Non-convex rate dependent strain gradient crystal plasticity and deformation patterning

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A rate dependent strain gradient crystal plasticity framework is presented where the displacement and the plastic slip fields are considered as primary variables. These coupled fields are determined on a global level by solving simultaneously the linear momentum balance and the slip evolution equation, which is derived in a thermodynamically consistent manner. The formulation is based on the 1D theory presented in Yalcinkaya et al. (2011), where the patterning of plastic slip is obtained in a system with non-convex energetic hardening through a phenomenological double-well plastic potential. In the current multi-dimensional multi-slip analysis the non-convexity enters the framework through a latent hardening potential presented in Ortiz and Repetto (1999) where the microstructure evolution is obtained explicitly via a lamination procedure. The current study aims the implicit evolution of deformation patterns due to the incorporated physically based non-convex potential.

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1. Introduction

At the microscopic scale, deformed crystalline materials usually show heterogeneous plastic deformation, where the amount of plastic strain varies spatially. At moderate strain levels, regular cellular dislocation structures have been observed. Typical examples of dislocation microstructures are dislocation cells and dislocation walls (see e.g. Rauch and Schmitt (1989), Gardey et al. (2005) and Yalcinkaya et al. (2009)). Patterning typically refers to the self organization of dislocations, yielding regions with a high dislocation density (dislocation walls) that envelop areas with a low dislocation density (dislocation cell interiors), also regarded as domains of high and low plastic slip accumulation, respectively.

In addition to the cellular microstructures at meso-scale, clear band formation and related plastic flow localization in irradiated materials (see e.g. Sauzay et al. (2010)) at lower scales and macroscopic plastic slip bands such as Lüders bands (see e.g. Shaw and Kyriakides (1998)) are also commonly observed structures due to plastic deformation. These microstructures macroscopically e.g. manifest themselves through softening of the material or through plastic anisotropy under strain path changes.

The softening of the material and macroscopic anisotropic effects under strain path changes (see e.g. Peeters et al. (2000) and Yalcinkaya et al. (2009)), resulting from evolving dislocation microstructures, have been an interesting topic for the materials science community and the metal forming industry for decades. Starting with the studies on the cold-worked sub-structure of polycrystals using transmission electron microscopy in the 1960s (e.g. Bailey and Hirsch (1960), Keh et al. (1963) and Swann (1963)), a vast amount of experimental results have been collected, and several promising theoretical models were presented dealing with dislocation (or slip) patterning. Nevertheless, a complete descriptive understanding of the occurring phenomena has not been reached and the necessary input for computational models is still subject of ongoing discussions.

In the context of the computational modeling of plastic slip patterning (or dislocation sub-structure formation), different approaches have been pursued in the literature which can be categorized into three main groups: (i) models using directly the mechanics of single dislocations or populations of dislocations, (ii) phase field modeling of dislocation patterning, (iii) the incremental variational formulation of inelasticity by applying relaxation concepts for fine scale microstructure evolution. See Yalcinkaya et al. (2011) for a global overview of the available approaches.

In the present paper we develop a rate dependent strain gradient crystal plasticity finite element framework for the simulation of dislocation microstructure evolution, where non-convexity is introduced as an intrinsic property of the plastic free energy of the material. The objective of the developed constitutive model is to simulate deformation patterning and the associated macroscopic material behavior in a thermodynamically consistent manner. Hence, the influence of latent hardening on the dislocation
microstructure evolution is studied through a physically based latent hardening potential proposed by Ortiz and Repetto (1999). The non-convex formulation, inspired by the physics of interacting dislocations is relevant in multi-slip deformation states, accounting for the interaction of slip systems.

In the model, the plastic slip and the displacement are taken as degrees of freedom. These fields are determined on a global level by solving simultaneously the linear momentum balance and the slip evolution equation. The latter, expressed through a thermodynamically consistent slip law is a crucial part of the model. At first glance, the slip law (see Eq. (18)) is similar to the one encountered in classical rate dependent crystal plasticity approaches (e.g. Hutchinson (1976), Peirce et al. (1982) and Yalcinckaya et al. (2008)), however the contribution of the actual stress state differs. Three stress contributions can be distinguished: (1) the conventional resolved shear stress directly related to the external loading, (2) an internal stress depending on the higher order gradient of the plastic slip, which is characteristic for strain gradient crystal plasticity models (e.g. Evers et al. (2004), Yefimov et al. (2004) and Bayley et al. (2006)) and (3) the stress which occurs through a non-convex free energy and which is affecting the accumulation of the plastic deformation. The latter contribution eventually triggers the patterning of the dislocation slip field.

The paper is organized as follows. First, in Section 2, the rate dependent strain gradient crystal plasticity and its finite element solution is briefly discussed. Then, in Section 3, the incorporation of non-convexity into the model is presented, using a physically based latent hardening potential. A detailed analysis of the latent hardening based non-convex function is performed in this section in order to clarify the conditions enabling microstructure evolution. In Section 4, numerical examples are presented in order to demonstrate the capability of the proposed model. First, the size effect related to plastic slip gradients and rate dependent deformation evolution in the context of convex strain gradient crystal plasticity is studied. Then, the rate dependent microstructure evolution via the physically motivated latent hardening non-convex potential is addressed in this section. Finally, some concluding remarks are given in Section 5.

2. Strain gradient crystal plasticity and finite element implementation

In this section, the theoretical framework of the slip based strain gradient crystal plasticity is presented and its incorporation into a finite element formulation is addressed briefly. First, the thermodynamical consistency and the derivation of the governing system equations are discussed. In a geometrically linear context, with small displacements, strains and rotations, (the Lagrangian approach coincides with the Eulerian formalism), the time dependent displacement field is denoted by \( \mathbf{u} = \mathbf{u}(\mathbf{x}, t) \), where the vector \( \mathbf{x} \) indicates the position of a material point. The strain tensor \( \varepsilon \) is defined as \( \varepsilon = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \), and the velocity vector is represented as \( \mathbf{v} = \dot{\mathbf{u}} \). The strain is decomposed additively as

\[
\varepsilon = \varepsilon^p + \varepsilon^f
\]

into an elastic part \( \varepsilon^p \) and a plastic part \( \varepsilon^f \). The plastic strain rate can be written as a summation of plastic slip rates on the individual slip systems, \( \dot{\varepsilon}^f = \sum_\alpha \dot{\gamma}_\alpha \mathbf{P}^\alpha \) with \( \mathbf{P}^\alpha = \frac{1}{2}(\mathbf{s}^\alpha \otimes \mathbf{n}^\alpha + \mathbf{n}^\alpha \otimes \mathbf{s}^\alpha) \) the symmetrized Schmid tensor, where \( \mathbf{s}^\alpha \) and \( \mathbf{n}^\alpha \) are the unit slip direction vector and unit normal vector on slip system \( \alpha \), respectively. The state variables are chosen to be given by the set

\[
\text{state} = \{ \varepsilon^p, \gamma, \nabla \gamma \}
\]

where \( \gamma \) contains the plastic slips on the different slip systems \( \alpha \) and \( \nabla \gamma \) represents the gradient of the slips on these slip systems.

