The influence of the dissipation due to the plastic spin on the size effects describable by means of isotropic strain gradient plasticity

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SUMMARY. Within the context of work-conjugate, higher-order strain gradient plasticity (see, e.g., [1]), it has been recently shown [2, 3] that, even in the small displacement range, it may be important to constitutively prescribe the dissipation due to the plastic spin in the isotropic modelling of strain gradient plasticity, as earlier envisaged by Gurtin in section 12 of [4]. In this work, we wish to further investigate on such a modelling possibility.

With reference to the so-called energetic and dissipative strain gradients (see, e.g., [5]), and the related size effects, we mainly aim at getting an insight on the role of the material parameters involved in both the free energy and the dissipation function.

About the form of the free energy, we are concerned with its contribution due to geometrically necessary dislocations [6], a function of Nye's dislocation density tensor [7, 8] also called the defect energy (e.g., [4]): a few studies on this, providing significantly different results, are available in the literature [9, 10, 11, 12]. Here, just to appreciate how much the results are influenced by different choices, we analyse a quite simple power-law expression for the free energy which, for appropriate choices of its exponent particularises to the quadratic and the one-homogeneous forms, already exploited by various authors.

Instead, it is much more difficult to find a dissipation function (governing the isotropic hardening) able to account, in the continuum average, for the dissipation due to the motion of dislocations [13]. We will try to reach our goal by determining the influence of the various material length scales and parameters which is possible to include in the modelling.

For what concerns the material parameter χ ruling the influence of the dissipation due to plastic spin, we shall show that it strongly affects the energetic size effect which is possible to describe. In particular, if χ is set as proposed in [3], i.e., as a function of both energetic and dissipative length scales, and other standard material parameters, then, it turns out that the energetic size effect mainly consists of strengthening (i.e., an increase in the initial yield stress) accompanied with diminishing size, contrary to what usually found within strain gradient plasticity, i.e., that the energetic size effect is related to the strain hardening variation. Actually, in *crystal* plasticity, while the dissipative size effect seems always to consist of some strengthening, the energetic size effect is strongly related to the number and relative orientations of families of active slip systems [2], and provides an increase in strain hardening without strengthening only when plasticity develops on a very limited number of systems (typically in single slip). Hence, χ should be set as in [3] or differently, depending on whether the *isotropic* modelling is intended to approximate the multislip behaviour of crystals or not.

1 INTRODUCTION

We consider strain gradient plasticity models for the description of the mechanical behaviour exhibited by metallic components undergoing inhomogeneous plastic flow, in the size range between a few tens of micrometers to a few hundreds of nanometers. As nowadays well documented in the literature (see, e.g., Fleck et al. [14]), diminishing size within such a range leads to some peculiar size effects (classified as "second-order" effects by Geers et al. [15]), with smaller being stronger.

Adopting the terminology of Hirschberger and Steinmann [16], we classify the theory presented here as gradient plasticity based on the plastic strain (in contrast with the theories where also the gradient of the elastic strain plays a role, as in Fleck and Hutchinson [17]), characterised by

- an *external* variable approach (as we define some appropriate measures of the plastic parts of the first and second gradients of the displacement as *primary* variables with conjugated stresses entering the higher-order balance equations which substitute the so-called Karush-Kuhn-Tucker conditions, not implicitly enforced)

- a *compatible* formulation (as, for instance, we derive the higher-order equilibrium equations by imposing that the plastic part of the second gradient of the displacement is the gradient of the plastic strain).

This notwithstanding, the theory proposed does not belong to any specific category analysed by Hirschberger and Steinmann [16], because they neglect the possibility to distinguish between *energetic* and *dissipative* strain gradient dependences within the external variable approach, as we do here, so that a dissipation inequality leading to a flow rule can be constitutively designed.

Since we believe that the defect energy should be expressed in terms of Nye's tensor (some reasons for this are given in [3, 2]), the observation that Nye's tensor depends on equal footing upon the plastic strain and plastic spin suggests that also the latter should enter the dissipative potential (see, e.g., [4]). In fact, in [3] it has been shown that neglecting the dissipation due to plastic spin in an isotropic strain gradient model may lead to a poor description of the micro-plasticity.

In this work, at the light of the way recently proposed by Del Piero [18] to derive the balance equations from the principle of virtual work, we will discuss shortcomings and benefits of alternative constitutive choices of *primary* kinematic variables employed to account for the dissipation due to the plastic spin; moreover, we shall appreciate the strong coupling of those choices with the constitutive assumptions for the defect energy in determining the modelling capability.

