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A minimal gradient-enhancement of the classical continuum theory of crystal plasticity. Part I: The hardening law

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A simple gradient-enhancement of the classical continuum theory of plasticity of single crystals deformed by multislip is proposed for incorporating size effects in a manner consistent with phenomenological laws established in materials science. Despite considerable efforts in developing gradient theories, there is no consensus regarding the minimal set of physically based assumptions needed to capture the slip-gradient effects in metal single crystals and to provide a benchmark for more refined approaches. In order to make a step towards such a reference model, the concept of the tensorial density of geometrically necessary dislocations generated by slip-rate gradients is combined with a generalized form of the classical Taylor formula for the flow stress. In the governing equations in the rate form, the derived internal length scale is expressed through the current flow stress and standard parameters so that no further assumption is needed to define a characteristic length. It is shown that this internal length scale is directly related to the mean free path of dislocations and possesses physical interpretation which is frequently missing in other gradient-plasticity models.

Key words: gradient plasticity, geometrically necessary dislocations, single crystal, strain-hardening, internal length scale, size effect

1. Introduction

The classical continuum theory of single crystals deformed plastically by multislip at arbitrary strain, established by Hill and Rice [1–3] and reformulated by Asaro [4], involves no internal length scale. To incorporate size effects, a number of strain-gradient theories of crystal plasticity have been proposed that use different sets of basic assumptions and exhibit a different degree of complexity; compare, for instance, representative papers [5–25]. This list is not intended to be complete, and might be considerably extended by gradient plasticity approaches to continua other than single crystals deformed by multislip. While plasticity of such continua is essentially be-

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yond the scope of this article, at least some of preceding works should be mentioned [26–30] along with more recent contributions to crystal plasticity [31–40]. Clear ordering of the existing theories from the point of view of decreasing simplicity and increasing accuracy in predicting the real behaviour of materials is not yet available. Despite the progress made in various theoretical aspects, the number of realistic 3D examples calculated with the use of a full set of slip systems in a framework of gradient plasticity of crystals is still rather limited. All this indicates a current need for developing a verifiable gradient-enhanced crystal plasticity model based on a possibly small set of physically based assumptions needed to capture the slip gradient effects in single crystals.

The following major question is addressed here: how to include the effect of slip-rate gradients in a possibly simple way such that the internal length scale possesses a physical meaning. Accordingly, rather than to begin with comparing the specific features of the existing gradient theories of crystal plasticity – such reviews can be found elsewhere, cf. [41–45] – in the introduction we concentrate on the concepts that are most fundamental for handling the above question. In particular, we wish to incorporate certain basic phenomenological laws established in materials science in the field of plasticity of metals.

In the phenomenological description of dislocation strengthening during plastic flow, a fundamental role is played by the *average* density of dislocations, ρ. Starting from the famous relationship $\tau \propto \sqrt{\rho}$ for the flow stress τ, cf. Taylor [46], average dislocation density ρ is omnipresent in the materials science literature on plasticity of metals; cf. excellent reviews by Kocks and Mecking [47], Sauzay and Kubin [48] and Niewczas [49]. It is thus natural and justified to incorporate ρ into a gradient-enhanced plasticity theory as a measurable material parameter of primary importance. This is also desirable in view of a length scale $1/\sqrt{\rho}$ provided by ρ and related to the commonly observed phenomenon of dislocation patterning.

The concept of geometrically necessary dislocations (GNDs) in the description of nonuniform plastic slip in crystalline solids is classical and well established, following Nye [50]. Dislocation density ρ, understood as a *total* dislocation density in a representative volume element of a crystal, is frequently split, following [6, 29, 51], into the sum of the contribution ρ_{S} of the statistically stored dislocations (SSDs, independent of strain gradients) and the average density ρ_{G} of GNDs (dependent on plastic strain gradients). That well-known procedure is adopted in the present work, however, with the distinction that the above split is applied *incrementally*, to the dislocation density *rates*, $\dot{\rho} = \dot{\rho}_{\mathrm{S}} + \dot{\rho}_{\mathrm{G}}$. This modification, apparently minor at first glance, will be shown to lead, perhaps unexpectedly, to another internal length scale directly linked to the mean free path of dislocations.

Consequently, it is the average density *rate* $\dot{\rho}_{\rm G}$ of GNDs that represents the basic constitutive variable to be determined from slip-rate gradients, rather than an accumulated density $\rho_{\rm G}$. Nye's dislocation density tensor [50] will also be considered in the rate form, generalized to finite deformations as follows. Recall that a general analytic tool to characterize GNDs is the curl of either the elastic or plastic part of total distortion, which measures the field incompatibility of elastic or plastic deformation, respectively; see Kroner [52] for an exposition of the background. In the literature dealing with finite deformation, the curl was included in the theory in different versions. Cermelli and Gurtin [53] discussed that matter in historical perspective and proposed the dislocation density tensor $\mathbf{G}$ that acts in the intermediate configuration. Gurtin [54] has shown that in the rate framework being of special interest here, it is the plastically convected derivative of $\mathbf{G}$ that is a linear function of slip-rate gradients projected on the respective slip planes and can be split further into a sum of terms involving the rates of densities of edge and screw dislocations on individual slip-systems. However, working with multiple GND densities and associated multiple length scales is too complicated in the minimal gradient-enhanced framework aimed at here, and it will rather be viewed as a possible extension. A relation between the plastically convected derivative of $\mathbf{G}$ and an *average* density rate $\dot{\rho}_{\rm G}$ of GNDs being generated by slip-rate gradients is not immediate and will be discussed in the sequel.

When studying the recent literature, one might get an impression that it is obligatory to describe the GND effect using a non-standard balance law. However, such a non-standard balance law is not a law of nature, as its particular form depends on the mathematical definition of the adopted class of continua. In particular, the expression for *external power* can be extended to virtual variations of scalar, vector or tensor variables, defining in that way different classes of continua corresponding to different (quasi-)balance laws [55, 56]. The dilemma mentioned by Mughrabi [57] and concerning the choice between various theories it still actual. Moreover, the choice of a particular class of continua is to be accompanied by a separate choice of constitutive assumptions [55, 56].

While more complex approaches developed in the literature can be expected to describe the hardening behaviour of metal crystals with better accuracy, the present aim is to capture the essence of the physical effect of slip-rate gradients in crystal plasticity in a possibly simple way. Therefore, we will proceed in the framework of classical continua, characterized by the external power in the standard form involving no virtual variations other than the usual variations of spatial displacements. The corresponding balance equations take the classical form, independently of constitutive assumptions that involve slip-rate gradients. Accordingly, there is no necessity here to introduce higher-order stresses or microforce balance equations. Moreover, in the present approach the split of the stress power into dissipative and energetic parts remains arbitrary, subject to the second law of thermodynamics only, since it does not affect the incremental hardening rule for isothermal monotonic deformations, similarly as in the non-gradient case, cf. [58, Remark 2].

It will become clear later that the present approach differs in essential aspects from the other available models of gradient plasticity of single crystals considered as classical continua. For instance, in the approach developed in [59, 60], the physical background is similar, but the final incremental hardening rule is of conventional type. It is clearly distinct from our non-conventional hardening rule with an extra term involving the *current slip-rate gradients* and an explicit intrinsic length scale. In the approaches by Nix and Gao and others [6, 18], another intrinsic length scale appears in the dislocation-strengthening formula at an accumulated slip-gradient rather than at its rate counterpart as here, and in consequence it has a substantially different value.

All attempts are made below to reduce the number of free parameters in the final computational model as much as possible. The preceding theoretical framework is developed in a more general way and is based on certain constitutive functions left arbitrary to enhance its applicability. The resulting new extension of the Hill and Rice [3] classical theory of single crystal plasticity to slip-rate gradient effects requires *no extra parameters* in comparison to the non-gradient theory. It will be shown that the derived internal length scale is expressed through τ and standard parameters of a non-gradient hardening law and, remarkably, possesses physical interpretation which is frequently missing in other gradient-plasticity models.

That minimal model requires, of course, a verification whether the simplifications involved are not too severe. Since there is no freedom to adjust the internal length scale, the primary challenge is to verify the predicted size effect by comparison with experimental observations. This will be done in Part II [61] of this paper by comparing the results of 3D finite element simulations of spherical indentation in a Cu single crystal with the experimentally observed indentation size effect.

2. A minimal gradient-enhancement of classical crystal plasticity

2.1. Main concept

The following question is addressed: given the conventional incremental strain-hardening law in the local continuum theory of crystal plasticity at constant temperature [3, 4],

$$\dot{\tau}^{\mathrm{c}}_{\alpha} = \sum_{\beta} h_{\alpha\beta}\,\dot{\gamma}_{\beta} \qquad \text{if} \quad \nabla\dot{\gamma}_{\alpha} \equiv 0, \tag{2.1}$$

how to include the effect of slip-rate gradients $\nabla\dot{\gamma}_\alpha$ in a possibly simple way such that the internal length scale possesses a physical meaning. In spite of simplicity of the subsequent reasoning, its major outcome has not been found in the literature.