The chosen variables describing the state are to be regarded as meso-scale internal state variables. At that scale, the glide plane slip and their gradients are natural candidates. They both describe the physical state on a slip plane in the mean field sense. The slip characterizes the average plastic deformation accumulated on a glide plane, whereas their gradients characterize the amount of geometrically necessary dislocations that accompany that process, also an important characteristic of the mean dislocation configuration. The use of these state variables naturally entails the other quantities in the constitutive description, like the gradient of the dislocation density, see Eq. (18), where the divergence of the microstress directly involves the gradient of GND.

Obviously, there are more choices possible for the state variables. At the meso-scale, the choice made is quite appropriate in representing a spatio-temporal ensemble of microscopic states. The meso-scale state variables are measures of the current dislocation state in the material relative to which energy storage and hardening in the material are modeled. Microscopic processes like phase transitions or dislocation interaction may survive coarse-graining (from the micro-scale to the meso-scale), resulting in non-convex contributions to the free energy as in phase field models and a transition from spatial or material homogeneity or inhomogeneity. The use of like-quantities as meso-scale state variables is quite common in crystal plasticity. Several examples can be found in the literature, e.g. Rice (1971), using a continuum slip-model, which characterizes the state of the crystal in terms of the shear strains on each slip system. Later on Perzyna (1988) considered plastic slips together with the slip resistance as internal state variables. For the considered problems with monotonic loading histories, the adopted mesoscopic state variables are well capable of bridging the microscopic and mesoscopic states of the material.

Following the arguments of Gurtin (e.g. Gurtin (2000) and Gurtin (2002)), the power expended by each independent rate-like kinematical descriptor is expressible in terms of an associated force consistent with its own balance. However, the basic kinematical fields of rate variables, namely \( \dot{\varepsilon}, \dot{\mathbf{u}} \) and \( \dot{\gamma} \) are not spatially independent. It is therefore not immediately clear how the associated force balances are to be formulated, and, for that reason, these balances are established using the principle of virtual power.

Assuming that at a fixed time the fields \( \mathbf{u}, \varepsilon^p \) and \( \gamma^p \) are known, we consider \( \mathbf{u}, \varepsilon^f \) and \( \gamma^f \) as virtual rates, which are collected in the generalized virtual velocity \( \mathbf{V} = \{ \dot{\mathbf{u}}, \dot{\varepsilon}^f, \dot{\gamma}^f \} \). \( P_{\text{ext}} \) is the power expended on the domain \( \Omega \) and \( P_{\text{int}} \) a concomitant expenditure of power within \( \Omega \), given by

\[
P_{\text{ext}}(\Omega, \mathbf{V}) = \int_\Omega \mathbf{t}(\mathbf{n}) \cdot \dot{\mathbf{u}} d\mathbf{S} + \int_\Omega \sum_\alpha \left( \mathbf{X}^\alpha \gamma^\alpha \right) d\mathbf{S} \]

\[
P_{\text{int}}(\Omega, \mathbf{V}) = \int_\Omega \mathbf{\sigma} : \dot{\varepsilon}^f d\Omega + \int_\Omega \sum_\alpha \left( \mathbf{\pi}^\alpha \gamma^\alpha \right) d\Omega + \int_\Omega \sum_\alpha \left( \mathbf{\xi}^\alpha \cdot \nabla \gamma^\alpha \right) d\Omega \quad (3)
\]

where the stress tensor \( \mathbf{\sigma} \), the scalar internal forces \( \mathbf{\pi}^\alpha \) and the microstress vectors \( \mathbf{\xi}^\alpha \) are the thermodynamical forces conjugate to the internal state variables \( \varepsilon^f, \mathbf{\varepsilon} \) and \( \gamma^f \), respectively. In \( P_{\text{ext}} \), \( \mathbf{t}(\mathbf{n}) \) is the macroscopic surface traction while \( \mathbf{\gamma}(\mathbf{n}) \) represents the macroscopic surface traction conjugate to \( \gamma^f \) at the boundary \( S \) with \( \mathbf{n} \) indicating the boundary normal. As explained in the following, the relation of the conjugate stress quantity to the free energy, depends whether the stress is energetic or dissipative. If the stress is energetic then it is directly calculated as the partial derivative of the free energy with respect to the corresponding internal variables. If the stress is dissipative then such a relation cannot be identified.

The principle of virtual power states that for any generalized virtual velocity \( \mathbf{\gamma} \) the corresponding internal and external power are balanced, i.e.
\[ P_{\text{ext}}(\Omega, \mathcal{V}) = P_{\text{int}}(\Omega, \mathcal{V}) \quad \forall \mathcal{V} \]

Considering a generalized virtual velocity without slip, the virtual velocity field can be chosen arbitrarily and this leads to the classical macroscopic force balance,

\[ \mathbf{V} \cdot \boldsymbol{\sigma} = 0 \]  

(5)

and considering arbitrary virtual slip fields without a generalized virtual velocity leads to the microscopic force balances,

\[ \mathbf{V} \cdot \varepsilon^s + \tau^s - \pi^s = 0 \]  

(6)

on each slip system \( s \), where \( \tau^s \) is the resolved Schmid stress on the slip systems given by

\[ \tau^s = \sigma \cdot \mathbf{P}^s. \]

The local internal power expression can be written as

\[ P_i = \mathbf{\sigma} : \mathbf{\varepsilon} + \sum_s \left( \pi^s \mathbf{\varepsilon} + \mathbf{\varepsilon} \cdot \mathbf{\nabla} \mathbf{\varepsilon} \right) \]

(7)

The local dissipation inequality results in

\[ D = P_i - \dot{\psi} = \mathbf{\sigma} : \mathbf{\varepsilon} + \sum_s \left( \pi^s \mathbf{\varepsilon} + \mathbf{\varepsilon} \cdot \mathbf{\nabla} \mathbf{\varepsilon} \right) - \dot{\psi} \geq 0 \]  

(8)

The material is assumed to be endowed with a free energy with different contributions according to

\[ \dot{\psi} = \dot{\psi}_e + \dot{\psi}_s + \dot{\psi}_{\text{CVc}}. \]

