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Effects of initial orientation, sample geometry and friction on anisotropy and crystallographic orientation changes in single crystal microcompression deformation: A crystal plasticity finite element study

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Abstract

The study presents crystal plasticity finite element simulations of cylindrical Cu single crystal micropillar compression tests. The aim is to study the influence of the stability of the initial crystal orientation, sample geometry (diameter-to-length ratio) and friction on the anisotropy and crystallographic orientation changes during such tests. Initial anisotropy (initial orientation) has a strong influence on the evolution of crystallographic orientation changes and also, to a minor extent, on the sample shape during compression. Pronounced orientation changes occur at an early stage of compression (at engineering strains of 0.2), entailing as a rule a large orientation spread within the initially uniformly oriented sample. A non-zero friction has a stabilizing effect on the course of the compression test even in cases where strong orientation changes occur. The evolution of orientation changes during compression is in part due to rigid body rotations (shape inclination due to buckling) rather than exclusively to crystallographic reorientation. Orientations that are crystallographically unstable and non-symmetric during compression tend to entail shape instability of the pillars at an earlier stage than observed for more stable cases.

Keywords: Column; Pillar; Compression; Orientation; Misorientation

1. Introduction and motivation

Mechanical size effects discovered recently during microscale compression tests of crystalline metallic single crystals [1] are currently attracting great attention. The main experimental observation is that the mechanical properties observed during such tests become remarkably different compared with bulk specimens when the sample dimensions of the pillars approach the micrometer scale. Uchic et al. [1] tested three different materials: Ni, Ni_3Al–1% Ta and a Ni-based superalloy. By mapping the engineering stress–strain curves during microscale compression the authors observed that the yield stresses dramatically increased as the diameters of the test pillars decreased. The group of Nix and Greer [2,3] performed similar tests on gold pillars but used two different sample fabrication methods. The authors found a similarly significant flow stress increase as in Ref. [1], and proposed that a dislocation starvation effect could have been responsible for this. Their hypothesis suggests that due to the small dimensions of the specimens the dislocations that are present at the onset of plastic deformation leave these specimens before dislocations can multiply: this results in dislocation starvation. The authors propose that if this state is reached, very high stresses would be required to nucleate new dislocations, either at the sample surface or in the bulk of the crystal, leading to the observed near-theoretical strengths. Similar observations were reported by Dimiduk et al. [4] and Volkert and Lilleoden [5].

Afrin and Ngan performed similar microcompression experiments using a nanoindenter at room temperature

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on Ni_3Al specimens [6]. Their columns, which were also produced via focused ion-beam milling, had a diameter of 2 μm.

By using finite element simulations with an isotropic constitutive law Zhang et al. [7] proposed some guidelines from a continuum mechanics point of view in terms of geometry and system set-up to design accurate microcompression tests. This is a sensible approach since finite element simulations are well suited to study details of the influence of the external boundary conditions and their possible changes during compression encountered in such tests. Points of particular interest in the paper were the effects of the strain-hardening behavior, the initial height and the Coulomb friction coefficient.

The motivation for the present study consists in merging some aspects of the different investigations quoted above into one simulation procedure. This means that we combine the advantages of an anisotropic crystallographic law for the constitutive description of the material in conjunction with a full consideration of crystallographic orientation effects and orientation evolution with proper boundary condition treatment via a crystal plasticity finite element simulation.

The aim of this approach is to address the compression deformation of cylindrical single crystal micropillars with respect to the role of the initial crystal orientation, evolution of deformation-induced orientation changes, sample geometry (diameter-to-length ratio), crystalline anisotropy and Coulomb friction on the course of such tests. Similar crystal plasticity finite element simulation approaches have been previously shown to be successful for investigating the relationship between mechanical boundary conditions and orientation effects at small scales, e.g. for the case of single crystal deformation [8], bicrystal deformation [9–11], oligocrystal deformation [12] and nanoindentation [13,14]. The results are used to investigate our hypothesis that even in the case of an homogeneous initial crystallographic orientation and homogeneous initial boundary conditions at the beginning of a compression test, gradual formation of orientation gradients can take place within an initially uniformly oriented specimen during loading.

2. Simulation procedure

2.1. Introduction

The finite element method is well suited to the treatment of complex boundary conditions in materials mechanics. Its concept is based on dividing (continuum) space into small domains with simple geometry which allows one to approximate the response to a given local constitutive behavior in such domains under the boundary conditions imposed jointly by external and internal constraints. Of importance in this paper is the use of a crystalline elastic and plastic anisotropic constitutive law [15].

In classical isotropic continuum mechanics, crystallographic rotations, and hence orientation effects, do not play a role since an antisymmetric portion associated with the dyadic nature of crystallographic dislocation slip (i.e. shear only along discrete directions on discrete planes) does not exist. This means that isotropic constitutive approaches to materials micromechanics are less useful in cases where the crystalline nature of matter plays an important role in terms of anisotropy and deformation-induced orientation changes including the formation of orientation gradients. An overview of the different approaches to the incorporation of crystalline anisotropy into finite element schemes is given in Refs. [15–20].

In this investigation the crystal plasticity finite element method is used to systematically study the intrinsic parameters (e.g. initial orientation and the evolution of deformation-induced orientation changes upon mechanical loading) and extrinsic effects (e.g. sample geometry and the contact conditions) involved in microcompression tests.

2.2. Constitutive model

2.2.1. Flow rule

In order to describe the flow kinematics the finite deformation defined by the deformation gradient, F, is multiplicatively decomposed into two contributions, namely the elastic and rotational part of the deformation gradient, F^*, and the plastic part of the deformation gradient, F_p [15]. The latter quantity describes an intermediate configuration accounting only for the deformation induced by the plastic slip in the lattice, i.e. $\det F_p = 1$. The elastic and rotational portion of the deformation gradient, F^*, captures both the stretch and the rotation of the lattice. The flow rule was used in the form:

$$\dot{F}_p = L_p F_p, \tag{1}$$

and the plastic velocity gradient, L_p, as:

$$L_p = \sum_{\alpha} \dot{\gamma}_\alpha (m_0^\alpha \otimes n_0^\alpha), \tag{2}$$

where m_0^α and n_0^α are the orthonormal vectors describing the slip direction and the slip plane normal of the slip system α in the reference configuration, respectively. $\dot{\gamma}_\alpha$ describes the shear rates on the slip systems α.

2.2.2. Hardening mechanism

The phenomenological hardening law is based on a crystal plasticity model which was suggested by Rice [15], Hutchinson [21] and Peirce et al. [16,17] for the face-centered cubic (fcc) lattice. The kinetic law on a slip system α follows:

$$\dot{\gamma}_\alpha = \dot{\gamma}_0 \left| \frac{\tau_\alpha}{s_\alpha} \right|^{1/m} \operatorname{sign}(\tau_\alpha), \tag{3}$$

where $\dot{\gamma}_\alpha$ is the shear rate on the slip system subjected to the resolved shear stress τ_α having a slip resistance of s_α. $\dot{\gamma}_0$ and m are material parameters and stand for the reference shear rate and for the rate sensitivity of slip, respectively. The influence of any slip system β on the hardening behavior of system α is given by: