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ON THE ACCOUNTING OF DISLOCATION INTERNAL STRESS IN CONTINUUM PLASTICITY

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Summary We discuss existing gradient plasticity proposals that are intended to represent internal stress effects of dislocation distributions, and show by a common and simple example that all such proposals overestimate the strain energy or stress of a dislocated medium by the introduced phenomenology. Based on the above observation, we propose a model of crystal plasticity of unrestricted nonlinearity, both in material response and kinematics, that does not have the above defect. The model phenomenologically accounts for short-range interactions through the usual strength-based hardening assumptions of conventional crystal plasticity and calculates the long-range stress and evolution of so-called geometrically necessary dislocation distributions, at the desired scale of resolution, in a mechanically rigorous manner. We present computational results for a simplified version of the model. The development of microstructure is a natural consequence of the model.

The analysis of metal plasticity based on a (physically) rigorous connection to its origins in the mechanics of defects in elastic solids is a complex matter. The primary source of complexity arises in achieving an adequate theory that can describe the dynamics of crystal defects, namely dislocation distributions, as it arises from the interaction of the stress fields of these defects as well as applied loads. Also, simply calculating the stress field of a dislocation distribution in a body undergoing finite deformations and whose crystal elastic response is non-convex is not a trivial matter. Moreover, even if such a theory could be developed, its physical resolution would have to be in the nanometer scale, whereas the effects of the physical mechanisms described above are manifest in plasticity even at the micron scale and above. Consequently, a coarse-graining technique for nonlinear evolutionary systems becomes essential, once a fine-scale theory of plasticity/dislocation mechanics has been constructed.

It is fair to say that there are no modeling approaches available presently that can rigorously deal with all of the aspects mentioned above. Gradient plasticity approaches (Aifantis, 1987; Fleck and Hutchinson, 1997; Gao et al. 1999; Acharya and Bassani, 2000; Busso et al. 2000; Menzel and Steinmann, 2000; Gurtin, 2002) are being developed to deal with such challenges. The approaches amongst these that address single crystal plasticity are based on modifications of conventional single crystal plasticity theory (Rice, 1971; Asaro, 1983; Bassani, 1994) that add the prediction of size dependent response to the list of capabilities of the conventional theory. The description of short-range interactions of dislocations leading to work hardening is phenomenological in these approaches, but is calibrated robustly for practical and scientific applications so as to yield good predictive capability with respect to the various other features of single crystal response apart from work-hardening. It should also be mentioned that work-hardening is the most complex feature of plastic response and, as of now, there are no fundamental treatments of the problem that may be called a theory.

As to the issue of handling the evolving stress field in the body that provides the driving force for its inelasticity, conventional as well as gradient approaches utilizes the same technique whose conceptual connection to the actual stress field of the dislocation distribution in the body is not so clear.

As a perceived improvement of this situation, some gradient plasticity theories have been proposed where the incompatibility of the plastic distortion, a continuum measure of so-called geometrically necessary dislocations (GND), is included in the list of dependencies of the free energy of the solid along with the elastic distortion. The incompatibility being a measure of dislocation density, under the *assumption* that the conventional theory is unable to represent the strain energy and internal stress contribution of the GND distribution, such a device may be expected to be a better reflection of the strain energy and stress content of the body.

However, we show that the internal stress, and consequent strain energy, of a dislocation distribution that is represented by the incompatibility of the constitutively specified plastic distortion is automatically taken into account by the conventional theory employing an elasto-plastic constitutive assumption in which the strain energy and stress depend only on the elastic distortion. Consequently, an added contribution to the strain energy due to the incompatibility is unnecessary, and can be shown to be strictly erroneous in many situations.

However, it remains a fact that conventional plasticity fails to represent strain energy and stress effects of dislocation distributions in a realistic manner. Combining this observation with the conclusion of the previous paragraph, this failure may only be attributed to an inadequate prescription of the plastic distortion in the conventional theory. A theory of nonequilibrium dislocation mechanics that addresses the issues of calculating the stress field of a dislocation density distribution in a nonlinear material under finite deformations and the evolution of such a density giving rise to plasticity has recently been proposed (Acharya, 2001; 2003; 2004). While its complete range of predictive capability still remains to be explored, initial results seem to be promising. This theory, however, is for plasticity at the smallest scales. Apart from its intrinsic value for the analysis of inelasticity at scales of a tenth of microns to a tenth of a nanometer, it is envisioned that it will serve as the fine theory for coarse-graining to achieve a proper theory of macroscopic plasticity, when such a coarse-graining technique for nonlinear evolutionary equations becomes available in the scientific literature.

As a practical expedient, in this work we adopt the ideas of field dislocation mechanics pertaining to calculating the stress field and evolution of GND distributions and append them to the gradient plasticity approach of Acharya and Beaudoin (2000). The rationale behind this approach is that the gradient plasticity approach is thought to be adequate for the modeling of short-range interactions of unresolved dislocation distributions (statistically stored dislocations, SSD), and the long-range stress field and kinetic effects of the dislocation distribution at scales that are resolved by the calculation (so-called geometrically-necessary dislocations, GND) are fundamentally accounted for by the additional dislocation mechanics component of the theory. The 'combined' model does not suffer from the inconsistency mentioned earlier with respect to accounting of strain energy of dislocation distributions.

We describe this finite deformation 'combined' model of single crystal plasticity, and show computational results for a simplified version that includes all the important conceptual details of the model.

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