Discrete dislocation and nonlocal crystal plasticity modelling

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Chapter 2

Nonlocal crystal plasticity formulations versus classical single crystal plasticity

Abstract

The aim of this chapter is to illustrate the variety of attempts to generalize classical (local) single-crystal plasticity by nonlocal terms to incorporate the size dependence of material response. To make a clear transition from the local crystal plasticity to non-local formulations, a summary of the local framework will be given first. Afterwards, an overview of the recently developed nonlocal continuum crystal plasticity theories of Shu and Fleck (1999), Gurtin (2002), Acharya and Bassani (2000) will be presented.

2.1 Classical single-crystal plasticity: Summary

The classical crystal plasticity framework was established by the early 1970s (see e.g. Rice, 1971; Hill and Rice, 1972; Mandel, 1973) and further elaborated for numerical applications by Asaro (1983) and by Cuitiño and Ortiz (1992). In this study, the interest will be confined to small displacement gradients, and Cartesian tensor notation is used throughout.

The total strain rate $\dot{\boldsymbol{\varepsilon}}$ in such a constitutive model is decomposed into the elastic strain rate $\dot{\boldsymbol{\varepsilon}}^{\mathrm{e}}$ and the plastic strain rate $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^{\mathrm{e}} + \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}. \tag{2.1}$$

The plastic strain rate, $\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}$, is taken to be composed of the contributions of the active individual slip systems. A slip system α ($\alpha = 1, \ldots, N$) is defined by a pair of unit vectors $(\boldsymbol{s}^{(\alpha)}, \boldsymbol{m}^{(\alpha)})$ in the direction of slip and the slip plane normal, respectively. Hence,

$$\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \sum_{\alpha} \boldsymbol{P}^{(\alpha)} \dot{\gamma}^{(\alpha)}, \tag{2.2}$$

where $\dot{\gamma}^{(\alpha)}$ is the shear rate on the slip system α and $\boldsymbol{P}^{(\alpha)}$ is a symmetric second-rank crystallographic tensor,

$$\boldsymbol{P}^{(\alpha)} = \frac{1}{2}(\boldsymbol{s}^{(\alpha)} \otimes \boldsymbol{m}^{(\alpha)} + \boldsymbol{m}^{(\alpha)} \otimes \boldsymbol{s}^{(\alpha)}). \tag{2.3}$$

The elastic properties of the material are assumed to be unaffected by plastic slip and, therefore, the elastic constitutive relation can be specified by the rate form of Hooke's law

$$\dot{\boldsymbol{\sigma}} = \boldsymbol{\mathcal{L}} : \dot{\boldsymbol{\varepsilon}}^{\mathrm{e}}, \tag{2.4}$$

with $\dot{\boldsymbol{\sigma}}$ the standard stress rate and $\boldsymbol{\mathcal{L}}$ the elastic modulus tensor. Thus, combining (2.1)–(2.4) one gets

$$\dot{\boldsymbol{\sigma}} = \boldsymbol{\mathcal{L}} : \left[\dot{\boldsymbol{\varepsilon}} - \sum_{\alpha} \boldsymbol{P}^{(\alpha)} \dot{\gamma}^{(\alpha)}\right]. \tag{2.5}$$

To complete the constitutive law (2.5) one needs to specify the shear rate $\dot{\gamma}^{(\alpha)}$. Before doing so, we define the Schmid resolved shear stress on slip system α by

$$\tau^{(\alpha)} = \boldsymbol{P}^{(\alpha)} : \boldsymbol{\sigma}. \tag{2.6}$$

For a viscoplastic material (i.e. rate-dependent plasticity) $\dot{\gamma}^{(\alpha)}$ is taken to depend upon the resolved shear stress according to the power law relation

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \left[\frac{\tau^{(\alpha)}}{g^{(\alpha)}}\right] \left|\frac{\tau^{(\alpha)}}{g^{(\alpha)}}\right|^{1/m-1}. \tag{2.7}$$