(9)

The time derivative of the free energy is expanded and Eq. (8) is elaborated to

\[ D = \mathbf{\sigma} : \mathbf{\varepsilon} + \sum_s \left( \pi^s \mathbf{\varepsilon} + \mathbf{\varepsilon} \cdot \mathbf{\nabla} \mathbf{\varepsilon} \right) - \frac{\partial \dot{\psi}_e}{\partial \mathbf{\varepsilon}} \]

\[ : \mathbf{\varepsilon} + \sum_s \left( \pi^s + \frac{\partial \dot{\psi}_s}{\partial \mathbf{\varepsilon}} \right) \mathbf{\varepsilon} + \sum_s \left( \frac{\partial \dot{\psi}_{\text{CVc}}}{\partial \mathbf{\varepsilon}} \right) \mathbf{\nabla} \mathbf{\varepsilon} \geq 0 \]  

(10)

The stress \( \mathbf{\sigma} \) and the microstress vectors \( \varepsilon^s \) are regarded as energetic quantities having no contribution to the dissipation

\[ \mathbf{\sigma} = \frac{\partial \dot{\psi}_e}{\partial \mathbf{\varepsilon}}, \]

(11)

\[ \varepsilon^s = \frac{\partial \dot{\psi}_s}{\partial \mathbf{\varepsilon}}, \]

whereas \( \pi^s \) does have a dissipative contribution,

\[ D = \sum_s \left( \pi^s + \frac{\partial \dot{\psi}_s}{\partial \mathbf{\varepsilon}} \right) \mathbf{\varepsilon} + \sum_s \left( \frac{\partial \dot{\psi}_{\text{CVc}}}{\partial \mathbf{\varepsilon}} \right) \mathbf{\nabla} \mathbf{\varepsilon} \geq 0 \]

(12)

The multipliers of the plastic slip rates are identified as the set of dissipative stresses \( \sigma_{\text{dis}}^s \)

\[ \sigma_{\text{dis}}^s = \pi^s + \frac{\partial \dot{\psi}_s}{\partial \mathbf{\varepsilon}} \]  

(13)

In order to satisfy the reduced dissipation inequality at the slip system level the following constitutive equation is proposed

\[ \sigma_{\text{dis}}^s = q^s \text{sign}(\dot{\gamma}^s) \]

(14)

where \( q^s \) represents the mobilized slip resistance of the slip system under consideration

\[ q^s = \frac{\gamma_0}{\sigma_{\text{dis}}^s} \]  

(15)

where \( \gamma_0 \) is the resistance to dislocation slip which is assumed to be constant and \( \gamma_0 \) is the reference slip rate. Substituting (15) into (14) gives

\[ \dot{\gamma}^s = \frac{\gamma_0}{\sigma_{\text{dis}}^s} \]  

(16)

Substitution of \( \sigma_{\text{dis}}^s \) according to (13) into (16) reveals,

\[ \dot{\gamma}^s = \frac{\gamma_0}{\sigma_{\text{dis}}^s} \left( \pi^s + \frac{\partial \dot{\psi}_s}{\partial \mathbf{\varepsilon}} \right) \]

(17)

Using the microforce balance (6) results in the plastic slip equation

\[ \dot{\gamma}^s = \frac{\gamma_0}{\sigma_{\text{dis}}^s} \left( \tau^s + \mathbf{\varepsilon} \cdot \mathbf{\nabla} \mathbf{\varepsilon} - \frac{\partial \dot{\psi}_s}{\partial \mathbf{\varepsilon}} \right) \]

(18)

Comparing Eqs. (16) and (18) resolves \( \sigma_{\text{dis}}^s = \tau^s + \mathbf{\varepsilon} \cdot \mathbf{\nabla} \mathbf{\varepsilon} - \frac{\partial \dot{\psi}_s}{\partial \mathbf{\varepsilon}} \).

In the current non-convex strain gradient crystal plasticity framework the driving force for the dislocation slip evolution is \( \sigma_{\text{dis}}^s \) which physically means that, in addition to the resolved shear stress \( \tau^s \), the back stress due to the gradients of the geometrically necessary dislocation densities \( \mathbf{\varepsilon} \cdot \mathbf{\nabla} \mathbf{\varepsilon} \), and the internal force leading to the accumulation of plastic slip \( \frac{\partial \dot{\psi}_s}{\partial \mathbf{\varepsilon}} \) is affecting the plastic flow. In classical crystal plasticity frameworks it is only the resolved shear stress \( \tau^s \) which determines the plastic flow while in strain gradient type of models it is the effective resolved shear stresses \( \tau_{\text{eff}}^s \) which physically represents the radius of the dislocation domain contributing to the internal stress field. If the dislocation interaction is limited to nearest neighbor interactions only, then \( R \) equals the dislocation spacing. Moreover, \( v \) is Poisson’s ratio, \( E \) is Young’s modulus and the plastic slip dependent free energy \( \psi_s \) will be defined in the following section.

In order to solve the initial boundary value problem for this rate dependent strain gradient crystal plasticity framework, a fully coupled finite element solution algorithm is used in which both the displacement \( \mathbf{u} \) and plastic slips \( \dot{\gamma}^s \) are considered as primary variables. These fields are determined in the solution domain by solving simultaneously the linear momentum balance (5) and the slip evolution Eq. (18), which constitute the local strong form of the balance equations:

\[ \mathbf{V} \cdot \boldsymbol{\sigma} = 0 \]

(19)

\[ \dot{\gamma}^s - \frac{\gamma_0}{\sigma_{\text{dis}}^s} \mathbf{\varepsilon} + \frac{\gamma_0}{\sigma_{\text{dis}}^s} \mathbf{\nabla} \mathbf{\varepsilon} + \frac{\gamma_0}{\sigma_{\text{dis}}^s} \frac{\partial \dot{\psi}_s}{\partial \mathbf{\varepsilon}} = 0 \]

(20)

In order to obtain variational expressions representing the weak forms of the governing equations given above, these equations are multiplied by weighting functions \( \delta u \) and \( \delta \dot{\gamma}^s \) and integrated over the domain \( \Omega \). Using the Gauss theorem (\( S \) is the boundary of \( \Omega \)) results in

\[ G_u = \int_\Omega \mathbf{V} \delta u : \boldsymbol{\sigma} d\Omega - \int_S \delta u \cdot \mathbf{t} dS \]