Notation We use lightface letters for scalars. Bold face is used for first-, second-, and third-order tensors, in most cases respectively represented by small Latin, small Greek, and capital Latin letters. In some exceptions, for the sake of clarity, we make use of indices, referred to an orthogonal cartesian system. " $\cdot$ " represents the scalar product of vectors and tensors (e.g., $a = \boldsymbol{b} \cdot \boldsymbol{u} \equiv b_i u_i$, $b = \boldsymbol{\sigma}\cdot\boldsymbol{\varepsilon} \equiv \sigma_{ij}\varepsilon_{ij}$, $c = \boldsymbol{T}\cdot\boldsymbol{S} \equiv T_{ijk}S_{ijk}$). For any tensor $\boldsymbol{\rho}$, the scalar product by itself is $|\boldsymbol{\rho}|^2 \equiv \boldsymbol{\rho}\cdot\boldsymbol{\rho}$. " $\times$ " is adopted for the vector product: $\boldsymbol{t} = \boldsymbol{m} \times \boldsymbol{n} \equiv e_{ijk} m_j n_k = t_i$, with e_{ijk} the alternating symbol (one of the exceptions, as it is a third-order tensor represented by a small Latin letter), and, for $\boldsymbol{\zeta}$ a second-order tensor: $\boldsymbol{\zeta} \times \boldsymbol{n} \equiv e_{jlk}\zeta_{il} n_k$. For the composition of tensors of different order the lower-order tensor is on the right and all its indices get saturated, e.g.: for $\boldsymbol{\sigma}$ a second-order tensor and $\boldsymbol{n}$ a vector, $\boldsymbol{t} = \boldsymbol{\sigma}\boldsymbol{n} \equiv \sigma_{ij} n_j = t_i$; for $\boldsymbol{T}$ a third-order tensor and $\boldsymbol{n}$ a vector, $\boldsymbol{T}\boldsymbol{n} \equiv T_{ijk} n_k$; for $\mathbb{L}$ a fourth-order tensor and $\boldsymbol{\varepsilon}$ a second-order tensor, $\boldsymbol{\sigma} = \mathbb{L}\boldsymbol{\varepsilon} \equiv L_{ijkl}\varepsilon_{kl} = \sigma_{ij}$. Moreover, $(\nabla \boldsymbol{u})_{ij} \equiv \partial u_i / \partial x_j \equiv u_{i,j}$, $(\operatorname{div} \boldsymbol{\sigma})_i \equiv \sigma_{ij,j}$, and $(\operatorname{curl} \boldsymbol{\gamma})_{ij} \equiv e_{jkl}\gamma_{il,k}$ designate, respectively, the gradient of the vector field $\boldsymbol{u}$, the divergence of the second-order tensor $\boldsymbol{\sigma}$, and the curl of the second-order tensor $\boldsymbol{\gamma}$, whereas $(\operatorname{dev} \boldsymbol{\varsigma})_{ij} \equiv (\varsigma_{ij} - \delta_{ij}\varsigma_{kk}/3)$ (with $\boldsymbol{\delta}$ the Kronecker symbol), $(\operatorname{sym} \boldsymbol{\varsigma})_{ij} \equiv (\varsigma_{ij} + \varsigma_{ji})/2$, and $(\operatorname{skw} \boldsymbol{\varsigma})_{ij} \equiv (\varsigma_{ij} - \varsigma_{ji})/2$ denote, respectively, the deviatoric, symmetric, and skew parts of the second-order tensor $\boldsymbol{\varsigma}$.

2 THE MODEL

We are concerned with the mechanical response of a body occupying a space region Ω, whose external surface S, of outward normal $\boldsymbol{n}$, consists of two *complementary* parts: S_T, where the tractions $\boldsymbol{t}^0$ are known and *dislocations are free to exit the body*, and S_U, where the displacement $\boldsymbol{u}^0$ is known and *dislocations are blocked*. More general higher-order boundary conditions can be easily incorporated in the theory, but they are irrelevant for what follows.

2.1 *The Principle of Virtual Work*

We base the theoretical framework on the principle of virtual work, in which, by following Del Piero [18], the main assumption consists in the belief that the virtual work on any region Π of Ω be provided by two contributions, one consisting of volume density of body forces $\boldsymbol{b}$ and the other determined by contact actions on the boundary of Π; it is assumed that such contact actions consist of two fields $\boldsymbol{t}$ and $\boldsymbol{\tau}$ associated with the displacement $\boldsymbol{u}$ and the plastic distortion $\boldsymbol{\gamma}$, the latter being plastic part of the displacement gradient:

$$\nabla \boldsymbol{u} = (\nabla \boldsymbol{u})_{\text{el}} + \boldsymbol{\gamma} \tag{1}$$

Hence, with $\delta\epsilon = \dot{\epsilon}\delta t$ a compatible variation of the kinematic field ϵ, the virtual work on Π is defined as:

$$\mathcal{W}(\Pi, \delta\boldsymbol{u}, \delta\boldsymbol{\gamma}) = \int_{\Pi} \boldsymbol{b} \cdot \delta\boldsymbol{u}\, dV + \int_{\partial\Pi} \Big(\boldsymbol{t} \cdot \delta\boldsymbol{u} + \boldsymbol{\tau} \cdot \delta\boldsymbol{\gamma}\Big) dA \tag{2}$$

