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Influence of strain gradients on lattice rotation in nano-indentation experiments: A numerical study

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ABSTRACT

In this paper the texture evolution in nano-indentation experiments was investigated numerically. To achieve this, a three-dimensional implicit finite-element model incorporating a strain-gradient crystal-plasticity theory was developed to represent accurately the deformation of a body-centred cubic metallic material. A hardening model was implemented to account for strain hardening of the involved slip systems. The surface topography around indents in different crystallographic orientations was compared to corresponding lattice rotations. The influence of strain gradients on the prediction of lattice rotations in nano-indentation was critically assessed.

1. Introduction and motivation

Indentation is an experimental method widely used to characterise the mechanical response of small volumes of materials [1–3]. Although indentation experiments are easy to perform, interpreting the obtained data is a challenge due to the inherent heterogeneity of the deformation fields, complex stress/strain distributions in the tested material and the non-trivial contact conditions during the process. Consequently, numerical simulation techniques are frequently used to study the underlying mechanics in indentation experiments. For instance, deformation-induced lattice rotations below an indent have attracted attention as there exists a close connection between crystallographic shear, the main mechanism governing the deformation, and the resulting lattice spin [4].

Some studies have attempted to characterise the observed phenomena, with the use of different techniques such as the non-destructive 3D synchrotron diffraction method [5], 3D electron back-scattered diffraction (EBSD) [4] and transmission electron microscopy (TEM) [6,7].

In this regard, a limited number of numerical studies attempted to analyse physical deformation mechanisms leading to lattice rotations [8,9]. Wang et al. [10] demonstrated lattice rotations for a single crystal of Cu with different orientations using a 3D elastic–viscoplastic crystal-plasticity (CP) finite-element (FE) method. Zaafarani et al. proposed a physically based crystal-plasticity model based on dislocation-rate formulations to explain the potential reasons for deformation-induced patterns consisting of multiple narrow zones with alternating crystalline rotations [11]. However, the model consistently overestimated the extent of lattice rotations in the experiment.

Strain-gradient plasticity theories [12–16] that account for the effects of geometrically necessary dislocations (GNDs) [17] on plastic flow had some success in explaining size effects observed in torsion [18], bending [19] and indentation [20–22]. In this paper, a 3D non-local elastic–viscoplastic crystal-plasticity finite-element model for the nano-indentation of Ti–15V–3Al–3Sn–3Cr (Ti–15–3–3–3) is developed to demonstrate the influence of strain gradients on the reorientation of the crystalline lattice and resulting deformation patterns. The relationship between the anisotropy of surface profiles around nano-indents and local texture changes is studied.

This paper is organised as follows: a brief self-contained description of constitutive equations of the strain-gradient crystal-plasticity theory is presented in Section 2. Details of the developed finite-element model of nano-indentation are presented in Section 3. Section 4 demonstrates the predictive capabilities of the model for lattice rotations and surface profiles for different crystallographic orientations. We finally offer concluding remarks in Section 5.

2. Theory

An enhanced modelling scheme for a strain-gradient crystal-plasticity (EMSGCP) theory proposed by Demiral [23] was used in

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the simulations. Below, the constitutive relations of the theory are summarised.

The deformation gradient $\boldsymbol{F}$ is decomposed multiplicatively into elastic ($\boldsymbol{F}^e$) and plastic ($\boldsymbol{F}^p$) parts as follows:

$$\boldsymbol{F} = \boldsymbol{F}^e \boldsymbol{F}^p. \tag{1}$$

$\boldsymbol{F}^p$ evolves according to the flow rule

$$\dot{\boldsymbol{F}}^p = \boldsymbol{L}^p \boldsymbol{F}^p, \tag{2}$$

where the plastic velocity gradient $\boldsymbol{L}^p$ corresponds to

$$\boldsymbol{L}^p = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha \boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha. \tag{3}$$

In Eq. (3), $\dot{\gamma}^\alpha$ is the shearing rate on the slip system α, which is represented by the slip direction $\boldsymbol{s}^\alpha$ and the slip plane normal $\boldsymbol{m}^\alpha$. We choose a power-law representation for $\dot{\gamma}^\alpha$, as

$$\dot{\gamma}^\alpha = \dot{\gamma}_0^\alpha \, \mathrm{sgn}(\tau^\alpha) \left| \frac{\tau^\alpha}{g_T^\alpha} \right|^n, \tag{4}$$

where $\dot{\gamma}_0^\alpha$ is the reference strain rate, n is the macroscopic rate-sensitivity parameter, τ^α is the resolved shear stress, g_T^α is the strength of the slip system α at the current time, and sgn(*) is the signum function of *.

In the EMSGCP theory, the initial strength of slip systems, i.e., the *critical resolved shear stress* (CRSS), is governed by pre-existing GNDs in the workpiece together with statistically stored dislocations (SSDs) (Eq. (5)), i.e., $g_T^\alpha|_{t=0} = g_S^\alpha|_{t=0} + g_G^\alpha|_{t=0}$. Here, a subscript G indicates GNDs and S implies SSDs. In this theory, $g_S^\alpha|_{t=0}$ and $g_G^\alpha|_{t=0}$ were linked with initial SSD ($\rho_S^\alpha|_{t=0}$) and GND ($\rho_G^\alpha|_{t=0}$) densities as $g_S^\alpha|_{t=0} = K\sqrt{\rho_S^\alpha|_{t=0}}$ and $g_G^\alpha|_{t=0} = K\sqrt{\rho|_{t=0}(\overline{S}/\overline{V})^2}$ via the constant, K, similar to the Taylor relation. The GND density term was expressed as a function of the normalised surface-to-volume ($\overline{S}/\overline{V}$) ratio (hence, dimensionless) for the component under study [24].