(21)

\[ G_{\dot{\gamma}^s} = \int_\Omega \delta \dot{\gamma}^s \dot{\gamma}^s d\Omega - \int_\Omega \frac{\gamma_0}{\sigma_{\text{dis}}^s} \mathbf{\varepsilon} + \frac{\gamma_0}{\sigma_{\text{dis}}^s} \mathbf{\nabla} \mathbf{\varepsilon} + \frac{\gamma_0}{\sigma_{\text{dis}}^s} \frac{\partial \dot{\psi}_s}{\partial \mathbf{\varepsilon}} d\Omega \]

\[ + \int_S \delta \dot{\gamma}^s \frac{\gamma_0}{\sigma_{\text{dis}}^s} \frac{\partial \dot{\psi}_s}{\partial \mathbf{\varepsilon}} d\Omega - \int_S \gamma_0 \frac{\varepsilon}{\sigma_{\text{dis}}^s} \mathbf{\nabla} \mathbf{\varepsilon} dS \]
where the unknown fields of the displacement and slips and the associated weighting functions within each element are approximated by their nodal values multiplied with the interpolation shape functions stored in the $N^N_u$ and $N^N_s$ matrices, using a standard Galerkin approach:

$$\begin{align*}
\delta_u &= N^N_u \delta_u, \quad u = N^N_u u \\
\delta_s &= N^N_s \delta_s, \quad \gamma = N^N_s \gamma^s
\end{align*}$$ (22)

where $u$, $\delta_u$, $\gamma$ and $\delta_s$ are columns containing the nodal variables. Bilinear interpolation functions for the slip field and quadratic interpolation functions for the displacement field are used. An implicit backward Euler time integration scheme is used for $\gamma^s$ in a typical time increment $[\tau_n, \tau_{n+1}]$ which gives $\gamma^s = [\gamma^s_{n+1} - \gamma^s_n]/\Delta \tau$.

The discretized element weak forms read

$$\begin{align*}
G_u &= \delta_s^T \int_\Omega (B^u)^T \sigma d\Omega - \int_\Gamma N^T \sigma d\Gamma \\
G_s &= \delta_s^T \int_\Omega N^T N \left[ \frac{\sigma^s}{C} - \frac{\tau^s}{\Delta \tau} \right] d\Omega - \int_\Gamma \frac{\sigma^s}{C} N^T \sigma d\Gamma
\end{align*}$$

$$+ \delta_s^T \int_\Gamma \frac{\tau^s}{C} N^T \frac{\partial \sigma^s}{\partial \gamma^s} d\Gamma + \int_\Omega \frac{\sigma^s}{C} N^T \frac{\partial \sigma^s}{\partial \gamma^s} d\Omega - \int_\Gamma N^T \sigma d\Gamma$$ (23)

The weak forms of the balance Eqs. (23) are linearized with respect to the variations of the primary variables $u$ and $\gamma^s$ and solved by means of a Newton–Raphson solution scheme for the increments of the displacement field $\Delta \mathbf{u}$ and the plastic slips $\Delta \gamma^s$. The procedure results in a system of linear equations which can be written in the following matrix format,

$$\begin{pmatrix}
K_{uu} & K_{us} \\
K_{su} & K_{ss}
\end{pmatrix}
\begin{pmatrix}
\Delta \mathbf{u} \\
\Delta \gamma^s
\end{pmatrix}
= 
\begin{pmatrix}
-\mathbf{R}^u + \mathbf{R}^s \\
\mathbf{R}^s + \mathbf{R}^u
\end{pmatrix}$$ (24)

where $K_{uu}$, $K_{ss}$, $K_{su}$ and $K_{us}$ represent the global tangent matrices while $\mathbf{R}^u$ and $\mathbf{R}^s$ are the global residual columns. The contributions $\mathbf{R}^u$ and $\mathbf{R}^s$ originate from the boundary terms.

3. Latent hardening based non-convex plastic potential

In metal crystals the active slip systems influence the hardening of the inactive slip systems (see e.g. Kocks and Brown (1966) and Franciosi (1985)). This is an important concept in the hardening of the material and also in crystal plasticity as it controls the shape of the single crystal yield surface. In most of the crystal plasticity frameworks the latent hardening is included in a hardening module appearing in the evolution equations of the slip resistance or so-called critical slip system shear strength. It is also possible to incorporate this effect through a latent hardening plastic potential. In this section, the latent hardening based non-convex plastic potential proposed by Ortiz and Repetto (1999) is examined, whereby the conditions for the occurrence of plastic slip patterning are studied.

In physically deformed crystals one of the main presumed reasons for dislocation microstructure formation, is latent hardening accompanied with non-convexity of the energy function due to slip system interactions. Such a function is proposed by Ortiz and Repetto (1999) which gives parabolic-like hardening in single slip and latent (off-diagonal) hardening in multi-slip (see Fig. 1 for two slip systems)

$$\psi_f = \frac{2}{3} \tau_0 \gamma_0 \left[ \sum_p \sum_{p'} a^{p p'} |\gamma_p| |\gamma_{p'}| \right]^{3/4}$$ (25)

where $\tau_0$ and $\gamma_0$ are a reference resolved shear stress and a reference slip value, respectively, and $a^{p p'}$ are interaction coefficients. For the values of the matrix $a^{p p'}$, a simple geometrical model is used proposed by Cuitino and Ortiz (1993),

$$a^{p p'} = \frac{2}{\pi} \sqrt{1 - (\mathbf{n}^p \cdot \mathbf{n}^{p'})^2}$$ (26)

where $\mathbf{n}^p$ and $\mathbf{n}^{p'}$ are normals on the slip planes of the systems considered. Using (26), slip systems do not self-harden in a multi-slip context. The reasoning leading to (26) is based on the fact that the typical resolved shear stress required to deform a well-annealed crystal in single slip tends to be small compared to the stress required for multi-slip. For the purpose of understanding the morphology of dislocation structures, self-hardening can be neglected at first instance. Ortiz and Repetto (1999) and Ortiz et al. (2000) employ (25) and (26) in the context of crystal plasticity to obtain lamellar dislocation structures via a sequential lamination procedure. The purpose here is to study patterning driven by this latent hardening based non-convex potential. It is also possible to construct the $a^{p p'}$ matrix from dislocation dynamics simulations. In that case the implementation is suitable for a more physically based framework in terms of dislocation densities. In the current framework the physical numbers in the off-diagonal entries of the hardening modulus would affect the value of the potential $\psi_f$ as $\tau_0$ and $\gamma_0$ would do, which would eventually only slightly affect the quantitative nature of the patterning.

