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ON THE INTRINSIC EVOLUTION OF MATERIAL INHOMOGENEITIES

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Abstract. *The evolution of a distribution of material inhomogeneities (defects, dislocations, etc.) is investigated. Adopting our recently developed model of the anelastic evolution law of a defective solid crystal body and using the classical methods of the theory of hyperbolic waves we analyze such phenomena as the long-term relaxation of defects and the dislocation pile-up.*

1 INTRODUCTION

In this short note we shall discuss the evolution of inhomogeneities of uniform material bodies made of triclinic crystals and such that there exists a global reference configuration in which all material points are simultaneously stress-free.

In the realm of pure elasticity the mechanical properties of a material point X are completely characterized by the density $W(\mathbf{F}, X)$ of the stored energy per unit reference volume, where $\mathbf{F}$ denotes the deformation gradient from the reference configuration evaluated at the point X. If the body is *materially uniform*[1] there exist smoothly distributed *uniformity maps* $\mathbf{P}(X)$ (hypothetical deformations) from $\mathbb{R}^3$ (which one may view in this context as 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 a (right-handed) orthonormal basis $\mathbf{e}_I$, the mappings $\mathbf{P}(X)$ induce in the reference configuration a frame field

$$\mathbf{f}_\alpha(X) \equiv P^I_\alpha(X)\mathbf{e}_I, \tag{2}$$

called a *uniform reference*. 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[2]. If in addition there exists a stress-free global reference configuration it follows that the unique uniform reference is in a *state of constant strain*[3], i.e., all uniformity maps are proper rotations assuming that the archetype is also stress-free. In other words, in the given reference configuration

$$P^I_\alpha(X) = Q^I_\alpha(X), \tag{3}$$

where all $Q^I_\alpha(X)$ are proper orthogonal tensors. A 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*[2] are given in the Cartesian coordinate system by

$$\Gamma^I{}_{KJ}(X) = -Q^I_{\alpha,J}(X)Q^\alpha_K(X) \tag{4}$$

where "comma" indicates partial differentiation.

A uniform reference $\mathbf{f}_\alpha$ does not, in general, correspond to any globally defined configuration of the body, i.e., it is not integrable. The unique material connection (4) has zero curvature but its torsion

$$T^I_{\ KJ} \equiv \Gamma^I_{\ KJ} - \Gamma^I_{\ JK} \tag{5}$$

does not necessarily vanish.

As long as the material body is elastic the given uniform reference remains unchanged as there are no elastic deformations which may change the existing material inhomogeneities. On the other hand, anelastic processes involve mechanisms which, in general, modify the distribution of inhomogeneities. Such processes can be modelled by allowing the uniform reference to evolve. As the uniform reference changes the corresponding material connection (4) changes and so does its torsion (5).

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 postulate, therefore, that regardless of the state of stress the torsion is the driving force of the intrinsic (on its own momentum) evolution of inhomogeneities. Thus, we suggest an evolution law of the form

$$\dot{\mathbf{P}}(X,t) = f(\mathbf{T}(X,t), \mathbf{P}(X,t)) \tag{6}$$

where $\mathbf{T}$ is the torsion tensor of the instantaneous material connection. Assuming that the evolution law is independent of any particular global reference configuration one can show[4] that it takes the form

$$\mathbf{L} = f(\widehat{\mathbf{T}}), \tag{7}$$

where the *inhomogeneity velocity gradient*[5]

$$\mathbf{L} \equiv \mathbf{P}^{-1}\dot{\mathbf{P}} \tag{8}$$

measures the temporal rate of change of uniform references, and $\widehat{\mathbf{T}}$ is the torsion tensor, both seen from the perspective (pulled back) of $\mathbb{R}^3$ (the reference material point). Restricting the form of the evolution law to the linear relation

$$\mathbf{L} = \mathbf{C}\widehat{\mathbf{T}}, \tag{9}$$

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

$$(P^{-1})^{\alpha}_{I}\dot{P}^{I}_{\beta} = C^{\alpha\ \ \sigma\lambda}_{\beta\rho}(P^{-1})^{\rho}_{M}P^{N}_{\sigma}P^{K}_{\lambda}T^{M}_{NK}. \tag{10}$$

2 TWO-DIMENSIONAL EVOLUTION

To illustrate the range of phenomena which can be captured by this simple model let us consider a planar case, that is, a class of problems for which the uniform reference is independent at all times of one of the Cartesian coordinates. By doing so we gain a significant computational simplicity afforded by the explicit representation of the rotation by means of a single angular parameter, say θ.