In formula (2.1), $\tau^{\rm c}_\alpha$ is the current critical value of the resolved shear stress τ_α on the α-th slip system, whose rate $\dot{\tau}^{\rm c}_\alpha$ is understood as the *one-sided* material time derivative in the *forward* sense. The rate $\dot{\tau}^{\rm c}_\alpha$ is linearly related by the current hardening moduli matrix $(h_{\alpha\beta})$ to the rate $\dot{\gamma}_\beta$ of average shear (called slip) on any slip-system β in the representative volume element under consideration. The slip-rates are taken here to be non-negative, $\dot{\gamma}_\beta \geq 0$, so that slipping on crystallographically the same slip-system but in opposite directions is treated as activity of two distinct slip systems (the back-stress effect is thus not excluded).

Without loss of generality, also when $\nabla\dot{\gamma}_\alpha \neq 0$, the multiplicative split of $h_{\alpha\beta}$ and the effective slip-rate $\dot{\gamma}$ can be introduced,

$$h_{\alpha\beta} = \theta\, q_{\alpha\beta}, \qquad \dot{\gamma} = \sum_\alpha \dot{\gamma}_\alpha, \tag{2.2}$$

where θ is an isotropic hardening modulus, and dimensionless parameters $q_{\alpha\beta}$ describe unequal hardening of distinct slip systems. Accordingly, an isotropic part τ of critical resolved shear stresses $\tau^{\rm c}_\alpha$ is defined incrementally as follows

$$\dot{\tau} = \theta\dot{\gamma} \qquad \text{if} \quad \nabla\dot{\gamma}_\alpha \equiv 0. \tag{2.3}$$

When all rate-dependent or viscous effects are disregarded then τ is identified with the flow stress, the common concept in the materials science literature. However, only in the special case of fully isotropic hardening when all $q_{\alpha\beta} = 1$, we would have $h_{\alpha\beta} = \theta$ and $\tau^{\rm c}_\alpha = \tau$.

The basic phenomenological law of metal plasticity in materials science is a one-to-one relationship between the flow stress τ and average dislocation density ρ, taken most frequently in the surprisingly universal although approximate form $\tau \propto \sqrt{\rho}$ [46]. Instead of assuming the Taylor square-root formula from the outset, we begin with a more general relationship for the isotropic flow stress in the form

$$\tau = \tau_\rho(\rho), \tag{2.4}$$

where ρ is the *total* density of all dislocations of a given Burgers vector modulus b, in an average sense for the representative volume element of the crystal. Mathematically, τ_ρ is a continuous and (possibly piecewise) differentiable real function, otherwise arbitrary at the moment, of a single scalar argument ρ as an internal state variable. To retain desirable generality of the framework, we prefer to keep at the moment the freedom to choose a specific function τ_ρ for fitting experimental data, for instance, for including an initial yield stress $\tau_0 > 0$, an imperfect square-root relation, or a non-constant strengthening coefficient in the Taylor formula, cf. [48, 62].

To include the GND density effect in a simple way, in the approach initiated by ASHBY [51] and developed by FLECK *et al.* [29], NIX and GAO [6] and others, ρ is split into contributions of statistically stored and geometrically necessary dislocations. In distinction to studies of direct relationships between τ and ρ, the attention is focused here on the *rate* form of equation (2.4). Accordingly, $\dot{\rho}$ is split into the sum of two *rate*-contributions: $\dot{\rho}_{\mathrm{S}}$ as the rate of average density of statistically stored dislocations (SSDs, independent of slip-rate gradients) and $\dot{\rho}_{\mathrm{G}}$ as the rate of average density of geometrically necessary dislocations (GNDs, induced by slip-rate gradients), viz.

$$\dot{\rho} = \dot{\rho}_{\mathrm{S}} + \dot{\rho}_{\mathrm{G}}. \tag{2.5}$$

This is motivated by the fact that the basic constitutive equations of crystal plasticity are anyway formulated in the rate form, cf. formula (2.1), in order to be applicable along any straining path. Moreover, dislocation density rates are related to the shear rates on slip-systems that in the finite-deformation setting have more clear meaning as constitutive *rate*-variables than their time integrals, cf. [2, 54].

For SSD and GND density rates, $\dot{\rho}_{\mathrm{S}}$ and $\dot{\rho}_{\mathrm{G}}$, we adopt the well-known formulae. The rate of net storage of SSDs is taken to be the same as in the absence of GNDs when $\dot{\rho} = \dot{\rho}_{\mathrm{S}}$, viz.

$$\dot{\rho}_{\mathrm{S}} = \frac{1}{b\lambda}\dot{\gamma} - \dot{\rho}_{\mathrm{r}}. \tag{2.6}$$

In formula (2.6) (see KOCKS and MECKING [47] for a detailed discussion), b is the Burgers vector modulus, λ the dislocation mean free path, and $\dot{\rho}_{\mathrm{r}}$ the dynamic recovery term. The first term describes multiplication and the second annihilation of SSDs. The inverse of λ is classically defined as the mean length of dislocation stored ($\mathrm{d}L$) per area swept ($\mathrm{d}A$) in differential form [47]

$$\frac{1}{\lambda} = \frac{\mathrm{d}L}{\mathrm{d}A}. \tag{2.7}$$

The rate of creation of GNDs does not depend explicitly on $\dot{\gamma}$ but depends on gradients of $\dot{\gamma}_\alpha$-s through

$$\dot{\rho}_{\mathrm{G}} = \frac{1}{b}\dot{\chi}. \tag{2.8}$$

In formula (2.8), which represents the rate form of that in the basic papers by ASHBY [51], FLECK *et al.* [29] and NIX and GAO [6], $\dot{\chi}$ is the 'effective' plastic strain gradient rate, to be discussed in more detail later on.

By combining Eqs. (2.5), (2.6) and (2.8), we have

$$\dot{\rho} = \frac{1}{b\lambda}(\dot{\gamma} + \lambda\dot{\chi} - b\lambda\dot{\rho}_{\mathrm{r}}). \tag{2.9}$$

Consequently, denoting a current value of the derivative of function τ_ρ by $\tau'_\rho = (\mathrm{d}\tau_\rho/\mathrm{d}\rho)(\rho)$, taking time derivative of Eq. (2.4) and substituting Eq. (2.9), we obtain

$$\dot{\tau} = \tau'_\rho\dot{\rho} = \frac{\tau'_\rho}{b\lambda}\,(\dot{\gamma} + \lambda\dot{\chi} - b\lambda\dot{\rho}_{\mathrm{r}}). \tag{2.10}$$

Suppose first that the dislocation annihilation term $\dot{\rho}_{\mathrm{r}}$ can be neglected; its contribution will be discussed in Subsection 2.2. Then, from Eq. (2.9) and for consistency of formula (2.10) with Eq. (2.3) in the non-gradient case $\dot{\chi} = 0$, it follows that

$$\dot{\rho} = \frac{1}{b\lambda}(\dot{\gamma} + \lambda\dot{\chi}) \qquad \text{and} \qquad \theta = \frac{\tau'_\rho}{b\lambda} \qquad \text{if} \quad \dot{\rho}_{\mathrm{r}} = 0. \tag{2.11}$$

Finally, by combining equations (2.10) and (2.11), we arrive at the *isotropic part* of an incremental hardening law in the form

$$\dot{\tau} = \theta\dot{\gamma} + \frac{\tau'_\rho}{b}\dot{\chi} = \theta\,(\dot{\gamma} + \ell\dot{\chi}) \qquad \text{with} \quad \ell = \frac{\tau'_\rho}{b\theta} \quad \text{for} \quad \theta \neq 0 \tag{2.12}$$

and

$$\ell = \lambda \qquad \text{if} \quad \dot{\rho}_{\mathrm{r}} = 0. \tag{2.13}$$

Note that the *effective* multiplier $\theta\ell = \tau'_\rho/b$ of $\dot{\chi}$ is a state-dependent quantity defined directly by the constitutive function τ_ρ in Eq. (2.4).

Remark 1. It turns out that the dislocation mean free path λ, which is a standard length-scale parameter in the physically-based dislocation theory of plasticity *without* macroscopic strain gradients, coincides with the internal length-scale ℓ in the *gradient-enhanced hardening rate equation* for the isotropic flow stress, if the dislocation annihilation term $\dot{\rho}_{\mathrm{r}}$ vanishes. This remarkable conclusion drawn from an arbitrary relationship between the flow stress and total dislocation density has not been found in the literature.

As the most important inspiration and specification of Eq. (2.4), the classical Taylor formula [46]

$$\tau = a\mu b\sqrt{\rho} \tag{2.14}$$

is used, where the strengthening coefficient a along with elastic shear modulus μ and Burgers vector modulus b are treated as known constants for a given material. From formulae (2.14) and $(2.11)_2$ we obtain the following specifications

$$\tau'_\rho = \frac{a\mu b}{2\sqrt{\rho}} = \frac{(a\mu b)^2}{2\tau} = \frac{\tau}{2\rho} \tag{2.15}$$

and

$$\lambda = \frac{\tau}{2\rho b\theta} = \frac{a\mu}{2\theta\sqrt{\rho}} = \frac{a^2\mu^2 b}{2\tau\theta} \qquad \text{if} \quad \dot{\rho}_\mathrm{r} = 0 \quad \text{and} \quad \theta \neq 0. \tag{2.16}$$

The above expression for the dislocation mean free path λ is well known in the dislocation theory of crystal plasticity, cf. Kocks and Mecking [47, Eqs. (11) and (12)]. Here, on account of equality (2.13), the same expression (2.16) appears in the different context as the formula for the internal length scale ℓ in the isotropic part (2.12) of an incremental hardening law of the gradient-enhanced crystal plasticity.

Remark 2. $\ell = \lambda$ as above differs from the characteristic internal length scale $\hat{\ell}$ derived also from the Taylor formula (2.14) but interpreted as follows [6, 57]

$$\frac{\tau}{\tau_\mathrm{S}} = \sqrt{1+\hat{\ell}\chi}, \qquad \hat{\ell} = \frac{1}{b\rho_\mathrm{S}} = b\left(\frac{a\mu}{\tau_\mathrm{S}}\right)^2, \qquad \rho_\mathrm{G} = \frac{\chi}{b}, \tag{2.17}$$

where χ is the 'effective' plastic strain gradient and τ_S is the flow stress related to the dislocation density ρ_S in the absence of GNDs. The difference is due to the fact that $\hat{\ell}$ was defined using *accumulated* quantities while ℓ appears here in the *rate* equation (2.12). Clearly, the difference is substantial since $2\theta \neq \tau_\mathrm{S}$ except at a single point on a hardening curve.

2.2. Effect of dislocation annihilation

Suppose now that the SSD annihilation term $\dot{\rho}_\mathrm{r}$ in Eq. (2.6) is not disregarded but taken proportional to $\dot{\gamma}$,

$$\dot{\rho}_\mathrm{r} = k_\mathrm{r}\dot{\gamma}, \qquad k_\mathrm{r} = \frac{2y_c}{b}\rho, \tag{2.18}$$

where $k_\mathrm{r} \geq 0$ is a state-dependent parameter. This is consistent with the present treatment of the critical resolved shear stresses as rate-independent, which implies that a time-dependent part of $\dot{\rho}_\mathrm{r}$ does not affect $\dot{\tau}$ and is thus disregarded here. The second formula (2.18) follows Essmann and Mughrabi [63], with the simplification that we do not distinguish at the moment (however, see Subsection 2.4) between different types of dislocations and treat y_c as a mean critical distance of dislocation annihilation. From Eq. (2.9) and for consistency of formula (2.10) with Eq. (2.3) in the non-gradient case $\dot{\chi} = 0$, we obtain

$$\dot{\rho} = \frac{1}{b\lambda}\big((1 - k_{\mathrm{r}} b\lambda)\dot{\gamma} + \lambda\dot{\chi}\big) \quad \text{and} \quad \theta = \frac{\tau_\rho'}{b\lambda}(1 - k_{\mathrm{r}} b\lambda) \tag{2.19}$$

in place of formulae (2.11). From Eq. (2.10) it follows that the key equation (2.12) remains unchanged, while ℓ is no longer identified with λ as in Eq. (2.13) but is now linked to λ through

$$\ell = \frac{\lambda}{1 - k_{\mathrm{r}} b\lambda} \qquad \text{if} \quad \dot{\rho}_{\mathrm{r}} = k_{\mathrm{r}}\dot{\gamma}. \tag{2.20}$$

Formulae (2.19) on substituting relation (2.20) take the simple form

$$\dot{\rho} = \frac{1}{b\ell}(\dot{\gamma} + \ell\dot{\chi}) \quad \text{and} \quad \theta = \frac{\tau_\rho'}{b\ell}. \tag{2.21}$$

Equation (2.20) means that ℓ is related to the mean free path of dislocations λ by a state-dependent multiplier that is not less than unity and can be much larger. In fact, straightforward transformation of formula (2.20) yields

$$\frac{\ell}{\lambda} = 1 + k_{\mathrm{r}} b\ell. \tag{2.22}$$

The last term, $k_{\mathrm{r}} b\ell$, is clearly state-dependent and non-negative for $\ell > 0$ so that $\ell/\lambda \geq 1$.

Let us analyze relationship (2.22) further when function τ_ρ is specified by the Taylor formula (2.14). Then expression (2.16) no longer holds for λ but is valid instead for ℓ in Eq. (2.12), that is

$$\ell = \frac{a^2\mu^2}{2\tau\theta}\, b. \tag{2.23}$$

Remarkably, the derived internal length scale ℓ in the gradient-enhanced hardening law (2.12) is thus expressed through standard quantities that appear in a non-gradient hardening law.

On substituting relationships (2.14), (2.18) and (2.23) into (2.22), we obtain

$$\frac{\ell}{\lambda} = 1 + \frac{y_c}{b}\frac{\tau}{\theta}. \tag{2.24}$$

Hence, ℓ/λ can be much larger than unity if θ decreases below τ. Nevertheless, an explicit relation between ℓ and λ is maintained.

Substitution of Eq. (2.23) in the above formula yields

$$\lambda = \frac{a^2\mu^2 b^2}{2(b\theta + y_c\tau)\tau}. \tag{2.25}$$

Thus, if strain hardening saturates at large strains so that $\rho \to \rho_\infty < \infty$, $\tau \to \tau_\infty < \infty$ and $\theta \to 0$, λ approaches asymptotically a finite value,

$$\lambda \to \lambda_\infty = \frac{a^2\mu^2 b^2}{2y_c\tau_\infty^2} = \frac{1}{2y_c\rho_\infty} \qquad \text{as } \theta \to 0 \text{ at large plastic strain,} \tag{2.26}$$

while ℓ after initial decreasing at small and moderate strain (when $\tau\theta$ increases) can eventually increase at large plastic strain (when $\tau\theta$ decreases).

In turn, at small strain and stress at the beginning of 'stage II' when $\theta \approx \theta_0 = \text{const}$ and $\tau \ll \theta_0 b/y_c$, we have

$$\lambda \approx \ell \approx \frac{a^2\mu^2}{2\tau\theta_0}b = \frac{a\mu}{2\theta_0\sqrt{\rho}} \qquad \text{if } \theta \approx \theta_0 \gg \frac{y_c}{b}\tau \text{ at small plastic strain,} \tag{2.27}$$

which is a well-known relationship for the mean free path of dislocations in stage II [47]. For typical values of $a \approx 0.3$ and $\theta_0 \approx \mu/200$, we obtain that $\lambda \approx \ell$ decreases initially with increasing dislocation density according to an approximate relationship $\lambda \approx \ell \approx 30/\sqrt{\rho}$. The well-acknowledged similitude relation for the characteristic wavelength d (or average cell size) of dislocation patterns, assuming the strengthening relation (2.14), reads

$$d = \frac{K\mu b}{\tau} = \frac{K}{a\sqrt{\rho}}, \tag{2.28}$$

where the similitude coefficient K for fcc metals is found in the literature to be a constant within a range of $K = 5\div 10$; see Sauzay and Kubin [48] for a review. In particular, for $K \approx 9$ and $a \approx 0.3$ the resulting relation is $d \approx 30/\sqrt{\rho}$ which is fully analogous to the relation obtained above for $\lambda \approx \ell$ in terms of $\sqrt{\rho}$. Hence, we conclude that in 'stage II' at small plastic strain and sufficiently small stress, in the circumstances specified above, $\ell \approx \lambda$ approximates also the characteristic wavelength d (or average cell size) of dislocation patterns, i.e. $\ell \approx \lambda \approx d$. It is beyond the scope of this paper to discuss in more detail a general relation between d and λ and ℓ at large strains.

Remark 3. The above discussion admits a conclusion that the internal length scale ℓ in the rate form (2.12) of the isotropic part of a gradient-enhanced crystal plasticity theory can be given a direct physical meaning using the Taylor formula (2.14) in the range of small plastic strain and sufficiently low dislocation density so that dislocation annihilation is negligible. In that range, the value of $\ell \propto 1/\sqrt{\rho}$ is estimated to be close to the dislocation mean free path λ and correlated with the characteristic wavelength $d \propto 1/\sqrt{\rho}$ of dislocation patterns.

2.3. Anisotropic hardening

We now turn back to a generic anisotropic hardening law (2.1) which was our starting point. In the non-gradient case, formula (2.1) can be rearranged by using formulae (2.2) and the isotropic part (2.3) of the incremental hardening law as follows

$$\begin{aligned}\dot\tau^{\mathrm{c}}_\alpha &= \theta\sum_\beta q_{\alpha\beta}\dot\gamma_\beta = \theta\dot\gamma + \theta\sum_\beta (q_{\alpha\beta}-1)\dot\gamma_\beta \\ &= \dot\tau + \theta\sum_\beta (q_{\alpha\beta}-1)\dot\gamma_\beta \qquad \text{if} \quad \dot\chi = 0.\end{aligned} \tag{2.29}$$

The gradient-enhancement of the above formula is the simplest if restricted to the isotropic part $\dot\tau$ of $\dot\tau^{\mathrm{c}}_\alpha$ only, with the formulae (2.4) and (2.12) applied as they stand. Then, substitution of equation (2.12) into the last expression for $\dot\tau^{\mathrm{c}}_\alpha$ in Eq. (2.29) yields

$$\dot\tau^{\mathrm{c}}_\alpha = \theta\,(\dot\gamma + \ell\dot\chi) + \theta\sum_\beta (q_{\alpha\beta}-1)\dot\gamma_\beta = \theta\Big(\sum_\beta q_{\alpha\beta}\dot\gamma_\beta + \ell\dot\chi\Big). \tag{2.30}$$

Finally, by using formula for ℓ from Eq. (2.12) we arrive at *the minimal gradient-enhancement of an anisotropic hardening law* (2.1), in two alternative forms

$$\dot\tau^{\mathrm{c}}_\alpha = \sum_\beta h_{\alpha\beta}\dot\gamma_\beta + \frac{\tau'_\rho}{b}\dot\chi = \theta\Big(\sum_\beta q_{\alpha\beta}\dot\gamma_\beta + \ell\dot\chi\Big) \tag{2.31}$$

with

$$\ell = \frac{\tau'_\rho}{b\theta} \qquad \text{for} \quad \theta \neq 0, \tag{2.32}$$

no matter whether the contribution of the dislocation annihilation term $\dot\rho_{\mathrm{r}}$ is included or not.

Recall that ℓ is expressed by formula (2.23) if τ_ρ is specified by the Taylor formula (2.14). In this important specific case the effective multiplier $\theta\ell = \tau'_\rho/b$ of $\dot\chi$ in formula (2.31) becomes inversely proportional to τ with a constant coefficient, independently of further specification of the hardening law discussed in Section 2.5. Explicitly, Eq. (2.31) on substituting formula (2.14) reduces to

$$\dot\tau^{\mathrm{c}}_\alpha = \sum_\beta h_{\alpha\beta}\dot\gamma_\beta + \frac{a^2\mu^2 b}{2\tau}\dot\chi. \tag{2.33}$$

REMARK 4. Formula (2.31) represents the minimal gradient-enhancement of a conventional incremental hardening law (2.1) describing anisotropic hardening of a single crystal. It has been obtained by including GND effects in the isotropic hardening part only. The internal length scale ℓ defined by Eq. (2.32) and specified by formula (2.23) is expressed through standard quantities that appear in a non-gradient hardening law, so that no further assumption is needed to define a characteristic length. The variable ℓ is related to the dislocation mean free path λ by formula (2.24) and coincides with λ when the dislocation annihilation term $\dot{\rho}_{\mathrm{r}}$ is disregarded. In the latter case ℓ has a physical meaning summarized in Remark 3.

2.4. Extension to multiple densities of dislocations

One of possible extensions of the above minimal gradient-enhanced framework of crystal plasticity is to begin with the Taylor formula (2.14) replaced with its generalized form [64]

$$\tau_\alpha^{\mathrm{c}} = \mu b \sqrt{\sum_\beta a_{\alpha\beta}\rho_\beta}, \tag{2.34}$$

where $a_{\alpha\beta}$ are parameters (e.g., constants) and ρ_α denotes the density of dislocations associated with α-th slip system. Differences in parameters $a_{\alpha\beta}$ correspond to different strength of classical types of junctions and can be estimated using dedicated dislocation dynamics simulations, e.g., Madec *et al.* [65]. It is also possible to distinguish between edge and screw dislocations by increasing the number of β's and adjusting the meaning of ρ_β and $a_{\alpha\beta}$ accordingly.

Equations (2.5), (2.6), (2.18) and (2.8) can be replaced with their analogs applied to dislocation accumulation on each slip system separately,

$$\begin{aligned} \dot{\rho}_\alpha &= \dot{\rho}_{\mathrm{S}\alpha} + \dot{\rho}_{\mathrm{G}\alpha}, \qquad & \dot{\rho}_{\mathrm{S}\alpha} &= \frac{1}{b\lambda_\alpha}\dot{\gamma}_\alpha - \dot{\rho}_{\mathrm{r}\alpha}, \\ \dot{\rho}_{\mathrm{r}\alpha} &= \frac{2y_\alpha}{b}\rho_\alpha\dot{\gamma}_\alpha, \qquad & \dot{\rho}_{\mathrm{G}\alpha} &= \frac{1}{b}\dot{\chi}_\alpha, \end{aligned} \tag{2.35}$$

where λ_α is the mean free path of dislocations on α-th slip system,

$$\frac{1}{\lambda_\alpha} = \frac{\mathrm{d}L_\alpha}{\mathrm{d}A_\alpha}, \tag{2.36}$$

and $\dot{\chi}_\alpha$ is the effective gradient of slip rate on the α-th slip system.

By combining Eqs. (2.35) it follows that

$$\dot{\rho}_\alpha = \frac{1}{b\lambda_\alpha}\big((1 - 2y_\alpha\rho_\alpha\lambda_\alpha)\dot{\gamma}_\alpha + \lambda_\alpha\dot{\chi}_\alpha\big). \tag{2.37}$$

On taking time derivative of Eq. (2.34) with $a_{\alpha\beta}$ assumed constant and substituting Eqs. (2.37), we obtain

$$\dot{\tau}^{\mathrm{c}}_{\alpha} = \frac{\mu^2 b^2}{2\tau^{\mathrm{c}}_{\alpha}} \sum_{\beta} a_{\alpha\beta}\dot{\rho}_{\beta} = \frac{\mu^2 b}{2\tau^{\mathrm{c}}_{\alpha}} \sum_{\beta} a_{\alpha\beta}\Big(\frac{1-2y_{\beta}\rho_{\beta}\lambda_{\beta}}{\lambda_{\beta}}\dot{\gamma}_{\beta} + \dot{\chi}_{\beta}\Big). \tag{2.38}$$

Consistency of the above equation with Eq. (2.1) in the non-gradient case $\dot{\chi}_{\beta} \equiv 0$ implies the following correspondences

$$h_{\alpha\beta} = \frac{\mu^2 b}{2\tau^{\mathrm{c}}_{\alpha}\ell_{\beta}} a_{\alpha\beta} \qquad \text{with} \qquad \ell_{\beta} = \frac{\lambda_{\beta}}{1-2y_{\beta}\rho_{\beta}\lambda_{\beta}}. \tag{2.39}$$

It is worth noting that for $a_{\alpha\beta}$ = const as assumed above, hardening moduli $h_{\alpha\beta}$ vary proportionally to the inverses of $\tau^{\mathrm{c}}_{\alpha}$ and ℓ_{β}, in analogy to the isotropic counterpart (2.23).

Finally, by combining Eqs. (2.38) and (2.39), we obtain

$$\dot{\tau}^{\mathrm{c}}_{\alpha} = \frac{\mu^2 b}{2\tau^{\mathrm{c}}_{\alpha}} \sum_{\beta} a_{\alpha\beta}\Big(\frac{1}{\ell_{\beta}}\dot{\gamma}_{\beta} + \dot{\chi}_{\beta}\Big) = \sum_{\beta} h_{\alpha\beta}(\dot{\gamma}_{\beta} + \ell_{\beta}\dot{\chi}_{\beta}). \tag{2.40}$$

The conclusions are to some extent analogous to those drawn after Eqs. (2.12), (2.13) and (2.20). Dislocation mean free paths λ_{β}, taken separately for distinct slip systems, are length-scale parameters in the dislocation theory of plasticity without macroscopic strain gradients. In the hardening rate equations (2.40) of gradient-enhanced crystal plasticity, they play themselves the role of the internal length-scale parameters ℓ_{β} if the dislocation annihilation terms $\dot{\rho}_{\mathrm{r}\beta}$ are neglected. If $\dot{\rho}_{\mathrm{r}\beta} \neq 0$ obey Eq. $(2.35)_3$ then ℓ_{β} is related to λ_{β} by a state-dependent multiplier dependent also on β. When $\dot{\chi}_{\beta} \equiv 0$ then the local hardening law (2.1) is obviously recovered in each case.

The gradient-enhanced hardening law (2.40) derived above can be maximally simplified by reducing the GND contribution to that in Eq. (2.31). To do this, on using the multiplicative split $(2.2)_1$, the right-hand side expression (2.40) is rewritten as follows

$$\dot{\tau}^{\mathrm{c}}_{\alpha} = \theta \sum_{\beta} (q_{\alpha\beta}\dot{\gamma}_{\beta} + q_{\alpha\beta}\ell_{\beta}\dot{\chi}_{\beta}). \tag{2.41}$$

Latent-hardening coefficients $q_{\alpha\beta}$ are usually regarded to be not far from unity (frequently, following Kocks [66], the diagonal terms are taken equal to 1 and off-diagonal terms between 1 and 1.4), while differences between ℓ_{β}'s for different slip systems are hardly accessible from experiment. This motivates a crude simplification

$$q_{\alpha\beta}\ell_{\beta} \approx \ell. \tag{2.42}$$

When the effective plastic strain gradient rate $\dot{\chi}$ is defined by

$$\dot{\chi} = \sum_{\beta} \dot{\chi}_{\beta} \tag{2.43}$$

then after substituting the simplification (2.42) into Eq. (2.40) we recover Eq. $(2.31)_2$ on another route.

Further extensions of the main concept elaborated above are left for future investigations.

2.5. The master curve

Changes of hardening modulus θ along any deformation path, with or without strain gradients, must somehow be determined. In the non-gradient case, an isotropic hardening relationship is frequently prescribed as a stress-strain relationship, viz.

$$\tau = \tau_{\gamma}(\gamma) \quad \text{and} \quad \theta = \tau_{\gamma}'(\gamma) \qquad \text{if} \quad \dot{\chi} \equiv 0, \tag{2.44}$$

where τ_{γ} is a given continuous real function and a prime denotes its derivative. Typical examples of τ_{γ} include power-law or exponentially saturating strain-hardening.

In the gradient-enhanced framework, the current values of τ and θ no longer depend only on γ. Since τ has been assumed in Eq. (2.4) to depend solely on total dislocation density ρ as a single internal state parameter, the current isotropic hardening modulus θ, which is generally a function of state, can also be considered as a function of ρ. However, that function need not be specified directly, rather, θ can be alternatively determined as a function of τ. In fact, in the materials science literature, without addressing the strain-gradient issue, it is quite common to consider θ, or the product $\tau\theta$, as a function of τ, cf. [47, 49]. Accordingly, as the 'master curve' for describing strain hardening we adopt the relationship between θ and τ defined by a given constitutive function θ_{τ}, viz.

$$\theta = \theta_{\tau}(\tau). \tag{2.45}$$

The formula (2.45) defines an indirect relationship between θ and ρ through $\theta = \theta_{\tau}(\tau_{\rho}(\rho))$ and, what is of primary importance here, is applicable both in the absence or presence of slip-rate gradients. In the latter case, ρ, τ and θ depend on the history of both $\dot{\gamma}$ and $\dot{\chi}$.

Once the master curve is specified as above then the characteristic length ℓ defined by formula (2.32) for given functions θ_{τ} and τ_{ρ} becomes a function of total dislocation density ρ, viz.

$$\ell = \tilde{\ell}(\rho) = \frac{\tau_{\rho}'(\rho)}{b\,\theta_{\tau}(\tau_{\rho}(\rho))}. \tag{2.46}$$

Consequently, for an invertible relationship between τ and ρ, the characteristic length ℓ can be expressed as a function of τ.

In the non-gradient case, the simplest approximation of 'stage III' behaviour is obtained by a linear decrease of θ with τ starting from some τ_0, which is described by

$$\theta_\tau = \theta_0 \Big(1 - \frac{\tau}{\tau_{\max}}\Big), \qquad \tau \geq \tau_0 \geq 0, \tag{2.47}$$

where τ_0, θ_0 and $\tau_{\max}$ are constant parameters. In the case of $\tau_0 = 0$ and $\dot{\chi} \equiv 0$, comparison with Eq. (2.44) leads to the Voce strain-hardening law:

$$\tau_\gamma = \tau_{\max}\Big(1 - \exp\Big(-\frac{\theta_0 \gamma}{\tau_{\max}}\Big)\Big) \qquad \text{if} \quad \dot{\chi} \equiv 0. \tag{2.48}$$

In contrast to formula (2.48), formula (2.47) is applicable as it stands also if $\dot{\chi} \neq 0$. Hence, it is the formula (2.47) that is adopted in the calculations reported in Part II.

When τ_ρ is specified by the classical Taylor formula (2.14) and θ_τ by formula (2.47) then from Eq. (2.23) we obtain an explicit relationship between ℓ and τ, viz.

$$\ell = \frac{a^2 \mu^2 b \, \tau_{\max}}{2\theta_0} \frac{1}{(\tau_{\max} - \tau)\tau}. \tag{2.49}$$

Finally, suppose for simplicity that $q_{\alpha\beta}$ are given constants (a standard assumption is to take $q_{\alpha\beta} = 1$ for $\beta = \alpha$ and $q_{\alpha\beta} = q \geq 1$ for $\beta \neq \alpha$, although according to FRANCIOSI and ZAOUI [67] up to five latent hardening parameters may be required to describe physically different interactions between slip-systems).

Knowledge of $q_{\alpha\beta}$ for given constitutive functions τ_ρ and θ_τ closes the system of governing equations – (2.2), (2.4), (2.31), (2.32), (2.45) – from which current values of τ^{c}_α can be determined for any given history of all $\dot{\gamma}_\alpha$ and $\dot{\chi}$ at arbitrarily large deformation. If function τ_ρ is specified by the Taylor formula (2.14) and function θ_τ by the Voce-like hardening law (2.47) then the resulting computational gradient-enhanced model of crystal plasticity is defined by the reduced system of governing equations – (2.2), (2.33), (2.47) – with a few material constants, all of them having the standard meaning in non-gradient strain-hardening laws.

It remains to define the effective slip-rate gradient $\dot{\chi}$ in terms of gradients of slip-rates $\dot{\gamma}_\alpha$.

2.6. Effective slip-rate gradient

To complete the above framework of gradient-enhanced crystal plasticity, we need to define $\dot{\chi}$ that enters the hardening rate equation (2.31) as the 'effective' plastic slip-rate gradient which induces the GND density rate (2.8). Since the slip-rate gradient orthogonal to the respective slip plane corresponds to a *compatible* strain-rate field, it does not contribute to the actual GND density rate. Therefore, the modulus $|\nabla\dot{\gamma}|$ of the gradient of effective slip-rate $\dot{\gamma}$ is generally *not* adequate as a candidate for $\dot{\chi}$, so that other choices are to be considered.

The concept of effective slip-rate gradient is discussed first in the framework of the geometrically linear theory throughout the current Section 2.6; the extension to the finite deformation framework is given later in Section 3.2. Recall that the density of dislocations is understood in an average sense within a representative volume element of the crystal, large enough for the effects of all dislocations within it to be averaged. Nye's [50] dislocation density tensor, denoted frequently in the literature by bold $\boldsymbol{\alpha}$ in the geometrically linear framework (not to be confused with plain α used as a slip-system index), assigns to a unit normal $\mathbf{n}$ to a lattice plane the net (resultant) Burgers vector $\mathbf{B_n}$ of *geometrically necessary* dislocations piercing a unit area of the plane,

$$\mathbf{B_n} = \boldsymbol{\alpha}\mathbf{n}. \tag{2.50}$$

It is important to recognize that the second-order tensor $\boldsymbol{\alpha}$ does *not* incorporate statistically stored dislocations as it 'quantifies a special set of dislocations whose geometric properties are not canceled by other dislocations in the crystal' [8].

According to the continuum theory of defects (the background is presented in historical perspective by Kroner [52]), $\boldsymbol{\alpha}$ is a measure of incompatibility of the plastic distortion field $\boldsymbol{\beta}^{\mathrm{p}}$, and simultaneously of incompatibility of elastic distortion field $\boldsymbol{\beta}^{\mathrm{e}}$ due to compatibility of the field of the total displacement gradient $\nabla\mathbf{u}$,

$$\boldsymbol{\alpha} = \operatorname{curl}\boldsymbol{\beta}^{\mathrm{p}} = -\operatorname{curl}\boldsymbol{\beta}^{\mathrm{e}}, \qquad \nabla\mathbf{u} = \boldsymbol{\beta}^{\mathrm{e}} + \boldsymbol{\beta}^{\mathrm{p}}. \tag{2.51}$$

When defining the curl operator, at the moment in the small strain formalism, we adopt the following convention[1]

$$\operatorname{curl}\boldsymbol{\beta}^{\mathrm{p}} = \epsilon_{jkl}\partial_k\beta^{\mathrm{p}}_{il}\,\mathbf{e}_i\otimes\mathbf{e}_j \tag{2.52}$$

in Cartesian components on an orthonormal basis $\mathbf{e}_i$, where ϵ_{jkl} denotes the (Levi-Civita) permutation symbol, the summation convention is used, and ∂_k denotes the partial derivative with respect to spatial coordinate x_k in the Euclidean space. Consistency between the net Burgers vector in formula (2.50) and

[1]A note of caution: other conventions using a transpose or minus sign are also met in the literature. The tensor notation is used where direct juxtaposition means simple contraction, a central dot denotes double contraction in the sense $\mathbf{A}\cdot\mathbf{B} = A_{ij}B_{ij}$, $\otimes$ a dyadic product, and $\times$ a vector product. A superimposed -1, T or $-$T *over* a tensor symbol denotes an inverse, transpose or transposed inverse, respectively.

that found from a circuit on a plane containing an incompatible field $\boldsymbol{\beta}^{\mathrm{p}}$ follows by applying Stoke's theorem and interpreting $\boldsymbol{\alpha}$ as an average over a unit planar area.