Here, $\dot{\gamma}_0$ is a reference shear rate, m is the rate sensitivity parameter, and $g^{(\alpha)}$ is the slip system hardness. Since usually $m << 1$, slip on a system α is possible if the actual resolved shear stress $|\tau^{(\alpha)}|$ is close to $g^{(\alpha)}$. The slip system hardness $\dot{g}^{(\alpha)}$ evolves with the slip on all glide systems. Its rate of change is expressed by (Hill, 1966)

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta}\dot{\gamma}^{(\beta)}, \tag{2.8}$$

in terms of the matrix of hardening moduli $h_{\alpha\beta}$ that generally depend upon the history of slip. The diagonal elements $h_{\alpha\alpha}$ of the hardening moduli matrix reflect the self-hardening, while the off-diagonal elements govern the latent hardening effects. Even though there are several general considerations about these moduli, the hardening matrix is the most elusive parameter of the constitutive model to define. As a consequence, there is a variety of hardening models that propose different forms of the $h_{\alpha\beta}$, from very simple (e.g. Koiter, 1953; Hutchinson, 1970) to quite sophisticated ones (e.g. Peirce *et al.*, 1982; Cuitiño and Ortiz, 1992).

2.2 Nonlocal continuum crystal plasticity formulations

The formulation above does not contain a length scale, and therefore is not able to pick up size-dependent behaviour. This motivates the development of more sophisticated (nonlocal) models that incorporate such a length scale and, therefore, should be able to capture size effects. There is no unified concept yet about the structure of such nonlocal theories. This fact triggers a variety of ways of developing a nonlocal theory and how to introduce the nonlocality into the theory. Therefore, there are a number of nonlocal (or strain-gradient) crystal plasticity theories available in the literature now. In this section a summary of three nonlocal theories is presented, highlighting some features of the chosen approaches.

2.2.1 Shu-Fleck theory

The formulation of the nonlocal theory by Shu and Fleck (1999) involves higher-order stresses that are work conjugate to the strain gradients. To incorporate these higher-order stresses into the theory the classical equilibrium condition is extended to the form

$$\int_V [\sigma_{ij}\delta\varepsilon_{ij} + \tau_{ijk}\delta\eta_{ijk}]\, dV = \int_S [T_i\delta u_i + r_i\delta u_{i,n}]\, dS\,, \tag{2.9}$$

where $u_{i,n}$ is the normal derivative of the displacement u_i at the surface S, r_i is the higher order traction vector, τ_{ijk} is the so-called double stress (to be defined later) and the strain gradient

$$\eta_{ijk} = \varepsilon_{ij,k}. \tag{2.10}$$

The strain ε_{ij} is the sum of the elastic and plastic strains as previously defined in (2.1) in the local plasticity formulation. The definition of the plastic strain rate adopted in the theory is also the same as in (2.2) of the local formulation. In the same spirit, the rate of the plastic part of the strain gradient (2.10) is defined by

$$\dot{\eta}^{\mathrm{p}}_{ijk} = \sum_{\alpha}[\dot{\gamma}_S^{(\alpha)}\Psi_{Sij}^{(\alpha)} + \dot{\gamma}_M^{(\alpha)}\Psi_{Mij}^{(\alpha)}], \tag{2.11}$$

where

$$\Psi^{(\alpha)}_{Sijk} \equiv P^{(\alpha)}_{ij} s^{(\alpha)}_k, \quad \Psi^{(\alpha)}_{Mijk} \equiv P^{(\alpha)}_{ij} m^{(\alpha)}_k \tag{2.12}$$

are third-order orientation tensors. $\dot{\gamma}^{(\alpha)}_S$ and $\dot{\gamma}^{(\alpha)}_M$ are called 'microslip rate gradients' along the slip direction $s^{(\alpha)}_i$ and the slip normal $m^{(\alpha)}_i$, respectively.