Adopting an orthonormal basis in the reference crystal and a Cartesian coordinate system x, y, z in the fixed reference configuration, and assuming that at all times t and all material points (x, y, z) the uniform reference is a stress-free state enables us to represent the uniformity maps $\mathbf{P}$ (3) as the following matrices:

$$[\mathbf{P}](x, y, z) = \begin{pmatrix} \cos\theta(x,y,t) & \sin\theta(x,y,t) & 0 \\ -\sin\theta(x,y,t) & \cos\theta(x,y,t) & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{11}$$

where $\theta = \theta(x, y, t)$ measures the counterclockwise rotation between the x-axis and the first uniformity basis vector $\mathbf{f}_1$. The Christoffel symbols of the second kind of the material connection $\Gamma^{I}{}_{KJ}$ induced by the rotations $[\mathbf{P}]$ can now be calculated directly from equation (4) as:

$$\Gamma^{1}{}_{21} = -\Gamma^{2}{}_{11} = \theta_{,x} \tag{12a}$$

$$\Gamma^{1}{}_{22} = -\Gamma^{2}{}_{12} = \theta_{,y} \tag{12b}$$

$$\Gamma^{1}{}_{12} = \Gamma^{2}{}_{21} = 0 \tag{12c}$$

Hence, the non-vanishing components of the torsion tensor are:

$$T^{1}{}_{12} = -T^{1}{}_{21} = -\theta_{,x} \tag{13a}$$

$$T^{2}{}_{12} = -T^{2}{}_{21} = -\theta_{,y}\,. \tag{13b}$$

Similarly, the non-vanishing components of the inhomogeneity velocity gradient $\mathbf{L}$ (8) at the reference crystal are:

$$L^{1}{}_{2} = -L^{2}{}_{1} = \theta_{,t}\,. \tag{14}$$

Thus, the linear evolution law (9) reduces, after rather tedious but elementary calculations, to the single quasi-linear homogeneous partial differential equation for the angle of rotation θ

$$\theta_{,t} + (a\cos\theta - b\sin\theta)\theta_{,x} + (a\sin\theta + b\cos\theta)\theta_{,y} = 0, \tag{15}$$

where a and b are the material constants $2C^{1}{}_{21}{}^{12}$ and $2C^{1}{}_{22}{}^{12}$, respectively. We may further simplify its form by writing it as a single nonlinear balance law for the new variable β

$$\beta_{,t} + c(\sin\beta)_{,x} - c(\cos\beta)_{,y} = 0, \tag{16}$$

where $\beta \equiv \theta + \theta_0$, $c = \frac{1}{\sqrt{a^2+b^2}}$, and θ_0 is such that $\tan\theta_0 = \frac{b}{a}$.

The *characteristic curves*[6] of this equation are solutions of the following system of ordinary differential equations:

$$\frac{dt}{ds} = 1, \tag{17a}$$

$$\frac{dx}{ds} = c\cos\beta, \tag{17b}$$

$$\frac{dy}{ds} = -c\sin\beta, \tag{17c}$$

$$\frac{d\beta}{ds} = 0, \tag{17d}$$

As evident from equation (17a) the parameter s can be identified with time t. More importantly, equation (17d) implies that β is actually constant along characteristics. Consequently, the right-hand sides of equations (17b) and (17c) are constant, and the characteristics are straight lines. As the solution is constant along characteristics its long-term behavior depends on whether or not the characteristics tend to converge (intersect) or diverge. This, in turn, is determined by the choice of material constants a and b, and the initial condition. Indeed, if for some choice of the material constants the characteristics of an initial condition $\beta_0(x, y)$ intersect, we observe the creation of dislocations pile-ups. On the other hand the divergence (spreading) of characteristics represents the tendency of the dislocations to dissipate.

For the sake of being even more specific and to be able to illustrate better any of the above mentioned types of evolutions let us restrict further our analysis to the one-dimensional case by assuming that the uniform references depend only on one Cartesian coordinate, say y. This renders the evolution equation (16) particularly simple:

$$\beta_{,t} + c\beta_{,y} \sin\beta = 0. \tag{18}$$

The general Cauchy problem for such a balance law has, as it is well known[7], no smooth global solution even for smooth compactly supported initial condition. A solution stays temporarily smooth but eventually develops singularities. The blow-up of a smooth solution, which in the context of our model we identify with the dislocations pile-up, occurs when the $\beta_{,y}$ becomes unbounded. It is easy to show by integrating along characteristics that this is possible provided

