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EVOLUTION OF CRYSTAL STRESS DISTRIBUTION ON ELASTOPLASTIC DEFORMATION OF POLYCRYSTALLINE SOLIDS

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ABSTRACT

Stress tensor of plastically deforming polycrystalline solids can be obtained from the development of synchrotron X-ray diffraction experiment techniques. The mechanism behind the stress tensor evolution of plastic deformation of polycrystalline solids is presented in this study. The elastoplastic behavior of polycrystals is investigated using a simulation model that is calibrated with the X-ray diffraction experiment results of a copper specimen under uniaxial tension. The preferred crystal stress direction and its evolution pattern are examined by identifying the angular distance between the crystal stress direction and the single crystal yield surface vertices as well as the applied loading direction. It is confirmed that crystal stress tends to move toward the closest vertex of the single crystal yield surface to the applied loading direction, as plasticity develops.

Keywords: Polycrystalline solids, plasticity, crystal stress, single crystal yield surface, finite element analysis

1. INTRODUCTION

The study of crystal stress distribution in polycrystalline solids enables further understanding of the behavior of materials, such as plasticity, fatigue, and crack propagation. The deformation of polycrystalline solids is dependent on the crystal stress distribution at the micro-scale. Therefore, the investigation of the crystal stress behavior is necessary for better understanding the underlying mechanisms of the material behavior. In this research, the stress distribution change before and after yielding of deforming copper polycrystals is investigated over crystal orientation space using a method extended from Miller et al. (2008). In particular, the crystal behavior during plastic flow originated along crystallographic slip systems is the primary interest in this study.

Miller et al. (2008) describes a procedure to obtain crystal stress distribution function over a crystal orientation space from experiment and simulation data. The crystal stress orientation distribution function is constructed using the crystal strain obtained from the experiment and in a form of crystal strain pole figures for a set of families of crystals. Then, distribution of a crystal

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strain tensor over a complete crystal orientation space can be constructed from the crystal strain pole figures by an inversion procedure. The crystal-based finite element method which mimics the actual experiments is used to obtain the stress tensors for crystals in a virtual specimen. The crystal stress distribution function is then constructed over a crystal orientation space.

In this research, insights on the crystal stress evolution mechanism during plastic flow using simulated data are provided. The crystal stress distribution after the full development of plasticity is described by investigating coaxiality that represents the angular distance between the crystal stress direction and the vertex direction of the single crystal yield surface (SCYS) or the applied loading direction (Ritz et al. 2010; Han et al. 2012). Evolutions of crystal stress and its direction related to the SCYS vertex and the applied loading directions are investigated. The analysis is performed over the entire orientation space as well as along typical crystallographic fibers to examine the crystal orientation dependence of preferred crystal stress evolution.

2. METHODOLOGIES FOR DESCRIBING CRYSTAL STRESS DISTRIBUTION

The methodology for generating the crystal stress distribution from modeling is described. A detailed description on the method can be found in Miller et al. (2008) and Han et al. (2012), so only brief description of the method is presented here.

2.1. Finite element formulation

The crystal-based finite element method where a grain is represented by one or more finite elements is described. The weak form of the residual of equilibrium equation is given as:

$$R_u = -\int_B \mathrm{tr}(\sigma'^{\mathrm{T}} \mathrm{grad}\,\psi)\mathrm{d}B + \int_B \pi \mathrm{div}\,\psi \mathrm{d}B + \int_{\partial B} t\cdot\psi \mathrm{d}\Gamma + \int_B \iota\cdot\psi \mathrm{d}B \tag{1}$$

Cauchy stress can be decomposed into deviatoric and spherical parts: $\sigma = \sigma' - \pi\mathbf{I}$, where π is pressure, **I** is the second order identity tensor, $\langle\cdot\rangle'$ designates a deviatoric component. t is traction acting on the surface of the domain, ι is body force and ψ is a weight function. The residual is transformed to a discretized form following the standard finite element procedure in Marin and Dawson (1998b).

