

Strain gradient crystal plasticity : thermomechanical formulations and applications

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1 Introduction

Since the pioneering work of [3] (see [4] for a review), strain gradient plasticity has aroused increasing interest in the mechanics of materials community, leading to a large panel of non local plasticity models. However, comparisons between these models remain seldom [19], and the full thermomechanical framework is usually not provided. The attention is focused here on models incorporating modified or additional balance equations and therefore additional boundary conditions in order to solve practical boundary value problems. The reader is referred to [1] for models sticking to classical structure of the boundary value problem.

The aim of the present work is to bring together and to some extent reconcile three main trends of strain gradient plasticity models applied to metal single crystals : the gradient of internal variable, second grade and Cosserat approaches. In particular, the thermodynamical setting for all three models will be described in a unified way, in order to make actual differences between theories really visible. For simplicity and clarity, the analysis is restricted to single slip and rate-independent constitutive equations. Extensions to the general viscoplastic multislip case are straightforward, based on multicriterion elastoviscoplasticity.

Each model presentation follows the three following main steps :

- The *principle of virtual power* is applied to derive balance equations and appropriate boundary conditions. This requires the choice of the number of degrees of freedom (*order* of the theory) and the precision (*grade* of the theory) of the retained theory. The key functions to be defined in each theory are the *power density of internal forces* p^i and the *power density of contact forces* p^c , body forces being excluded here for simplicity.

- The *energy principle* introduces internal energy e and Helmholtz free energy ψ as a function of state and internal variables.
- The *entropy principle* is exploited to derive state laws and intrinsic dissipation D .

The results of the application of each step are reported here. The reader is referred to [10] for an example of detailed derivation in the case of second grade thermoelasticity. The presentation is restricted to the small perturbation framework under isothermal conditions (except in sections 3.2 and 3.3). Vectors and tensors are denoted by boldface letters.

The impact of the previous modifications of the classical thermomechanical framework on heat equation and conduction is briefly analysed, since it may well be the key point to choose between concurrent formulations.

2 Second grade and Cosserat crystal plasticity

Two recent enhancements of classical crystal plasticity, based on the mechanics of generalized continua, are presented in this section. The main motivation of both models lies in the taking into account of the dislocation density tensor in the constitutive modeling. The stress is laid on the common features and main differences arising from the original choice of extended continuum.

2.1 Second grade constitutive framework

Following the second gradient modeling framework settled by Mindlin [16], Fleck and Hutchinson [6] have proposed a crystal plasticity model incorporating characteristic lengths associated with the effect of so-called geometrically necessary dislocations, and also of gradient of slip normal to the slip plane. The degrees of freedom and modeling quantities of the theory are the displacement field and its first and second gradients :

$$(\mathbf{u}, \nabla \mathbf{u}, \nabla \nabla \mathbf{u}) \quad (1)$$

The corresponding strain measures are the second order strain tensor $\boldsymbol{\varepsilon}$, with its classical definition, and its gradient $\boldsymbol{\eta} = \nabla \boldsymbol{\varepsilon}$. They are split into elastic and plastic contributions :

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p, \quad \boldsymbol{\eta} = \boldsymbol{\eta}^e + \boldsymbol{\eta}^p \quad (2)$$

Note that it is not assumed that $\boldsymbol{\eta}^p$ is equal to the gradient of plastic strain : *plastic strain gradient* is not the *gradient of plastic strain* in the theory developed in [6]. Two stress tensors are associated with the previous strain measures and appear in the power densities of internal and contact forces :

$$p^i = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + M : \dot{\boldsymbol{\eta}}, \quad p^c = t \cdot \dot{u} + m \cdot D_n u \quad (3)$$

where D_n and D_t are the normal and tangent gradient operators acting on a surface with normal vector \mathbf{n} . The traction and double force vectors on the surface are denoted by \mathbf{t} and m . The balance and boundary conditions then read :

$$\operatorname{div} \boldsymbol{\tau} = 0, \quad \text{with } \boldsymbol{\tau} = \boldsymbol{\sigma} - \operatorname{div} M \quad (4)$$

$$\mathbf{t} = \boldsymbol{\tau} \cdot \mathbf{n} + 2RM : (\mathbf{n} \otimes \mathbf{n}) - D_t(M \cdot \mathbf{n}), \quad m = M : (n \otimes n) \quad (5)$$