By enforcing that the virtual work is left unchanged by rigid body translation and rotation, i.e., $\mathcal{W}(\Pi, \boldsymbol{c}, \boldsymbol{0}) = 0$ and $\mathcal{W}(\Pi, \boldsymbol{c} \times \boldsymbol{x}, \boldsymbol{0}) = 0$ for any constant vector $\boldsymbol{c}$, and by using the Cauchy tetrahedron theorem, one deduces (see, e.g., [18]) the existence of the standard symmetric Cauchy stress $\boldsymbol{\sigma}$ such that

$$\text{div}\, \boldsymbol{\sigma} + \boldsymbol{b} = \boldsymbol{0} \ \text{ in } \ \Pi \tag{3}$$

$$\boldsymbol{\sigma}\boldsymbol{n} = \boldsymbol{t} \ \text{ on } \ \partial\Pi \tag{4}$$

so that the virtual work can be rewritten as:

$$\mathcal{W}(\Pi, \delta\boldsymbol{u}, \delta\boldsymbol{\gamma}) = \int_{\Pi} \boldsymbol{\sigma} \cdot \ \text{sym}\, \nabla\delta\boldsymbol{u}\, dV + \int_{\partial\Pi} \boldsymbol{\tau} \cdot \delta\boldsymbol{\gamma}\, dA \tag{5}$$

Now, since we wish to account for the dissipation due to plastic spin, we do *not* impose

$$\mathcal{W}(\Pi, \boldsymbol{0}, \boldsymbol{\varpi}) = 0 \tag{6}$$

for any *constant* skew-symmetric second order tensor $\boldsymbol{\varpi}$, as instead done by Del Piero [18] in order to obtain the model of Gurtin and Anand [5].

Hence, all the remaining (higher-order) balance equations have to be derived by making an hypothesis which allows the transformation of the area integral in equation (5) into a volume integral. To this purpose, we define the following body forces $\tilde{\boldsymbol{\beta}}$ [18]:

$$\tilde{\boldsymbol{\beta}} = -\lim_{r\to 0}\left(\frac{1}{|B(\boldsymbol{x}, r)|}\int_{\partial B(\boldsymbol{x}, r)} \boldsymbol{\tau}\, dA\right) \tag{7}$$

where $B(\boldsymbol{x}, r)$ is the sphere centered in $\boldsymbol{x}$ of radius r and volume $|B(\boldsymbol{x}, r)|$. This allows the deduction of the existence of a third-order stress tensor $\boldsymbol{S}$ such that

$$\text{div}\, \boldsymbol{S} + \tilde{\boldsymbol{\beta}} = \boldsymbol{0} \ \text{ in } \ \Pi \tag{8}$$

$$\boldsymbol{S}\boldsymbol{n} = \boldsymbol{\tau} \ \text{ on } \ \partial\Pi \tag{9}$$

Because of the different nature of the hypothesis used to derive these equations with respect to that behind the derivation of (3) and (4), one may call them pseudo-balance equations, as proposed by Del Piero [18].

Then, the virtual work becomes:

$$\mathcal{W}(\Pi, \delta\boldsymbol{u}, \delta\boldsymbol{\gamma}) = \int_{\Pi} \Big(\boldsymbol{\sigma} \cdot \ \text{sym}\, \nabla\delta\boldsymbol{u} + \boldsymbol{S} \cdot \nabla\delta\boldsymbol{\gamma} - \tilde{\boldsymbol{\beta}} \cdot \delta\boldsymbol{\gamma}\Big) dV \tag{10}$$

Now, we decompose $\tilde{\boldsymbol{\beta}}$ into the opposites of its symmetric and skew-symmetric parts

$$\text{sym}\, \tilde{\boldsymbol{\beta}} = -\boldsymbol{\xi} \qquad \text{skw}\, \tilde{\boldsymbol{\beta}} = -\boldsymbol{\omega} \tag{11}$$

and *assume* that $\boldsymbol{S}$ admits the decomposition

$$\boldsymbol{S} = \boldsymbol{S}^{(\text{def})} + \boldsymbol{T}^{(\varepsilon)} \tag{12}$$

such that

$$S^{(\text{def})}_{ijk} = e_{kjh}\zeta_{ih} \qquad T^{(\varepsilon)}_{ijk} = T^{(\varepsilon)}_{jik} \tag{13}$$

in which $\boldsymbol{\zeta}$ is called the defect stress. The virtual work turns out ot read:

$$\mathcal{W}(\Pi, \delta\boldsymbol{u}, \delta\boldsymbol{\gamma}) = \int_{\Pi} \Big(\boldsymbol{\sigma} \cdot \ \text{sym}\, \nabla\delta\boldsymbol{u} + \boldsymbol{\zeta} \cdot \ \text{curl}\, \delta\boldsymbol{\gamma} + \boldsymbol{\xi} \cdot \ \text{sym}\, \delta\boldsymbol{\gamma} + \boldsymbol{\omega} \cdot \ \text{skw}\, \delta\boldsymbol{\gamma} + \boldsymbol{T}^{(\varepsilon)} \cdot \ \text{sym}\, \nabla\delta\boldsymbol{\gamma}\Big) dV \tag{14}$$

