate can then be expressed as,

$$(\tau + \underline{\mathbf{l}} \cdot \underline{\boldsymbol{s}} \cdot \underline{\mathbf{n}})\dot{\gamma} - R\dot{q} \geq 0, \quad (95)$$

where  $\tau = \underline{\mathbf{l}} \cdot \underline{\boldsymbol{\sigma}} \cdot \underline{\mathbf{n}}$  is the resolved shear stress. In the absence of a hardening variable,  $q$ , for simplicity, the following generalised Schmid law can be defined (for positive  $\dot{\gamma}$ ):

$$|\tau - x| = \tau_c, \quad \text{with} \quad x = -\underline{\mathbf{l}} \cdot \underline{\boldsymbol{s}} \cdot \underline{\mathbf{n}}, \quad (96)$$

meaning that plastic flow occurs when the effective resolved shear stress  $|\tau - x|$  reaches the critical resolved shear stress  $\tau_c$ . A kinematic hardening component,  $x$ , naturally arises in the formulation for which a more specific form is given next. The curl of the plastic deformation is then given by

$$\text{curl } \underline{\mathbf{H}}^p = \underline{\mathbf{l}} \otimes (\underline{\mathbf{n}} \times \nabla\gamma). \quad (97)$$

For a two-dimensional case, one finds

$$[\text{curl } \underline{\mathbf{H}}^p] = \begin{bmatrix} 0 & 0 & \gamma_{,2}n_1n_2 - \gamma_{,1}n_2^2 \\ 0 & 0 & -\gamma_{,2}n_1^2 + \gamma_{,1}n_1n_2 \\ 0 & 0 & 0 \end{bmatrix}. \quad (98)$$

In the particular case when  $\underline{\mathbf{l}} = \underline{\mathbf{e}}_1$ ,  $\underline{\mathbf{n}} = \underline{\mathbf{e}}_2$ , the only non-vanishing component of the dislocation density tensor is

$$(\text{curl } \underline{\mathbf{H}}^p)_{13} = -\gamma_{,1}. \quad (99)$$

Let us consider at this stage the simple quadratic potential:

$$\rho\psi(\underline{\boldsymbol{\varepsilon}}^e, \text{curl } \underline{\mathbf{H}}^p) = \frac{1}{2}\underline{\boldsymbol{\varepsilon}}^e : \underline{\mathbf{C}} : \underline{\boldsymbol{\varepsilon}}^e + \frac{1}{2}A(\text{curl } \underline{\mathbf{H}}^p) : (\text{curl } \underline{\mathbf{H}}^p), \quad (100)$$

so that

$$\underline{\boldsymbol{\sigma}} = \underline{\mathbf{C}} : \underline{\boldsymbol{\varepsilon}}^e, \quad \underline{\mathbf{M}} = A \text{curl } \underline{\mathbf{H}}^p, \quad (101)$$

where  $\underline{\mathbf{C}}$  is the four-rank tensor of the elastic moduli, assumed isotropic hereafter, and  $A$  is a higher order modulus. According to the balance equation (85), it follows that

$$\underline{\boldsymbol{s}} = -\text{curl } \underline{\mathbf{M}} = -\text{curl } \text{curl } \underline{\mathbf{H}}^p. \quad (102)$$

For single slip, the double curl of plastic deformation is defined as

$$\text{curl } \text{curl } \underline{\mathbf{H}}^p = \underline{\mathbf{l}} \otimes ((\underline{\mathbf{n}} \times \gamma_{,ij}\underline{\mathbf{e}}_i) \times \underline{\mathbf{e}}_j). \quad (103)$$