A detailed derivation of these equations can be found in [11]. The free energy density is a function of elastic strain and strain gradient and possibly of hardening variable(s) $q : \psi(\varepsilon^e, \eta^e, q)$. The state laws are deduced from the analysis of the entropy principle :

$$\sigma = \rho \frac{\partial \psi}{\partial \varepsilon^e}, \quad M = \rho \frac{\partial \psi}{\partial \eta^e}, \quad R = \rho \frac{\partial \psi}{\partial q} \quad (6)$$

The remaining intrinsic dissipation reads :

$$D = \sigma : \dot{\varepsilon}^p + M : \dot{\eta}^p - R \dot{q} \quad (7)$$

The authors in [6] and [22] propose a simplified version of elasticity constitutive equations including the usual four-rank tensor of elasticity moduli \mathbf{C} and an additional intrinsic length scale l_e :

$$\sigma = \mathbf{C} : \varepsilon^e, \quad M = l_e^2 \mathbf{C} : \eta^e \quad (8)$$

The dissipative processes are modeled by a potential function $f(\sigma, \mathbf{M}, R)$ of the thermodynamical forces :

$$\dot{\varepsilon}^p = \dot{\lambda} \frac{\partial f}{\partial \sigma}, \quad \dot{\eta}^p = \dot{\lambda} \frac{\partial f}{\partial \mathbf{M}}, \quad \dot{q} = -\dot{\lambda} \frac{\partial f}{\partial R} \quad (9)$$

where $\dot{\lambda}$ is the plastic multiplier. The theory presented in [6, 21, 22] considers the general case of viscoplasticity, we translate it here in the particular case of rate-independent plasticity for simplicity.

Let us now specify the previous framework in the case of a single crystal undergoing single slip in direction \mathbf{l} in the slip plane of normal \mathbf{v} . The usual Schmid law is extended to incorporate not only resolved shear stresses but also resolved hyperstresses, related by a constitutive length l_p :

$$f = |\tau| + \frac{|m|}{l_p} - R, \quad \text{with} \quad \tau = \sigma : (\mathbf{l} \otimes \mathbf{v}), \quad m = \mathbf{M} : (\mathbf{l} \otimes \mathbf{v} \otimes \mathbf{l}) \quad (10)$$

The plastic strain and strain gradient rates follow from the normality rules (9) :

$$\dot{\varepsilon}^p = \dot{\gamma}^p \mathbf{l} \otimes \mathbf{v}, \quad \dot{\eta}^p = \dot{\gamma}^S \mathbf{l} \otimes \mathbf{v} \otimes \mathbf{l} \quad (11)$$

For the sake of simplicity, we have introduced only the effect of slip gradient in the slip direction \mathbf{l} , although the original model also contains a contribution of slip gradient in the normal direction \mathbf{v} . The first type of strain gradient effect is associated with the density of so-called geometrically necessary dislocations, the second one remains unclear. It must be noticed that the *slip gradient variable* γ^S does not coincide with the *gradient of slip* $\nabla \gamma^p$. Both are related to the plastic multiplier $\dot{\lambda}$ according to (9) :

$$\dot{\lambda} = \dot{\gamma}^p \operatorname{sign} \tau = l_p \dot{\gamma}^S \operatorname{sign} m \quad (12)$$

For monotonous loading, the slip gradient variable γ^S turns out to be equal to the amount of slip γ^p divided by l_p .

2.2 Cosserat single crystal plasticity

In the continuum theory of dislocations, the notion of geometrically necessary dislocations is associated with that of dislocation density tensor introduced by Nye [18]. The famous Nye

relation links the dislocation density tensor and lattice curvature. Accordingly, introducing the influence of dislocation density tensor in the single crystal constitutive equations amounts to including lattice curvature effects. This is the main motivation of the Cosserat crystal plasticity model detailed in [9]. It can be noticed that the dislocation density tensor is also related to the curl of plastic deformation, which in turn gives also a motivation for the previous second grade approach.