According to the standard theory of crystal plasticity, the rate of plastic distortion associated with the α-th slip system reads $\dot{\boldsymbol{\beta}}^{\mathrm{p}}_{\alpha} = \dot{\gamma}_{\alpha}\mathbf{s}_{\alpha} \otimes \mathbf{m}_{\alpha}$, where $(\mathbf{s}_{\alpha}, \mathbf{m}_{\alpha})$ is a fixed pair of orthogonal unit vectors that define the slip direction and slip-plane normal, respectively, assumed unaffected by plastic distortion of the material. On substituting $\dot{\boldsymbol{\beta}}^{\mathrm{p}} = \sum_{\alpha} \dot{\boldsymbol{\beta}}^{\mathrm{p}}_{\alpha}$ into Eqs. (2.51) and (2.52), the rate of Nye's tensor can be decomposed as follows:

$$\dot{\boldsymbol{\alpha}} = \sum_{\alpha} \mathbf{s}_{\alpha} \otimes (\nabla\dot{\gamma}_{\alpha} \times \mathbf{m}_{\alpha}) = b \sum_{\alpha} \dot{\rho}_{\mathrm{G}\alpha} \mathbf{s}_{\alpha} \otimes \bar{\mathbf{t}}_{\alpha}. \tag{2.53}$$

The last expression provides another interpretation of the former one and is obtained by identifying $\bar{\mathbf{t}}_{\alpha}$ with vector $(\nabla\dot{\gamma}_{\alpha} \times \mathbf{m}_{\alpha})$ normalized to unit length. The sense of $\bar{\mathbf{t}}_{\alpha}$ can be chosen such that $\dot{\rho}_{\mathrm{G}\alpha} \geq 0$. Accordingly, $\dot{\rho}_{\mathrm{G}\alpha}$ is the rate of increasing length, per unit volume, of *non-redundant, straight* lines of geometrically necessary dislocations on the α-th slip system, of a given Burgers vector magnitude b and a general direction $\bar{\mathbf{t}}_{\alpha}$ lying within the respective slip plane ($\bar{\mathbf{t}}_{\alpha} \cdot \mathbf{m}_{\alpha} = 0$, $|\bar{\mathbf{t}}_{\alpha}| = 1$). A more detailed analysis is omitted here; useful relevant comments can be found in [8], in particular, on the indeterminacy of GND solutions consistent with a given Nye dislocation density tensor.

In the search for a single, *effective* slip-rate gradient $\dot{\chi}$ to be substituted in formula (2.8) for the average density rate of GNDs, we consider the following inequalities

$$|\dot{\mathbf{B}}_{\mathbf{n}}| \leq \|\dot{\boldsymbol{\alpha}}\| \leq b \sum_{\alpha} |\dot{\rho}_{\mathrm{G}\alpha}|. \tag{2.54}$$

Here, $\|\mathbf{A}\|$ denotes the Euclidean norm of a second-order tensor $\mathbf{A}$ (or the Frobenius norm of its matrix),

$$\|\mathbf{A}\| = \sqrt{\mathbf{A} \cdot \mathbf{A}} = (\mathrm{tr}(\overset{\mathrm{T}}{\mathbf{A}}\mathbf{A}))^{1/2}. \tag{2.55}$$

The spectral norm of $\mathbf{A}$ denoted by $\|\mathbf{A}\|_2$ is bounded from above by $\|\mathbf{A}\|$, hence from Eq. (2.50) it follows that

$$\max_{|\mathbf{n}|=1} |\dot{\mathbf{B}}_{\mathbf{n}}| = \|\dot{\boldsymbol{\alpha}}\|_2 \leq \|\dot{\boldsymbol{\alpha}}\|. \tag{2.56}$$

This implies the left-hand side inequality (2.54). The right-hand side inequality (2.54) follows from equation $(2.53)_2$ by using the triangle inequality,

$$\Big\|\sum_{\alpha} \dot{\rho}_{\mathrm{G}\alpha} \mathbf{s}_{\alpha} \otimes \bar{\mathbf{t}}_{\alpha}\Big\| \leq \sum_{\alpha} |\dot{\rho}_{\mathrm{G}\alpha}| \, \|\mathbf{s}_{\alpha} \otimes \bar{\mathbf{t}}_{\alpha}\| = \sum_{\alpha} |\dot{\rho}_{\mathrm{G}\alpha}|, \tag{2.57}$$

on account of the assumed normalization $|\mathbf{s}_{\alpha}| = |\bar{\mathbf{t}}_{\alpha}| = 1$.

The right-hand side expression (2.54), in view of the interpretation of $\dot{\rho}_{\mathrm{G}\alpha}$ given above and in accord with Eq. (2.43), appears as a natural candidate for $\dot{\chi}$, which is denoted by $\dot{\chi}_{\Sigma}$. With the sign convention for $\bar{\mathbf{t}}_{\alpha}$ such that $\dot{\rho}_{\mathrm{G}\alpha} \geq 0$, we obtain

$$\dot{\chi}_{\Sigma} = b \sum_{\alpha} \dot{\rho}_{\mathrm{G}\alpha}, \qquad \dot{\rho}_{\mathrm{G}\alpha} \geq 0, \qquad \dot{\rho}_{\mathrm{G}} = \sum_{\alpha} \dot{\rho}_{\mathrm{G}\alpha}. \tag{2.58}$$

However, the choice of $\dot{\chi}_{\Sigma}$ as an effective slip-rate gradient $\dot{\chi}$ to be substituted in formulae (2.8) and (2.9) has also some deficiencies. First, the value of $\dot{\chi}_{\Sigma}$ need not be uniquely determined by $\dot{\boldsymbol{\alpha}}$ alone. Second, $\dot{\chi}_{\Sigma}$ used as $\dot{\chi}$ in equation (2.9) does not reflect the possibility that $\dot{\boldsymbol{\alpha}}$ may induce additional annihilation of existing SSDs. For example, some segments of *existing* dislocation loops (not incorporated into $\boldsymbol{\alpha}$) may move away from the crystal region under consideration, in order to provide the required net contribution to $\dot{\boldsymbol{\alpha}}$ by some $\dot{\rho}_{\mathrm{G}\alpha} > 0$, accompanied with $\dot{\rho}_{\mathrm{S}\alpha} < 0$ not accounted for in Eq. (2.6). Third, $\dot{\boldsymbol{\alpha}}$ may correspond to annihilation of some existing GNDs, so that the corresponding value of some $\dot{\rho}_{\mathrm{G}\alpha}$ might be negative, in contrast to definition (2.58). Therefore, $\dot{\chi}_{\Sigma}$ substituted in formulae (2.8) and (2.9) as an effective slip-rate gradient $\dot{\chi}$ is likely to overestimate the actual rate of increase of average dislocation density.

In view of relations (2.54) and in the light of the above discussion, we propose to complete the minimal gradient-enhancement of crystal plasticity in the small strain framework by the simple definition

$$\dot{\chi} = \varphi(\nabla\dot{\gamma}_{\alpha}) \quad \text{specified by} \quad \varphi(\nabla\dot{\gamma}_{\alpha}) = \|\dot{\boldsymbol{\alpha}}\| = \Big\| \sum_{\alpha} \mathbf{s}_{\alpha} \otimes (\nabla\dot{\gamma}_{\alpha} \times \mathbf{m}_{\alpha}) \Big\| \tag{2.59}$$

as the primary option for predominantly *monotonic* deformation processes. For instance, in the monotonic plastic bending we have $\|\dot{\boldsymbol{\alpha}}\| = \dot{\kappa}$ and $\dot{\rho}_{\mathrm{G}} = \dot{\kappa}/b$, where κ is the curvature due to plastic bending, in agreement with the well-known formula for lattice curvature caused by creating a family of parallel edge dislocations of strength b [51].

In cyclic deformation processes, reverse plastic bending may be caused either by creation of new GNDs or by annihilation of existing ones, in addition to SSD annihilation. A specific form of the free energy function, which was not needed in the simple approach developed above, may be required to define the gradient-induced back-stress effect after a strain-rate reversal. The extension of the present approach to cyclic deformation processes is thus not immediate and requires further work, going beyond the scope of this paper.

