Deformation patterning in three-dimensional large-strain Cosserat plasticity

T. Blesgen

Bingen university, Berlinstraße 109, D-55411 Bingen, Germany

Abstract

In the framework of the rate-independent large-strain Cosserat theory of plasticity explicit analytic solutions are computed in three space dimensions. It is shown that the micro-rotations can be computed by solving stationary Allen-Cahn equations. While the material parameters are within a certain range, this explains the occurrence of pattering leading to a partitioning of the domain into subsets with approximately constant rotations.

Key words: Plasticity, Cosserat theory, pattern formation, Allen-Cahn equation

1. Introduction

This article focuses on the theoretical investigation of rotation deformation zones predicted by the large-strain rate-independent Cosserat theory of visco-plasticity. The results extend and confirm the two-dimensional findings in Blesgen (2013). Therein, it had been shown that for suitable boundary conditions *deformation patterning* arises. This term refers to the occurrence of Cosserat deformation zones, i.e. the formation of cells in the material with approximately constant micro-rotations as a consequence of deformation. The proposed mechanism may explain the formation of grains and subgrains in solids. Earlier studies of this topic include the articles by Zeghadi et al. (2005), Forest et al. (2000), Vardoulakis et al. (1995) and Oda et al. (1999), where the plasticity of polycrystals and the kinetics of the individual grains were investigated.

From its construction, the Cosserat model is a gradient model. In that, in contrast to other established models in elasto-plasticity as Hill (1998),

Email addresses: `t.blesgen@fh-bingen.de` (T. Blesgen)

Miehe (1988) and Simo (1988a,b), it automatically induces a length scale, with the effect that the localisation zones always have a finite width.

This paper is organised in the following way. Section 2 recalls the formalism of the rate-independent large-strain Cosserat theory in the case that plasticity occurs along given slip systems only. In Section 3, analytic solutions to a three-dimensional shear problem are computed, first for a purely plastic case without elastic deformations, secondly for a purely elastic case without plasticity. In both cases, using a parametrisation of the rotation group SO(3) by Euler angles, it is shown that the rotations can be computed by solving an Allen-Cahn system, a model originally derived for studying phase transitions. The article ends with a discussion of the results.

2. The finite-strain Cosserat model of visco-plasticity

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with Lipschitz boundary serving as the reference configuration of the undeformed material. The total deformation of the solid is controlled by the diffeomorphism $\varphi : \Omega \to \Omega_t$ where $\Omega_t \subset \mathbb{R}^3$ is the deformed solid at time $t \geq 0$. Because of $\varphi(\cdot, 0) = \mathrm{Id}$ it holds $\det(D\varphi(t)) > 0$ for all $t \geq 0$.

By the Cosserat approach, the deformation tensor $F := D\varphi$ is multiplicatively decomposed into the plastic part F_p and the elastic part F_e. In turn, F_e is split into a rotation component R_e and a stretching component U_e,

$$F = F_\mathrm{e} F_\mathrm{p} = R_\mathrm{e} U_\mathrm{e} F_\mathrm{p}. \tag{1}$$

It holds $U_\mathrm{e} \in \mathrm{GL}(\mathbb{R}^3)$ and $R_\mathrm{e} \in \mathrm{SO}(3)$, where GL is the general linear group of invertible matrices, and

$$\mathrm{SO}(d) := \{R \in \mathrm{GL}(\mathbb{R}^d) \mid \det(R) = 1,\ R^t R = \mathrm{Id}\}$$

denotes the special orthogonal group. In general, U_e is not symmetric and positive definite, in particular the decomposition $F_\mathrm{e} = R_\mathrm{e} U_\mathrm{e}$ is *not* the polar decomposition. By

$$K_\mathrm{e} := R_\mathrm{e}^t D_x R_\mathrm{e} = (R_\mathrm{e}^t \partial_{x_k} R_\mathrm{e})_{1 \leq k \leq 3} \tag{2}$$

the third-order (right) curvature tensor is denoted, $\kappa = (\kappa_0, \ldots, \kappa_{I_\mathrm{p}})$ designates the vector of stored dislocation densities, $\sigma_Y > 0$ is the yield stress.