A parallel is drawn between the following equations (13) to (24) and the corresponding equations (1) to (12) of the second gradient theory. The degrees of freedom and modeling variables of the Cosserat theory are the displacement u , the micro-rotation ϕ and their gradients :

$$(u, \phi, \nabla u, \nabla \phi) \quad (13)$$

from which the Cosserat deformation and curvature second rank tensors are deduced :

$$e = \nabla u + \varepsilon \cdot \phi = e^e + e^p, \quad \kappa = \nabla \phi = \kappa^e + \kappa^p \quad (14)$$

The third order permutation tensor is denoted by ε and its components give the sign of the permutation (ijk) of $(1, 2, 3)$. The power densities of internal and contact forces are used to derive two balance equations, namely balance of momentum and balance of moment of momentum. They involve the second rank tensors of force stresses σ and couple stresses M :

$$p^i = \sigma : \dot{e} + M : \dot{\kappa}, \quad p^c = t \cdot \dot{u} + m \cdot \dot{\phi} \quad (15)$$

$$\operatorname{div} \sigma = 0, \quad \operatorname{div} M - \varepsilon : \sigma = 0 \quad (16)$$

$$t = \sigma \cdot n, \quad m = M \cdot n \quad (17)$$

The traction and couple vectors acting on a surface element are denoted by t and m . The free energy $\psi(e^e, \kappa^e, q)$ is a function of elastic deformation and curvature, and internal variable(s) q :

$$\sigma = \rho \frac{\partial \psi}{\partial e^e}, \quad M = \rho \frac{\partial \psi}{\partial \kappa^e}, \quad R = \rho \frac{\partial \psi}{\partial q} \quad (18)$$

This leads to the following intrinsic dissipation :

$$D = \sigma : \dot{e}^p + M : \dot{\kappa}^p \quad (19)$$

The elasticity constitutive equations require two symmetric four-rank tensor of elastic moduli, C and D having the dimension of MPa and MPa.m² respectively :

$$\sigma = C : e, \quad M = D : \kappa \quad (20)$$

In contrast to the single plastic potential used in the second grade model, we resort here to two dissipation potentials $f_1(\sigma, R, q)$ and $f_2(M, R, q)$. This corresponds to a multi-criterion framework, introduced by Koiter and Mandel, involving two plastic multipliers :

$$\dot{e}^p = \dot{\lambda}_1 \frac{\partial f_1}{\partial \sigma}, \quad \dot{\kappa}^p = \dot{\lambda}_2 \frac{\partial f_2}{\partial M}, \quad \dot{q} = -\dot{\lambda} \frac{\partial f_1}{\partial R} \quad (21)$$

Note that the choice of the proper plastic multiplier to be used in the evolution equation for hardening variable (21)₃ depends on the specific type of hardening laws and number of internal variables. Let us specify the potentials retained to model Cosserat crystal plasticity :

$$f_1 = |\tau| - R, \quad f_2 = |m| - l_p R_c, \quad \text{with } \tau = \sigma : (l \otimes v), \quad m = M : (\xi \otimes l) \quad (22)$$

where $\xi = \mathbf{v} \times \mathbf{l}$ and l_p is a characteristic length. Accordingly, this model requires at least two hardening variable q and q_c , the thermodynamical forces of which are R and R_c . A coupling must exist between hardening variables for the model to give rise to size effects, as explained in the example of section 4.2. In contrast, in the specific second gradient model of section 2.1, coupling is introduced directly by a single criterion and plastic multiplier. Within the present Cosserat model, the flow rules become :

$$\dot{\mathbf{e}}^p = \dot{\gamma}^p \mathbf{l} \otimes \mathbf{v}, \quad \dot{\boldsymbol{\kappa}}^p = \frac{\dot{\theta}}{l_p} \boldsymbol{\xi} \otimes \mathbf{l} \quad (23)$$

$$\dot{\lambda}_1 = \dot{\gamma}^p \operatorname{sign} \tau, \quad \dot{\lambda}_2 = \frac{\dot{\theta}}{l_p} \operatorname{sign} m \quad (24)$$

The meaning of the second plastic multiplier therefore is that of a scalar curvature rate, i.e. the ratio of a rotation rate by a characteristic length.

Until now, the physical meaning of micro-rotation ϕ has not been specified. It is in fact intended to coincide with the notion of crystal lattice rotation, so that the Cosserat directors are simply lattice directions defined in the released isoclinic configuration introduced in [13]. The definitions of Cosserat relative deformation (14) and plastic deformation rate (23) imply that the skew-symmetric part of elastic deformation e^e measures the difference between lattice and Cosserat rotation. The constraint that e^e be symmetric must therefore be added for the microrotation to have the wanted physical meaning. This can be achieved by choosing very high elastic constants linking the skew-symmetric parts of stress and of elastic deformation. Skew-symmetric reaction stresses then remain.