By exploiting the standard definitions for the total strain

$$\boldsymbol{\varepsilon} = \ \text{sym}\, \nabla\boldsymbol{u}\ ,$$

Nye's dislocation density tensor [7, 8]

$$\boldsymbol{\alpha} = \ \text{curl}\, \boldsymbol{\gamma}\ , \tag{15}$$

and plastic strain and spin

$$\boldsymbol{\varepsilon}^p = \ \text{sym}\, \boldsymbol{\gamma} \qquad \boldsymbol{\theta}^p = \ \text{skw}\, \boldsymbol{\gamma}\ , \tag{16}$$

the (*internal*) virtual work can be re-written in a more readable form:

$$\mathcal{W}_i(\Pi) = \int_{\Pi} \Big(\boldsymbol{\sigma} \cdot \delta\boldsymbol{\varepsilon} + \boldsymbol{\zeta} \cdot \delta\boldsymbol{\alpha} + \boldsymbol{\xi} \cdot \delta\boldsymbol{\varepsilon}^p + \boldsymbol{\omega} \cdot \delta\boldsymbol{\theta}^p + \boldsymbol{T}^{(\varepsilon)} \cdot \delta\nabla\boldsymbol{\varepsilon}^p\Big) dV \tag{17}$$

Finally, by defining the following stress, which will result to be conjugated to the plastic strain rate through the plastic potential,

$$\boldsymbol{\rho} = \boldsymbol{\xi} + \ \text{dev}\, \boldsymbol{\sigma} \tag{18}$$

the equilibrium equations (3) and (8) for the whole body free from standard body forces read:

$$\text{div}\, \boldsymbol{\sigma} = \boldsymbol{0} \quad \text{in} \quad \Omega \tag{19}$$

$$\boldsymbol{\rho} - \ \text{dev}\, \boldsymbol{\sigma} - \ \text{div}\, \boldsymbol{T}^{(\varepsilon)} + \ \text{sym}\, [\ \text{dev}\, (\ \text{curl}\, \boldsymbol{\zeta})] = \boldsymbol{0} \quad \text{in} \ \ \Omega \tag{20}$$

$$\boldsymbol{\omega} + \ \text{skw}\, (\ \text{curl}\, \boldsymbol{\zeta}) = \boldsymbol{0} \quad \text{in} \ \ \Omega \tag{21}$$

with boundary conditions:

$$\boldsymbol{\sigma}\boldsymbol{n} = \boldsymbol{t}^0 \ \text{on}\ S_T \tag{22}$$

$$\boldsymbol{T}^{(\varepsilon)}\boldsymbol{n} + \ \text{sym}\, [\ \text{dev}\, (\boldsymbol{\zeta} \times \boldsymbol{n})] = \boldsymbol{0} \quad \text{on} \ \ S_T \tag{23}$$

$$\text{skw}\, (\boldsymbol{\zeta} \times \boldsymbol{n}) = \boldsymbol{0} \quad \text{on} \ \ S_T \tag{24}$$

Discussion The plastic spin dissipation could be accounted for also by means of constitutive choices respectful of the invariance (6), as proposed in [18]. To this purpose, first of all, we impose (6) and obtain that $\dot{\boldsymbol{\theta}}^p$ cannot directly enter the (internal) virtual work (or, in other words, this sets $\boldsymbol{\omega} \equiv \mathbf{0}$). Then, we remove the assumption (12), and replace it with the following decomposition which allows us to account for the dissipation due to the gradient of the plastic spin:

$$\boldsymbol{S} = \boldsymbol{S}^{(\text{def})} + \boldsymbol{T}^{(\varepsilon)} + \boldsymbol{T}^{(\vartheta)} \tag{25}$$

where

$$S_{ijk}^{(\text{def})} = e_{kjh}\zeta_{ih} \qquad T_{ijk}^{(\varepsilon)} = T_{jik}^{(\varepsilon)} \qquad T_{ijk}^{(\vartheta)} = -T_{jik}^{(\vartheta)} \tag{26}$$

Note that there is no redundancy in this decomposition of $\boldsymbol{S}$ because of the completely different constitutive choices that we have in mind for $\boldsymbol{\zeta}$ and $\boldsymbol{T}^{(\vartheta)}$, the former related to part of the free energy, the latter describing part of the dissipation (analogously to the prescriptions of next subsections 2.2 and 2.3).

The assumption (25)-(26) leads to the following form of the (internal) virtual work, substituting (17):

$$\mathcal{W}_i(\Pi) = \int_\Pi \Big(\boldsymbol{\sigma} \cdot \delta\boldsymbol{\varepsilon} + \boldsymbol{\zeta} \cdot \delta\boldsymbol{\alpha} + \boldsymbol{\xi} \cdot \delta\boldsymbol{\varepsilon}^p + \boldsymbol{T}^{(\varepsilon)} \cdot \delta\nabla\boldsymbol{\varepsilon}^p + \boldsymbol{T}^{(\vartheta)} \cdot \delta\nabla\boldsymbol{\theta}^p \Big) dV \tag{27}$$

The pseudo-balance equation (20) remains the same, while the equation (21) has to be replaced by

$$\text{skw}\ (\ \text{curl}\ \boldsymbol{\zeta}) - \ \text{div}\ \boldsymbol{T}^{(\vartheta)} = \mathbf{0} \quad \text{in}\ \ \Omega \tag{28}$$

This modelling is extremely appealing because both it respects (6) and it seems to even better follow the view by which the internal work should be affected by the *different* plastic rotation of two neighbour *macroscopic* material points.