3. Finite deformation framework

The major physical reason for describing *incremental* kinematics of metal single crystals using the finite-deformation framework is the phenomenon of mutual spin (called the plastic spin) of the material and the crystallographic lattice. The plastic spin influences the incremental constitutive relationships in a non-negligible manner when the current hardening moduli are of the order of the current stress, irrespectively of whether the current strains are small or not. In the geometrically exact treatment of finite deformation plasticity, such common concepts like slip-rate, plastic strain-rate, resolved shear stress, unloading criterion and normality flow rule require a precise analysis [3]. The classical concepts are briefly recapitulated below in Section 3.1, followed by a discussion of the effective plastic slip-rate gradient in Section 3.2. It is pointed out that in the present minimal gradient-enhancement of classical crystal plasticity, in contrast to the more refined theories, there is no need to introduce higher-order stresses or balance laws other than in classical continua.

3.1. Classical continuum deformed plastically by multislip

We adopt the convention that slip-rates $\dot{\gamma}_\alpha \geq 0$ that represent incremental plastic simple shears on the corresponding slip systems are referenced to the undistorted crystallographic lattice at zero stress, in the so-called intermediate *local* configuration. Consequently, $\dot{\gamma}_\alpha$'s are invariant with respect to elastic distortion $\mathbf{F}^*$ of the lattice. The collective effect $\mathbf{L}^{\mathrm{p}}$ of plastic slip-rates $\dot{\gamma}_\alpha$, which defines the rate of accumulated plastic deformation gradient $\mathbf{F}^{\mathrm{p}}$, reads [2]

$$\mathbf{L}^{\mathrm{p}} = \sum_\alpha \dot{\gamma}_\alpha \, \mathbf{s}_\alpha \otimes \mathbf{m}_\alpha \,, \qquad \dot{\mathbf{F}}^{\mathrm{p}} = \mathbf{L}^{\mathrm{p}}\mathbf{F}^{\mathrm{p}}, \tag{3.1}$$

where a fixed pair of orthogonal unit vectors $(\mathbf{s}_\alpha, \mathbf{m}_\alpha)$ for the α-th slip system defines the slip direction and slip-plane normal, respectively, in the stress-free configuration of the crystallographic lattice, assumed undistorted by plastic slips. As a consequence, the plastic flow is isochoric, $\det \mathbf{F}^{\mathrm{p}} = 1$. An average dislocation density is taken per unit volume of the undistorted lattice. The skew part of $\mathbf{L}^{\mathrm{p}}$ is called the plastic spin.

The total isothermal deformation gradient, $\mathbf{F}$, taken relative to a fixed stress-free reference configuration of the material, includes $\mathbf{F}^{\mathrm{p}}$ and $\mathbf{F}^*$ in a multiplicative manner [26], where $\mathbf{F}^*$ is decomposed into the elastic stretch $\mathbf{U}^{\mathrm{e}}$ and rotation $\mathbf{R}^*$ of the lattice, viz.

$$\mathbf{F} = \mathbf{F}^*\mathbf{F}^{\mathrm{p}}, \qquad \mathbf{F}^* = \mathbf{R}^*\mathbf{U}^{\mathrm{e}}, \qquad (\mathbf{U}^{\mathrm{e}})^2 = \mathbf{C}^{\mathrm{e}} = \overset{\mathrm{T}}{\mathbf{F}}{}^*\mathbf{F}^*. \tag{3.2}$$

Let $\mathbf{S}$ and $\mathbf{S}^*$ denote the Piola stress tensors relative to the reference configuration of the material and the intermediate local configuration, respectively, and $\mathbf{M}$ the Mandel stress [68], related mutually and to the Cauchy stress $\boldsymbol{\sigma}$ through

$$\mathbf{M} = \overset{\mathrm{T}}{\mathbf{F}}{}^*\mathbf{S}^*, \qquad \mathbf{S}^* = \mathbf{S}\overset{\mathrm{T}}{\mathbf{F}}{}^{\mathrm{p}}, \qquad \mathbf{S}\overset{\mathrm{T}}{\mathbf{F}} = (\det \mathbf{U}^{\mathrm{e}})\boldsymbol{\sigma}. \tag{3.3}$$

The total stress-power $\mathbf{S}\cdot\dot{\mathbf{F}}$, per unit volume in the reference configuration, is decomposed accordingly into elastic ($\dot{w}^{\mathrm{e}}$) and plastic ($\dot{w}^{\mathrm{p}}$) parts,

$$\mathbf{S}\cdot\dot{\mathbf{F}} = \dot{w}^{\mathrm{e}} + \dot{w}^{\mathrm{p}}, \qquad \dot{w}^{\mathrm{e}} = \mathbf{S}^{*}\cdot\dot{\mathbf{F}}^{*}, \qquad \dot{w}^{\mathrm{p}} = \mathbf{M}\cdot\mathbf{L}^{\mathrm{p}}. \tag{3.4}$$

This is an identity that follows by combining the equations $(3.1)_2$, $(3.2)_1$ and $(3.3)_{1,2}$.

REMARK 5. It is advantageous for wider applicability of the present constitutive framework to keep another common split of the stress-power into dissipative and energetic parts *arbitrary*, subject to the second law of thermodynamics only, similarly as in the non-gradient case, cf. [58, Remark 2]. That split can be left unspecified as it does not influence the conventional strain-hardening law (2.1) nor its gradient-enhancement (2.31). Physically based knowledge of dissipative and energetic parts separately can be helpful in determining hardening moduli $h_{\alpha\beta}$ themselves, however, it is not the subject of this paper. In the present framework, only the evolution equations for τ_α^{c} are affected by slip-rate gradients, while τ_α are still defined in the classical manner recalled below.

The generalized resolved shear stress τ_α on the α-th slip-system (the Schmid stresss) is defined such that $\tau_\alpha\dot{\gamma}_\alpha$ is precisely the rate of plastic working due to slip on system α per unit volume in a stress-free configuration [3, 4]:

$$\tau_\alpha = \mathbf{M}\cdot(\mathbf{s}_\alpha\otimes\mathbf{m}_\alpha) = (\det\mathbf{U}^{\mathrm{e}})\,\boldsymbol{\sigma}\cdot(\mathbf{F}^{*}\mathbf{s}_\alpha\otimes\overset{-\mathrm{T}}{\mathbf{F}^{*}}\mathbf{m}_\alpha), \qquad \dot{w}^{\mathrm{p}} = \sum_\alpha \tau_\alpha\dot{\gamma}_\alpha. \tag{3.5}$$

Since elastic compressibility is included, τ_α is interpreted as the resolved Kirchhoff stress $\boldsymbol{\tau} = (\det\mathbf{U}^{\mathrm{e}})\boldsymbol{\sigma}$ rather than the resolved Cauchy stress $\boldsymbol{\sigma}$. It can be checked that the factor $(\det\mathbf{U}^{\mathrm{e}})$ in the definition (3.5) of τ_α is needed to avoid inconsistency in sensitivity of the yield criterion $\tau_\alpha = \tau_\alpha^{\mathrm{c}}$ at given τ_α^{c} to an otherwise purely elastic variation of volumetric strain. The difference between resolved $\boldsymbol{\tau}$ and resolved $\boldsymbol{\sigma}$ affects thus the loading/unloading criterion and also the normality flow rule, although only slightly for metals under ordinary pressures. The definition (3.5) of τ_α is the only one that is precisely compatible with the normality flow rule in the sense of HILL and RICE [3] and MANDEL [68], which can be reformulated in the specific subgradient form as

$$\mathbf{L}^{\mathrm{p}} \in \partial\{\mathbf{M} \mid \tau_\alpha \le \tau_\alpha^{\mathrm{c}}\ \forall\alpha\} \tag{3.6}$$

in the rate-independent case.

3.2. Effective slip-rate gradient

The basic equations from Section 2.6 are now reformulated in the finite deformation framework. This is done following CERMELLI and GURTIN [53] to much extent, noting the difference in the convention of defining the curl here as the transpose of that in the reference. The dislocation density tensor, denoted now by $\mathbf{G}$, gives analogously the net Burgers vector $\mathbf{B}^{\#}_{\mathbf{n}}$ of *geometrically necessary* dislocations piercing a unit area of an undistorted lattice plane of a unit normal $\mathbf{n}^{\#}$, viz.

$$\mathbf{B}^{\#}_{\mathbf{n}} = \mathbf{G}\mathbf{n}^{\#}. \tag{3.7}$$

In the finite deformation framework adopted, both $\mathbf{B}^{\#}_{\mathbf{n}}$ and $\mathbf{n}^{\#}$ are referenced to the undistorted crystallographic lattice considered in the *intermediate local* configuration. Accordingly, by constructing the Burgers circuit either in the reference or current configuration of the material, and transforming the resulting Burgers vector by pushing forward or pulling back, respectively, to the intermediate local configuration, in place of Eq. (2.51) we obtain [53]

$$\mathbf{G} = \mathbf{F}^{\mathrm{p}} \overset{\mathrm{T}}{\mathrm{Curl}}\, \mathbf{F}^{\mathrm{p}} = (\det \mathbf{F}^{*}) \overset{-1}{\mathbf{F}^{*}} \overset{\mathrm{T}}{\mathrm{curl}}\, \overset{-1}{\mathbf{F}^{*}}. \tag{3.8}$$

The transposed curl in the reference configuration of the material, $\overset{\mathrm{T}}{\mathrm{Curl}}$, is defined by

$$\overset{\mathrm{T}}{\mathrm{Curl}}\, \mathbf{F}^{\mathrm{p}} = \epsilon_{jkl} \partial_k F^{\mathrm{p}}_{il}\, \mathbf{e}^{\mathrm{R}}_{j} \otimes \mathbf{e}^{\#}_{i} \tag{3.9}$$

in analogy to Eq. (2.52). Here, a distinction is made between bases $\mathbf{e}^{\mathrm{R}}_{j}$ and $\mathbf{e}^{\#}_{i}$ in the reference and intermediate local configurations, respectively, put in opposite order to that in Eq. (2.52) which implies the transpose. ∂_k denotes now the partial derivative with respect to material coordinate X_k in the Euclidean reference space. A similar definition (omitted here) holds for the transposed curl in the current configuration.