3 Gradient of internal variable approach

The motivation of the non local plasticity models proposed by Aifantis [3] is originally not the introduction of so-called geometrically necessary dislocation densities, but rather dislocation patterning during deformation. It is shown that this class of models can be regarded as a gradient of internal variable approach depicted in [14]. In the previous Aifantis models, the internal variable is the scalar dislocation density (so-called density of statistically stored dislocations) or the cumulative plastic strain. When applied to the slip variable γ^p [24], so indirectly to a density of geometrically necessary dislocation, it builds a link with the models of previous sections. In particular, it appears that the gradient of internal variable approach gives rise, as a special case, to the well-known Laplacian term $\Delta\gamma^p$, the physical meaning of which remains to be explained in each specific situation. This model remains different from the second grade and Cosserat models in so far as it is not directly related to the dislocation density tensor.

3.1 Enriched power of internal and contact forces

The same structure of model presentation as for the second grade and Cosserat models is kept in this section, so that direct comparison is possible at each step. The degrees of freedom and modeling quantities are the displacement, the internal variable γ^p and their gradients :

$$(\mathbf{u}, \gamma^p, \nabla \mathbf{u}, \nabla \gamma^p) \quad (25)$$

A short presentation of this thermomechanical setting has been reported in [12] in the case of cumulative plastic strain as internal variable (see also [23]). The classical strain tensor $\boldsymbol{\varepsilon}$,

single strain measure of the model, is decomposed into elastic and plastic contributions as usual. However, the power density of internal forces must be extended as a linear form of the modeling quantities :

$$p^i = \sigma : \dot{\epsilon} + \alpha \dot{\gamma}^p + B \cdot \nabla \dot{\gamma}^p, \quad p^c = t \cdot \dot{u} + \alpha^c \dot{\gamma}^p \quad (26)$$

This leads to two sets of balance equations and associated boundary conditions :

$$\operatorname{div} \sigma = 0, \quad \alpha = \operatorname{div} B \quad (27)$$

$$t = \sigma \cdot n, \quad \alpha^c = B \cdot n \quad (28)$$

The term $\alpha \dot{\gamma}^p + B \cdot \nabla \dot{\gamma}^p = \operatorname{div}(\dot{\gamma}^p B)$ represents a nonlocal power of internal forces of first degree. The second balance equation $\alpha = \operatorname{div} B$ can also be interpreted as a definition of α . The value of γ^p or the dual force α^c must be prescribed at the boundary of the considered solid. The free energy is a function of elastic strain, $\nabla \gamma^p$ and internal variables q (including γ^p if necessary) : $\psi(\epsilon^e, \nabla \gamma^p, q)$. The state laws and intrinsic dissipation take the form :

$$\sigma = \rho \frac{\partial \psi}{\partial \epsilon^e}, \quad B = \rho \frac{\partial \psi}{\partial \nabla \gamma^p}, \quad R = \rho \frac{\partial \psi}{\partial q} \quad (29)$$

$$D = \sigma : \dot{\epsilon}^p + \alpha \dot{\gamma}^p - R \dot{q} \quad (30)$$

The classical elastic constitutive relations are unchanged. A potential function $f(\sigma, \alpha, R)$ is used to derive the flow and hardening rules :

$$\dot{\epsilon}^p = \dot{\lambda} \frac{\partial f}{\partial \sigma}, \quad \dot{\gamma}^p = \dot{\lambda} \frac{\partial f}{\partial \alpha}, \quad \dot{q} = -\dot{\lambda} \frac{\partial f}{\partial R} \quad (31)$$

In a case of a single crystal undergoing single slip, the yield criterion is again an extension of Schmid law, from which the flow rules are deduced :

$$f = |\tau + \alpha| - R = |\tau + \operatorname{div} B| - R, \quad \text{with} \quad \tau = \sigma : (l \otimes v) \quad (32)$$

$$\dot{\epsilon}^p = \dot{\gamma}^p l \otimes v, \quad \dot{\gamma}^p = \dot{\lambda} \operatorname{sign}(\tau + \operatorname{div} B) \quad (33)$$

