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# Modelling the Evolution of Inhomogeneities

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**Abstract.** A model of an anelastic evolution law of a defective continuum is discussed, emphasizing the role of the Clausius-Duhem inequality in selecting admissible processes.

## 1 Introduction

This short note is a sequel to a recent work [9] in which a model of the anelastic evolution law of a defective solid crystal body was proposed. Assuming that the material body is made of triclinic crystals and that the evolution process does not change the material symmetry group, we further discuss the situation in which the evolution is driven primarily by the density of the distribution of inhomogeneities represented by the torsion of the unique material connection. The dependence on stress and other internal parameters could also be considered. As we deal here with the general case of a two-dimensional evolution we feel that it is necessary to discuss also, however briefly, its thermodynamic context, in particular, the role of the Clausius-Duhem inequality. Especially, that now, in contrast to the situation analyzed in [9], where only constant strain states [7] were allowed to participate, the choice of the distribution of inhomogeneities may be such that residual stresses are present. Postulating, as we did in [9], that the evolution law, at least in principle, is independent of the Eshelby stress and depends only on the torsion of the unique material connection, we show that in two-dimensions the torsion tensor can be presented in terms of the Eshelby stress tensor and its derivatives. Re-writing the thermodynamic residual inequality in terms of the divergence of the Eshelby stress allows us to discuss the consequences of the Clausius-Duhem inequality for the choice of processes allowed. The analysis presented here does not pretend to be complete. The only objective of this work is to show, using a very particular example, how the constitutive problem of modelling the evolution of defects can be approached. Also, no attempt is made to compare this work with any other contemporary theory, e.g., [1], [12], [14]. More complete analysis of the approach advocated in this note will be presented elsewhere [5].

## 2 Evolution law

In the realm of pure elasticity the mechanical properties of a material point  $X$  are completely characterized by the density of the stored energy function per unit reference volume, say  $W(\mathbf{F}, X)$ , where  $\mathbf{F}$  denotes the deformation gradient from the reference configuration evaluated at the point  $X$ . Assuming that the body is *materially uniform* [15] implies that there exist smoothly distributed *uniformity maps*  $\mathbf{P}(X)$  (hypothetical, volume-preserving deformations) from  $\mathbb{R}^3$ , an archetype of a material point, to the tangent space of the reference configuration at each point  $X$ , and a real valued function  $\widehat{W}$  such that

$$W(\mathbf{F}, X) = \widehat{W}(\mathbf{F}\mathbf{P}(X)) \tag{1}$$

for all deformation gradients  $\mathbf{F}$  and any material point  $X$ . Given a Cartesian coordinate system on  $\mathbb{R}^3$  defined by an right-handed orthonormal basis  $\mathbf{e}_I$ , the mappings  $\mathbf{P}(X)$  induce in the reference configuration a frame field

$$\mathbf{f}_\alpha(X) \equiv P_\alpha^I(X)\mathbf{e}_I, \quad (2)$$

called a *uniform reference frame*. We remind the reader that the uniform reference  $\mathbf{f}_\alpha$  is, in general, non-integrable, i.e., does not correspond to any globally defined configuration of the body. When the body is made of triclinic crystals, and the material symmetry group is trivial the uniform reference is unique. This is in contrast to the case when the material symmetry group is continuous and the uniform reference can be selected modulo the smooth pointwise action of the symmetry group [15]. A unique uniform reference induces trivially a smooth distant parallelism which, in the triclinic case, must be global. The Christoffel symbols of the second kind of the corresponding unique *material connection* [15] are given in the Cartesian coordinate system by

$$\Gamma_{KJ}^I(X) \equiv -P_{\alpha,J}^I(X)P_K^\alpha(X) \quad (3)$$

where "comma" indicates partial differentiation. The unique material connection (3) has zero curvature but its torsion

$$T_{KJ}^I \equiv \Gamma_{KJ}^I - \Gamma_{JK}^I \quad (4)$$

does not necessarily vanish.

As long as the material body deforms elastically the given uniform reference remains unchanged. Indeed, there are no elastic deformations which may change the form and the distribution of the existing material inhomogeneities. On the other hand, anelastic processes involve mechanisms which, in general, modify the pattern of inhomogeneities. It appears that such processes can be modelled by allowing the uniform reference to evolve. As the uniform reference changes the corresponding material connection (3) changes and so does its torsion (4).

