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On the large-deformation- and continuum-based formulation of models for extended crystal plasticity

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Abstract

The purpose of this work is the application of continuum thermodynamics to the extension of standard crystal plasticity to account for the effects of the development of geometrically necessary dislocations (GNDs) on the material behavior. To this end, following Nye, Kondo, and many others, local deformation incompatibility in the material is adopted as a measure of the density of GNDs. Their development results in additional energy being stored in the material, resulting in additional kinematic-like hardening effects. The current approach generalized previous ones in that the thermodynamic formulation is based on the notion of generalized energy flux. A detailed comparison of the current approach and its results with previous such approaches and their results is given.

Keywords: Continuum thermodynamics; Non-local crystal plasticity; Multiscale modeling; Continuum dislocation theory

1. Introduction

The lengthscale- or size-dependence of material behavior in materials and structures in which characteristic continuum dimensions approach characteristic microstructural lengthscales (e.g., grain size) is by now well-documented (at least in fcc-based systems), having been repeatedly confirmed in different experiments. For example, in torsion tests on thin wires with diameters between 12 and 170 μm, Fleck et al. (1994) observed increasing hardening with the decreasing wire-thickness. Stölken and Evans (1998) observed this as well in bending experiments on thin beams as the beam thickness decreases from 50 to 12.5 μm. Microindentation tests on single crystals displayed the same tendency. In the case of indentation tests, Stelmashenko et al. (1993) showed that the measured indentation hardness increases as the depth of the indentation decreases from 10 to 1 μm. All these tests show the same tendency, i.e., the smaller the specimen size, the larger the increase in hardening. Since standard plasticity models do not account for such a lengthscale or size-dependent

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hardening behavior, they predict flow stresses independent of this. In addition, tests exhibiting size-dependence behavior have in common the fact that, in contrast to conventional tests (e.g., tensile tests), material anisotropy and the imposed kinematic constraints (e.g., at grain boundaries) lead to instability of the initially homogeneous deformation field and to the emergence of energetically more-favorable localized inhomogeneous deformation in the form of, e.g., dislocation substructures (e.g., Ortiz et al., 2000).

As has been pointed out in many works, the phenomena of increasing hardening due to increasing deformation inhomogeneity can be explained (e.g., Ashby, 1970) by the fact that such deformation is accommodated locally via the generation of additional, so-called geometrically necessary dislocations (GNDs). These arise via the net build-up of single-sign "polar" or "excess" dislocations at local obstacles to dislocation motion, e.g., precipitates or grain boundaries, facilitating local inhomogeneous and incompatible deformation which would otherwise take the form of energetically less-favorable local lattice deformation. In contrast to the build-up of "non-polar" or "neutral" dislocation dipoles, then, that of "polar" or "charged" GNDs results in a net Burgers vector. Together with the random trapping of dislocation dipoles resulting in so-called statistically stored dislocations (SSDs), then, the buildup of GNDs leads to a further increase in the total dislocation density. As such, the emergence of GNDs results in both additional hardening in the system and its lengthscale-dependence (Ashby, 1970). In his pioneering work, Nye (1953) (or in the large-deformation context: Kondo et al., 1952) introduced the dislocation density tensor whose three diagonal components can be interpreted as excess screw contributions, and the six off-diagonal components as excess edge contributions, to the dislocation density. Since the production of excess dislocations implies local closure failure, they result in Burgers vector production and in local incompatibility in the deformation field. Consequently, such incompatibility can be taken as a continuum measure of the presence of such dislocations. In the small deformation context, Nye established in addition a relation between the dislocation density and the lattice curvature tensors. In particular, he showed that edge-type GNDs result in the lattice bending, and screw-type GNDs lead to lattice twisting. Exactly this connection between the dislocation density tensor and the lattice curvature has been used in Sun et al. (1998) or El-Dasher et al. (2003) to determine the GND density with the help of electron back scattering diffraction and (lattice) orientation image microscopy. In addition, the correlation between decrease of specimen size and the increase of local deformation inhomogeneity and so of local deformation incompatibility would imply that the GND density increases with decreasing specimen size, leading to the observed correlation between speciment size and additional hardening.

Even in such "simple" tests as microtorsion or microbending, GND development due to local deformation incompatibility results in size-dependent material behavior. More generally, phenomena such as precipitate hardening of metallic materials (higher yield stresses in the case of smaller particle but unchanged volume-fraction precipitation/matrix: Ashby, 1970) and the Hall–Petch effect (hardening of polycrystals by decreasing the grain size) can be explained using the GND concept. In both cases, local deformation incompatibility results from the contrast in kinematic and/or material properties at phase boundaries (e.g., at the interface between the precipitates and matrix, or at grain boundaries), and is accommodated by GND development. Since a decreasing particle or grain size implies a higher percentage of such interfaces, a fine-precipitate or fine-grained material is generally harder. In addition to their role in hardening, GNDs may also play a significant role in deformation localization in metallic materials. In single crystals, for example, one observes the development of slip bands parallel to the active slip plane, and that of kink bands incline to the active slip plane (e.g., Flouriot et al., 2003). In contrast to slip-band formation, kink-band formation involves local lattice rotation and bending, resulting in local lattice curvature. To accommodate such local deformation inhomogeneity in the form of lattice curvature, GNDs accumulate at kink-band boundaries. Because kink band formation always involves strong lattice curvature, it is energetically less favorable than slip band formation, which involves none. That is the reason why slip bands are observed much more frequently than kink bands. Because it does not account for the presence of GNDs and their effect on the material behavior, standard crystal plasticity does not distinguish between the different nature of slip and kink bands. Indeed, it predicts similar resistance against the developing of the both types of shear bands in spite of their different nature (Asaro and Rice, 1979).

The fact that standard crystal plasticity accounts only for the effect of the history of crystallographic slip, i.e., of SSDs, on the hardening behavior, has motivated a number of workers to propose a number of extensions to standard phenomenological plasticity and crystal plasticity. Prominent among these is the Mindlin-