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Dislocation density distribution around an indent in single-crystalline nickel: Comparing nonlocal crystal plasticity finite-element predictions with experiments

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Abstract

We present a physics-based constitutive model of dislocation glide in metals that explicitly accounts for the redistribution of dislocations due to their motion. The model parameterizes the complex microstructure by dislocation densities of edge and screw character, which either occur with monopolar properties, i.e. a single dislocation with positive or negative line sense, or with dipolar properties, i.e. two dislocations of opposite line sense combined. The advantage of the model lies in the description of the dislocation density evolution, which comprises the usual rate equations for dislocation multiplication and annihilation, and formation and dissociation of dislocation dipoles. Additionally, the spatial redistribution of dislocations by slip is explicitly accounted for. This is achieved by introducing an advection term for the dislocation density that turns the evolution equations for the dislocation density from ordinary into partial differential equations. The associated spatial gradients of the dislocation slip render the model nonlocal. The model is applied to wedge indentation in single-crystalline nickel. The simulation results are compared to published experiments (Kysar et al., 2010) in terms of the spatial distribution of lattice rotations and geometrically necessary dislocations. In agreement with experiment, the predicted dislocation fluxes lead to accumulation of geometrically necessary dislocations around a vertical geometrical border with a high orientation gradient below the indenter that is decisive for the overall plastic response. A local model variant without dislocation transport is not able to predict the influence of this geometrical transition zone correctly and is shown to behave markedly softer.

Keywords: Crystal plasticity; Microstructure; Dislocations; Geometrically necessary dislocations; Indentation

1. Introduction

The indentation of metals is widely used for material characterization and the derivation of mechanical properties [1–7]. Although the actual deformation process is simple, the boundary conditions and kinematics involved are complex. Accordingly, structure formation below indents is complex too, rendering the derivation of the corresponding structure–property relationship challenging. Hence, a thorough understanding of the underlying substructure evolution associated with indentation is of great importance.

One reason for the complexity of the deformation state is its strong variation both in space and time. Since the load of the indenter is locally applied, high gradients in the stress, strain and rotation fields naturally arise. As demonstrated by using 2-D and 3-D electron backscatter diffraction (EBSD) methods for a sphero-conical indenter, the loading of the material under the indenter changes with increasing indentation depth and induces a rapid change in the activated slip systems in space and time [8–14].

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Variations in the plastic deformation also lead to a heterogeneous distribution of dislocations: regions of high plastic slip activity naturally contain more dislocations than weakly deformed regions. This relation between slip and the statistically stored dislocation (SSD) density can be described well by a local dislocation-based constitutive model [15–17]. If all dislocation loops are statistically equally distributed within and among the slip systems, then on average the signed character of the single dislocation segments mutually compensate and the ensemble of dislocations is neutral in the sense that no net Burgers vector (or plastic incompatibility) arises. A gradient in plastic slip, however, gives rise to an imbalance of dislocation segments of positive and negative sign, thus building up an excess of signed dislocations, also referred to as geometrically necessary dislocation (GND) density [18–25]. It is these GNDs that accommodate gradients in the lattice rotation field. However, they cannot confidently be predicted by a local constitutive law, since their origin—namely the redistribution of dislocations—is inherently nonlocal [26–30].

Initiated by the work of Walgraef and Aifantis [31], a new simulation approach has emerged in recent years; the so-called continuum density-based dislocation dynamics (CDDD) models treat dislocations as continuously defined dislocation density that evolves in time but also proceeds in space [32–35]. While similar in spirit, they differ in the degree of detail for the description of the dislocation density. A very detailed description is achieved when dislocations are represented by a higher-order dislocation density tensor that retains information about the line direction and the curvature [36]. With this description it is possible to formulate evolution laws for the dislocation density based only on the motion and balance equations of dislocations. When supplemented by a kinetic law, this formulation captures the kinematics of crystal plasticity in fine detail [37]. In order to reduce the substantial computational effort associated with such approaches, various simplifications were suggested to reduce this large configuration space: the restriction to two excess densities of edge and screw character plus their mean curvature and the total dislocation content [34], a single, but spatially variable line direction plus its mean curvature [35], the use of four density measures of straight edge and screw dislocations of opposite signs [31,33], or one excess density and the total dislocation density when restricting the model to two dimensions [38].