3.1. Conditions for plastic slip patterning

One of the basic problems in plasticity is to determine the plastic slip localization or the arrangements of dislocations under their mutual interactions and under the action of an applied stress. This problem has been addressed from various perspectives. Some scientists employ dislocation dynamics simulations e.g. Lubarda et al. (1993), Groma and Pavley (1993) and Kubin and Canova (1992) while others follow reaction–diffusion solutions for continuous distributions of dislocations such as Walgraef and Alfantis (1985) and Alfantis (1987). Another approach is to consider the problem from an energy perspective where dislocations seek configurations with a minimum free energy (see e.g. Kuhlmann-Wilsdorf and Van der Merwe (1982), Holt (1980) and Kuhlmann-Wilsdorf (2001)). In the context of finite plasticity theories some authors obtain laminate type dislocation microstructures through an incremental minimization procedure of a non-convex potential via a relaxation procedure (see e.g. Ortiz and Repetto (1999), Hackl and Kochmann (2008) and Kochmann and Hackl (2011)). From a thermodynamics point of view, a patterned microstructure will develop if it has a lower energy than a state with a homogeneous plastic deformation distribution. Yalcinkaya et al. (2011) studied this aspect on a double-well potential and showed that plastic slip patterning occurs at relatively low strain rates due to the existence of an unstable region in the double-well potential, where the microstructure evolves in a patterned way to lower its free energy. Convex energy potentials preserve stability and do not trigger patterning. Therefore, the presence of non-convexity is the first condition for a heterogeneous microstructure evolution to develop, yielding a lower energy than the homogeneous state. Note that there might be some exceptions in case of non-monotonic loading histories. For instance, during cyclic loading the evolution of dislocation microstructures may result in different observations in terms of energy as studied in e.g. Laird et al. (1988). It is stated that the deformation which occurs in the structures at a low number of cycles does not seem to be consistent with low energy arrays, however with sufficient cycling lower energy arrays seem to become established. The existence of a lower energy state is only one of the reasons that contribute to patterning. This is what is investigated in this paper. This does not exclude that also other physical mechanisms related to the dislocation
interactions may contribute to the formation of particular dislocation configurations.

In what follows, the latent hardening function (25) including (26), which is assumed to be the driving force for the evolution of dislocation microstructures, is examined in this sense. For this purpose, a single crystal in 2D having 2 slip systems oriented $\theta_1$ and $\theta_2$ with respect to the x axis is considered. A pure shear deformation is applied with a macroscopic strain field $\gamma_{ik}$, whose components are written in Cartesian coordinates as

$$e_{im} = \begin{bmatrix} 0 & \gamma \\ \gamma & 0 \end{bmatrix}$$

which satisfies the plastic incompressibility condition $\text{tr}(e_{im}) = 0$. Assume that the plastic deformation is patterned in the solution domain and that there exist two states with volume fraction $f$ and $1-f$. The weighted average strain of the two phases should be equal to the macroscopic strain, i.e.

$$f\epsilon_1 + (1-f)\epsilon_2 = e_{im}$$

where

$$\epsilon_1 = e_{i1}(\gamma_1^1, \gamma_1^2, \theta_1, \theta_2)$$

$$\epsilon_2 = e_{i2}(\gamma_2^1, \gamma_2^2, \theta_1, \theta_2)$$

are symmetric and incompressible. Note only the plastic deformation is considered in this analysis because the latent hardening based plastic potential depends solely on the plastic slips. Including the elastic strains would increase the number of unknowns, and it would make the problem impossible to solve analytically. With respect to the existence of a patterned solution, this would hardly affect the results. Using (29), Eq. (28) reduces to a set of 2 linear equations with 5 unknowns $\gamma_1^1, \gamma_1^2, \gamma_2^1, \gamma_2^2, f$. For a fixed value of $f$ and given two of the unknown slips, $\gamma_1^1$ and $\gamma_1^2$, the value of the other plastic slips $\gamma_2^1$ and $\gamma_2^2$ can be calculated according to

$$\gamma_2^1 = -\frac{f}{1-f} \gamma_1^1 + \frac{P_{11}}{P_{22}P_{11} - P_{12}P_{21}} \frac{1}{1-f}$$

$$\gamma_2^2 = -\frac{f}{1-f} \gamma_1^2 + \frac{P_{11}}{P_{22}P_{11} - P_{12}P_{21}} \frac{1}{1-f}$$

with

$$P_{11} = P^1(1, 1), \quad P_{12} = P^1(1, 2), \quad P_{21} = P^2(1, 1), \quad P_{22} = P^2(1, 2).$$

The energy of this assumed patterned state can be calculated as,

$$\bar{\psi}_l = f\psi_{\gamma_1^1}(\gamma_1^1, \gamma_1^2, \theta_1, \theta_2) + (1-f)\psi_{\gamma_2^1}(\gamma_2^1, \gamma_2^2, \theta_1, \theta_2)$$

which is plotted in Fig. 2. The latent hardening energy corresponding to the macroscopic shear strain $\epsilon_{im}$ is calculated via (25) and (26) in terms of the plastic slips $\gamma_1^1$ and $\gamma_1^2$ on given slip systems as,

$$\psi_l = \psi_{\gamma_1^1}(\gamma_1^1, \gamma_1^2, \theta_1, \theta_2)$$

The purpose of the analysis in this section is to investigate if there exists a domain of a latent hardening based energy for the assumed patterned case $\bar{\psi}_l$ smaller than the macroscopic latent hardening based energy $\psi_l$, (reflecting the homogeneous non-patterned state), which would energetically allow for patterning of the plastic slip field. Therefore this analysis can be regarded as a prerequisite for the patterning simulations in the next section. To this end, $\bar{\psi}_l$ is calculated for different values of $\gamma_1^1$ and $\gamma_1^2$, and for specific (selected) orientations and volume fractions.

If a macroscopic shear deformation tensor $\epsilon_{im}$ with $\gamma = 0.02$ is applied on a combination of slip systems with orientations $\theta_1 = 60^\circ$ and $\theta_2 = 120^\circ$, the amount of slips on the two slip systems for the local homogeneous state equals 0.04. Using these values for the slips and the orientations, the locally homogeneous latent hardening plastic potential is calculated via Eqs. (25) and (26).

Assuming $\gamma_0 = 1$ MPa and $\gamma_1 = 1$ the characterizing latent hardening energy for the non-patterned state equals $\psi_l = 0.0057$ MPa. Presuming the existence of patterned states for different values of $f$ and ($\gamma_1^1, \gamma_1^2$), the values of $\gamma_1^1$ and $\gamma_1^2$ are calculated via (30) and the latent hardening energy follows from (31). In order to obtain a patterned microstructure the energy of the patterned state should be smaller than the energy of the local homogeneous state $\bar{\psi}_l < \psi_l$. As it can be observed in Fig. 2 there are many combinations satisfying this inequality for different values of the volume fraction $f$ and the plastic slip values $\gamma_1^1$ and $\gamma_1^2$.