Starting point of the analysis is the unconstrained minimisation problem

$$
\begin{aligned}
E_\beta(R_{\rm e},\gamma) = \int_\Omega \Big[& W_{\rm st}(R_{\rm e}^t D\varphi F_{\rm p}(\gamma)^{-1}) + W_{\rm c}(K_{\rm e}) + \varrho\Big(\sum_{a=1}^{I_{\rm p}} |\gamma_a - \gamma_a^0|\Big)^2 \\
& + \sum_{a=1}^{I_{\rm p}} |\gamma_a - \gamma_a^0| \Big(\sigma_Y - 2\varrho \sum_{a=1}^{I_{\rm p}} \kappa_a^0\Big)\Big] \, {\rm d}x \to \min, \qquad (3) \\
R_{\rm e}|_{\partial\Omega} = & R_D.
\end{aligned}
$$

This problem originates from Eqn. (16) in Blesgen (2013) after using the identity (6) on the dislocation densities stated below, plugging in the simple quadratic energy density of stored dislocations

$$
V(\kappa) := \varrho\Big(\sum_{a=1}^{I_{\rm p}} \kappa_a\Big)^2, \qquad (4)
$$

and generalising to $I_{\rm p} \geq 1$ slip systems.

In (3), E_β represents the mechanical energy of a deformed solid. In deriving this functional, it is assumed that plastic deformations occur only along given slip systems, controlled by a set of parameters $\gamma = (\gamma_1, \ldots, \gamma_{I_{\rm p}})$ according to

$$
F_{\rm p}(\gamma) = {\rm Id} + \sum_{a=1}^{I_{\rm p}} \gamma_a m_a \otimes n_a. \qquad (5)
$$

In (5), $m_a, n_a \in \mathbb{R}^3$ denote the slip vectors and slip normals with $|m_a| = |n_a| = 1$, $m_a \cdot n_a = 0$ for all slip systems $1 \leq a \leq I_{\rm p}$.

For two sets of initial parameters $\kappa^0 = (\kappa_1^0, \ldots, \kappa_{I_{\rm p}}^0)$, $\gamma^0 = (\gamma_1^0, \ldots, \gamma_{I_{\rm p}}^0)$ of the previous time step t, the new quantities $(R_{\rm e}, \gamma)$ at time $t+h$ are computed as minimisers of E_β. Then,

$$
\kappa_a := \kappa_a^0 - |\gamma_a - \gamma_a^0|, \qquad 1 \leq a \leq I_{\rm p} \qquad (6)
$$

is set and (κ, γ) serve as initial values of the next time step. This concept of time-discrete minimisation problems goes back to Ortiz et al. (1999). It allows to apply variational methods for the investigation of deformation processes.

Starting from a material free of dislocations, $\kappa(\cdot, 0) = 0$, as a consequence of the hardening law (6), $\sum_{a=1}^{I_{\rm p}} \kappa_a(t+h) \leq \sum_{a=1}^{I_{\rm p}} \kappa(t) \leq 0$ for all times t. Therefore, in (3), $-2\varrho \sum_{a=1}^{I_{\rm p}} \kappa_a^0 \geq 0$ specifies the increase of the yield stress σ_Y due to stored dislocations.

In deriving (3), the deformations are restricted to the shear case

$$D\varphi(t) = \mathrm{Id} + \sum_{a=1}^{I_\mathrm{p}} \beta_a(t) m_a \otimes n_a \qquad \text{in } \overline{\Omega} \tag{7}$$

for given $\beta = (\beta_1, \ldots, \beta_{I_\mathrm{p}})$. Eqn. (7) not only fixes φ at $\partial\Omega$, but states in addition that in the interior of Ω, the deformation follows this prescribed boundary deformation, i.e. states the validity of the Cauchy-Born rule.

Eqn. (3) is formulated for the traction-free case only. It is assumed further that no external volume forces and no external volume couples are applied to the solid.

The stretching energy W_st and the curvature energy W_c are introduced as, cf. Neff (2006), Blesgen (2013),

$$W_\mathrm{st}(U_\mathrm{e}) := \mu\|\mathrm{sym}(U_\mathrm{e} - \mathrm{Id})\|^2 + \mu_c\|\mathrm{skw}(U_\mathrm{e})\|^2 + \frac{\lambda}{2}|\mathrm{tr}(U_\mathrm{e} - \mathrm{Id})|^2, \tag{8}$$

$$W_\mathrm{c}(K_\mathrm{e}) := \mu_2\|\nabla R_\mathrm{e}\|^2 \tag{9}$$

for positive material parameters ϱ, μ, λ, μ_c, $\mu_2 := \mu L_c^2$ with the internal length scale $L_c > 0$, $\mathrm{sym}(A) := 0.5(A + A^t)$, $\mathrm{skw}(A) := 0.5(A - A^t)$, the trace operator $\mathrm{tr}(A) := \sum_i A_{ii}$ and the Frobenius matrix norm

$$\|A\| := \sqrt{\mathrm{tr}(A^t A)}. \tag{10}$$

In the two-dimensional analysis in Blesgen (2013), the canonical one-to-one parametrisation