When the material connection is unique, as it is in the case of the body made of triclinic crystals, the torsion can be recognized as the true measure of the density of the distribution of inhomogeneities. We have, therefore, postulated in [9] that regardless of the state of stress maintaining the current distribution of inhomogeneities, the torsion is the driving force of the intrinsic (on its own momentum) evolution of inhomogeneities. On the other hand, if the material symmetry group is a continuous group, the material connection is non-unique and the torsion alone does not characterize well the distribution of defects. In fact, it is not the torsion but the corresponding G-structure and its characteristic objects which provide proper characterization of the state of inhomogeneities [3], [6]. For example, in the case of a fully isotropic body such characterization can be provided by the curvature of the corresponding Riemmanian connection [15]. In fact, investigating the self-driven evolution of defects in a fully isotropic body it was postulated in [8] that the material evolution depends on the curvature of the corresponding Riemmanian connection and its gradient. In the case of the triclinic crystal body these two approaches (using torsion or curvature) are geometrically completely equivalent. Different constitutive formulations lead, however, to qualitatively different results.

In this work we concentrate on the evolution law of the form

$$\dot{\mathbf{P}}(X, t) = f(\mathbf{T}(X, t), \mathbf{P}(X, t)) \quad (5)$$

where  $\mathbf{T}$  is the torsion tensor of the instantaneous material connection. Assuming that the form of the evolution law must not depend of any particular global reference configuration one can show [9] that it takes the form

$$\mathbf{L} = f(\widehat{\mathbf{T}}), \quad (6)$$

where the *inhomogeneity velocity gradient* [11]

$$L_{\beta}^{\alpha} \equiv (P^{-1})^{\alpha}_I \dot{P}^I_{\beta} \quad (7)$$

measures the temporal rate of change of uniform references seen from the perspective of the reference crystal, and

$$\widehat{T}^{\alpha}_{\beta\gamma} = (P^{-1})^{\alpha}_I P^K_{\beta} P^L_{\gamma} T^I_{KL} \quad (8)$$

is the torsion tensor pulled back to  $\mathbb{R}^3$ , an archetype of a material point. Restricting the form of the evolution law to the linear relation

$$\mathbf{L} \equiv \mathbf{C}\widehat{\mathbf{T}}, \quad (9)$$

where  $\mathbf{C}$  is a fifth order tensor of material constants, we obtain the following component representation of the law of evolution (9):

$$(P^{-1})^{\alpha}_I \dot{P}^I_{\beta} = C^{\alpha}_{\beta\rho}{}^{\sigma\lambda} (P^{-1})^{\rho}_M P^N_{\sigma} P^K_{\lambda} T^M_{NK}. \quad (10)$$

We feel that it is only appropriate to finish this introductory section by relating - for the benefit of the reader - the terminology of the approach being presented here, fundamentally rooted in the geometric theory of inhomogeneities [15], [3], [2], to more traditional approaches of finite-strain anelasticity like, for example, multiplicative plasticity [13]. In the plasticity approach the integrable deformation gradient  $\mathbf{F}$  is multiplicatively decomposed into elastic and anelastic (plastic) parts, say  $\mathbf{F}_e$  and  $\mathbf{F}_p$ , respectively, so that

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p. \quad (11)$$

Note that neither partial deformation gradient is integrable. In turn, analogously to the velocity gradient  $\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}$ , the *plastic distortion rate* tensor

$$\mathbf{L}_p \equiv \dot{\mathbf{F}}_p \mathbf{F}_p^{-1} \quad (12)$$

is introduced. It relates to the motion of dislocations through the shear rates of the corresponding slip systems. In our approach, the roles of the elastic  $\mathbf{F}_e$  and plastic  $\mathbf{F}_p$  deformations gradients are played by  $\mathbf{F}\mathbf{P}$  and  $\mathbf{P}^{-1}$ , respectively. Thus, the *intermediate configuration* of multiplicative plasticity corresponds to our uniform reference and the plastic distortion rate  $\mathbf{L}_p$  and the inhomogeneity velocity gradient  $\mathbf{L}$  are naturally related by

$$\mathbf{L}_p = -\mathbf{P}^{-1}\mathbf{L}\mathbf{P}. \quad (13)$$

Note, however, that while the inhomogeneity velocity gradient  $\mathbf{L}$  is a true material tensor the plastic distortion rate tensor  $\mathbf{L}_p$  unnecessarily relies on a non-physical intermediate configuration. Although the density of inhomogeneities (torsion) tensor  $\mathbf{T}$  has no clear counterpart in the plasticity theory [13] other similar to ours objects describing the density of defects are used in other approaches, e.g., the geometric dislocation tensor in Cermelli-Gurtin theory of single-crystal viscoplasticity [1], [12] or the dislocation density tensor of the structurally based theory of defects [4].

