MODELING SIZE-EFFECTS IN SINGLE CRYSTALS AT FINITE STRAINS: INDENTATION OF FCC CRYSTALS

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Summary A new finite element method for analyzing size-effects in single crystals at finite strains is developed and applied to wedge indentation of an FCC crystal. The method is based on a higher order strain gradient crystal plasticity theory where hardening is included due to the addition of gradient terms in both the free energy as well as through a dissipation potential. Size-dependence of hardness measurements are shown to originate from two sources: 1) a blunted indenter tip, and 2) hardening due to strain gradients.

INTRODUCTION

Strengthening size-effects in metals on the micron scale are well captured by higher order strain gradient plasticity theories (see e.g. [1,2]). One example is metal indentation on the micron scale, where it is experimentally well documented that hardness measurements increases for decreasing indentation size (see e.g. [3]). It is widely accepted that the main cause of size-effects in metals is due to storage of geometrically necessary dislocations (GNDs) as a consequence of plastic strain gradients. For wedge indentation GND densities up to the order of $10^{15}\mathrm{m}^{-2}$ have been measured directly by Kysar and co-workers [4].

In this paper a computational effective finite element implementation of a finite strain gradient crystal plasticity theory is presented. The model is applied to the problem of wedge indentation of an FCC crystal oriented such that a plane study is possible. For indentation with a sharp wedge indenter into a non-hardening single crystal, dimensional analysis dictates that hardness, H, here defined as contact force per unit contact area, has the following functional dependence on model parameters:

$$H = \tau_0 \cdot F\left[\frac{\tau_0}{E}, \nu, m, \phi, \frac{\dot{\delta}/a}{\dot{\gamma}_0}, \frac{L_d}{a}\right] \tag{1}$$

Here, τ_0 is the slip resistance, E and ν are Young's modulus and Poisson's ratio respectively, m is a visco-plastic power-law exponent, $180^o - 2\phi$ is the included wedge angle, $\dot{\gamma}_0$ is a reference slip rate, and a is the contact length. The indentation rate, $\dot{\delta}$, is here taken to be proportional to the contact length, a, such that for any given analysis, $\dot{\delta}/(a\dot{\gamma}_0)$ is constant. In the absence of gradient-effects, hardness is independent of the contact length (and hence of indentation depth). However, if a constitutive material length parameter, L_d, is accounted for to model the effect of GNDs in a strain gradient theory, the hardness depends on contact size, as signified by the last term in the above expression.

MATERIAL MODEL AT FINITE STRAINS

A finite strain theory of strain gradient crystal plasticity along the lines of [1,2], together with minimum principles similar to those recently proposed by Fleck and Willis [5] for isotropic plasticity, are developed. The deformation gradient is decomposed into an elastic part, $\boldsymbol{F}^*$, and a plastic part, $\boldsymbol{F}^p$

$$\boldsymbol{F} = \boldsymbol{F}^* \cdot \boldsymbol{F}^p \tag{2}$$

The lattice vectors defining the slip direction, $\boldsymbol{s}^{(\alpha)}$, and the slip normal, $\boldsymbol{m}^{(\alpha)}$, for a slip system (α), are stretched and rotated according to

$$\boldsymbol{s}^{*(\alpha)} = \boldsymbol{F}^* \cdot \boldsymbol{s}^{(\alpha)} \qquad\qquad \boldsymbol{m}^{*(\alpha)} = \boldsymbol{m}^{(\alpha)} \cdot \boldsymbol{F}^{*-1} \tag{3}$$

With the velocity gradient given by $\boldsymbol{L} = \dot{\boldsymbol{F}} \cdot \boldsymbol{F}^{-1} = \boldsymbol{L}^* + \boldsymbol{L}^p$, the plastic strain rate can be expressed by

$$\dot{\boldsymbol{\epsilon}}^p = \sum_\alpha \dot{\gamma}^{(\alpha)} \boldsymbol{\mu}^{*(\alpha)} = \frac{1}{2}\left(\boldsymbol{L}^p + \boldsymbol{L}^{pT}\right) \tag{4}$$

where $\dot{\gamma}^{(\alpha)}$ are the slip rates and $\boldsymbol{\mu}^{*(\alpha)} = (\boldsymbol{s}^{*(\alpha)}\boldsymbol{m}^{*(\alpha)} + \boldsymbol{m}^{*(\alpha)}\boldsymbol{s}^{*(\alpha)})/2$ is the Schmid orientation tensor.

The principle of virtual work in the deformed geometry is given by ([1,2])

$$\int_V \left(\boldsymbol{\sigma} : \delta\dot{\boldsymbol{\epsilon}} + \sum_\alpha (Q^{(\alpha)} - \tau^{(\alpha)})\delta\dot{\gamma}^{(\alpha)} + \sum_\alpha \xi^{(\alpha)} \boldsymbol{s}^{*(\alpha)} \cdot \delta(\boldsymbol{\nabla}\dot{\gamma}^{(\alpha)})\right) dV = \int_S \left(\boldsymbol{T} \cdot \delta\dot{\boldsymbol{u}} + \sum_\alpha r^{(\alpha)}\delta\dot{\gamma}^{(\alpha)}\right) dS \tag{5}$$