4. Numerical analysis

In this section, two different numerical examples are presented to study the behavior of the proposed rate dependent strain gradient crystal plasticity models. The first example deals with a conventional convex free energy in terms of plastic slip gradients and elastic strains, where the effects of the applied shear rate and the internal length parameter $R$ are analyzed. Then, the influence of the physically based non-convex latent hardening plastic potential on the mechanical behavior of the material is discussed.

4.1. Convex strain gradient crystal plasticity

In this subsection, the plastic potential $\psi_{\gamma_1^1}$ is assumed to be zero therefore having no influence on patterning and the hardening of

![Fig. 1. Two different views of $\bar{\psi}_l$ (MPa) for different amounts of slip on two slip systems oriented with respect to the x axis as 60° and 120° where $\gamma_0 = 1$ and $\gamma_1 = 1$ MPa.](image-url)
the material. The incorporated hardening is only due to the gradients of the plastic slip. This is referred to as convex strain gradient crystal plasticity because there is no plastic potential inducing a lack of convexity.

To reveal the main characteristics of this convex strain gradient viscous crystal plasticity model, a constrained plane strain shear problem of an infinite strip, induced by periodic boundary conditions, is studied in the first example. A strip, with height \( H \) (in \( y \) direction) is bounded by rigid walls that are impenetrable for dislocations, i.e. a no slip condition applies (\( \gamma_y = 0 \)) at top and bottom edges. These so-called micro clamped boundary conditions for the plastic slips invoke an inhomogeneous plastic deformation state (e.g. as present near grain boundaries in polycrystals or at the surface of a thin film). The displacements at \( y = 0 \) are suppressed (\( u_x = 0 \) and \( u_y = 0 \)) and prescribed at \( y = H \) as \( u_x = u(t) \) and \( u_y = 0 \). In addition, in \( x \) direction all field quantities are taken to be independent of \( x \). Consequently, the field quantities on the left side are assumed to be identical to those on the right side (\( u_l = u_r \) and \( \gamma_{y,l} = \gamma_{y,r} \)).

Locally, two slip systems with orientations 60° and 120° with respect to the horizontal axis are considered. The material is assumed to be elastically isotropic with Young’s modulus \( E = 210 \) GPa, Poisson’s ratio \( \nu = 0.33 \), slip resistance for both slip systems \( s = 35 \) MPa, and a reference slip rate \( \dot{\gamma}_0 = 15 \) s\(^{-1}\). Results presented in the following correspond to a discretization with 1 \( \times \) 100 rectangular elements. One element in the \( x \)-direction is sufficient, given the uniformity in this direction.

The examples addressed in this subsection are carried out for different applied shear rates and \( R/H \) ratios for varying \( R \) and constant height \( H \), where the relative effect of the internal length scale

![Fig. 2. \( \bar{\psi} \) (MPa) in terms of a set of given \( \gamma_1 \) and \( \gamma_2 \) for different values of \( f \) with \( \theta_1 = 60^\circ \) and \( \theta_2 = 120^\circ \).](image_url)
parameter \( R \) determining \( A \), acting on the higher order microstresses \( \xi \) (see equations (11) and (19)), is analyzed.

First, the resulting shear stress versus the applied macroscopic shear \( \Gamma \) is presented in Fig. 3 for different overall shear rates \( \dot{\Gamma} \), using \( R = 0.35 \mu m \), and \( H = 20 \mu m \). \( \Gamma \) is the macroscopic shear defined as \( \Gamma = u/H \). In this case, the average of the local strain \( \varepsilon_{12} \) should be half of the macroscopic shear \( \Gamma \). If the elastic deformation is small, the average value of the local plastic shear strain \( \varepsilon_{p12}^{p} \) will be roughly equal to half of the macroscopic shear \( \Gamma \) as well. When the applied macroscopic shear rate increases, the material shows a stiffer (dominantly elastic) response. Note that a considerable viscosity effect is predicted in these results. This is due to Eq. (18) which is identical to the power law relations in rate dependent classical crystal plasticity frameworks with a power exponent \( m = 1 \) which basically defines the viscosity, as studied in Yalcinkaya et al. (2011). Other values of \( m \) or introducing a lower viscosity would change the results quantitatively, but not qualitatively. The viscosity is not needed for numerical convergence, nor for obtaining the patterns in the following examples. The reason of this choice is to keep the framework as simple as possible with a minimum number of parameters. In Fig. 4, the local rate dependent plastic shear strain evolution is presented at a macroscopic shear level of \( \dot{\Gamma} = 0.02 \). There is a clear boundary layer width dependence on the applied shear rate. For high values of the applied shear rate, e.g. \( \dot{\Gamma} = 2.5s^{-1} \) we observe a sharp boundary layer, while for low values of the shear rate, e.g. \( \dot{\Gamma} = 0.025s^{-1} \), the boundary layer thickness is more diffuse. This type of rate dependent dislocation slip profile is also observed in Yalcinkaya et al. (2011) where a high strain rate causes that the plastic slip has not enough time to evolve.

The next example in this subsection concerns the influence of the internal length scale parameter \( R \) on the mechanical behavior for a fixed height \( H = 20 \mu m \). The value of \( R \) is taken as 0.35 \( \mu m \), 0.7 \( \mu m \) and 1.75 \( \mu m \) corresponding to a \( R/H \) ratio equal to 0.0175, 0.035 and 0.0875 respectively. The shear stress versus the applied macroscopic shear response is plotted in Fig. 5 for different values of \( R \) at \( \dot{\Gamma} = 0.025s^{-1} \). Note that the formulation is intrinsically viscous, corresponding to models using a linear drag law for dislocation motion to determine the slip. Fig. 5 illustrates a significant effect of the internal length parameter where the strip is exhibiting a stiffer response for larger values of \( R \). The results are consistent with many strain gradient models (e.g. Shu et al. (2001), Evers et al. (2004) and Yalcinkaya et al. (2011)) in which the influence of the length scale was shown. Physically, this effect results from the fact that large \( R \) values induce a large internal stress and hence penalize high plastic slip gradients (see Fig. 6) spreading the geometrically necessary dislocation densities. In this convex example, the slip gradient is the dominating factor in the plastic and hardening behavior of the material and therefore a clear size effect is observed. In Fig. 6 a clear dependence of the boundary layer evolution on \( R \) is presented at \( \dot{\Gamma} = 0.02 \). With increasing \( R \) an increased influence of the boundary conditions is observed with a more diffuse boundary layer.

