A GEOMETRICAL THEORY OF DISCRETE DISLOCATIONS IN LATTICES, WITH APPLICATIONS TO DISLOCATION DYNAMICS AND CRYSTAL PLASTICITY

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Abstract

The mechanics of crystal lattices containing dislocations can be expressed in terms of fields that are supported on the lattice itself, e. g., the displacement field and the energy density; and fields that are defined on certain ancillary lattices, e. g., the eigendeformation fields which describe the dislocations. In the harmonic approximation, the energy is a quadratic form in the displacement field and the eigendeformations. At fixed dislocation density, the displacement field of the crystal lattice follows by energy minimization. We show that the structure of the resulting mechanics of defective lattices can be streamlined and given a compelling interpretation in terms of a discrete version of homology and differential calculus. The resulting differential operators generalize the conventional differential operators of exterior calculus in a manner which reflects and takes full account of the structure of the crystal lattice. Based on this mathematical framework, we generalize to lattices classical constructs and relations from the geometrical theory of continuously distributed dislocations, such as the notion of Burgers circuit and slip system; and Frank's and Kröner's formulae. We also show how the forest-hardening model can be phrased in terms of certain topological invariants. We illustrate the versatility of the theory by means of a number of selected applications, including: core energies of bcc dislocations; the dislocation field of an expanding nanovoid; and the dislocation structures selected by the forest mechanisms and the attendant hardening rates.

EXTENDED SUMMARY

The classical geometrical theory of continuously distributed dislocations relies on the notion of Burgers circuit to characterize the distribution of dislocations in an otherwise linear elastic continuum (cf, e. g., [3]). Thus, if $\beta^e : \mathbb{R}^3 \to gl(\mathbb{R}^3, \mathbb{R}^3)$ is the elastic deformation field, the formula

$$\mathbf{b}(C) = \oint_C \beta^e \mathbf{dx} \tag{1}$$

gives the total Burgers vector of all the dislocations encircled by the closed loop C, or Burgers circuit. In particular, two circuits C_1 and C_2 are equivalent if one can be mapped homotopically to the other without changing the total Burgers vector $\mathbf{b}(C)$ along the way. In particular, this requires that $\mathbf{b}(C_1) = \mathbf{b}(C_2)$. This introduces an equivalence relation among loops in $\mathbb{R}^3$, each of which represents a dislocation bundle. The equivalence classes consisting of loops having a common point have a group structure in which the group operation between two loops consists of traversing the loops consecutively. The resulting *fundamental group* provides an intrinsic characterization of the topology of the dislocation ensemble. Alternatively, the geometry of the dislocation ensemble is described by Nye's dislocation density tensor

$$\alpha = \beta^e \times \nabla \tag{2}$$

since, by Stoke's theorem

$$\mathbf{b}(C) = \oint_C \beta^e \mathbf{dx} = \int_S (\beta^e \times \nabla) \boldsymbol{n} dS \tag{3}$$

where S is any surface having C as boundary and $\boldsymbol{n}$ is the (consistently oriented) unit normal to S. In crystals, the dislocation motion is confined to crystallographically determined slip planes, which requires that the displacement gradient be of the form

$$\nabla \boldsymbol{u} = \beta^e + \beta^p \tag{4}$$

with β^e absolutely continuous and the plastic deformation β^p defining a measure supported on discrete crystallographic planes. The energy of the crystal is then variously given by

$$E = \int \frac{1}{2} c_{ijkl} \beta^e_{ij} \beta^e_{kl} dx = \int \frac{1}{2} c_{ijkl} (u_{i,j} - \beta^p_{ij})(u_{k,l} - \beta^p_{kl}) dx \tag{5}$$

At fixed β^p, the displacement field follows by energy minimization. It is also of interest to determine the energy minimizing dislocation structures that arise under suitable constraints and loading conditions, and the energy stored in the dislocation structures.

This classical picture suffers from a number of fundamental shortcomings, all of which can be traced to the idealization of the crystal as a continuum and the corresponding jettisoning of its lattice structure. Thus, perfect or Volterra dislocations have infinite energy per unit length. This type of divergence can be eliminated by the introduction of a core cut-off radius, but this fix is ad-hoc and not rooted in fundamental theory. Other maladies that afflict the continuum theory are the absence of any natural minimum separation between slip planes, and the extraneous nature of the Burgers vectors.

A satisfactory resolution of these deficiencies *a fortiriori* requires an acknowledgement from the outset of the discrete nature of crystals and the formulation of a mechanics of defective crystal lattices. In this framework, the familiar notion of continuum is replaced by that of a Bravais lattice of points. This substitution immediately begs a number of fundamental questions, namely:

i) What is the discrete analog of a Burgers circuit?

ii) What is the discrete analog of the *grad*, *curl* and *div* operators?

iii) What is the discrete analog of line integrals, surface integrals, unit normals and Stokes theorem?

iv) What is the discrete analog of a slip system?

among others. In the present work we address these issues systematically with the aid of basic tools from algebraic topology, such as CW complexes and homology; from differential calculus, such as differential complexes and integration; and from analysis, such as the Fourier transform and Γ-convergence. The picture that emerges gives rigorous mathematically expression to: the notion of a perfect or defect-free lattice, in which, in particular, every loop is the boundary of an area and can be shrunk to a point, and every close surface is the boundary of a volume and can be likewise shrunk to a point; the notion of discrete differential operators and integrals, including Stoke's theorem; the notion of a crystallographic slip system, with well-defined Burgers vectors and a minimum spacing between slip planes; and the notion of dislocation densities, dislocation entanglements such as junctions, and the topological transitions attendant to the formation and dissolution of junctions. These tools provide a powerful framework for the formulation of a discrete dislocation dynamics in crystal lattices. The theory supplies a full three-dimensional generalization of some existing theories of crystallographic slip on a single plane [2, 1]. We illustrate the versatility of the theory by means of a number of selected applications, including: core energies of bcc dislocations; the dislocation field of an expanding nanovoid; and the dislocation structures selected by the forest mechanisms and the attendant hardening rates.

References

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