

A Geometrical Theory of Discrete Dislocations in Lattices, with Applications to Dislocation Dynamics and Crystal Plasticity

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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 Kroner'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.

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