$$R_\mathrm{e} = R_\mathrm{e}(\tilde{\alpha}) = \begin{pmatrix} \cos\tilde{\alpha} & -\sin\tilde{\alpha} \\ \sin\tilde{\alpha} & \cos\tilde{\alpha} \end{pmatrix}, \qquad \tilde{\alpha} \in [0, 2\pi)$$

of SO(2) had been used. In three space dimensions however, SO(3) is a manifold and all charts are only locally invertible. In this article, Euler angles are applied, i.e. for $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{R}^3$ it is set

$$\begin{aligned} R_\mathrm{e}(\alpha) &:= Q_3(\alpha_3) Q_2(\alpha_2) Q_1(\alpha_1) \\ &:= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha_3 & \sin\alpha_3 \\ 0 & -\sin\alpha_3 & \cos\alpha_3 \end{pmatrix} \begin{pmatrix} \cos\alpha_2 & 0 & -\sin\alpha_2 \\ 0 & 1 & 0 \\ \sin\alpha_2 & 0 & \cos\alpha_2 \end{pmatrix} \begin{pmatrix} \cos\alpha_1 & \sin\alpha_1 & 0 \\ -\sin\alpha_1 & \cos\alpha_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{11}$$

The right hand side of (11) defines a rotation for any argument $\alpha \in \mathbb{R}^3$ and the mapping $\alpha \mapsto R_\mathrm{e}(\alpha) \in \mathrm{SO}(3)$ is onto, but possesses critical points where its inverse is not unique. The ansatz (11) does not prefer one of the three spatial coordinates and, in contrast to other parametrisations by Euler angles where two elementary rotations Q_k are along the same coordinate axis, satisfies (15) below.

Letting $s_k := \sin(\alpha_k)$, $c_k := \cos(\alpha_k)$ for $k = 1, 2, 3$, Eqn. (11) leads to

$$R_{\mathrm{e}}(\alpha) = \begin{pmatrix} c_1c_2 & s_1c_2 & -s_2 \\ c_1s_2s_3 - s_1c_3 & c_1c_3 + s_1s_2s_3 & c_2s_3 \\ s_1s_3 + c_1s_2c_3 & s_1s_2c_3 - c_1s_3 & c_2c_3 \end{pmatrix}. \tag{12}$$

In order to recast ∇R_{e}, the identity

$$\frac{\partial Q_k(\alpha_k)}{\partial \alpha_k} = Q_k(\alpha_k) Z_k, \quad k = 1, 2, 3,$$

with the basis $\{Z_1, Z_2, Z_3\}$ of $\mathfrak{so}(3)$, the Lie Algebra corresponding to SO(3),

$$Z_1 := \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad Z_2 := \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \qquad Z_3 := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix},$$

infers for any $k = 1, 2, 3$

$$\begin{aligned} \|\partial_{x_k} R_{\mathrm{e}}(\alpha)\|^2 &= \|\partial_{x_k}(Q_3(\alpha_3)Q_2(\alpha_2)Q_1(\alpha_1))\|^2 \\ &= \left\| Q_3Z_3Q_2Q_1 \frac{\partial \alpha_3}{\partial x_k} + Q_3Q_2Z_2Q_1 \frac{\partial \alpha_2}{\partial x_k} + Q_3Q_2Q_1Z_1 \frac{\partial \alpha_1}{\partial x_k} \right\|^2. \end{aligned} \tag{13}$$

Unfortunately, in general $Q_i(\alpha)$ and Z_j, $i, j \in \{1, 2, 3\}$ do not commute. Furthermore, the Frobenius norm $\|\cdot\|$ is not even submultiplicative, i.e. $\|AB\| \not\leq \|A\|\|B\|$ for general tensors A, B. Therefore, explicit and lengthy computations are inevitable. By direct inspection of the terms in (13),

$$\begin{aligned} (Q_3Z_3Q_2Q_1)(\alpha) &= \begin{pmatrix} 0 & 0 & 0 \\ s_1s_3 + c_1s_2c_3 & -c_1s_3 + s_1s_2c_3 & c_2c_3 \\ s_1c_3 - c_1s_2s_3 & -c_1c_3 - s_1s_2s_3 & -c_2s_3 \end{pmatrix}, \\ (Q_3Q_2Z_2Q_1)(\alpha) &= \begin{pmatrix} -c_1s_2 & -s_1s_2 & -c_2 \\ c_1c_2s_3 & s_1c_2s_3 & -s_2s_3 \\ c_1c_2c_3 & s_1c_2c_3 & -s_2c_3 \end{pmatrix}, \\ (Q_3Q_2Q_1Z_1)(\alpha) &= \begin{pmatrix} -s_1c_2 & c_1c_2 & 0 \\ -s_1s_2s_3 - c_1c_3 & c_1s_2s_3 - s_1c_3 & 0 \\ -s_1s_2c_3 + c_1s_3 & c_1s_2c_3 + s_1s_3 & 0 \end{pmatrix}. \end{aligned} \tag{14}$$

