A Mathematical Theory of Defective Crystals

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Content

- Theory of Material Inhomogeneities
- Possible Generalizations

- Structurally Based Theory of Defective Crystals
- Properties of States with Constant ddt.

- References

Theory of Material Inhomogeneities

The mechanical properties of a material point X of the body B (a differentiable manifold) are completely characterized by the density of the stored energy function per unit reference (configuration) volume, $W(\mathbf{F}, X)$, where:

- A configuration of B is a (global) chart $u : B \to \mathbb{R}^3$.
- $\mathbf{F}$ denotes the deformation gradient $\nabla u : TB \to \mathbb{R}^3$.

The body B is said to be *materially uniform* if it is made of the same material at all points. This means that there exist smoothly distributed *uniformity maps* $\mathbf{P}(X)$ from the reference crystal $\mathbf{V}$ to $T_X B$ and a real-valued function $\widehat{W}$, such that

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

for all deformations $\mathbf{F}$, $\det \mathbf{F} > 0$, and every material point X.

Given a basis $\mathbf{E}_\alpha$ $(\alpha = 1,2,3)$ in the reference crystal $\mathbf{V}$ and a (right-handed) coordinate system $\mathbf{e}_I$ $(I = 1,2,3)$ in $\mathbb{R}^3$ the mappings $\mathbf{P}(X)$ induce in the reference configuration a frame field

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

called a *uniform reference.*

A uniform reference is *not unique* if the strain energy function W has a not-trivial continuous symmetry group:

- $\mathbf{G} \in GL(\mathbb{R},3)$ is a symmetry of the function W at X if $W(\mathbf{FG};X) = W(\mathbf{F};X)$ for all $\mathbf{F}$.
- If B is materially uniform the group $\widehat{\mathbf{G}} \equiv \mathbf{P}^{-1}\mathbf{GP}$ is material point independent.
- $\overline{\mathbf{P}} \equiv \mathbf{P}\widehat{\mathbf{G}} = \mathbf{GP}$ induces another uniform reference.

- A collection of all uniform references is a $\widehat{\mathbf{G}}$-structure on B.
- A collection of all $\mathbf{P}$ maps defines a transitive Lie groupoid.

Any uniform reference induces on B a smooth distant parallelism. The Christoffel symbols of the corresponding *material connection* are given in the Cartesian coordinate system by

$$\Gamma^I{}_{KJ}(X) = -P^I_{\alpha,J}(X)P^\alpha_K(X). \tag{3}$$

- Material connection is not unique unless the symmetry group $\widehat{\mathbf{G}}$ is discrete.
- Every material connection has zero curvature but its torsion $T^I{}_{KJ} \equiv \Gamma^I{}_{KJ} - \Gamma^I{}_{JK}$ does not necessarily vanish.
- If a torsion of a material connection vanishes the corresponding uniform reference is a gradient of a global configuration.
- 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*.

Generalizations

- Higher-grade materials (diffusive phenomena, interactions between cracks, disclinations):

$$W(\mathbf{F}, \nabla\mathbf{F}, X). \tag{4}$$

- Micromorphic media (Cosserat media, liquid crystals):

$$W(\mathbf{F}, \mathbf{H}, \nabla\mathbf{H}; X), \tag{5}$$

  where the tensor $\mathbf{H} = H^I_\alpha \mathbf{e}_I \otimes \mathbf{E}_\alpha$ represents the extra microstructure describing, for example, a homogeneous deformation of small grains embedded in the elastic matrix B.

- Homogeneity is now characterized by three different connections.

Structurally Based Theory of Defective Crystals

- A *crystal state* Σ is defined by prescribing the domain Ω and the frame field $\mathfrak{l}_i : \Omega \rightarrow \mathbb{R}^3$, $i = 1, 2, 3$.

- The *dislocation density tensor* (ddt.) is given at a point by

$$S_{ij} = \frac{1}{n} \nabla \wedge d_i \cdot d_j \tag{6}$$

where $d_i(\cdot)$ denotes the dual to $\mathfrak{l}_i(\cdot)$ frame field and n is the corresponding determinant.