In the particular case of  $\underline{\mathbf{l}} = \underline{\mathbf{e}}_1$ ,  $\underline{\mathbf{n}} = \underline{\mathbf{e}}_2$ , we obtain

$$\text{curl } \text{curl } \underline{\mathbf{H}}^p = \gamma_{,12}\underline{\mathbf{e}}_1 \otimes \underline{\mathbf{e}}_1 - \gamma_{,11}\underline{\mathbf{e}}_1 \otimes \underline{\mathbf{e}}_2, \quad (104)$$

so that the back-stress takes the form

$$x = A(\text{curl } \text{curl } \underline{\mathbf{H}}^p) : (\underline{\mathbf{l}} \otimes \underline{\mathbf{n}}) = -\gamma_{,11}. \quad (105)$$

## 5 Conclusions

The elastoviscoplasticity theory of single crystals is the single well-established anisotropic nonlinear mechanical theory. Indeed, the multiplicative decomposition of the deformation gradient into elastic and plastic parts is only possible when a triad of directors can be unambiguously defined for the considered materials. Mandel showed that lattice directions in a single crystal determine privileged directors for the material. Such directors are more difficult to define for a composite material or for a polycrystal (Mandel, 1982). The benefit is that the kinematic aspects of plastic deformation in single crystals is well-accepted today and that research can be focused on the development of relevant evolution equations for the internal variables like dislocation densities.

Discrete dislocation dynamics simulations are currently used as guidelines to develop advanced constitutive equations, as explained in the chapter by B. Devincre in part I. The transition from the single crystal to polycrystalline material volume elements can be done by means of analytical and computational homogenization methods, like simulations of the response of polycrystalline aggregates, see chapter by H. Proudhon in part III.

2D and 3D field measurement techniques have been used to validate the plasticity theory. For large metallic grains, the theory is essentially validated by the early contribution (Teodosiu et al., 1993) and subsequent comparisons between lattice rotation and total strain field measurements by means of EBSD and grids. More recent techniques give access to 3D data (Proudhon et al., 2010; Vaxelaire et al., 2010; Ludwig et al., 2009).

Difficulties arise when tackling size effect problems in crystal plasticity. The introduction of the dislocation density tensor in modern crystal plasticity theory gives rise to the prediction of size effects that are in qualitative agreement with many experimental results. However, quantitative agreement is not met yet. The determination of scaling laws, like the Hall-Petch scaling  $1/\sqrt{d}$  (with  $d$ , the grain size) or Orowan's scaling  $1/d$  for distances  $d$  between precipitates, are still not correctly retrieved by most strain gradient plasticity models because of the expensive nonlinear 3D computations required or because of the inadequate enhanced constitutive equations. These research issues are discussed in the contribution (Cordero et al., 2010) and in the references quoted therein.

## References

### References

- Arsenlis A. and Parks D. M. (1999). *Crystallographic aspects of geometrically-necessary and statistically stored dislocation density*. Acta Materialia, vol. 47, pp 1597–1611.
- Besson J., Cailletaud G., Chaboche J.-L., Forest S., and Blétry M. (2009). *Non-Linear Mechanics of Materials*. Series: Solid Mechanics and Its Applications, Vol. 167, Springer, ISBN: 978-90-481-3355-0, 433 p.
- Bilby B.A., Bullough R., Gardner L.R.T., and Smith E. (1957). *Continuous distributions of dislocations IV: Single glide and plane strain*. Proc. Roy. Soc. London, vol. A236, pp 538–557.
- Bittencourt E., Needleman A., M.E. Gurtin, and Van der Giessen E. (2003). *A comparison of nonlocal continuum and discrete dislocation plasticity predictions*. Journal of the Mechanics and Physics of Solids, vol. 51, pp 281–310.
- Cermelli P. and Gurtin M.E. (2001). *On the characterization of geometrically necessary dislocations in finite plasticity*. Journal of the Mechanics and Physics of Solids, vol. 49, pp 1539–1568.
- Cordero N.M., Gaubert A., Forest S., Busso E., Gallerneau F., and Kruch S. (2010). *Size effects in generalised continuum crystal plasticity for two-phase laminates*. Journal of the Mechanics and Physics of Solids, vol. 58, pp 1963–1994.
- Fivel M. and Forest S. (2004a). *Plasticité cristalline et transition d'échelle : cas du monocristal*. Techniques de l'Ingénieur, M4016, 23 pages.
- Fivel M. and Forest S. (2004b). *Plasticité cristalline et transition d'échelle : cas du polycristal*. Techniques de l'Ingénieur, M4017, 11 pages.