Unfortunately, our preliminary calculations (done in a similar way as in [3], with analogous constitutive choices for the free energy and for the dissipative potential — see also the following subsections) have shown that this model is not as good as that coming from the choices leading to (17) in representing the mechanical response of a strain gradient *crystalline* strip under simple shear. Hence, we leave this open issue for future developments and keep working on the model (17)–(24), substantially equivalent to that sketched in section 12 of Gurtin [4].

2.2 *The free energy*

The free energy reads

$$\frac{1}{2}\mathbb{L}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) \cdot (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) + \mathcal{D}(\boldsymbol{\alpha}) \tag{29}$$

where $\mathbb{L}$ is the elastic stiffness and $\mathcal{D}(\boldsymbol{\alpha})$ is the defect energy. Of course, the Cauchy stress and the defect stress respectively read:

$$\boldsymbol{\sigma} = \mathbb{L}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) \tag{30}$$

$$\boldsymbol{\zeta} = \frac{\partial \mathcal{D}(\boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}} \tag{31}$$

which is the transpose of what Gurtin [19] called the defect stress.

Choice (29) for the free energy makes it meaningful the following form of the (internal) virtual work, in the place of (14):

$$\mathcal{W}_i(\Pi) = \int_\Pi \Big(\underbrace{\boldsymbol{\sigma} \cdot (\delta\boldsymbol{\varepsilon} - \delta\boldsymbol{\varepsilon}^p) + \boldsymbol{\zeta} \cdot \delta\boldsymbol{\alpha}}_{\text{energetic}} + \underbrace{\boldsymbol{\rho} \cdot \delta\boldsymbol{\varepsilon}^p + \boldsymbol{\omega} \cdot \delta\boldsymbol{\theta}^p + \boldsymbol{T}^{(\varepsilon)} \cdot \delta\nabla\boldsymbol{\varepsilon}^p}_{\text{dissipative}} \Big) dV \tag{32}$$

The constitutive choice for the defect energy The defect energy can be chosen as:

$$\mathcal{D}(\boldsymbol{\alpha}) = \frac{1}{M+1}\mu(\ell|\boldsymbol{\alpha}|)^{M+1} \tag{33}$$

in which μ is the shear modulus in the case of an isotropic linear elastic behaviour, and ℓ is an *energetic* material length scale quantifying the size effect due to GNDs long-range interactions. The third material parameter M governs the nonlinearity: $M = 1$ leads to the quadratic form exploited by many authors (e.g., [19] and [3]), while $M \to 0$ leads to a defect energy homogeneous of degree 1 on Nye's tensor, as proposed by Ohno and Okumura [10] and Garroni et al. [11], even though (i) Ohno and Okumura take a significantly different version, where the interactions among different systems are unaccounted for and (ii) the reasoning of Garroni et al. is related to an infinite dislocation density, never to be reached in real materials. Moreover, let us put an argument against the one-homogeneous form of the defect energy: such a form, in fundamental deformation modes as the simple shear, ideally governed by scalar fields, would predict a constant defect stress, independently upon the Nye tensor, that is, disregarding the length of dislocation pile-ups; such a model, expected to describe some strengthening, seems to be in contrast with the purposes of the defect energy to account for GNDs.

Choice (33) leads to

$$\boldsymbol{\zeta} = \mu\ell^2(\ell|\boldsymbol{\alpha}|)^{M-1}\boldsymbol{\alpha}$$

Fleck and Willis [20] consider the free energy extension to be a function of $\boldsymbol{\varepsilon}^p$ and $\nabla\boldsymbol{\varepsilon}^p$, which can in case turn out to be a function of curl $\boldsymbol{\varepsilon}^p$, not $\boldsymbol{\alpha}$, as it neglects the plastic spin. In any case, Fleck and Willis do not suggest any specific form of their free energy extension, while they point out that it could even be a function of the history of $\boldsymbol{\varepsilon}^p$ and $\nabla\boldsymbol{\varepsilon}^p$. Analogously, the defect energy $\mathcal{D}(\boldsymbol{\alpha})$ could also be chosen as a function of the history of Nye's tensor, with the requirement that $\delta\mathcal{D} = \boldsymbol{\zeta}\cdot\delta\boldsymbol{\alpha}$, but this possibility seems to us out of the physical picture by which Nye's tensor accounts for an average of the stress field due to the jumps in displacement inherent to the presence GNDs *at rest*.

2.3 *The constitutive choice for the dissipative stresses*

The dissipative stresses must be defined in such a way that the following "dissipative inequality" holds (see, e.g., Gurtin and Anand [5] for the analogous case related to plastically irrotational materials):

$$\boldsymbol{\rho}\cdot\delta\boldsymbol{\varepsilon}^p + \boldsymbol{\omega}\cdot\delta\boldsymbol{\theta}^p + \boldsymbol{T}^{(\varepsilon)}\cdot\delta\nabla\boldsymbol{\varepsilon}^p \geq 0 \tag{34}$$

A prescription consistent with this requirement which usually allows a satisfactory description of the evolution of the yield stress and the strain hardening/softening (see Gurtin and Anand [5]) reads:

$$\mathcal{V}(\dot{\boldsymbol{\varepsilon}}^p, \dot{\boldsymbol{\theta}}^p, \nabla\dot{\boldsymbol{\varepsilon}}^p) = \frac{\sigma_0\dot{\varepsilon}_0}{N+1}\left(\frac{\dot{E}^p}{\dot{\varepsilon}_0}\right)^{N+1} \tag{35}$$

with the assumption

$$\dot{E}^p := \sqrt{\frac{2}{3}|\dot{\boldsymbol{\varepsilon}}^p|^2 + \chi|\dot{\boldsymbol{\theta}}^p|^2 + \frac{2}{3}L^2|\nabla\dot{\boldsymbol{\varepsilon}}^p|^2} \tag{36}$$

σ_0, $\dot{\varepsilon}_0$, N, and χ are non-negative material parameters, as well as L that is a *dissipative* material length scale, so-called because related to dissipative higher-order stresses. Of course, definition (36) is phenomenological, and we do not see how to do anything more physically based at this scale for many reasons, among which the fact that it is still unclear how to describe in average the relevant features of the short-range interactions among dislocations (Roy et al. [13], Kröner [21]). In [3], it has been shown that the parameter χ governing the dissipation due to plastic spin can be identified on the basis of the comparison with an isotropic model obtained from a *crystal* model in which any direction is assumed to be an active slip system. Such a criterium provides:

$$\chi = \left[\frac{3}{2} + \frac{\sigma_0}{\mu\varepsilon_0}\Big(\frac{L}{\ell}\Big)^2\right]^{-1} \tag{37}$$

Of course, this may be useful if the isotropic modelling is intended to approximate the behaviour of a single grain in multislip. However, in other circumstances the effect due to the plastic spin should be even more important.

The dissipative stresses result:

$$\boldsymbol{\rho} = \frac{\partial \mathcal{V}(\dot{\boldsymbol{\varepsilon}}^p, \dot{\boldsymbol{\theta}}^p, \nabla\dot{\boldsymbol{\varepsilon}}^p)}{\partial \dot{\boldsymbol{\varepsilon}}^p} = \frac{2}{3}\frac{\sigma_0}{\dot{\varepsilon}_0}\left(\frac{\dot{E}^p}{\dot{\varepsilon}_0}\right)^{N-1}\dot{\boldsymbol{\varepsilon}}^p \tag{38}$$

$$\boldsymbol{\omega} = \frac{\partial \mathcal{V}(\dot{\boldsymbol{\varepsilon}}^p, \dot{\boldsymbol{\theta}}^p, \nabla\dot{\boldsymbol{\varepsilon}}^p)}{\partial \dot{\boldsymbol{\theta}}^p} = \chi\frac{\sigma_0}{\dot{\varepsilon}_0}\left(\frac{\dot{E}^p}{\dot{\varepsilon}_0}\right)^{N-1}\dot{\boldsymbol{\theta}}^p \tag{39}$$

$$\boldsymbol{T}^{(\varepsilon)} = \frac{\partial \mathcal{V}(\dot{\boldsymbol{\varepsilon}}^p, \dot{\boldsymbol{\theta}}^p, \nabla\dot{\boldsymbol{\varepsilon}}^p)}{\partial \nabla\dot{\boldsymbol{\varepsilon}}^p} = \frac{2}{3}L^2\frac{\sigma_0}{\dot{\varepsilon}_0}\left(\frac{\dot{E}^p}{\dot{\varepsilon}_0}\right)^{N-1}\nabla\dot{\boldsymbol{\varepsilon}}^p \tag{40}$$

Standard arguments allow the plastic potential to be written in terms of an equivalent stress measure Σ:

$$\mathcal{V} = \frac{\Sigma \dot{E}^p}{N+1}\,, \qquad \Sigma = \sqrt{\frac{3}{2}|\boldsymbol{\rho}|^2 + \frac{1}{\chi}|\boldsymbol{\omega}|^2 + \frac{3}{2L^2}|\boldsymbol{T}^{(\varepsilon)}|^2} \tag{41}$$

Discussion For isotropic solids the most general definition of $\dot{E}^p$ involves three dissipative length scales instead of just L (see, e.g., Fleck and Hutchinson [17]). Moreover, Fleck and Willis [20] have proposed a form (including the possibility of describing anisotropic bodies) combining all the relevant components of the plastic strain and its gradient into a positive definite matrix. Furthermore, as proposed by Molinari and Ravichandran [22], and recently reconsidered by Evans and Hutchison [23], the material length scales may change with the amount of plasticity, and this is seems to be particularly relevant in the isotropic modelling of polycrystal plasticity.

The so-called visco-plastic case (ensured by setting $N > 0$) provides a big benefit: plasticity is developed at any stress level, albeit in small quantity if N is close to 0, so that there is no need to impose any higher-order boundary condition at the internal surfaces between elastic and plastic domains (i.e., the moving elastic-plastic boundaries), problem that one has to face in the rate-independent limit (i.e., $N \to 0$). In such a case, σ_0 may even be replaced by a hardening function σ_Y such that

$$\dot{\sigma}_Y = \mathcal{F}(\sigma_Y)\dot{E}^p \qquad\qquad \sigma_Y(E^p = 0) = \sigma_0 \tag{42}$$

where the function $\mathcal{F}$ governs the strain hardening/softening in such a way that $\sigma_Y > 0$ always and σ_0 is, in the case $N \to 0$, the value of the equivalent stress Σ at which yield starts (that is a sort of internal isotropic hardening for the dissipative stresses).

One can consider a more general P-norm for the definition of the rate of *effective* plastic strain [17, 23]:

$$\dot{E}^p := \left[\Big(\frac{2}{3}|\dot{\boldsymbol{\varepsilon}}^p|^2\Big)^{P/2} + \Big(\chi|\dot{\boldsymbol{\theta}}^p|^2\Big)^{P/2} + L^P\Big(\frac{2}{3}|\nabla\dot{\boldsymbol{\varepsilon}}^p|^2\Big)^{P/2}\right]^{1/P}$$

Evans and Hutchinson [23], based on their observations of scaling trends, propose to abandon the computationally convenient and long beaten path $P = 2$, in favor of the choice $P = 1$. In [2], a different conclusion, supporting the choice $P = 2$, has been drawn within the framework of crystal plasticity.

2.4 *The "flow rule" in terms of kinematic quantities*

By writing the stresses in terms of kinematic quantities consistently with the foregoing constitutive choices, equations (20)-(21) assume the meaning of the *flow rule*. In the viscoplastic case, in which the extension (42) is neglected, we have:

$$\frac{2\sigma_0}{3\dot{\varepsilon}_0}\left\{\left(\frac{\dot{E}^p}{\dot{\varepsilon}_0}\right)^{N-1}(\dot{\varepsilon}^p_{ij} - L^2\dot{\varepsilon}^p_{ij,kk}) - L^2\left[\left(\frac{\dot{E}^p}{\dot{\varepsilon}_0}\right)^{N-1}\right]_{,k}\dot{\varepsilon}^p_{ij,k}\right\} + 2\mu\varepsilon^p_{ij}$$
$$- \mu\ell^2\left(\ell\sqrt{\gamma_{pl,k}\gamma_{pk,l} - \gamma_{pk,l}\gamma_{pk,l}}\right)^{M-1}\left[\varepsilon^p_{ij,kk} - \frac{1}{2}(\gamma_{ik,jk} + \gamma_{jk,ik}) + \frac{1}{3}\delta_{ij}(\gamma_{kl,kl} - \gamma_{ll,kk})\right]$$
$$= 2\mu(\varepsilon_{ij} - \delta_{ij}\varepsilon_{kk}) \quad (43)$$

$$\chi\frac{\sigma_0}{\dot{\varepsilon}_0}\left(\frac{\dot{E}^p}{\dot{\varepsilon}_0}\right)^{N-1}\dot{\theta}^p_{ij} - \mu\ell^2\left(\ell\sqrt{\gamma_{pl,k}\gamma_{pk,l} - \gamma_{pk,l}\gamma_{pk,l}}\right)^{M-1}\left[\theta^p_{ij,kk} - \frac{1}{2}(\gamma_{ik,jk} - \gamma_{jk,ik})\right] = 0 \quad (44)$$

Integrating the system (43)-(44) (together with the other equations and boundary conditions defining the problem) is far harder than obtaining the solution of the analogous problem within the deformation theory context. Hence, by assuming that for monotonic loading the deformation theory provide results close to those obtainable by means of the flow theory, the former modelling will be used next to discuss the outcome of the theory proposed. Let us refer to [3] for the precise equations of the deformation theory, albeit the higher-order balance equations in terms of stresses (20)-(21) are left unchanged in passing from the flow theory to the deformation theory.

3 SIMULATIONS IN SIMPLE SHEAR AND CONCLUDING REMARKS

The concluding remarks are based on the results of the simulations of the simple shear of a strip constrained between two bodies in which dislocations cannot penetrate. The details of such simulations are totally skipped here for the sake of brevity and because most of them can be evicted from what has been done in [3, 2].

The results show that the value of the parameter χ governing the dissipation due plastic spin strongly affects the capability of describing the size effects.

Setting χ as in (37) leads to a model where both the energetic and the dissipative size effects mostly consist of strengthening, without an appreciable variation of strain hardening with diminishing size. This is almost always the case for the dissipative effect, but it is remarkable for the energetic effect. This result is corroborated by previous analyses in multislip of single crystals [2], which showed the same peculiarity (let us remind that equation (37) was obtained for "infinite-multislip"). Also, the numerical results show that this energetic strengthening seems to hold for any relevant value of the material parameters M and N governing the nonlinearity, as in the constitutive prescriptions (33) and (35), and this was not a priori obvious since equation (37) was obtained in the linear case.

Moreover, we have found that the behaviour is extremely sensitive to the exponent M in the power-law put forward for the defect energy. Also, we have confirmed the expectation, based on the observation after equation (33), that values of M close to 0, independently upon how χ is set, lead to energetic strengthening, inhibiting the capability to describe conspicuous strain hardening variations.

The above conclusions suggest that the actual forms of defect energy and plastic potential are of fundamental importance, and a large effort should by put in order to obtain simple and effective forms of them, for instance, by extensively comparing the results of Discrete Dislocation simulations (e.g., [24, 25]) with those obtained from a robust finite element implementation of strain gradient models.

Moreover, it would be interesting to investigate on the effect of the plastic spin on the mechanical response of polycrystals, also by accounting for the behaviour of grain boundaries, by appropriately extending the technology developed by Fleck and Willis [26, 20].