The free energy can be taken as a quadratic function of $\nabla \gamma^p$, so that, in the case of isotropic or cubic material symmetry :

$$B = c \nabla \gamma^p, \quad \operatorname{div} B = c \Delta \gamma^p \quad (34)$$

The term $\operatorname{div} B$ therefore introduces a sort of kinematical hardening (see also [15]). Under monotonous loading conditions such that τ remains positive, the well-known relation found in Aifantis models is retrieved ($c > 0$) :

$$\tau = R - c \Delta \gamma^p \quad (35)$$

3.2 Alternative formulation : Enlarged entropy flux

The three presented thermomechanical frameworks share the common feature that the power of internal forces has not the classical form and contains additional terms, the mechanical meaning of which is not necessarily obvious. This explains why an alternative formulation based on the introduction of an extra-entropy flux has been preferred in the past, that preserves the classical structure of internal work. Let us present this formulation in the case of the previous gradient

of internal variable approach. The free energy still is a function $\psi(\varepsilon^e, \nabla\gamma^p, q, T)$, T being the absolute temperature, but the power density p^i keeps its classical form. The energy principle then reads :

$$\rho\dot{e} = p^i - \operatorname{div} Q = \sigma : \dot{\varepsilon} - \operatorname{div} Q \quad (36)$$

where Q is the heat flux vector. The entropy principle in its global form on a volume V with boundary ∂V reads :

$$\int_V \rho\dot{\eta} dV + \int_{\partial V} \Phi \cdot n dS \geq 0, \quad \text{with} \quad \Phi = \frac{Q}{T} + k \quad (37)$$

where Φ is the total entropy flux vector and k an extra-entropy flux [17]. The entropy density is denoted by η . The use of the divergence theorem leads to the expression :

$$\int_V D^{tot} dV \geq 0, \quad \text{with} \quad D^{tot} = \rho\dot{\eta} + \operatorname{div} \left(\frac{Q}{T} + k \right) \quad (38)$$

Using the state laws (29) complemented by the relation $\eta = -\partial\psi/\partial T$, the total dissipation density reduces to :

$$TD^{tot} = \sigma : \dot{\varepsilon}^p - B \cdot \nabla\dot{\gamma}^p - R\dot{q} - \frac{Q}{T} \cdot \nabla T + T \operatorname{div} k \quad (39)$$

The only possible choice that eliminates the $\nabla\dot{\gamma}^p$ term is

$$k = \dot{\gamma}^p \frac{B}{T} \quad (40)$$

(see also [14]) which gives

$$TD^{tot} = \sigma : \dot{\varepsilon}^p + \dot{\gamma}^p \operatorname{div} B - R\dot{q} - \Phi \cdot \nabla T \quad (41)$$

where the intrinsic and thermal parts of dissipation appear clearly. The positiveness of dissipation is then ensured by the choice of a potential $f(\sigma, \alpha = \operatorname{div} B, R)$ for the intrinsic part and a generalized Fourier law for the thermal part :

$$\Phi = \frac{Q}{T} + k = -\frac{K}{T} \cdot \nabla T \quad (42)$$

3.3 Heat equation

There are two main differences between the thermomechanical framework based on the extension of internal work and that relying on extra-entropy flux : it is not ensured in the latter case, that the heat is flowing always from hot to cold, this requires $-Q \cdot \nabla T$ positive, and the heat equations differ in the same amount as they are approaching an adiabatic process. According to the first scheme, the heat equation reads :

$$\rho T\dot{\eta} = D - \operatorname{div} Q \quad (43)$$

where the intrinsic dissipation is given by (30). In contrast, the presence of an extra-entropy flux modifies the heat equation as follows :

$$\rho T\dot{\eta} = D - \operatorname{div}(Q + Tk) \quad (44)$$

When considering a locally quasi-adiabatic process ($|\operatorname{div} Q| \ll D$), one notices that heat equation (43) leads to the classical equation $\rho T \dot{\eta} = D$, whereas heat equation (44) remains due to (42) a partial differential equation in T

$$\rho T \dot{\eta} = D - \operatorname{div}(Tk) = D + \operatorname{div}(K \cdot \nabla T) \quad (45)$$

as for a fully heat conducting process, because the divergence of the transient power vector Tk according to (40) need not vanish necessarily at vanishing $\operatorname{div} Q$. Thus, if a significant $\operatorname{div}(Tk)$ is present in a locally quasi-adiabatic process, then $\operatorname{div}(K \cdot \nabla T)$ must not vanish. But a locally quasi-adiabatic process is a very fast process, so that $|\nabla \cdot (K \cdot \nabla T)|$ will become in such a process much smaller than the mechanical dissipation power D . If this is right, conversion of the aforementioned implication says that $\operatorname{div}(Tk)$ cannot be significant in a very fast process, where, on the other hand, a transient power is present naturally. Thus, the existence of an extra entropy flux (k) seems to be difficult in the theory of gradients of mechanical internal variables.

