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THERMODYNAMIC COARSE-GRAINING OF DISLOCATION MECHANICS AND THE SIZE-DEPENDENT CONTINUUM PLASTICITY

***S. Dj. Mesarovic, R. Baskaran, S. Akarapu and H. M. Zbib**

School of Mechanical and Materials Engineering, Washington State University,
Pullman, WA 99164-2920, USA.
**mesarovic@mme.wsu.edu*   Web: *www.mme.wsu.edu/people/faculty/sm.html*

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ABSTRACT

Classical crystal plasticity is size-invariant. Yet, numerous experiments indicate that in small volumes, where motion of dislocations is restricted, the size effects are appreciable. The classical theory is also incapable of incorporating boundary conditions for slip, which is apparent from the weak form of governing equations. Yet, when interfaces impenetrable to dislocations are present, homogeneous boundary conditions for slip are indicated.

Qualitatively, the size effects arise from pile-ups of geometrically necessary dislocations [1] against the boundaries. Such high-energy configurations require additional work to produce an increment of plastic deformation, relative to the work needed in large volumes where dislocations move without hard obstacles.

Following the pioneering work of Fleck and Hutchinson [2], numerous *heuristic* gradient theories have been proposed (e.g., [3]). Typically, these involve intuitivly chosen higher order gradients and physically ambiguous length scales.

Here, we present a micromechanical theory *derived* from dislocation mechanics, by coarse-graining dislocation energies to achieve the thermodynamic equivalence between the dislocation model and the continuum theory.

We define the *microstructural energy* as the elastic strain energy associated with the presence of geometrically necessary dislocations, or, equivalently – the strain energy associated with incompatible elastic deformation. The recently developed integral version [4] of Kroner's [5] continuum theory of dislocations provides an efficient method of calculating this energy, whether dislocations are represented as continuum density fields, or, as discrete line discontinuities. With such mathematical tool in hand, we consider strain energies computed from different descriptions of dislocations:

(i) *Discrete representation*, whereby dislocations are discrete line discontinuities in an otherwise perfect continuum,

(ii) *Semi-discrete representation*, obtained by smearing out the Burgers discontinuity in the slip plane, but keeping the discrete discontinuities across slip planes, and,

(iii) *Continuous representation*, whereby dislocations are represented by a continuous tensor field – the Nye's [6] dislocation density tensor $\boldsymbol{\alpha}$, which derives from the continuous slip fields.

Then, we note that a diluted form of this energy – the one computed from the continuous representation – is already included in the classical crystal plasticity.

Therefore, the energy missing from the classical crystal plasticity is the error in microstructural energy arising from replacing the actual, discrete representation, with the continuous Nye's tensor field.

After computing an approximation to this error for several simple configurations, we express it in terms of continuum fields and formulate the crystal plasticity theory that describes the size effects. The internal virtual work δW can be written as

$$\delta W = \int_V \left(\boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon} + \sum_\alpha \tau^\alpha \delta\gamma^\alpha + \mathbf{m} : \delta\boldsymbol{\alpha} \right) dV - \int_S dS \; \boldsymbol{\mu} : \delta\boldsymbol{\alpha} , \qquad (1)$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are the stress and the elastic strain, γ^α and τ^α are the slip on the slip system α and its work-conjugate [3, 4], while $\mathbf{m}$ and $\boldsymbol{\mu}$ are the volume (V) and boundary (S) work-conjugates if $\boldsymbol{\alpha}$. In addition to the energy terms common to many existing gradient theories – the quadratic form of Nye's densities, the current theory also contains an additional boundary energy term.

The microstructural constitutive laws, relating $\boldsymbol{\alpha}$ to $\mathbf{m}$ and $\boldsymbol{\mu}$, are derived from dislocation mechanics; neither curve-fitting parameters nor physically ambiguous lengths are present in the theory.

The theory features multiple characteristic lengths, h^α, each associated with an active slip system. Physically, these represent average spacing between discrete slip planes in each slip system and evolve with deformation.

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