The evolution of slip resistance during loading is the result of hardening due to the SSDs (Δg_S^α) and GNDs (Δg_G^α) on the slip system.

$$g_T^\alpha = g_S^\alpha|_{t=0} + g_G^\alpha|_{t=0} + \sqrt{(\Delta g_S^\alpha)^2 + (\Delta g_G^\alpha)^2},$$
$$\Delta g_S^\alpha = \sum_{\beta=1}^{N} h_{\alpha\beta} \, \Delta\gamma^\beta, \; \Delta g_G^\alpha = \alpha_T \mu_s \sqrt{b n_G^\alpha}. \tag{5}$$

Here $h_{\alpha\beta}$, α_T, μ_s, b and n_G^α correspond to the slip-hardening modulus, the Taylor coefficient, the shear modulus, the Burger vector and the effective density of geometrically necessary dislocations, respectively. The hardening model proposed by Peirce et al. [25] is used to represent $h_{\alpha\beta}$, as follows:

$$h_{\alpha\alpha} = h_0 \mathrm{sech}^2 \left| \frac{h_0 \tilde{\gamma}}{g_T^\alpha|_{sat} - g_T^\alpha|_{t=0}} \right|, \; h_{\alpha\beta} = q h_{\alpha\alpha} (\alpha \neq \beta), \; \tilde{\gamma} = \sum_\alpha \int_0^t |\dot{\gamma}^\alpha| dt, \tag{6}$$

where h_0 is the initial hardening parameter, $g_T^\alpha|_{sat}$ is the saturation stress of the slip system α, q is the latent hardening ratio, which is assumed to be 1, and $\tilde{\gamma}$ is the Taylor cumulative shear strain on all slip systems. The effective GND density (n_G^α) is given by

$$n_G^\alpha = |\boldsymbol{m}^\alpha \times \sum_\beta s^{\alpha\beta} \nabla\gamma^\beta \times \boldsymbol{m}^\beta|, \tag{7}$$

where $s^{\alpha\beta} = \boldsymbol{s}^\alpha \boldsymbol{s}^\beta$ and $\nabla\gamma^\beta$ is the gradient of shear strain in each slip system. To calculate $\nabla\gamma^\beta$ the scheme proposed in Demiral et al. [24] is followed. The model was implemented in the implicit finite-element code ABAQUS/standard using the user-defined material subroutine (UMAT). Relevant details can be found in [21,24,26,27].

It should be noted that as the $\overline{S}/\overline{V}$ ratio is negligibly small in nano-indentation samples, the CRSS value of slip systems depends only on SSDs. Therefore, for the nano-indentation test, the EMSGCP theory naturally reduces to the mechanism-based strain-gradient crystal-plasticity theory proposed by Han et al. [28]. Note that in the classical CP theory the contribution from both incipient and evolving GNDs is not accounted for, i.e., instantaneous strength of the slip system is given by $g_T^\alpha = g_S^\alpha|_{t=0} + \Delta g_S^\alpha$.

Here, a β-Ti alloy with a b.c.c. crystalline structure is studied. In the following simulations only the {112} ⟨111⟩ slip system (Table 1) was considered [24].

3. Finite-element modelling of nano-indentation

A FE model of the indentation experiment was developed [24]. Dimensions of the workpiece sample used in the FE model were 10 μm × 10 μm × 6 μm. Eight-node linear brick elements (C3D8) were used to discretise the sample. A finer mesh with a minimum element size of 100 nm was used near the indenter tip as the strain gradients are typically the highest in the vicinity of the indenter. A conical indenter with $\theta = 90^\circ$ and a tip radius of 1.0 μm was modelled as a rigid body. The indenter was displaced in the negative y-direction with a maximum indentation depth of 375 nm followed by complete unloading. The total simulation time was 1.2 s with loading time of 1.0 s. The bottom face of the workpiece was constrained in all directions, its faces with normals in the x- and z-directions were constrained, respectively. Contact between the indenter and workpiece was assumed to follow Coulomb's friction law with $\mu = 0.05$ [23].

The material parameters used in the simulations are listed in Table 2. These are based on their exhaustive calibration by matching the surface profile of the indented surface along a path with the

Table 2
Material parameters for Ti-alloy single-crystal micropillars used in the model of the micropillar-compression experiment Demiral et al. [24].

Elastic constants (GPa)	CP parameters	EMSGCP parameters
$C_{11} = 127.740$	$\dot{\gamma}_0^\alpha = 10^{-4}\ \mathrm{s}^{-1}$	$\alpha_T = 0.7$
$C_{12} = 118.850$	$n = 15$	$\mu_s = 13.980$ GPa
$C_{44} = 43.997$	$g_T^\alpha|_{t=0} = 150$ MPa	$b = 2.803 \times 10^{-7}$ mm
	$g_T^\alpha|_{sat} = 170$ MPa	
	$h_0 = 10,000$ MPa	

Table 1
Available slip systems for Ti alloy single crystal for {112} ⟨111⟩ set.

Slip system	1	2	3	4	5	6	7	8	9	10	11	12
Direction	$11\bar{1}$	$1\bar{1}1$	$\bar{1}11$	111	$1\bar{1}1$	$11\bar{1}$	111	$\bar{1}11$	$\bar{1}11$	111	$11\bar{1}$	$1\bar{1}1$
Plane	112	$\bar{1}12$	$1\bar{1}2$	$11\bar{2}$	121	$\bar{1}21$	$1\bar{2}1$	$12\bar{1}$	211	$\bar{2}11$	$2\bar{1}1$	$21\bar{1}$