### 3 Two-dimensional evolution

To better illustrate our simple model and the range of phenomena it can capture we shall only consider uniform material bodies made of solid crystals and such that there exists a global reference in which all material isomorphisms  $\mathbf{P}$  (1) are, and remain during the evolution, independent of one Cartesian coordinates, say  $z$ . This is a natural generalization of the work presented in [9] where the material remaining in the state of contorted aelotropy was discussed only, and where the uniformity maps were selected as proper rotations. By restricting our analysis to a two-dimensional situation we gain a significant computational advantage afforded by the simplicity of the geometric relations in two dimensions.

Adopting an orthonormal basis in the reference crystal (an archetype of a material point) and a Cartesian coordinate system  $x, y, z$  in the fixed reference configuration enables us to represent the unimodular uniformity maps  $\mathbf{P}$  as the following matrices:

$$[\mathbf{P}](x, y, z) = \begin{pmatrix} a(x, y, t) & b(x, y, t) & 0 \\ c(x, y, t) & d(x, y, t) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (14)$$

where  $ad - bc = 1$  at all times and for all material points. The non-vanishing Christoffel symbols of the second kind of the material connection  $\Gamma_{KJ}^I$  induced by the mappings  $[\mathbf{P}]$  can now be calculated directly from (3) as:

$$\Gamma_{1J}^I = \begin{pmatrix} da_{,x} - cb_{,x} & -ba_{,x} + ab_{,x} \\ dc_{,x} - cb_{,x} & ad_{,x} - bc_{,x} \end{pmatrix}, \quad (15a)$$

$$\Gamma_{2J}^I = \begin{pmatrix} da_{,y} - cb_{,y} & -ba_{,y} + ab_{,y} \\ dc_{,y} - cb_{,y} & ad_{,y} - bc_{,y} \end{pmatrix}, \quad (15b)$$

where  $I, J = 1, 2$  and "comma" indicates partial differentiation. Hence, the non-vanishing components of the torsion tensor are:

$$T_{12}^1 = -T_{21}^1 = \frac{1}{2}[ab_{,x} - ba_{,x} - da_{,y} + cb_{,y}], \quad (16a)$$

$$T_{12}^2 = -T_{21}^2 = \frac{1}{2}[ad_{,x} - bc_{,x} - dc_{,y} + cd_{,y}]. \quad (16b)$$

Similarly, the non-vanishing components of the inhomogeneity velocity gradient  $\mathbf{L}$  at the reference crystal (7) are:

$$L_{\beta}^{\alpha} = \begin{pmatrix} d\dot{a} - b\dot{c} & d\dot{b} - b\dot{d} \\ a\dot{c} - c\dot{a} & a\dot{d} - c\dot{b} \end{pmatrix}, \quad (17)$$

where  $\alpha, \beta = 1, 2$ . Realizing that the pull back of the torsion tensor to  $\mathbb{R}^3$  has the same symmetries as the torsion itself and using repeatedly the fact that the uniformity maps are volume preserving ( $ad - bc = 1$ ) we can calculate non-vanishing components of  $\hat{\mathbf{T}}$  as:

$$\hat{T}_{12}^1 = -\hat{T}_{21}^1 = \frac{1}{2}[b_{,x} - d_{,y}], \quad (18a)$$

$$\hat{T}_{12}^2 = -\hat{T}_{21}^2 = \frac{1}{2}[a_{,x} + c_{,y}]. \quad (18b)$$

Thus, the linear evolution law (9) reduces, after rather tedious but elementary calculations, to the system of first order quasi-linear homogeneous partial differential equation

$$\begin{aligned}
 \dot{a} &= (Aa + Fb)[b_{,x} - d_{,y}] + (Ba + Gb)[a_{,x} + c_{,y}], \\
 \dot{b} &= (Ea - Ab)[b_{,x} - d_{,y}] + (Da - Bb)[a_{,x} + c_{,y}], \\
 \dot{c} &= (Ac + Fd)[b_{,x} - d_{,y}] + (Bc + Gd)[a_{,x} + c_{,y}], \\
 \dot{d} &= (Ec - Ad)[b_{,x} - d_{,y}] + (Dc - Bd)[a_{,x} + c_{,y}],
 \end{aligned} \tag{19}$$