With (13) and (14) one finds after rearrangements and simplifications

$$\|\partial_{x_k} R_{\mathrm{e}}(\alpha)\|^2 = 2\Big(\left|\partial_{x_k}\alpha_1\right|^2 + \left|\partial_{x_k}\alpha_2\right|^2 + \left|\partial_{x_k}\alpha_3\right|^2 \Big), \qquad k = 1, 2, 3. \tag{15}$$

For W_{c} given by (9), this implies

$$W_{\mathrm{c}}(K_{\mathrm{e}}(\alpha)) = \mu_2 \sum_{k=1}^{3} \|\partial_{x_k} R_{\mathrm{e}}(\alpha)\|^2 = 2\mu_2 \sum_{k=1}^{3} \Big(|\partial_{x_k}\alpha_1|^2 + |\partial_{x_k}\alpha_2|^2 + |\partial_{x_k}\alpha_3|^2 \Big)$$
$$= 2\mu_2 \Big(|\nabla\alpha_1|_2^2 + |\nabla\alpha_2|_2^2 + |\nabla\alpha_3|_2^2 \Big) =: 2\mu_2 |\nabla\alpha|_2^2, \tag{16}$$

where $|x|_2 := \big(\sum_{k=1}^{3} x_k^2\big)^{\frac{1}{2}}$ denotes the Euclidean norm in $\mathbb{R}^3$.

3. Analytic solutions of the 3D shear problem

The difficulty in the analytic treatment is that in many cases it is impossible to derive an explicit formulation of E_β without selecting I_{p} and the slip systems first. To simplify the further analysis, let

$$F_{\mathrm{p}}^{-1} = \mathrm{Id} - \sum_{a=1}^{I_{\mathrm{p}}} \gamma_a m_a \otimes n_a. \tag{17}$$

Eqn. (17) may be violated if $I_{\mathrm{p}} \geq 3$. From (17), it follows

$$U_{\mathrm{e}} = R_{\mathrm{e}}^t (F F_{\mathrm{p}}^{-1}) = R_{\mathrm{e}}^t \Big(\mathrm{Id} - \sum_{a=1}^{I_{\mathrm{p}}} (\gamma_a - \beta_a) m_a \otimes n_a \Big). \tag{18}$$

For later use, the first derivative of $\gamma \mapsto W_{\mathrm{st}}(U_{\mathrm{e}}(\alpha, \gamma))$ is now calculated. Within the matrix calculus, the chain rule reads

$$\frac{\partial}{\partial \gamma_k} W_{\mathrm{st}}(U_{\mathrm{e}}(\gamma)) = \mathrm{tr}\Big(\frac{\partial W_{\mathrm{st}}(U_{\mathrm{e}})^t}{\partial U_{\mathrm{e}}} \frac{\partial U_{\mathrm{e}}(\gamma)}{\partial \gamma_k} \Big), \qquad 1 \leq k \leq I_{\mathrm{p}}. \tag{19}$$

Based on (8), one finds

$$\frac{\partial}{\partial U_{\mathrm{e}}} W_{\mathrm{st}}(U_{\mathrm{e}}) = 2\mu \, \mathrm{sym}(U_{\mathrm{e}} - \mathrm{Id}) + 2\mu_c \, \mathrm{skw}(U_{\mathrm{e}}) + \lambda \, \mathrm{tr}(U_{\mathrm{e}} - \mathrm{Id}) \mathrm{Id} \tag{20}$$

and from (18)

$$\frac{\partial}{\partial \gamma_k} U_{\mathrm{e}}(\gamma) = -R_{\mathrm{e}}^t m_k \otimes n_k, \qquad 1 \leq k \leq I_{\mathrm{p}}.$$

Thus, (19) leads to

$$\frac{\partial}{\partial \gamma_k} W_{\mathrm{st}}(U_{\mathrm{e}}(\gamma)) = \mathrm{tr}\Big(\Big[2\mu_c \mathrm{skw}(U_{\mathrm{e}}) - 2\mu \, \mathrm{sym}(U_{\mathrm{e}} - \mathrm{Id}) - \lambda \mathrm{tr}(U_{\mathrm{e}} - \mathrm{Id}) \mathrm{Id} \Big] R_{\mathrm{e}}^t m_k \otimes n_k \Big). \tag{21}$$

The following observation is analogous to Blesgen (2013). It is central for the analysis.