$$c\beta_0' \cos\beta_0(y) < 0 \tag{19}$$

at some $y \in \mathbb{R}$, where $\beta_0(y) \equiv \beta(y,0)$ and where $k(y) \equiv c\cos\beta_0(y)$ is obviously constant along the characteristics. The actual breaking of a continuous solution will be observed at the critical time

$$t_c \equiv \min_y \frac{-1}{c\beta_0'(y)\cos\beta_0(y)}. \tag{20}$$

Such a singularity, once developed, will propagate, as implied by the Rankine-Hugoniot condition[7], with the speed

$$\upsilon = c\frac{[\cos\beta]}{[\beta]} \tag{21}$$

along the shock-curve $y = \Gamma(s)$, where $\frac{d}{ds}\Gamma(s) = \upsilon(y(s), s)$. The evolution of the amplitude $[\beta]$ of such a shock is given by the propagation condition[8]

$$\tilde{[\beta]} = c\left(\frac{[\cos\beta]}{[\beta]}[\beta_{,y}] + [\beta_{,y}\sin\beta]\right), \tag{22}$$

where $[f(\beta)] \equiv f(\beta^+) - f(\beta^-)$ denotes the jump of the quantity f across the shock-curve Γ, and where $\tilde{[\beta]}$ indicates differentiation along Γ. Using the method of singular surface[9] the propagation of such a singularity can be further analyzed by developing the infinite system of iterated compatibility conditions and solving it numerically[10].

3 EXAMPLES

To show the relation between the form of the initial condition and the choice of the material constants a and b we briefly discuss here some one-dimensional evolution initial-value problems.

(i) Suppose that $a = b = 1$ and let $\beta_0(y) = \arctan y$. As $\beta_{0,y} > 0$ the condition (19) is never satisfied proving that no pile-up of dislocation will ever occur. A simple analysis of characteristics shows, in fact, that the solution $\theta(y)$ tends asymptotically to $-\frac{\pi}{4}$ at every $y \in \mathbb{R}$.

(ii) Let $\beta_0(y) = -\arctan y$ and let us keep the same material constants. This initial condition, in contrast to the previous one, will develop, as easily attested by (19), into a shock. In fact, investigating the arrangement of characteristics and calculating the critical blow-up time (20) one arrives at the conclusion that the two shocks travelling in opposite directions (one front-shock and one back-shock) will develop at the same time $t_c = \frac{\sqrt{2}}{2}$.

(iii) Suppose $a = b = 1$ and select a symmetric, about $y = 0$, initial condition, e.g., $\beta_0(y) = \frac{\pi}{2}\text{sech}\, y$. An elementary analysis of characteristics shows that this solution will blow-up in finite time into a front shock. Changing the material constants to $a = -b = -1$ but keeping the initial condition unchanged will make very little difference. Indeed, rewriting the evolution equation for the new material constants as $\beta_{,t} + \frac{\sqrt{2}}{2}\beta_{,y}\cos\beta = 0$ one can easily conclude that the new solution also blows up in finite time. However, a different part of the initial condition contributes now to the pile-up, slowing down its occurrence and propagation considerably.

(iv) As the last example we consider the spherically symmetric planar problem. In other words, we seek solutions to the evolution equation (16) such that it is invariant at all times $t \geq 0$ with respect to rotations about the origin. Rewriting equation (16) in the polar coordinates (ϱ, ψ) we obtain

$$\beta_{,t} + c\beta_{,\varrho}\sin(\beta - \psi) - \frac{c}{\varrho}\beta_{,\psi}\cos(\beta - \psi) = 0, \tag{23}$$

where $\beta = \beta(\varrho, \psi, t)$. The solution β is truly rotationally invariant provided

$$(\beta - \psi)_{,\psi} = 0. \tag{24}$$

Hence,

$$\beta(\varrho, \psi, t) = \psi + F(\varrho, t), \tag{25}$$

where

$$F_{,t} + cF_{,\varrho}\sin F - \frac{c}{\varrho}\cos F = 0. \tag{26}$$

What we have now is a one-dimensional balance law with the source. The characteristic curves are no longer straight lines and the solution F is no longer constant along characteristics. The initial value problem is well posed only locally in time. As in the case of a conservation law the solution of (26) generally stays smooth only up to some critical time at which a singularity develops. Moreover, the source term may even cause the singular solution to become unbounded in finite time[8,11], and if dissipative enough it may prevent all together the breaking of some relatively week waves[12]. Note also that for the source term of (26) plays a prominent role close to the origin while it is negligible very far away from the center. Indeed, the proximity of defects increases the density of defects which, in turn, as expected, influences their evolution in a more significant way.

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