4 Applications

This section mentions recent applications of Cosserat crystal plasticity to handle size effects observed in metals. Most of them can also be described by the two other approaches presented in this work. We insist then of the advantages and shortcomings of each model.

4.1 Size effects in two-phase laminate microstructures

The collective behavior of dislocations in narrow channels in multiphase materials or films is associated with size effects like the dependence of Orowan stresses on channel width. This situation is encountered for instance in PSB of fatigued single crystals or in the γ -channels of nickel-base single crystals. In [20], an idealized laminate microstructure is considered under shear, for which one phase remains elastic whereas the second one deforms plastically. A simple dislocation analysis shows that plastic strain is not uniform due to the bowing of screw dislocations and the pileup formation near the interface. In contrast, classical crystal plasticity predicts uniform deformation, which is the actual limit state for thick layers. Due to the existence of interface conditions, deformation is not uniform when using a Cosserat model, and some Cosserat parameters can be identified explicitly looking at the dislocation solution. Similarly, boundary layers in a sheared single crystal layer has been analysed in [22] using both second gradient theory and discrete dislocation dynamics. The additional interface or boundary conditions play a central rôle in the development of non-homogeneous deformation in non-local models, so that explicit models including higher order gradients but keeping the standard structure of the boundary value problem, are not able to account for it.

The case of PSB formation is adequately handled by Ainfantis model involving dislocation densities [3], because this phenomenon has *a priori* nothing to do with the concept of geometrically necessary dislocations.

Another example of application dealing with constrained plasticity in γ -channels of nickel-base single crystal superalloys is provided in [7].

4.2 Grain size effects

The use of higher order or higher grade theories in the context of polycrystalline plasticity is the a straightforward manner to predict size effects, the Hall-Petch effect for grain size being

the most documented situation. In [21], the size-dependent deformation is studied using the second grade model of section 2.1. The case of polycrystalline aggregates with prediction of the influence of grain size on the tensile curves is tackled in [7] for Cosserat elastoplasticity, and in [2] for viscoplasticity. In the latter case, the authors use a model with explicit use of higher order gradients in the hardening law and the classical structure of the boundary value problem. This is sufficient for this type of applications.

4.3 Cracks in single crystals

The problem of the crack in a infinite medium has been addressed very often during the development of the mechanics of generalized continua in the 60s and 70s. Solutions are available for the elastic couple stress medium and fully non local elasticity. In the case of crystal plasticity, numerical solutions with the Cosserat continuum have been compared to Rice's solution for the classical continuum in [8]. The classical solution, derived for an elastoplastic single crystal without hardening, predicts the existence of sectors with constant stress separated by localization bands. The physical nature of the bands depends on crystal structure and orientation. Intense slip bands, kink bands and multislip bands can coexist. The use of the Cosserat continuum leads to the weakening and even elimination of kink bands at the crack tip. The existence of kink bands in actual experiment remains an unsettled question. This has lead some authors to eliminate this localization modes from Rice's solution [5] and so imitate the Cosserat solution.

The used of physically more realistic models at the crack tip than classical crystal plasticity is an important issue for the prediction of subsequent crack growth, especially in fatigue.