Lemma 1. *The mappings $\gamma \mapsto E_\beta(\alpha,\gamma)$ and $\gamma \mapsto W_{\rm st}(U_{\rm e}(\alpha,\gamma))$ are convex.*

Proof The convexity of $\gamma \mapsto W_{\rm st}(U_{\rm e}(\alpha,\gamma))$ is equivalent to the convexity of the real functions $g_\alpha(s) := W_{\rm st}(U_{\rm e}(\alpha, d+s\gamma))$ for all $\gamma, d \in \mathbb{R}^{I_{\rm p}}$ and $\alpha \in \mathbb{R}^3$. Computing the second derivative yields

$$
\begin{aligned}
g_\alpha''(s) =& 2\mu \Big\| {\rm sym}\Big(\sum_{a=1}^{I_{\rm p}} \gamma_a R_{\rm e}^t(\alpha) m_a \otimes n_a\Big)\Big\|^2 + 2\mu_c \Big\| {\rm skw}\Big(\sum_{a=1}^{I_{\rm p}} \gamma_a R_{\rm e}^t(\alpha) m_a \otimes n_a\Big)\Big\|^2 \\
&+ \lambda \Big| {\rm tr}\Big(\sum_{a=1}^{I_{\rm p}} \gamma_a R_{\rm e}^t(\alpha) m_a \otimes n_a\Big)\Big|^2
\end{aligned}
$$

proving the convexity of $W_{\rm st}(U_{\rm e}(\alpha,\cdot))$ for any α.

The convexity of $E_\beta(\alpha,\cdot)$ follows, since $\gamma \mapsto \varrho\big(\sum_{a=1}^{I_{\rm p}} \kappa_a^0 - |\gamma_a - \gamma_a^0|\big)^2$ and $\gamma \mapsto \sigma_Y |\gamma|$ are convex. □

3.1. The limiting case of ultra-soft materials

Thanks to Lemma 1, the minimisers of E_β can be determined analytically. As a result, for ultra-soft materials, e.g. in the limit $\varrho \searrow 0$, $\sigma_Y \searrow 0$, the plastic deformation coincides with the given total deformation,

$$
\gamma_a(t) = \beta_a(t), \qquad 1 \le a \le I_{\rm p}. \tag{22}
$$

Using (22), (16) and (8), after setting $\kappa^0 = \gamma^0 = 0$ for simplicity, (3) becomes (where $R_{\rm e}(\alpha_D) = R_D$)

$$
E_\beta(\alpha) = \int_\Omega \Big[2\mu_2 |\nabla\alpha|_2^2 + J(\alpha)\Big]\,{\rm d}x \to \min_{\alpha|_{\partial\Omega}=\alpha_D}, \tag{23}
$$

with the stretching energy density (noting $W_{\rm st}(U_{\rm e}) = W_{\rm st}(R_{\rm e})$ as $F_{\rm e} = {\rm Id}$)

$$
\begin{aligned}
J(\alpha) :=& W_{\rm st}(R_{\rm e}(\alpha)) \qquad\qquad (24)\\
=& \frac{\mu}{2}\Big[2(1-c_1c_3-s_1s_2s_3)^2 + 2(1-c_1c_2)^2 + (s_1c_3 - s_1c_2 - c_1s_2s_3)^2 \\
&\quad + 2(1-c_2c_3)^2 + (c_1s_3 - c_2s_3 - s_1s_2c_3)^2 + (c_1s_2c_3 - s_2 + s_1s_3)^2\Big] \\
&+ \frac{\mu_c}{2}\Big[(s_1c_3 + s_1c_2 - c_1s_2s_3)^2 + (c_1s_3 + c_2s_3 - s_1s_2c_3)^2 \\
&\quad + (c_1s_2c_3 + s_2 + s_1s_3)^2\Big] + \frac{\lambda}{2}\Big[3 - c_1c_2 - c_1c_3 - c_2c_3 - s_1s_2s_3\Big]^2.
\end{aligned}
$$

Any $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ optimal to (23) satisfies the Euler-Lagrange equations

$$0 = 4\mu_2 \triangle \alpha_k - \frac{\partial J(\alpha)}{\partial \alpha_k}, \qquad k = 1, 2, 3. \tag{25}$$

As a consequence to (25), optimal α are stationary in time (or long-time) limits of an Allen-Cahn equation, thus local minimisers of J. By direct inspection, $J(\alpha) \geq 0$ and $J(\alpha) = 0$ if and only if $\alpha = (0, 0, 0)$ or $\alpha = (\pi, \pi, \pi)$ which both parametrise the unique global minimiser $R_\mathrm{e} = \mathrm{Id}$ of J.