where  $A, B$  and  $D, E, F, G$  are the material constants  $2C_{11}^{1,12} = -2C_{22}^{1,12}$ ,  $2C_{11}^{2,12} = -2C_{22}^{2,12}$  and  $2C_{12}^{2,12}$ ,  $2C_{12}^{1,12}$ ,  $2C_{21}^{1,12}$ ,  $2C_{21}^{2,12}$ , respectively. These are the only material constants left due to the skew-symmetry of the torsion tensor and the form of the uniformity maps (14). Indeed, it is easy to check that the equations of the system (19) are not independent as  $\dot{a}d + a\dot{d} - \dot{b}c - b\dot{c} = 0$  due to the fact that the inhomogeneity gradient  $\mathbf{L}$  (17) takes values in the Lie algebra of traceless matrices. It is also worth pointing out that the system of evolution equations (19) is not strictly hyperbolic for all choices of material parameters. In fact, it is always degenerate as at least one eigenvalue vanishes [5].

## 4 Examples

For the sake of specificity and to illustrate better different types of evolution, we limit further our analysis by restricting the choice of the uniformity maps (14) to specific subalgebras of the algebra of traceless matrices. Namely, we assume that they take values either in the space of orthogonal matrices or in the space of the diagonal matrices.

1. **Contorted Aelotropy case:** Assuming that the uniform reference represents at all times and at all material points the state of constant strain, implies [7] that the uniformity maps must be represented as planar rotations:

$$\mathbf{[P]}(x, y, z) = \begin{pmatrix} \cos \theta(x, y, t) & \sin \theta(x, y, t) & 0 \\ -\sin \theta(x, y, t) & \cos \theta(x, y, t) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{20}$$

where  $\theta = \theta(x, y, t)$  measures the counterclockwise rotation between the  $x$ -axis and the vector  $\mathbf{f}_1$  (2). The general law of evolution (19) reduces, as it was shown in [9], to the single quasi-linear partial differential equation

$$\theta_{,t} + (E \cos \theta - D \sin \theta)\theta_{,x} + (E \sin \theta + D \cos \theta)\theta_{,y} = 0, \tag{21}$$

for the angle of rotation with the only two material constants left;  $G = -D$ ,  $F = -E$ . The equation is hyperbolic and it models, depending on the value of the material parameters and the form of the initial condition, such phenomena as dislocation pile-ups and dissipation of dislocations. The one-dimensional example and the spherically symmetric case were discussed in [9] using the method of characteristics.

2. **Diagonal case:** Let us suppose now that that we deal with the inhomogeneous material such that the distribution of inhomogeneities is modelled at all times by the uniformity maps represented by the diagonal matrices:

$$\mathbf{[P]}(x, y, z) = \begin{pmatrix} a(x, y, t) & 0 & 0 \\ 0 & 1/a(x, y, t) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{22}$$

Consequently, the inhomogeneity velocity gradient (17) takes value in the space of diagonal traceless matrices:

$$L_{\beta}^{\alpha} = \begin{pmatrix} \dot{a}/a & 0 & 0 \\ 0 & -\dot{a}/a & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (23)$$

Note that the corresponding plastic distortion rate tensor is just the negative of (23) and it represents a slip system on two perpendicular planes,  $x - y = 0$  and  $x + y = 0$ , with the identical shear rates [13] of  $\dot{a}/2a$ . The form of the inhomogeneity velocity gradient (23) forces most material constants, with the exception of  $A$  and  $B$ , to vanish as otherwise the general system of the evolution laws (19) would seem to be consistent. Hence, our system of the evolution equations reduces to the single quasi-linear differential equation for the parameter  $a$ :

$$\dot{a} = \frac{A}{2a} a_{,y} - \frac{B}{2} a a_{,x} = \left( -\frac{Ba}{2}, \frac{A}{2a} \right) \nabla a, \quad (24)$$

where  $\left( -\frac{Ba}{2}, \frac{A}{2a} \right)$  is called the *evolution vector*. The equation is again hyperbolic. It models the same class of phenomena as the contorted aelotropy evolution law (21). Note that the diagonal class of distributions of inhomogeneities was investigated also in the context of an isotropic material [8]. However, as we have mentioned earlier, the derivation of the equation of evolution was based on the assumption that the evolution is driven by the curvature of the appropriately defined Riemannian connection and its gradient. This led to the evolution law in the form of a (second-order) diffusive partial differential equation.