References

- [1] A. Acharya and J.L. Bassani. Lattice incompatibility and a gradient theory of crystal plasticity. *Journal of the Mechanics and Physics of Solids*, 48:1565–1595, 2000.
- [2] A. Acharya and A.J. Beaudoin. Grain size effects in viscoplastic polycrystals at moderate strains. *Journal of the Mechanics and Physics of Solids*, 48:2213–2230, 2000.
- [3] E.C. Aifantis. The physics of plastic deformation. *International Journal of Plasticity*, 3:211–248, 1987.
- [4] E.C. Aifantis. Gradient deformation models at nano, micro and macro scales. *J. of Engineering Materials and Technology*, 121:189–202, 1999.
- [5] W.J. Drugan. Asymptotic solutions for tensile crack tip fields without kink-type shear bands in elastic ideally-plastic single crystals. *Journal of the Mechanics and Physics of Solids*, 49:2155–2176, 2001.
- [6] N.A. Fleck and J.W. Hutchinson. Strain gradient plasticity. *Adv. Appl. Mech.*, 33:295–361, 1997.
- [7] S. Forest, F. Barbe, and G. Cailletaud. Cosserat modelling of size effects in the mechanical behaviour of polycrystals and multiphase materials. *International Journal of Solids and Structures*, 37:7105–7126, 2000.

- [8] S. Forest, P. Boubidi, and R. Sievert. Strain localization patterns at a crack tip in generalized single crystal plasticity. *Scripta Materialia*, 44:953–958, 2001.
- [9] S. Forest, G. Cailletaud, and R. Sievert. A Cosserat theory for elastoviscoplastic single crystals at finite deformation. *Archives of Mechanics*, 49(4):705–736, 1997.
- [10] S. Forest, J.-M. Cardona, and R. Sievert. Thermoelasticity of second-grade media. In G.A. Maugin, R. Drouot, and F. Sidoroff, editors, *Continuum Thermomechanics, The Art and Science of Modelling Material Behaviour, Paul Germain's Anniversary Volume*, pages 163–176. Kluwer Academic Publishers, 2000.
- [11] P. Germain. La méthode des puissances virtuelles en mécanique des milieux continus, première partie : théorie du second gradient. *J. de Mécanique*, 12:235–274, 1973.
- [12] J. Huang, K. Kalaitzidou, J.W. Sutherland, W.W. Milligan, E.C. Aifantis, R. Sievert, and S. Forest. Gradient plasticity : Implications to chip formation in machining. In A.-M. Habraken, editor, *4th International ESAFORM Conference on Material Forming*, pages 527–530. Université de Liège, Belgium, 2001.
- [13] J. Mandel. Equations constitutives et directeurs dans les milieux plastiques et viscoplastiques. *Int. J. Solids Structures*, 9:725–740, 1973.
- [14] G.A. Maugin. Internal variables and dissipative structures. *J. Non-Equilib. Thermodyn.*, 15:173–192, 1990.
- [15] A. Menzel and P. Steinmann. On the continuum formulation of higher order gradient plasticity for single and polycrystal. *Journal of the Mechanics and Physics of Solids*, 48:1777–1796, 2000.
- [16] R.D. Mindlin and N.N. Eshel. On first strain gradient theories in linear elasticity. *Int. J. Solids Structures*, 4:109–124, 1968.
- [17] I. Müller. *Thermodynamics*. Pitman Publishing Limited, London, 1985.
- [18] J.F. Nye. Some geometrical relations in dislocated crystals. *Acta Metall.*, 1:153–162, 1953.
- [19] R.H.J. Peerlings, M.G.D. Geers, R. de Borst, and W.A.M. Brekelmans. A critical comparison of nonlocal and gradient-enhanced softening continua. *Int. J. Solids Structures*, 38:7723–7746, 2001.
- [20] R. Sedláček and S. Forest. Non-local plasticity at microscale : A dislocation-based model and a Cosserat model. *physica status solidi (b)*, 221:583–596, 2000.
- [21] J.Y. Shu and N.A. Fleck. Strain gradient crystal plasticity :size-dependent deformation of bicrystals. *Journal of the Mechanics and Physics of Solids*, 47:297–324, 1999.
- [22] J.Y. Shu, N.A. Fleck, E. Van der Giessen, and A. Needleman. Boundary layers in constrained plastic flow : comparison of non local and discrete dislocation plasticity. *Journal of the Mechanics and Physics of Solids*, 49:1361–1395, 2001.

- [23] R. Sievert. Strain gradient and gradient of internal variable models. Technical Report BAM-V.2 01/4, Bundesanstalt für Materialforschung und Prüfung (BAM), Berlin, 2001.
- [24] B. Svendsen. Continuum thermodynamic models for crystal plasticity including the effects of geometrically-necessary dislocations. *J. Mech. Phys. Solids*, 2002, in press.