The simulation procedure begins with defining a multiplicative decomposition of kinematics which combines the elastic and plastic responses. It is assumed that crystallographic slip where the dislocation motion through the crystal lattice is the only source of plastic deformation. The detailed description on crystal plasticity adopted in this research can be found in Marin and Dawson (1998a).

A finite element mesh used in this study is shown in Fig. 1. Rhombic dodecahedral polyhedron is used to represent grains that composed by 48 equal size 10-noded tetrahedral elements. The finite

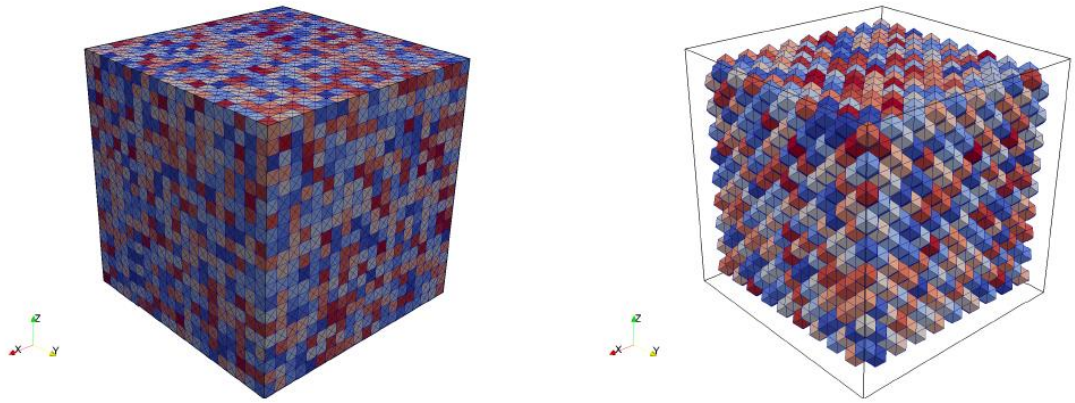

Figure 1: Finite element mesh. Total mesh (RVE) (left) and visualization of full dodecahedral grains by removing partial grains of RVE mesh (right).

element mesh in Fig. 1(a) contains 192,000 elements. In Fig. 1(b) shows the 2916 complete dodecahedra grains within the mesh by removing the partial dodecahedra near the boundary. The size of mesh was considered to be adequate for constructing the crystal strain distribution function.

2.2. Single crystal yield surface (SCYS) vertex and coaxiality

The crystal stress orientation function from experiments and simulations are investigated by generalized spherical harmonics analysis over the crystal orientation space in Miller et al. (2008). The core idea for identifying the mechanism behind the similarity between the experiment and simulation is that the crystal stress direction tends to move toward a SCYS vertex to accommodate the complex deformation compatibility among crystals as the plastic flow develops (Han et al. 2012). To measure the full crystal stress tensor over the orientation space became possible for plastically deforming polycrystals, the comparison and analysis of crystal stress evolution between experiment and simulation can be performed as in this research.

The evolution of the crystal stress direction is examined by evaluating the angle between the crystal stress direction and the SCYS vertex or the applied loading direction. The angle between stress tensors, coaxiality, is defined as:

$$\theta_a^b = \cos^{-1}\left(\frac{\sigma_a' : \sigma_b'}{\|\sigma_a'\|\|\sigma_b'\|}\right) \tag{2}$$

The superscript $\langle\cdot\rangle'$ designates a deviatoric (stress) component. Using this relation, the coaxiality between a crystal stress direction and the closest SCYS vertex is defined as θ_c^v, and the coaxiality between a crystal stress direction and the macroscopic applied loading direction is expressed as θ_c^m. The schematic of coaxiality is illustrated in Fig. 2.