- An *elastic deformation* is defined as a mapping $y : \Omega \rightarrow \mathbb{R}^3$ producing lattice vectors $\widehat{\mathfrak{l}}_i(\cdot)$ on $y(\Omega)$ such that

$$\widehat{\mathfrak{l}}_i(y(X)) = \nabla y \mathfrak{l}_i(X), \quad X \in \Omega. \tag{7}$$

- The focus of the theory is on objects which are *elastic invariants* like the Bürger's vector $\nabla \wedge d_i(\cdot)$ and the ddt.
- Deformations which preserve elastic invariants but are not elastic are called the *neutral deformations*, e.g., slip in planes where the lattice vectors are constant.
- It is necessary that the ddt. be singular if neutral deformations are to exist.

Basic constitutive assumptions

- Point values of the frame and the ddt. are enough to determine the value of the energy at a material point.
- The density of the energy function is constant in a crystal state with uniform (constant throughout the body) ddt.
- We focus on cases when ddt. is singular.

Properties of states with constant ddt.

- There exists an (associative) Lie group structure function

$$\psi : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3 \tag{8}$$

such that the frame field is right invariant. That is, constant ddt. implies that given the frame field $\mathfrak{l}_i(\cdot)$ such that $\mathfrak{l}_i(0) = \mathbf{e}_i$, the differential system

$$\mathfrak{l}_i(\psi(x,u)) = \nabla_1 \psi(x,u)\mathfrak{l}_i(x), \quad \psi(x,0) = \psi(0,x) = x, \tag{9}$$

has a unique invertible solution ψ with the property

$$\psi(u, \psi(v,w)) = \psi(\psi(u,v), w). \tag{10}$$

- The group property is available for any constant ddt. state.
- Elastic deformation of a crystal w constant ddt. produces a crystal state with constant ddt.

When ddt. is singular, one can choose a crystal state such that ψ is affine with respect to its first argument.

- The pair $\{\mathfrak{l}_i(\cdot), S\}$ defines a Lie algebra structure.
- Using the classification of 3-dimensional Lie algebras, one can assume that

$$S = \begin{pmatrix} * & * & 0 \\ * & * & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{11}$$

Theorem 1 *Given singular ddt., one can choose*

$$\psi(x, y) = y + e^{-y_3 C} x, \tag{12}$$

where C *has components* $C_{ir} \equiv \varepsilon_{rk3} S_{ik}$.

E.g., $S_{11} = S_{22} = 1$ corresponds to rotating the frames about $\mathbf{e}_3$.

We investigate the conditions which would allows us to introduce a "material symmetry" group in a fashion analogous to the continuum mechanics of simple materials.

The objective is to construct right invariant frame field $\{\mathfrak{l}_i(\cdot), i = 1, 2, 3\}$ such that $\mathfrak{l}_i(e) = L\mathbf{e}_i$, and the corresponding group composition function, say $\hat{\psi}$.

We propose the following construction:

- Given ddt. S define the affine group composition function ψ, and a frame field $\mathfrak{l}_i(\cdot)$ such that $\mathfrak{l}_i(0) = \mathbf{e}_i$.
- Define the elastic deformation $y : \mathbb{R}^3 \to \mathbb{R}^3$ by

$$y(x) = Lx + e.$$

- The state $\left\{\hat{\mathfrak{l}}_i(\cdot), \mathbb{R}^3\right\}$ elastically related by the deformation y to the canonical state $\left\{\mathfrak{l}_i(\cdot), \mathbb{R}^3\right\}$ is such that

$$\hat{\mathfrak{l}}_i(y(x)) = L\mathfrak{l}_i(x), \quad \text{and} \quad \hat{\mathfrak{l}}_i(e) = L\mathbf{e}_i. \tag{13}$$

- The group composition function for the new state is

$$\hat{\psi}(y(x), y(u)) = y(\psi(x, u)). \tag{14}$$

- The relevant symmetry group

$$F_e = LGL^{-1} \tag{15}$$

where the commutative group

$$G = \left\{g : g = e^{tC}, t \in \mathbb{R}\right\} \tag{16}$$

should be view as the symmetry group of the "canonical state" as

$$w(L, S) = w(Lg, S). \tag{17}$$

Final remarks

It can be shown, and this underscores both the validity of our original assumption as well as the the importance of our findings, that:

- there is no nontrivial elastic deformation which preserves the form of the canonical state,
- the state defined by the lattice vectors $(Fe^{tC}F^{-1})L(\cdot)$ is a *translation* of the state defined by the lattice vectors $L(\cdot)$.

References

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