It is straightforward to check that provided

$$\mu_c > 2(\lambda + \mu), \tag{26}$$

J defines a double well-potential, i.e. possesses local minimisers apart from $(0, 0, 0)$ and (π, π, π) on the non-discrete set

$$\begin{aligned} \mathcal{M} :=& \big\{(\alpha_1, 0, \pi) | \alpha_1 \in [0, 2\pi)\big\} \cup \big\{(\alpha_1, \pi, 0) | \alpha_1 \in [0, 2\pi)\big\} \\ & \cup \big\{(0, \alpha_2, \pi) | \alpha_2 \in [0, 2\pi)\big\} \cup \big\{(\pi, \alpha_2, 0) | \alpha_2 \in [0, 2\pi)\big\} \\ & \cup \big\{(0, \pi, \alpha_3) | \alpha_3 \in [0, 2\pi)\big\} \cup \big\{(\pi, 0, \alpha_3) | \alpha_3 \in [0, 2\pi)\big\} \subset [0, 2\pi)^3, \end{aligned} \tag{27}$$

with minimal energy $J(\mathcal{M}) = 8(\lambda + \mu) > 0$.

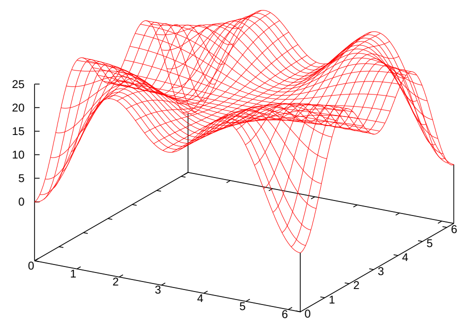

Figure 1: Plot of $J(\alpha_1, \alpha_2, 0)$ in $[0, 2\pi)^2$ for $\mu = \lambda = 1$, $\mu_c = 10$.

Fig. 1 renders J on the hypersurface $\alpha_3 = 0$ and illustrates the positions of the local minima.

3.2. The full problem in the elastic regime

As in section 3.1, the solution of the first time step is calculated, assuming $\gamma^0 = \kappa^0 = 0$. Computing the Euler-Lagrange equations w.r.t. γ of

$$E_\beta(\alpha, \gamma) = \int_\Omega \Big[2\mu_2 |\nabla \alpha|_2^2 + W_\mathrm{st}(U_\mathrm{e}(\beta, \alpha, \gamma)) + \varrho \Big(\sum_{a=1}^{I_\mathrm{p}} |\gamma_a| \Big)^2 + \sigma_Y \sum_{a=1}^{I_\mathrm{p}} |\gamma_a| \Big] \mathrm{d}x \to \min, \tag{28}$$

using

$$\partial^{\rm sub}|\gamma_k| = \begin{cases} +1, & \text{if } \gamma_k > 0, \\ -1, & \text{if } \gamma_k < 0, \\ [-1,+1], & \text{if } \gamma_k = 0, \end{cases}$$

it follows that no plastic flow occurs (i.e. $\gamma = \gamma_0$) if

$$\frac{\partial}{\partial \gamma_k} W_{\rm st}(U_{\rm e}(\beta,\alpha,\gamma))\Big|_{\gamma=0} \in [-\sigma_Y, +\sigma_Y] \qquad \text{for all } 1 \le k \le I_{\rm p}. \tag{29}$$

Plugging in $U_{\rm e}(\gamma=0) = R_{\rm e}^t\big(\mathrm{Id} + \sum_{a=1}^{I_{\rm p}} \beta_a m_a \otimes n_a\big)$ and using Eqn. (21), with

$$S := -2\mu_c\,\mathrm{skw}(R_{\rm e}) - 2\mu\,\mathrm{sym}(R_{\rm e} - \mathrm{Id}) - \lambda\,\mathrm{tr}(R_{\rm e} - \mathrm{Id})\mathrm{Id},$$

the condition (29) becomes

$$\begin{aligned} \mathrm{tr}\Big(\Big[2\mu_c \mathrm{skw}\Big(R_{\rm e}^t \sum_a \beta_a m_a \otimes n_a\Big) - 2\mu\,\mathrm{sym}\Big(R_{\rm e}^t \sum_a \beta_a m_a \otimes n_a\Big) \\ - \lambda \mathrm{tr}\Big(R_{\rm e}^t \sum_a \beta_a m_a \otimes n_a\Big)\mathrm{Id}\Big] R_{\rm e}^t m_k \otimes n_k\Big) + \mathrm{tr}\big(S R_{\rm e}^t m_k \otimes n_k\big) \in [-\sigma_Y, \sigma_Y]. \end{aligned} \tag{30}$$