Here, $\boldsymbol{\sigma}$ is the Cauchy stress tensor, $\dot{\boldsymbol{\epsilon}}$ is the strain rate, $Q^{(\alpha)}$ is the micro-stress on slip plane α and $\tau^{(\alpha)} = \boldsymbol{\sigma} : \boldsymbol{\mu}^{(\alpha)}$ is the Schmid stress. The higher order nature of the theory manifests itself through the terms $\xi^{(\alpha)}$, which are the higher order stress work conjugate to the resolved slip rate gradients, $\boldsymbol{s}^{*(\alpha)} \cdot \dot{\boldsymbol{\nabla}}\gamma^{(\alpha)}$. Denoting the outward unit normal by $\boldsymbol{n}$, the right hand side of the principle of virtual work includes the conventional traction vector $\boldsymbol{T} = \boldsymbol{\sigma} \cdot \boldsymbol{n}$, work conjugate to the displacement vector $\boldsymbol{u}$, and the higher order tractions $r^{(\alpha)} = \xi^{(\alpha)}\boldsymbol{s}^{(\alpha)} \cdot \boldsymbol{n}$, which are work conjugates to the slip rates $\dot{\gamma}^{(\alpha)}$.

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COMPUTATIONAL METHOD AND RESULTS

A finite element method based on minimum principles along the lines laid out by Fleck and Willis [5] are used to produce slip rate and velocity fields. The problem of micron scale blunt wedge indentation is investigated (see Fig. 1a). A wedge of included angle $180^0 - 2\phi$ with a flattened tip, of length a_0 is indented into a rectangular FCC single crystal of width, W, and height H, such that the line force exerted by the indenter along the [110] direction acts in the negative [001] direction. With this loading plane strain deformation takes place as shown by Rice [6] and Kysar and co-workers [4], and three effective in-plane slip systems oriented 54.7^o apart are activated. Each of these effective slip systems are made up of two crystallographic slip systems for which the slip directions and the slip normals have out-of-plane components, and effective in-plane slip parameters are derived from the crystallographic slip parameters.

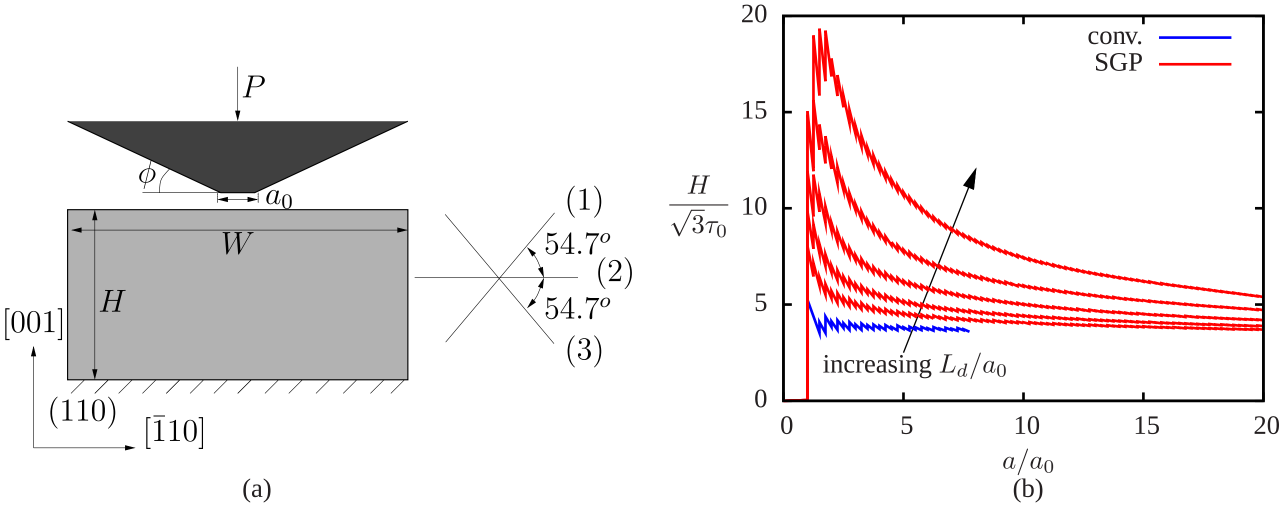

Figure 1: The indenter geometry is shown in a). For different dissipative length parameters, L_d, b) shows the hardness-contact length relation for the material length parameters: $L_d/a_0 = 0,\ 1/2,\ 1,\ 2,\ 4,\ 8.$

For an indenter of an included angle of 170^0 ($\phi = 5^o$), Fig. 1b shows the normalized hardness, as a function of contact length. The different curves in the figure correspond to different ratios between the material length scale, L_d, and the initial contact area, a_0. Conventional predictions with $L_d = 0$ are included for comparison. The irregular appearance of the hardness curves is due to the discreteness of the contact area in the finite element calculations. Deviations from a constant level of hardness (independent of indent size) in Fig. 1b originate from the following two reasons; I) The inclusion of material size-effects in the model; and II) the initial flat contact of length a_0. Hence, the results quantifies the material size-effect as well as the effect of a non-sharp indenter tip on hardness under wedge indentation.

CONCLUSIONS

A finite strain theory for strain gradient crystal plasticity is presented together with a numerically efficient finite element method. The problem of blunt tip wedge indentation is analyzed within a 2D setting, where effective in-plane slip parameters are rigorously developed from the crystallographic slip parameters. Deviations from size-independent results are shown to originate from the material size-effect as well as the blunted indenter tip.

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