## 5 Eshelby stress and thermodynamics

In this final section we discuss, within the constitutive framework we have presented so far, the consequences of the residual inequality of the Clausius-Duhem inequality [13], [11]:

$$tr (\mathbf{b}^T \mathbf{L}_p) \leq 0, \quad (25)$$

where  $\mathbf{b}^T$  denotes the transpose of the Eshelby stress tensor

$$\mathbf{b} \equiv -\frac{\partial W}{\partial \mathbf{P}} \mathbf{P}^T \quad (26)$$

[10] while  $\mathbf{L}_p$  is the plastic distortion rate tensor (13). The main obstacle in dealing effectively with this issue is that our evolution law seems to be independent of the Eshelby stress. As we show below, this is not completely true. Our first objective is to express, if possible, the torsion tensor of the unique material connection in terms of the Eshelby stress tensor. The underlying idea is that both objects represent, after all, the same distribution of inhomogeneities. To this end, we note that one of the consequences of the balance of linear momentum and the definition of the Eshelby energy-momentum tensor for the uniform material is, as shown in [10], that

$$b_{I;J}^J = b_K^J T_{JI}^K + b_I^J T_{JK}^K, \quad (27)$$

where  $(;)$  denotes covariant (material) differentiation. This differential equation is identically satisfied by the Eshelby stress tensor associated with a solution of an elastic boundary-value problem. In addition, analyzing the properties of the torsion tensor in two dimensions,

one can show that the torsion can be written in terms of its trace one-form

$$\omega_I = T_{IJ}^J. \quad (28)$$

Namely,

$$T_{JK}^I = \delta_K^I \omega_J - \delta_J^I \omega_K. \quad (29)$$

It is now easy to see that the trace of the (material) torsion tensor (28) can be expressed via the Eshelby stress tensor and its covariant divergence. Indeed, combining equations (27) and (29) one obtains that

$$\omega_I - b_I^J \omega_J = b_{I;J}^J. \quad (30)$$

Hence, equation (29) can be replaced by a relation presenting the torsion tensor as a function of the Eshelby stress tensor, its derivatives, and the components of the uniformity map. The presence of the uniformity map is the consequence of converting the covariant differentiation into the ordinary differentiation. Note that the representation of the torsion tensor through its trace one-form is available in dimension two only. Moreover, one can show [5] that in 3-dimension the Eshelby stress and the torsion tensor are not geometrically equivalent.

Having the relation between the torsion tensor and the Eshelby stress available let us look now at the specific evolution of the diagonal distributions as given by the uniformity maps (22). Elementary calculations show that the trace one-form of the torsion tensor takes the form:

$$\omega_I = \frac{b_{I,J}^J}{b_2^2 - b_1^1} \quad (31)$$

provided the Eshelby stress tensor is such that  $b_2^2 \neq b_1^1$ . In fact, having the Eshelby stress such that  $b_2^2 = b_1^1$  implies homogeneity [10]. Moreover, using the evolution equation (24) and the corresponding torsion tensor one obtains the following plastic distortion rate tensor  $\mathbf{L}_p$  (13):

$$L_{pIJ}^I = \frac{1}{a(b_2^2 - b_1^1)} \begin{pmatrix} -[Ab_{2,K}^K - Ba^2b_{1,K}^K] & 0 \\ 0 & [Ab_{2,K}^K - Ba^2b_{1,K}^K] \end{pmatrix}, \quad (32)$$

$I, J = 1, 2$ . Finally, the residual inequality (25) of the Clausius-Duhem inequality takes the form:

$$A \frac{b_{2,K}^K}{a} - Bab_{1,K}^K \leq 0. \quad (33)$$

The left hand side of this inequality is nothing else but the scalar product of two vectors; one being the divergence of the Eshelby tensor and the other, the evolution vector (24), representing the diagonal distribution of inhomogeneities as given by the evolution equation (24). Note also that the evolution vector sits always on a hyperbola parameterized by the material constant  $AB$ . Given an arbitrary stored energy function  $W(\mathbf{F}, X)$  and the corresponding Eshelby stress  $\mathbf{b}$ , in particular, its divergence, the residual inequality implies that the only processes  $\mathbf{P}(X, t)$  of the form (22) allowed are these for which the inequality (33) is satisfied - the evolution vector must be in the quadrant transversal to the one containing the Eshelby stress divergence.

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