For the yield condition, a new quantity —the overall effective stress $s^{(\alpha)}$ depending on the higher order stresses— is introduced. It is defined by

$$(s^{(\alpha)})^2 = (\tau^{(\alpha)})^2 + (Q^{(\alpha)}_S/\ell_S)^2 + (Q^{(\alpha)}_M/\ell_M)^2, \tag{2.13}$$

where the resolved shear stress $\tau^{(\alpha)}$ is defined in Eq. (2.6), $Q^{(\alpha)}_S = \tau_{ijk}\Psi^{(\alpha)}_{Sijk}$ and $Q^{(\alpha)}_M = \tau_{ijk}\Psi^{(\alpha)}_{Mijk}$ are resolved double stresses, with ℓ_S and ℓ_M being internal material length scales of the constitutive description. Yield occurs when the effective stress $s^{(\alpha)}$ attains a yield strength $s^{(\alpha)}_y$.

The slip rate $\dot{\gamma}^{(\alpha)}$ and microslip rate gradients $\dot{\gamma}^{(\alpha)}_S$ and $\dot{\gamma}^{(\alpha)}_M$ are defined in accordance with normality as

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}^{(\alpha)}_e \frac{\tau^{(\alpha)}}{s^{(\alpha)}}, \quad \dot{\gamma}^{(\alpha)}_S = \ell_S^{-2}\dot{\gamma}^{(\alpha)}_e \frac{Q^{(\alpha)}_S}{s^{(\alpha)}}, \quad \dot{\gamma}^{(\alpha)}_M = \ell_M^{-2}\dot{\gamma}^{(\alpha)}_e \frac{Q^{(\alpha)}_M}{s^{(\alpha)}}, \tag{2.14}$$

where $\dot{\gamma}^{(\alpha)}_e$ is the effective strain rate. The evolution of the yield strength is related to the effective strain history through

$$\dot{\gamma}^{(\alpha)}_e = \left[(\dot{\gamma}^{(\alpha)})^2 + \ell_S^2(\dot{\gamma}^{(\alpha)}_S)^2 + \ell_M^2(\dot{\gamma}^{(\alpha)}_M)^2\right]^{1/2}, \tag{2.15}$$

via the hardening relation

$$\dot{s}^{(\alpha)}_y = h_c(s^{(\alpha)}_y)\dot{\gamma}^{(\alpha)}_e \tag{2.16}$$

in terms of the slip system hardening modulus h_c.

To complete the theory, it is supplemented with the classical elastic stress rate-strain rate relation, Eq. (2.4) or

$$\dot{\sigma}_{ij} = \mathcal{L}_{ijkl}\dot{\varepsilon}^{\mathrm{e}}_{kl} \tag{2.17}$$

and, similar in spirit, an elastic relation between higher-order stresses and strains

$$\dot{\tau}_{ijm} = \ell_e^2\mathcal{L}_{ijkl}\dot{\eta}^{\mathrm{e}}_{klm}, \tag{2.18}$$

where ℓ_e is the elastic characteristic length.

In addition to the usual macroscopic boundary conditions that are expressed either in prescribing the displacements or tractions at the material surface, any nonlocal theory requires higher order boundary conditions. Which higher-order boundary condition is appropriate is usually a matter of choice, rather than an unambiguous mathematical relation that directly emerges from the physical behaviour at the boundaries. As seen in Eq. (2.9) for this particular nonlocal theory, either the normal component of the displacement gradient, $u_{i,n}$, or the higher-order traction r_i needs to be prescribed as the higher-order boundary conditions.

In order to apply the theory for a particular boundary value problem, a number of material parameters entering the theory, like the internal length scales (ℓ_e, ℓ_S, ℓ_M), slip system dependent yield strength $s_y^{(\alpha)}$ and hardening modulus $h_c^{(\alpha)}$, have to be fitted either to experimental observations or lower scale simulations — for instance, discrete dislocation plasticity simulations, see e.g. Shu *et al.* (2001).