The distribution of the plastic slips on each of the slip systems is illustrated in Fig. 7 for the same example with \( R = 0.35 \mu m \) and \( \dot{\Gamma} = 0.025s^{-1} \) at \( \dot{\Gamma} = 0.02 \). The amount of the slip on both slip
4.2. Non-convex strain gradient crystal plasticity

In this subsection the influence of the latent hardening plastic potential \( w_c \) (25) and (26) on the mechanical behavior and the deformation patterning is illustrated in the present rate dependent strain gradient crystal plasticity framework. In addition to \( w_c \), an elastic strain energy potential \( w_e \) and a plastic slip gradient free energy potential \( w_r \) are incorporated as well. The viscous formulation of the problem and the gradient free energy potential regularize the problem.

The paper of Ortiz and Repetto (1999) shows that in crystals exhibiting latent hardening the energy function is non-convex, which favors the development of microstructures. Therefore, uniform deformation fields are not the minimizers of the incremental work of deformation. In other words, in the context of classical variational formulations the crystals exhibiting latent hardening might not reach the expected solution, i.e. the minimum free energy is not achieved. It is possible to construct deformation mappings to recover the minimum value. Such deformation mappings make use of the existence of fine microstructures. Using a sequential lamination method, Ortiz and Repetto (1999) were able to characterize analytically several dislocation structures. The same procedure is followed later in Ortiz et al. (2000) where microstructures are regarded as instances of sequential lamination during deformation. The microstructures are explicitly constructed by recursive lamination and their subsequent equilibration.

Fig. 4. Rate dependent plastic shear strain \( \varepsilon_{12}^p \) distribution for the plane strain shear problem of an infinite strip at a global shear level of \( \Gamma = 0.02 \) for \( R = 0.35 \) and \( H = 20 \mu m \).

Fig. 5. The effect of the internal length scale parameter \( R \) on the stress vs. applied shear response for the plane strain shear problem of an infinite strip for \( H = 20 \mu m \) at \( \Gamma = 0.025s^{-1} \).

Fig. 6. The effect of the internal length scale parameter \( R \) on the plastic shear strain \( \varepsilon_{12}^p \) distribution for the plane strain shear problem of an infinite strip at a global shear level of \( \Gamma = 0.02 \) for \( H = 20 \mu m \) at \( \Gamma = 0.025s^{-1} \).

Fig. 7. The distribution of the plastic slip on both slip systems at a global shear level of \( \Gamma = 0.02 \) for \( R = 0.35 \) \( \mu m \) and \( \Gamma = 0.025s^{-1} \) at \( \Gamma = 0.02 \).
The numerical study in Section 3 proves that the latent hardening potential (26) is non-convex and satisfies the energetic conditions for plastic slip phase separation in the context of the present small strain rate dependent crystal plasticity formulation. Compared to the previous work of Ortiz and Repetto (1999) and Ortiz et al. (2000) relying on the explicit construction of cellular dislocation microstructures via a lamination procedure, the present framework is based on the implicit evolution of microstructures driven by the deformation. Throughout the incremental deformation process the state of the plastic slip enters energetically favorable regimes, (as illustrated in Section 3) which might eventually result in deformation heterogeneity.

The numerical study in this subsection concerns a plane strain pure shear problem of a square representative volume element (RVE) in order to have a direct link with the study in Section 3. Locally, two slip systems with orientations 60° and 120° with respect to the x axis are considered. The material is assumed to be elastically isotropic with Young’s modulus $E = 210$ GPa, Poisson’s ratio $\nu = 0.33$, slip resistance for both slip systems $s = 35$ MPa, and a reference slip rate $\dot{\gamma}_0 = 0.15$ s$^{-1}$. The reference slip strain and resolved shear stress in (26) are assumed to be $\dot{\gamma}_0 = 0.015$ and $\tau_0 = 50$ MPa, respectively.

In the square RVE the displacements and the plastic slips on the left edge are tied to the ones on the right edge and the ones on the bottom edge are tied to the ones on the top edge which makes it a fully periodic configuration. The vertical displacement at the right bottom corner and the horizontal displacement at the left top corner are prescribed, both equal to $u(t)$. The displacements at the left bottom corner are suppressed together with the horizontal displacement at the right bottom corner and vertical displacement at the left top corner. These boundary and loading conditions result in a pure shear deformation mode. The length of each edge of the square is $H = 20$ μm. Results presented in the following correspond to a discretization with $20 \times 20$ rectangular elements.

In Fig. 8 the shear stress versus applied macroscopic shear, defined as $\Gamma = 2u/H$, is plotted for an applied shear rate $\dot{\Gamma} = 0.025$ s$^{-1}$ and an internal length scale parameter $\lambda = 0.01$ μm. The curve does not exhibit a softening branch, stress-plateau and subsequent hardening as these were observed in the results of Yalcinkaya et al. (2011), which illustrate spinodal decomposition of the plastic slip field and macroscopic localization (e.g. Lüders band formation). It is consistent with the experimental observations during dislocation cell formation. The reason for this is the heterogeneous local distribution (and patterning) between the two slip systems. The patterns are now formed in a complementary manner on the coupled slip systems as shown in Fig. 10, to accommodate the overall shear. As a result, the fluctuations at the slip system level

![Fig. 8. Latent hardening based non-convex shear stress vs. applied macroscopic shear for a plane strain pure shear problem of a fully periodic RVE at $\dot{\Gamma} = 0.025$ s$^{-1}$.](image)

![Fig. 9. Shear strain (first figure), plastic shear strain (second figure), and plastic slip (last two figures) distributions at $\Gamma = 0.034$ for a plane strain pure shear problem of a fully periodic RVE at $\dot{\Gamma} = 0.025$ s$^{-1}$.](image)
have less effect on the macroscopic average behavior. In this case, the average of the local strain $e_{12}$ should be half of the macroscopic shear $C$. If the elastic deformation is small, the average value of the local plastic shear strain $e_{12}^p$ will be roughly equal to half of the macroscopic shear $C$ as well. The corresponding shear strain, plastic shear strain and plastic slips of the slip systems are plotted in Fig. 9. All plotted fields exhibit a strong patterned response due to the incorporated latent hardening potential. Note that the applied periodic boundary conditions lead to an initially homogeneous distribution of the strain and plastic slip fields. In order to properly trigger a small perturbation a small spatial fluctuation is applied to the Young’s modulus $E$ in the RVE. Giving a small spatial variation in one of the plastic parameters such as the slip resistance $s_a$ and $c_{0}$ would fit for this purpose as well. The amount of