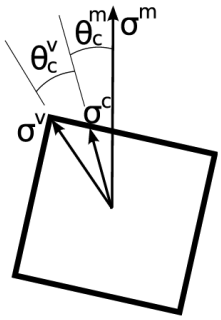

Figure 2: The schematic of crystal yield surface (SCYS). σ^c is the crystal stress, σ^v is the stress for a SCYS vertex, and σ^m is the macro-scale applied loading direction. The coaxiality between σ^c and σ^v or σ^m is defined by the angle σ_c^v and σ_c^m.

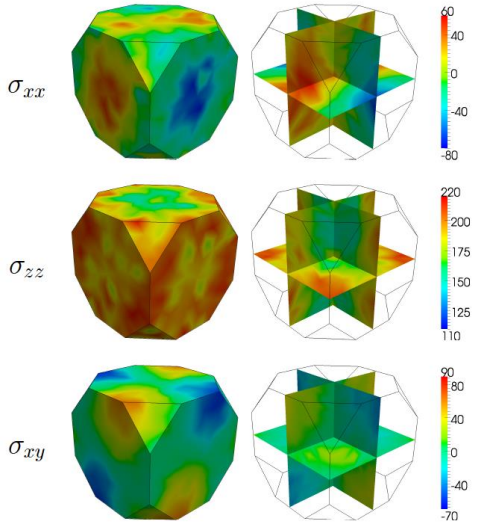

Figure 3: Crystal stress distribution over crystal orientation space after yielding ($\sum_{zz}$ = 180MPa, Unit: MPa)

3. ANALYSIS ON CRYSTAL STRESS EVOLUTION

Crystal stress distributions described over the fundamental region for cubic crystals in Rodrigues parameterization after yielding are shown in Fig. 3. In the Rodrigues orientation space, the axis direction ($\boldsymbol{n}$) in the Rodrigues parameterization is the same direction as that of the sample space. Vertical direction (z-axis) is the same as the tensile direction, and the symmetric pattern around the z-axis can be identified in the Fig. 3. It is shown that patterns of the crystal stress distributions after yielding represents the orientation dependence.

The hypothesis that the crystal stress evolves toward a vertex of SCYS is verified by investigating coaxialities of the crystal stress direction to the closest SCYS vertex (θ_c^v) and to the applied loading direction (θ_c^m) over the crystal orientation space. In Fig. 4, the values of θ_c^v reduces after yielding. It indicates that the crystal stresses are moving toward the SCYS vertices.

Even though the result of θ_c^m is not presented in this paper, the tendency of coaxiality evolution strongly indicates that the crystal stress direction is changed toward the SCYS vertex as plasticity develops.

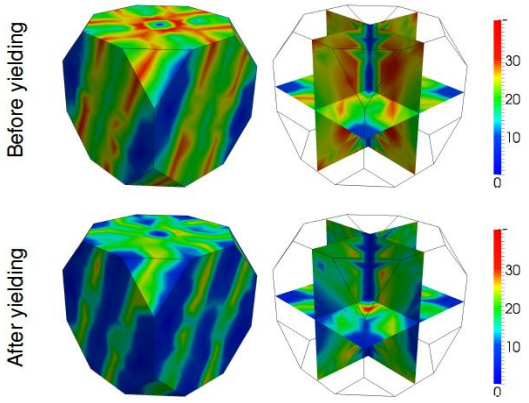

Figure 4: Coaxiality between crystal stresses and the closest SCYS vertex, θ_c^v (Unit: deg.)

4. CONCLUSION

Crystal stress distribution of copper polycrystals after elastoplastic deformation obtained from finite element simulation was analyzed, and the mechanism for the evolution of the stress direction was also investigated. The coaxiality between the crystal stress direction and the closest SCYS vertex or the macroscopic loading direction was examined. The dependence of the crystal stress direction on the crystal orientation was further analyzed by coaxiality distribution along crystallographic fibers in crystal orientation space. The patterns from the coaxiality analysis demonstrate that the crystal stress evolves toward the SCYS vertex and away from the macroscopic applied loading direction as plasticity develops.

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