- Gurtin M.E. (2002). *A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations*. Journal of the Mechanics and Physics of Solids, vol. 50, pp 5–32.
- Kröner E. (1969). *Initial studies of a plasticity theory based upon statistical mechanics*. In : Inelastic Behaviour of Solids, eds. Kanninen M.F., Adler W.F., Rosenfield A.R., and Jaffee R.I., pp 137–147. McGraw-Hill.
- Kröner E. and Teodosiu C. (1972). *Lattice defect approach to plasticity and viscoplasticity*. In : Problems of Plasticity, International Symposium on Foundations of Plasticity, Warsaw, ed. Sawczuk A. Noordhoff International Publishing Leyden.
- Ludwig W., King A., Reischig P., Herbig M., Lauridsen E.M., Schmidt S., Proudhon H., Forest S., Cloetens P., Rolland du Roscoat S., Buffière J.Y., Marrow T.J., and Poulsen H.F. (2009). *New opportunities for 3D materials science of polycrystalline materials at the micrometre lengthscale by combined use of X-ray diffraction and X-ray imaging*. Materials Science and Engineering A, vol. 524, pp 69–76.
- Mandel J. (1965). *Une généralisation de la théorie de la plasticité de W.T. Koiter*. Int. J. Solids Structures, vol. 1, pp 273–295.
- Mandel J. (1971). *Plasticité classique et viscoplasticité*. CISM Courses and Lectures No. 97, Udine, Springer Verlag, Berlin.
- Mandel J. (1973). *Equations constitutives et directeurs dans les milieux plastiques et viscoplastiques*. Int. J. Solids Structures, vol. 9, pp 725–740.
- Mandel J. (1982). *Définition d'un repère privilégié pour l'étude des transformations anélastiques du polycristal*. J. de Mécanique théorique et appliquée, vol. 1, pp 7–23.
- Nye J.F. (1953). *Some geometrical relations in dislocated crystals*. Acta Metall., vol. 1, pp 153–162.
- Proudhon H., Vaxelaire V., Labat S., Forest S., and Thomas O. (2010). *Finite element simulations of coherent diffraction in elastoplastic polycrystalline aggregates*. Comptes Rendus Physique, vol. 11, pp 293–303.
- Svendsen B. (2002). *Continuum thermodynamic models for crystal plasticity including the effects of geometrically-necessary dislocations*. J. Mech. Phys. Solids, vol. 50, pp 1297–1329.
- Teodosiu C. (1970). *A dynamic theory of dislocations and its applications to the theory of the elastic-plastic continuum*. In : Fundamental Aspects of Dislocation Theory, eds. Simmons J.A., de Wit R., and Bullough R., pp 837–876. Nat. Bur. Stand. (US) Spec. Publ. 317, II.
- Teodosiu C. (1982). *Elastic models of crystal defects*. Springer Verlag, Berlin.
- Teodosiu C., Raphanel J., and Tabourot L. (1993). *Finite element simulation of the large elastoplastic deformation of multi-crystals*. In : Large Plastic Deformations MECAMAT'91, eds. Teodosiu C. and Sidoroff F., pp 153–158. Balkema, Rotterdam.
- Teodosiu C. and Sidoroff F. (1976). *A theory of finite elastoviscoplasticity of single crystals*. Int. J. of Engng Science, vol. 14, pp 165–176.
- Vaxelaire V., Proudhon H., Labat S., Kirchlechner C., Keckes J., Jacques V., Ravy S., Forest S., and Thomas O. (2010). *Methodology for studying strain inhomogeneities in polycrystalline thin films during in situ thermal loading using coherent X-ray diffraction*. New Journal of Physics, vol. 12, pp 035018.