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References

[1] Gudmundson, P., "A unified treatment of strain gradient plasticity", *J. Mech. Phys. Solids*, **52**, 1379–1406 (2004).

[2] Bardella, L. and Giacomini, A., "Influence of material parameters and crystallography on the size effects describable by means of strain gradient plasticity", *J. Mech. Phys. Solids*, **56**, 2906–2934 (2008).

[3] Bardella, L., "A comparison between crystal and isotropic strain gradient plasticity theories with accent on the role of the plastic spin", *Eur. J. Mech. A-Solid.*, **28**, 638–646 (2009).

[4] Gurtin, M. E., "A gradient theory of small-deformation isotropic plasticity that accounts for the Burgers vector and for dissipation due to plastic spin", *J. Mech. Phys. Solids*, **52**, 2545–2568 (2004).

[5] Gurtin, M. E. and Anand, L., "A gradient theory of strain-gradient plasticity for isotropic, plastically irrotational materials. Part I: Small deformations", *J. Mech. Phys. Solids*, **53**, 1624–1649 (2005).

[6] Ashby, M. F., "The deformation of plastically non-homogeneous materials", *Philos. Mag.*, **21**, 399–424 (1970).

[7] Nye, J. F., "Some geometrical relations in dislocated crystals", *Acta Metall.*, **1**, 153–162 (1953).

[8] Arsenlis, A. and Parks, D. M., "Crystallographic aspects of geometrically-necessary and statistically-stored dislocation density", *Acta Mater.*, **47**, 1597–1611 (1999).

[9] Nicola, L., van der Giessen, E. and Gurtin, M. E., "Effect of defect energy on strain-gradient predictions of confined single-crystal plasticity", *J. Mech. Phys. Solids*, **53**, 1280–1294 (2005).

[10] Ohno, N. and Okumura, D., "Higher-order stress and grain size effects due to self-energy of geometrically necessary dislocations", *J. Mech. Phys. Solids*, **55**, 1879–1898 (2007).

[11] Garroni, A., Leoni, G. and Ponsiglione, M., "Gradient theory for plasticity via homogenization of discrete dislocations", *Preprint available at at http://cvgmt.sns.it/people* (2009).

[12] Xiang, Y., "Continuum approximation of the Peach-Köehler force on dislocations in a slip plane", *J. Mech. Phys. Solids*, **57**, 728–743 (2009).

[13] Roy, A., Peerlings, R. H. J., Geers, M. G. D. and Kasyanyuk, Y., "Continuum modeling of dislocations interactions: why discreteness matters?", *Mater. Sci. Eng./A*, **486**, 653–661 (2008).

[14] Fleck, N. A., Muller, G. M., Ashby, M. F. and Hutchinson, J. W., "Strain gradient plasticity: theory and experiments", *Acta Metall. Mater.*, **42**, 475–487 (1994).

[15] Geers, M. G. D., Brekelmans, W. A. M. and Janssen, P. J. M., "Size effects in miniaturized polycrystalline FCC samples: Strengthening versus weakening", *Int. J. Solids Struct.*, **43**, 7304–7321 (2006).

[16] Hirschberger, C. B. and Steinmann, P., "Classification of concepts in thermodynamically consistent generalized plasticity", *J. Eng. Mech.*, **135**, 156–170 (2009).

[17] Fleck, N. A. and Hutchinson, J. W., "Strain gradient plasticity", *Adv. Appl. Mech.*, **33**, 295–361 (1997).

[18] Del Piero, G., "On the method of virtual power in continuum mechanics", *J. Mech. Mater. Struct.*, **4**, 281–292 (2009).

[19] Gurtin, M. E., "A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations", *J. Mech. Phys. Solids*, **50**, 5–32 (2002).

[20] Fleck, N. A. and Willis, J. R., "A mathematical basis for strain-gradient plasticity theory. Part II: tensorial plastic multiplier", *J. Mech. Phys. Solids*, **57**, 1045–1057 (2009).

[21] Kröner, E., "Benefits and shortcomings of the continuous theory of dislocations", *Int. J. Solids Struct.*, **38**, 1115–1134 (2001).

[22] Molinari, A. and Ravichandran, G., "Constitutive modeling of high-strain-rate deformation in metals based on the evolution of an effective microstructural length", *Mech. Mater.*, **37**, 737–752 (2005).

[23] Evans, A. G. and Hutchinson, J. R., "A critical assessment of theories of strain gradient plasticity", *Acta Mater.*, **57**, 1675–1688 (2009).

[24] van der Giessen, E. and Needleman, A., "Discrete dislocation plasticity: a simple planar model", *Modell. Simul. Mater. Sci. Eng.*, **3**, 689–735 (1995).

[25] Segurado, J., Llorca, J. and Romero, I., "Computational issues in the simulation of two-dimensional discrete dislocation dynamics", *Modell. Simul. Mater. Sci. Eng.*, **15**, S361–S375 (2007).

[26] Fleck, N. A. and Willis, J. R., "Bounds and estimates for the effect of strain gradients upon the effective plastic properties of an isotropic two phase composite", *J. Mech. Phys. Solids*, **52**, 1855–1888 (2004).