2.2.2 Gurtin theory

The idea to develop a nonlocal theory of the type proposed by Gurtin (2000, 2002) is the fact that plastic deformation in crystalline solids originates from the collective motion of dislocations. It has been known for a long time that there is a natural material length scale related to the presence of so-called geometrically necessary dislocations (GNDs). As a measure of the GNDs the tensorial quantity α_{ij}, introduced by Nye (1953), is adopted:

$$\alpha_{ij} = e_{jkl} \sum_{\beta} \gamma_{,k}^{(\beta)} s_i^{(\beta)} m_l^{(\beta)}. \tag{2.19}$$

(e_{jkl} is the alternating tensor). This dislocation tensor can be viewed as a measure of lattice incompatibility due to the presence of dislocations.

Gurtin's theory is based on the assumption that the presence of the GNDs in a material leads to an increase of the free energy of the system. This argument is expressed by an additional quadratic term to the classical elastic free energy, which is dependent upon the GND density tensor as

$$\Psi = \frac{1}{2}\varepsilon_{ij}^{\mathrm{e}} \mathcal{L}_{ijlk} \varepsilon_{kl}^{\mathrm{e}} + \frac{1}{2}\ell^2 \pi_0 \alpha_{ij}\alpha_{ij}, \tag{2.20}$$

where ℓ is a material length parameter and π_0 is a material strength parameter. The assumption (2.20) also emphasizes that the elastic properties are not affected by the density of the GNDs.

The derivation of the balance laws is based on a principle of virtual work in which slips and slip gradients are introduced as independent fields:

$$\int_V \left[\sigma_{ij}\delta u_{ij}^{\mathrm{e}} + \sum_{\beta} \pi^{(\beta)} \delta\gamma^{(\beta)} + \sum_{\beta} \xi_i^{(\beta)} \delta\gamma_{,i}^{(\beta)}\right] dV = \int_S \sum_{\beta} q^{(\beta)} \delta\gamma^{(\beta)} dS + \int_S t_i \delta u_i dS \tag{2.21}$$

and where $\pi^{(\beta)}$ and $\xi_i^{(\beta)}$ are their respective work-conjugates. Independent variation of δu and $\delta\gamma^{(\beta)}$ yields the classical balance $\sigma_{ij,j} = 0$, a so-called microforce balance

$$\pi^{(\beta)} - \tau^{(\beta)} - \xi_{i,i}^{(\beta)} = 0, \tag{2.22}$$

with $\tau^{(\beta)}$ the resolved shear stress of (2.6), and two sets of boundary conditions. The first type of boundary conditions comprises the classical macroscopic ones for the displacements or tractions. The second set, implying that

$$q^{(\beta)} = \xi_i^{(\beta)} n_i \quad \text{or} \quad \gamma^{(\beta)} \tag{2.23}$$

be prescribed, represents additional (microscopic) boundary conditions for this theory. The constitutive equations for "internal forces" $\pi^{(\beta)}$ and the "microstress" $\xi_i^{(\beta)}$ are based on the free energy inequality

$$\dot{\psi} - \sigma_{ij}\dot{\varepsilon}^{e}_{ij} - \sum_{\beta}\left(\xi_i^{(\beta)}\dot{\gamma}^{(\beta)}_{,i} + \pi^{(\beta)}\dot{\gamma}_i^{(\beta)}\right) \leq 0, \tag{2.24}$$

which is derived from the second law of thermodynamics (for details see Cermelli and Gurtin, 2002; Gurtin, 2002). For the microstress, which serves as the backstress, one gets

$$\xi_i^{(\beta)} = e_{ipq} m_p^{(\beta)} T_{qr} s_r^{(\beta)} \tag{2.25}$$

with

$$T_{ji} = \frac{\partial \Psi}{\partial \alpha_{ij}} = \ell^2 \pi_0 \alpha_{ij} \tag{2.26}$$

being a defect stress tensor. Hence, by substituting (2.26) into (2.25) one can rewrite the definition of the microstress in the following form

$$\xi_i^{(\beta)} = \ell^2 \pi_0 e_{ipq} m_p^{(\beta)} \alpha_{rq} s_r^{(\beta)}. \tag{2.27}$$