![Fig. 10. Shear strain, plastic shear strain, and plastic slip distributions at $\tau = 0.034$ for a plane strain pure shear problem of a fully periodic RVE with a fluctuation applied to the central element (first four figures) and to the middle element on the right edge (last four figures) at $\tau = 0.025s^{-1}$.](image)
the perturbation is about 1% which does not make it unphysical, since the lattice orientation already triggers such a spatial orientation dependence larger than this value. In order to illustrate the influence of the selected spatial fluctuation of $E$ on the evolution of the plastic microstructure, two different types of fluctuations are applied in the next two examples. In Fig. 10 the field quantities are plotted for two additional cases with different fluctuations applied in Young's modulus. First, the fluctuation is given only to an element in the center of the RVE and in the second case the fluctuation is given to an element in the middle of the right edge. The applied fluctuation has certainly an effect on the distribution of the deformation patterns, however, the spacing of high and low strain areas and the amplitude do not depend on the applied fluctuation. The macroscopic stress versus strain diagram is not plotted in these two cases because it is identical to the previous case plotted in Fig. 8. Note that, the nucleation of the pattern depends on the size of the intrinsic heterogeneities that naturally depend on the mesh size, which is in agreement with mesh refinement in phase field models. The presented example illustrates one of the possible patterns that could be obtained via the actual framework, which has a substantial potential for the evolution of laminate structures.

It is remarked that the obtained deformation patterns depend considerably on the applied rate of deformation. Increasing the strain rate results in a stiffer stress versus strain response while the amplitude of the obtained patterns decreases. Even though the present paper aims to reveal the effect only qualitatively, this observation is in agreement with experimental studies (see e.g. Lee and Lin (2001)) where at higher loading rates the dislocation cell size becomes quite small, and even though the dislocation density is higher than for low strain rates the dislocation cells are less visible. On the other hand at low rates one can observe well-developed, pronounced dislocation cell structures. Another important parameter affecting the patterning of deformation fields is the internal length scale $R$ which should be small enough to obtain a stable numerical solution and pronounced patterns. These two factors and other material parameters play an important role in the convergence of the numerical solution as well. Due to the non-convexity of the latent hardening potential at each increment of the deformation some combinations of the parameters might give convergence problems and it is not always possible to reach the same state of deformation with different combinations of the rate of deformation and material parameters.

Even though the considered 2D material allows for much more strain heterogeneity than a 3D case would, as there are no constraints at the boundary planes in the missing dimension of the material, this is not the reason of the observed pronounced deformation patterns. Considering that the plastic slip patterns are obtained with soft boundaries, which does not apply any restriction to the regarding field, in the 1D case in Yalcinkaya et al. (2011) and the 2D case here, a similar approach in three dimensions would result in deformation patterning as well. Then, purposeful investigation on the non-convex potential should be pursued combined with comparison to real microstructure evolution observations.

As stated before the non-convex potential has been used to recover a cellular kind of dislocation microstructures by Ortiz and Repetto (1999) and Ortiz et al. (2000) via an external lamination procedure, while we try to obtain deformation patterns via a non-convex evolution problem. In the current examples we observe deformation patterning at low loading rates and a small internal length scale parameter due to the latent hardening based non-convexity. This shows agreement with the study in Section 3 illustrating the capability of the latent hardening function for deformation patterning.

Many authors addressed the microstructure evolution under shear loading in order to study e.g. the Bauschinger effect (see e.g. Rauch and Schmitt (1989), Nesterova et al. (2001), Peeters et al. (2001) and Gardey et al. (2005)). In these types of studies the applied deformation is at moderate to large strain levels, to achieve the dominating anisotropy effect caused by the evolution of well-developed dislocation microstructures. In our example, illustrating the deformation patterning under shear loading, the strain level is quite low compared to these studies, however the primary patterns are still obtained. The results have not been compared with the experimental studies and the model has not been validated yet. At this stage the examples illustrate solely the capability of the model to capture the deformation heterogeneity and the validation of the model with respect to experimental observations remains to be done.

Note that the current work only considers monotonic loading histories, however during cyclic loading some particular microstructure evolution is observed such as persistent slip bands (PSBs) in single slip and labyrinths in multi slip modes (see e.g. Sauzay and Kubin (2011) for an extensive overview). Depending on the given perturbation, the internal length scale parameter and most importantly the non-convex free energy function, microstructures with a different morphology could be obtained with the current model. As stated above, the validation of the model considering the experimental observations during monotonic loading has not been conducted yet. We have presented the influence of one of the physical mechanisms (latent hardening) which could affect the patterning during monotonic loading without a validation with respect to actual material data. The microstructure evolution under cyclic loading requires an additional analysis. Hence, it is yet too early to deal with the simulation of PSBs, labyrinths, or cell formation during cyclic loading at this stage. However, the model has a substantial potential to contribute to the formation and the evolution of microstructures. To model complex microstructures in cyclic loading, other mechanisms may be important as well.

5. Summary and conclusion

A plastic slip based rate dependent non-convex strain gradient crystal plasticity model is proposed and embedded in a FEM solution framework using displacements and plastic slips as degree of freedoms. A physically based latent hardening non-convex plastic potential (Ortiz and Repetto, 1999) is incorporated into the thermodynamically consistent viscous strain gradient crystal plasticity model based on the 1D formulation as presented in Yalcinkaya et al. (2011) in order to obtain deformation and plastic slip patterns due to slip system interactions in physically deforming crystals. The presented approach models the implicit evolution of deformation patterns through the intrinsic non-convexity of the free energy function. This kinetics driven method offers an alternative to the explicit construction of the microstructure evolution (e.g. in Ortiz and Repetto (1999)).

Selected examples demonstrate the ability of the model to obtain a deformation driven plastic slip microstructure evolution. While a convex theory explicitly illustrates the size dependent and rate dependent boundary layer development, the non-convex formulation, originating from the slip interaction phenomena in crystals, allows for deformation and plastic slip patterning.

In the model the destabilizing non-convex term in the free energy is mathematically stabilized through the gradient term in the free energy and the viscous nature of the thermodynamically consistent slip law. The obtained microstructure evolution is rate dependent, where the homogeneity or inhomogeneity of the deformation basically depends on the applied rate. Due to the non-convexity at each increment of the applied deformation, the convergence and the patterning of the field are sensitive to many parameters, where we have shown only the effect of the applied
fluctuation. A more detailed investigation of the dependence of the results on the loading type, loading rates, slip system orientations, material parameters, the mesh and boundary conditions would help for a deeper understanding of the observed microstructure evolution phenomena.

**References**