For $\gamma = 0$, any $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ optimal to (28) solves the Euler-Lagrange equations

$$0 = 4\mu_2 \triangle \alpha_k - \frac{\partial J_\beta(\alpha)}{\partial \alpha_k}, \qquad k = 1,2,3 \tag{31}$$

with the potential

$$J_\beta(\alpha) := W_{\rm st}(U_{\rm e}(\alpha, \beta, 0)). \tag{32}$$

To illustrate (30), two examples are considered.

Example (1): $I_{\rm p} = 1$, $m_1 = (1,0,0)^t$, $n_1 = (0,1,0)^t$

A direct evaluation of (30) yields that there is no plastic flow provided

$$\begin{aligned} & c_1 c_2\Big[(s_1 c_3 - c_1 s_2 s_3)(\mu_c + \mu) + s_1 c_2(\mu_c - \mu)\Big] \\ & + s_1 c_2\Big[(1 - c_1 c_3 - s_1 s_2 s_3)(\lambda + 2\mu) + (2 - c_1 c_2 - c_2 c_3)\lambda\Big] \\ & + s_2\Big[c_2 s_3(\mu + \mu_c) + (s_1 s_2 c_3 - c_1 s_3)(\mu - \mu_c)\Big] \\ & - \beta_1(t)\Big[(c_1^2 c_2^2 + s_2^2)(\mu + \mu_c) + s_1^2 c_2^2(\lambda + \mu)\Big] \in [-\sigma_Y, \sigma_Y]. \end{aligned} \tag{33}$$

For given material parameters λ, μ, μ_c, (33) is satisfied if σ_Y is large enough and then, (33) turns into a smallness condition on $\beta_1(t)$.

A sufficient condition for the validity of (33) independent of α is

$$4\lambda + 2\mu + \mu_c + (\lambda + \mu + \mu_c)|\beta_1(t)| \le \sigma_Y .$$

Example (2): $I_{\mathrm{p}} = 2$, $m_1 = m_2 = (1, 0, 0)^t$, $n_1 = (0, 1, 0)^t$, $n_2 = (0, 0, 1)^t$
Here, it holds

$$R_{\mathrm{e}}^t \sum_{a=1}^{I_{\mathrm{p}}} \beta_a m_a \otimes n_a = \begin{pmatrix} 0 & \beta_1 c_1 c_2 & \beta_2 c_1 c_2 \\ 0 & \beta_1 s_1 c_2 & \beta_2 s_1 c_2 \\ 0 & -\beta_1 s_2 & -\beta_2 s_2 \end{pmatrix} .$$

The condition (30) for $F_{\mathrm{p}} = \mathrm{Id}$ reads for the first slip system, e.g. for $k = 1$,

$$\begin{aligned} & c_1 c_2 \Big[s_1 c_3 (\mu_c + \mu) + (s_1 c_2 - c_1 s_2 s_3)(\mu_c - \mu) \Big] \\ & + s_2 \Big[c_2 s_3 (\mu_c + \mu) + (c_1 s_3 - s_1 s_2 c_3)(\mu_c - \mu) \Big] \\ & + s_1 c_2 \Big[(1 - c_1 c_3 - s_1 s_2 s_3)(\lambda + 2\mu) + (2 - c_1 c_2 - c_2 c_3)\lambda \Big] \qquad (34) \\ & - \beta_1(t) \Big[\mu + (c_1^2 c_2^2 + s_2^2)\mu_c + s_1^2 c_2^2 \lambda \Big] - \beta_2(t) s_1 c_2 s_2 \big[\lambda + \mu - \mu_c \big] \in [-\sigma_Y, \sigma_Y]. \end{aligned}$$

Similarly, for the second slip system $k = 2$,

$$\begin{aligned} & c_1 c_2 \Big[-(s_1 s_3 + c_1 s_2 c_3)(\mu_c + \mu) + s_2(\mu - \mu_c) \Big] \\ & + s_1 c_2 \Big[(c_1 s_3 - s_1 s_2 c_3)(\mu_c + \mu) + c_2 s_3 (\mu_c - \mu) \Big] \\ & + s_2 \Big[(1 - c_2 c_3)(\lambda + 2\mu) + (2 - c_1 c_2 - c_1 c_3 - s_1 s_2 s_3)\lambda \Big] \\ & + \beta_1(t) s_1 c_2 s_2 \big[\lambda + \mu - \mu_c \big] - \beta_2(t) \Big[c_2^2 (\mu + \mu_c) + s_2^2 \lambda \Big] \in [-\sigma_Y, \sigma_Y]. \qquad (35) \end{aligned}$$

If $\beta_1(t)$, $\beta_2(t)$ satisfy both (34), (35) simultaneously, no plastic flow occurs. A sufficient condition independent of α is

$$4\lambda + 2\mu + \mu_c + (\lambda + \mu + \mu_c)\big(|\beta_1(t)| + |\beta_2(t)|\big) \le \sigma_Y .$$

4. Discussion and concluding remarks

In this article solutions of a 3D shear problem within the framework of finite-strain Cosserat plasticity are computed analytically. Two complementary shear cases are studied, the first for solely plastic deformations without elasticity, the second for solely elastic deformations without plasticity. As the main result, in both scenarios it could be shown that the parametrisation α of the micro-rotations R_e is the long-time limit of an Allen-Cahn equation, cf. (25) for the purely plastic case and (31) for the purely elastic case. These findings are analogous to the 2D-case in Blesgen (2013). Since the Allen-Cahn equation was originally designed to model segregation phenomena and phase change processes in solids, this explains why a partitioning of Ω into subsets with (approximately) constant rotations occurs as a consequence to deforming the material. This is the aforementioned *deformation patterning.* The steepness of the transition layers depends on the size of μ_2.

Like in the 2D case, this phenomenon is limited to a certain parameter range of μ_2, e.g. there is no patterning in the limit $\mu_2 \to \infty$. For $\mu_2 > 0$, due to elliptic regularity theory, $\alpha_k \in H^2(\Omega)$, with $H^2(\Omega)$ the Sobolev space of two-times weakly differentiable functions in Ω. In contrast, for $\mu_2 = 0$, only $\alpha_k \in L^2(\Omega)$ is known, with $L^2(\Omega)$ the space of square-integrable functions, i.e. the rotations are not regular and boundary layer effects occur.

The presented patterning mechanism may explain why grains and subgrains in materials form. In experiments, the deviation of the rotation angles between neighbouring grains is usually small and restricted to a finite collection of angles. This may be accounted for by adding

$$\eta \, \mathrm{dist}(R_e, \mathcal{R}) \tag{36}$$

to E_β, where $\eta \geq 0$ is a parameter and $\mathcal{R}$ is the discrete lattice point group, i.e. the finite set of rotations favored by the material. Unfortunately, the resulting problem was too difficult to be solved here analytically.

The analytic solutions calculated in this article are also valuable as benchmark problems for numerical algorithms. Clearly, for more accurate predictions, the analysis must be extended to general deformations and more realistic dislocation models.

Appendix - List of symbols

$\Omega \subset \mathbb{R}^3$	reference domain, undeformed solid	(x,t)	space and time coordinates
$\sigma_Y > 0$	yield stress, (3)	$h > 0$	discrete time step
φ	deformation vector of the solid,	$F = D\varphi$	deformation tensor, (1)
F_e	elasticity tensor, (1)	F_p	plasticity tensor, (1)
R_e	rotation tensor, (1)	U_e	(right) stretching tensor, (1)
Id	identity tensor	K_e	(right) curvature tensor, (2)
W_{st}	stretching energy, (1)	W_c	curvature energy, (1)
λ, μ	Lamé parameters, (8)	μ_c	Cosserat couple modulus, (8)
ϱ	dislocation energy constant, (4)	μ_2	parameter μ scaled by L_c, (9)

L_c	internal length scale, (9)	$\|\cdot\|$	Frobenius matrix norm, (10)
$\mathrm{tr}(\sigma)$	trace of tensor σ, (10)	σ^t	transpose of tensor σ
$\mathrm{sym}(\sigma)$	symmetric part of σ, (8)	$\mathrm{skw}(\sigma)$	skew-symmetric part of σ, (8)
γ	single-slip parametrisation of F_p, (5)	γ^0	values of γ at time t, (3),
κ	dislocation density, (1)	κ^0	values of κ at time t, (3)
I_p	number of single slip systems	$\beta(t)$	shear parameter, (7)
α	parametrisation of R_e in 3D, (11)	Q_k	matrices of Euler angles, (11)
R_D	Dirichlet boundary values of R_e, (3)	α_D	Dirichlet boundary values of α, (23)
m_k	slip vector of k-th slip system	n_k	slip normal of k-th slip system
c_k, s_k	acronyms for $\cos(\alpha_k)$, $\sin(\alpha_k)$, (12)	J, J_β	double-well potentials, (24), (32).

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