By substituting $\pi^{(\beta)}$, governed by the equation

$$\pi^{(\beta)} = \varphi^{(\beta)} \mathrm{sgn}\dot{\gamma}^{(\beta)}, \tag{2.28}$$

into the microforce balance (2.22) and taking into account (2.27), one obtains the nonlocal yield condition

$$\tau^{(\beta)} = \varphi^{(\beta)} \mathrm{sgn}\dot{\gamma}^{(\beta)} + \ell^2 \pi_0 \sum_{\kappa} e_{ipq} e_{qkl} S^{(\beta\kappa)} \gamma^{(\kappa)}_{,ki} \tag{2.29}$$

involving second spatial derivatives of slip. Here, $\varphi^{(\beta)}$ is the slip resistance, and $\varphi^{(\beta)} > 0$; $S^{(\beta\kappa)} = s_j^{(\beta)} s_j^{(\kappa)}$ are the slip interaction coefficients. The first term in the yield condition (2.29) can be interpreted as a source of the dissipative hardening due to slip, while the second one represents so-called energetic hardening due to energy stored by the GNDs. The dissipative hardening is generally assumed to be local, but can be taken to be nonlocal as well. The nonlocal effect in the theory arises primarily from a free energy dependence on the GND density which, in turn, gives an energetic contribution to the nonlocal yield condition (2.29).

2.2.3 Acharya and Bassani theory

The nonlocal continuum plasticity formulation of Acharya and Bassani (2000) is the simplest one compared to the already discussed formulations of Shu-Fleck and Gurtin. Acharya and

Bassani have proposed a theory based on the notion of lattice incompatibility, as measured by Nye's (1953) dislocation density tensor α_{ij} defined in (2.19). The hypothesis is that this incompatibility enters the constitutive relation only as an additional contribution to the hardening of a slip system. Therefore, the hardening matrix in Eq. (2.8) is taken to depend both on slips $\gamma^{(k)}$ and on α_{ij}, and, thus, the rate of change of the slip system hardness reads

$$\dot{g}^{(\alpha)} = \sum_{\beta} h_{\alpha\beta}(\{\gamma^{(\mu)}\}, \alpha_{ij})\dot{\gamma}^{(\beta)}. \tag{2.30}$$

Note that the theory does not incorporate the kinematic (energetic) type of hardening as, for example, does Gurtin's theory. One of the important consequences of this is that the theory of Acharya and Bassani is not capable of predicting a Bauschinger effect.

Moreover, one of the still unresolved issues of the theory is the problem of including the nonlocal effects into the slip system hardening in case of multiple slip. The problem is that it is not clear how to apportion the effects of the GNDs across the individual slip systems. Exactly the same problem occurs in the theory of Gurtin when attempting to introduce nonlocality into the dissipative hardening description.

In single slip the hardening matrix collapses into a scalar h and the following slip system hardening rule has been adopted by Acharya and Bassani:

$$h(\gamma, \gamma_{,1}) = h_0 \left(\frac{\gamma}{\gamma_0} - 1\right)^{N-1} \left[1 + \ell^2 \left(\frac{\gamma_{,1}}{\gamma_0}\right)^2\right]^p. \tag{2.31}$$

Here ℓ is the material length scale introduced for dimensional consistency, N is the strain hardening exponent and p is a non-negative parameter smaller than one. The viscoplastic flow rule as well as the constitutive relations adopted here have the same form as those in the local theory in section 2.1.

One of the peculiarities of this simple theory is that it preserves the classical structure of local single crystal plasticity summarized in section 2.1 and does not require higher-order stresses or additional boundary conditions (which are not always physically transparent). On the other hand, like any other low-order continuum theory, the Acharya-Bassani theory cannot capture, for example, the formation of boundary layers in case of hindered plasticity. The reason is that, without the additional boundary conditions, it is not possible to trigger inhomogeneous plastic flow from a homogeneous initial state, so that the deformation remains uniform. The nonlocal plasticity theories of Shu-Fleck (1999) and Gurtin (2002), which both require higher order boundary conditions, are able to capture these boundary layers, as shown by Shu *et al.* (2001) and Bittencourt *et al.* (2003).