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Effect of phase interactions on crystal stress evolution over crystal orientation space under elastoplastic deformation of two-phase polycrystalline solids

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ABSTRACT

It has been known for decades that crystal stress directions move toward the vertices of the single crystal yield surface (SCYS) during plastic flow of polycrystalline solids to satisfy the deformation compatibility among crystals. The alignment of crystal stress with a SCYS vertex is affected not only by plastic anisotropy, but also by other factors such as elastic anisotropy, loading direction, and grain interactions. Among the factors contributing to the degree of alignment, the effect of phase interactions on the crystal stress evolution during plastic flow has not been extensively investigated. In this research, the effect of phase interactions on the crystal stress direction evolution is investigated using simulations of an elastoplastically deforming two-phase (Cu/Fe) polycrystalline solid calibrated to a neutron diffraction experiment. By mapping the simulated crystal stresses over the crystal orientation space, crystal-orientation-dependent nonuniform partitioning of the crystal stress between phases can be observed. An analysis of the distribution of angles between the SCYS vertex and the crystal stress based on the simulation of the two-phase material shows that the crystal stress evolution pattern during plastic flow is strongly affected by phase interactions. These interactions result in low alignment and greater dispersion angles between the crystal stresses and SCYS vertices, particularly in the strong phase.

1. Introduction

The development of high-energy diffraction techniques has enabled measurement and analysis of the strain evolution of crystals embedded within polycrystalline specimens under elastoplastic deformation. In particular, the in-situ crystal (lattice) strain in bulk polycrystalline solids can be obtained from neutron or X-ray diffraction experiments. Earlier work on diffraction measurements of polycrystalline solids includes (Turner et al., 1995; Holden et al., 1997; Clausen et al., 1998), and this has been an active area of research. State-of-the-art simulation tools can also be used to confirm the experimental results and to further investigate the complex behaviors of polycrystalline solids. A synergic approach combining state-of-the-art high-energy diffraction experiments and large-scale finite element simulation tools to investigate the elastoplastic behavior of polycrystalline solids (Miller et al., 2008) has been effective for exploring the behaviors of a wide range of these

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materials, including recent work such as Li and O'Dowd (2011) and Wollmershauser et al. (2012). In this research, simulation results calibrated to a neutron diffraction experiment (Han and Dawson, 2005) are used to investigate the crystal stress evolution characteristics of a two-phase (Cu/Fe) polycrystalline solid under elastoplastic deformation. In particular, the effect of phase interactions on the change in the crystal stress direction during plastic flow is studied.

The crystal stress evolution of polycrystalline solids during elastoplastic deformation is the result of complex behaviors among crystals, such as grain interactions and the effects of the elastic anisotropy, plastic anisotropy, and loading direction. In addition to these factors, phase interactions in multiphase materials contribute to crystal stress evolution, which is the primary focus of this study. It has been known for decades that the stress direction of polycrystalline solids during plastic flow tends to move toward one of the vertices of the single crystal yield surface (SCYS) (Kocks, 1960). When stress is placed on the facet of the SCYS, the deformation direction is uniquely defined by the facet. It is almost impossible to satisfy the complex deformation compatibility of a crystal embedded within polycrystalline aggregates using the unique deformation mode from only one active slip system, i.e., the “normality rule.” However, the crystal stress direction during plastic flow tends to move toward the edges of the SCYS where two facets meet, and thus two active slip systems exist, or toward the SCYS vertices, where multiple crystallographic slips are possible. Multislip at the SCYS vertices allows arbitrary deformation, which can effectively satisfy the compatibility of polycrystalline aggregates.

The plastic anisotropy is not the only factor that contributes to crystal stress evolution. During elastoplastic deformation, the elastic anisotropy also contributes. As a result of differences between the elastic and plastic anisotropies, the elastic anisotropy affects the alignment of the crystal stress directions with the SCYS vertices during elastoplastic deformation with well-developed plasticity (Maniatty and Yu, 1996).

The loading direction is also one of the major factors affecting the crystal stress evolution. The crystal stress direction does not generally tend to align with the applied loading (stress) direction but moves to the SCYS vertex. Among the SCYS vertices, the crystal stress moves to the closest SCYS vertex to the applied stress direction during plastic flow (Ritz et al., 2010; Han et al., 2012). However, depending on the crystal orientations relative to the applied loading direction, the alignment of the crystal stress and SCYS vertices, i.e., the coaxiality (Ritz et al., 2010), varies. The dependence of the crystal stress direction evolution on the crystal orientation relative to the loading direction has been confirmed using the coaxiality (Ritz et al., 2010; Han et al., 2012; Han and Chung, 2012; Han et al., 2013).

The complex deformation compatibility among polycrystalline aggregates fundamentally originates from grain interactions coupled with the normality rule. Furthermore, the degree of coaxiality depends on the characteristics of neighboring crystals, such as their orientations. Even with the same set of orientations of neighboring crystals, the stress evolution of a crystal is affected by the arrangement of the neighboring crystals (Han et al., 2012). The different elastic and plastic anisotropies resulting from different spatial arrangements of neighboring crystals contribute to crystal stress evolution.

The crystal stress evolution in multiphase materials with distinct phase properties can also be affected by phase interactions. Multiphase polycrystalline solids under elastoplastic deformation were investigated using high-energy diffraction experiments (Harjo et al., 2001; Han and Dawson, 2005; Hedström et al., 2010), and evidence of phase interactions was confirmed. In Han and Dawson (2005), two-phase polycrystalline solids composed of Cu and Fe phases were investigated by comparing neutron experiments with large-scale finite element simulations. In that paper, the crystal (lattice) strains measured experimentally were reproduced by the simulations, and further analysis confirmed a stress direction change during plastic flow. However, the mechanism behind this change was not presented for two-phase materials, and the effect of phase interactions on the coaxiality between the crystal stress and the SCYS vertex has not been reported, to the best of our knowledge.

Here, a two-phase (Cu/Fe) crystalline material with equal volume fractions is used to investigate the effect of phase interactions on crystal stress evolution during elastoplastic deformation. The stress distribution and coaxiality change for the two-phase material are compared with those of the single-phase counterparts. In the next section, the methodologies for obtaining the crystal stress/strain data from experiments and simulations are described, followed by descriptions of the coaxiality. Next, the results of a neutron diffraction experiment on the Cu/Fe crystal and the simulation are compared to validate the simulation results for further in-depth analysis. The stresses and coaxiality evolution patterns are then presented for single-phase and two-phase materials, and the effect of phase interactions on the crystal stress evolution during elastoplastic evolution is discussed.

2. Modeling and analysis methodologies

Modeling of two-phase Cu/Fe polycrystalline solids under elastoplastic deformation requires a description of the phase interactions; this is achieved by incorporating grain interactions. Widely used approaches to modeling polycrystalline solids using isostrain or isostress assumptions result in upper bound and lower bound solutions, respectively. The assumptions of Reuss (1929) and Voigt (1928) are the elastic versions of the isostrain and isostress solutions, and those of Taylor (1938) and Sachs (1983) are the plastic counterparts. However, these rather simple models do not incorporate grain interactions, so they do not adequately describe the behaviors of multiphase materials; this requires the spatial distribution of the phase connectivity and clustering.

A self-consistent model capable of simulating elastoplastic deformation (Lebensohn and Tomé, 1993) on the basis of Eshelby's solution (Eshelby, 1957) can be used to simulate a multiphase polycrystalline solid to a certain extent. However,