A straightforward rate $\dot{\mathbf{G}}$ of $\mathbf{G}$ in the finite deformation framework can be non-zero even if all slip-rate gradients vanish at the current instant. Therefore, as the finite-deformation counterpart to formula (2.53), we adopt the following expression

$$\overset{\diamond}{\mathbf{G}} = \sum_{\alpha} \mathbf{s}_{\alpha} \otimes (\nabla^{\#} \dot{\gamma}_{\alpha} \times \mathbf{m}_{\alpha}), \qquad \nabla^{\#} \dot{\gamma}_{\alpha} = \overset{-\mathrm{T}}{\mathbf{F}^{\mathrm{p}}}\, \nabla \dot{\gamma}_{\alpha}. \tag{3.10}$$

Here, $\nabla^{\#} \dot{\gamma}_{\alpha}$ is obtained from the reference gradient $\nabla \dot{\gamma}_{\alpha}$ by pushing it forward to the intermediate local configuration. As shown by CERMELLI and GURTIN [53], $\overset{\diamond}{\mathbf{G}}$ equals the plastically convected (Oldroyd) derivative of the dislocation density tensor $\mathbf{G}$, viz.

$$\overset{\diamond}{\mathbf{G}} = \dot{\mathbf{G}} - \mathbf{L}^{\mathrm{p}} \mathbf{G} - \mathbf{G} \overset{\mathrm{T}}{\mathbf{L}^{\mathrm{p}}} = \mathbf{F}^{\mathrm{p}} \frac{\partial}{\partial t} \left(\overset{-1}{\mathbf{F}^{\mathrm{p}}} \mathbf{G} \overset{-\mathrm{T}}{\mathbf{F}^{\mathrm{p}}} \right) \overset{\mathrm{T}}{\mathbf{F}^{\mathrm{p}}}. \tag{3.11}$$

Expression (3.10) is independent of the current value of $\mathbf{G}$, and evidently is not affected by a part of $\nabla^{\#}\dot{\gamma}_\alpha$ parallel to $\mathbf{m}_\alpha$, i.e. normal to the respective slip plane. Hence, by analogy to the rate form of Eq. (2.50), $\overset{\diamond}{\mathbf{G}}\mathbf{n}^{\#}$ represents the incremental net Burgers vector associated with GNDs being induced by in-plane gradients of slip-rates, irrespectively of the existing dislocation structure that does not influence the definition (3.10) of $\overset{\diamond}{\mathbf{G}}$.

The effective slip-rate gradient $\dot{\chi}$ is defined in the finite deformation framework, by analogy to the former expression (2.59) at small strain, as follows

$$\dot{\chi} = \|\overset{\diamond}{\mathbf{G}}\| = \Big\| \sum_\alpha \mathbf{s}_\alpha \otimes (\nabla^{\#}\dot{\gamma}_\alpha \times \mathbf{m}_\alpha) \Big\|. \tag{3.12}$$

This definition can be modified by specifying another suitable state dependent function φ of slip-rate gradients,

$$\dot{\chi} = \varphi(\nabla\dot{\gamma}_\alpha). \tag{3.13}$$

In view of the discussion presented in Section 2.6, definition (3.12) is adopted here as the primary option for predominantly *monotonic* deformation processes. As already mentioned, the extension of the present approach to cyclic deformation processes is not immediate and is not treated in the present paper.

3.3. Summary of the proposed gradient-enhancement of classical crystal plasticity

The proposed gradient-enhancement of the classical crystal plasticity theory is summarized in Box I. Once the Taylor formula (2.14) is adopted, the model takes a particularly simple form. The crucial (and non-standard) elements are the effective slip-rate gradient $\dot{\chi}$, the characteristic length ℓ, and the enhanced evolution law for the isotropic part τ of the critical resolved shear stresses.

Box I: Governing equations of the gradient-enhanced anisotropic hardening law for a single crystal.

Effective slip rate	$\dot{\gamma} = \sum_\alpha \dot{\gamma}_\alpha$
Effective slip-rate gradient	$\dot{\chi} = \varphi(\nabla\dot{\gamma}_\alpha) = \big\| \sum_\alpha \mathbf{s}_\alpha \otimes (\nabla^{\#}\dot{\gamma}_\alpha \times \mathbf{m}_\alpha) \big\|$
Voce-type hardening	$\theta = \theta_\tau(\tau) = \theta_0 \left(1 - \dfrac{\tau}{\tau_{\max}}\right)$
Characteristic length	$\ell = \dfrac{\tau'_\rho}{b\theta} = \dfrac{a^2\mu^2 b}{2\tau\theta}$
Isotropic part of critical resolved shear stresses	$\dot{\tau} = \theta\,(\dot{\gamma} + \ell\dot{\chi})$
Anisotropic hardening law	$\dot{\tau}^{\mathrm{c}}_\alpha = \theta \left(\sum_\beta q_{\alpha\beta}\dot{\gamma}_\beta + \ell\dot{\chi} \right)$

REMARK 6. The Taylor formula (2.14) can be replaced by an alternative relationship between ρ and τ, specified by a different function $\tau = \tau_\rho(\rho)$. Then,

in general, the dislocation density ρ, rather than τ, would be an independent variable to be integrated according to Eq. (2.21). However, one could also return to τ as an independent variable by using an inverse function of τ_ρ.

Remark 7. The Voce-type hardening law (2.47) can be replaced by any suitable hardening law $\theta = \theta_\tau(\tau)$ that specifies the isotropic hardening modulus θ as a function of the isotropic part τ of the critical resolved shear stresses.

Remark 8. The specific right-hand expression for $\dot{\chi}$ can be replaced by another suitable function $\dot{\chi} = \varphi(\nabla\dot{\gamma}_\alpha)$ of slip-rate gradients. The small-strain model is obtained simply by redefining the effective slip-rate gradient $\dot{\chi}$ by $\dot{\chi} = \|\dot{\boldsymbol{\alpha}}\|$, cf. Eq. (2.59), while the other formulae remain unaltered.

The critical resolved shear stresses τ^{c}_α governed by the resulting gradient-enhanced anisotropic hardening law (possibly in an extended version $(2.40)_2$) can be combined with virtually any crystal plasticity model, including a higher-order gradient model for more refined analysis or regularization purposes. In the present version, the derived gradient-enhanced incremental hardening law (2.31) introduces, through definition (3.13), slip-rate gradients $\nabla\dot{\gamma}_\alpha$ into the standard set of equations governing the rate-boundary value problem of crystal plasticity.

4. Conclusion

A new framework of gradient-enhanced plasticity of metal single crystals at arbitrary deformation has been developed. The equations of the proposed incremental anisotropic hardening law for a single crystal have been summarized in Box I. The key equation (2.31) represents an extremely simple gradient-enhancement of the conventional incremental strain-hardening law (2.1). It can hardly be simplified further, hence the adjective 'minimal' is used. In essence, only the evolution equation for the isotropic part τ of the critical resolved shear stresses τ^{c}_α is postulated to be affected by an average GND density rate induced by slip-rate gradients, without changing the remaining classical continuum framework. Moreover, the derived internal length scale ℓ is expressed through τ and standard parameters of a non-gradient hardening law, so that no further assumption is needed to define a characteristic length.

It has been shown that this internal length scale is closely linked to the mean free path of dislocations, a standard length-scale parameter in the physically-based dislocation theory of plasticity without macroscopic strain gradients. In fact, these two characteristic lengths coincide in the absence of the dislocation annihilation term. In Remark 3 the circumstances have been summarized in which the present internal length scale ℓ possesses a direct physical interpretation that is frequently missing in other gradient-plasticity models.

The model has been implemented in a finite element environment and applied to three-dimensional simulations of fcc single crystals. The results presented in Part II [61] of this paper show that the experimentally observed indentation size effect in a Cu single crystal is captured correctly in spite of the absence of any adjustable length-scale parameter in the proposed framework. Therefore, it is believed that a step has been made towards a simple reference model of gradient-enhanced crystal plasticity that might provide a benchmark for more refined approaches.

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