In our current approach, we develop a model that includes dislocation transport in a fashion similar to Arsenlis and Parks [33]. We apply this model to an existing microindentation experiment in single-crystalline Ni that was performed by Kysar et al. [39]. This experimental reference is chosen since the deformed volume in the experiment is, on the one hand, large enough so that statistical effects such as dislocation source sampling can be neglected; on the other hand, it is small enough so that dislocation transport is expected to play a significant role. We will analyze the effect of the dislocation transport in the simulations by means of a comparison with a local model variant without dislocation transport. The comparison to the experimentally obtained results then enables us to evaluate the generation of GNDs and their role in the mechanical response of the material.

The paper is organized as follows. In the next section we present the constitutive model with a description of the dislocation evolution equations, the dislocation kinetics and the integration into a finite strain framework. In Section 3 we introduce the setup of the experiment [39] and describe the implementation in the simulation. Section 4 presents the results both of the experiment and the simulations. A comparison of these results and a discussion follows in Section 5 with conclusions given in Section 6.

2. Constitutive model

2.1. Continuum mechanical framework of deformation

The description of the kinematics follows the established continuum mechanical framework of finite strain, as outlined, for instance, by Roters et al. [40]. The multiplicative decomposition of the deformation gradient

$$\boldsymbol{F} = \boldsymbol{F}_\mathrm{e}\boldsymbol{F}_\mathrm{p} \tag{1}$$

splits the deformation into a purely inelastic (or plastic) part, $\boldsymbol{F}_\mathrm{p}$, and a remaining "elastic" part, $\boldsymbol{F}_\mathrm{e}$, which accounts for elastic distortions of the crystal lattice and rigid body rotations [41]. Based on the right Cauchy–Green deformation tensor, an elastic strain measure is given by the Green–Lagrange strain tensor $\boldsymbol{E}_\mathrm{e}$:

$$\boldsymbol{E}_\mathrm{e} = \frac{1}{2}\left(\boldsymbol{F}_\mathrm{e}{}^\mathrm{T}\boldsymbol{F}_\mathrm{e} - \boldsymbol{I}\right), \tag{2}$$

with $\boldsymbol{I}$ the identity tensor. The second Piola–Kirchhoff stress $\boldsymbol{S}$ is related to this elastic strain tensor as its work-conjugate stress measure through:

$$\boldsymbol{S} = \det \boldsymbol{F}_\mathrm{e}\ \boldsymbol{F}_\mathrm{e}^{-1}\boldsymbol{\sigma}\boldsymbol{F}_\mathrm{e}^{-\mathrm{T}} = \mathbb{C} : \boldsymbol{E}_\mathrm{e} \tag{3}$$

with $\mathbb{C}$ being the fourth-order elasticity tensor and $\boldsymbol{\sigma}$ the Cauchy stress.

Plastic deformation is driven by $\boldsymbol{S}$ and in the present case is assumed to be mediated exclusively by dislocation glide on slip systems defined by two unit vectors $\boldsymbol{n}$ and $\boldsymbol{s}$ as the slip plane normal and slip direction with the latter being parallel to the respective Burgers vector $\boldsymbol{b}$ of length b. The shear rates $\dot{\gamma}^\xi$ resulting from corresponding changes in slipped area on systems $\xi = 1, \ldots, N$ contribute additively to the plastic velocity gradient $\boldsymbol{L}_\mathrm{p}$ [42]:

$$\boldsymbol{L}_\mathrm{p} = \sum_\xi \dot{\gamma}^\xi\ \boldsymbol{s}^\xi \otimes \boldsymbol{n}^\xi, \tag{4}$$

which in turn results in an evolution of the plastic deformation gradient at the rate:

$$\dot{\boldsymbol{F}}_\mathrm{p} = \boldsymbol{L}_\mathrm{p}\boldsymbol{F}_\mathrm{p}. \tag{5}$$

The driving force for dislocation motion is provided by the resolved shear stress τ^ξ: