Effect of Phase Interactions on Crystal Stress Evolution Under Elastoplastic Deformation

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ABSTRACT

Crystal stress direction evolution in two-phase polycrystalline solids under uniaxial compression is investigated using finite element simulations. Stress tensor evolution of the two-phase materials from simulations then are analyzed. Due to the nature of the two-phase materials of different stiffness and strength, the stress redistribution occurs as each phase enters the regime of fully developed plastic flow. Redistribution of stresses and repartitioning of two-phase polycrystalline solids during elastoplastic deformation are investigated. The mechanism behind the stress evolution is analyzed by quantifying proximity between stress directions and vertices of a single crystal yield surface. It is found from the analysis that, although crystal stress direction evolution in two-phase polycrystalline solids shares the similar trend as the single-phase polycrystals, the phase interactions in the two-phase materials affects the characteristics of the stress direction evolution.

1. INTRODUCTION

The crystal stress in polycrystalline aggregates during elastoplastic deformation is affected by both elastic and plastic anisotropy. During the pure elastic deformation, the crystal stress directions deviate from macroscopic (applied) stress even due to the interactions among crystals of anisotropic properties. Crystal stress direction in polycrystalline aggregates during plastic flow tends to move toward vertices of anisotropic single crystal yield surface (SCYS) to satisfy the heterogeneous deformation compatibility among crystals. The anisotropy of elasticity and plasticity are different, but, when the plasticity is well developed during elastoplastic deformation, the dominance of this tendency of alignment of crystal stress directions with SCYS vertices has been confirmed in the previous studies (Han et al., 2013). The previous studies were conducted for single-phase polycrystalline solids, and the tendency was not confirmed for multi-phase polycrystals. Thus, it is investigated herein that whether the same tendency of alignment of crystal stresses and SCYS vertices (coaxiality) is still valid for the two-phase polycrystals.

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2. ANAYSIS

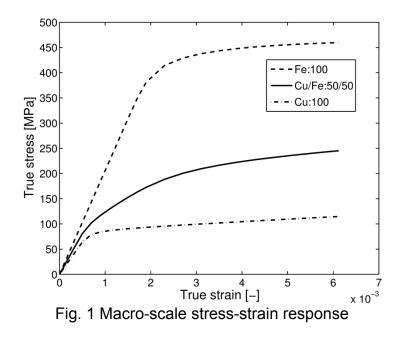
During plastic flow, crystal stresses within polycrystal aggregate tend to move toward vertices of the single crystal yield surface, which indicates the crystal orientation dependence of the crystal stresses. A parameter, *coaxiality* (θ_c^v), is used as a measure to represent the angular distance between the crystal stress direction and the vertex direction of the single crystal yield surface (SCYS).

$$\theta_c^{\nu} = \cos^{-1}\left(\frac{\sigma_c:\sigma_{\nu}}{\|\sigma_c\|\cdot\|\sigma_{\nu}\|}\right) \tag{1}$$

where subscript c and v denote crystal and SCYS vertex, respectively. There are factors such as elasticity and viscosity that reduce the coaxiality between the crystal stress and the SCYS, but the tendency of alignment of crystal stress direction with SCYS vertex directions has been identified. In particular, through modeling, the coaxiality was confirmed as an effective index for describing characteristics of crystal stress evolution when plasticity, due to crystallographic slip, is fully developed. Experimental confirmation is also conducted using high energy synchrotron diffraction experiment.

To obtain the stress tensor from modeling, the crystal-based finite element method is adopted. The finite element formulation adopted here (Marin and Dawson, 1998) follows a standard procedure of minimizing the residual form of the equilibrium equation. Three cases of polycrysatal virtual representative virtual specimens are investigated. Pure Cu (Cu:100)), Pure Fe (Fe:100), and random crystal mixture of two-phase crystals of Cu and Fe (Cu/Fe:50/50).

Uniaxial compression is applied to the specimens, and the results are presented in Fig. 1. The modeling parameters are determined based on the results shown in Han and Dawson (2005). Pure phase responses are used as references, and are compared with investigated to identify the effect of the phase interactions.



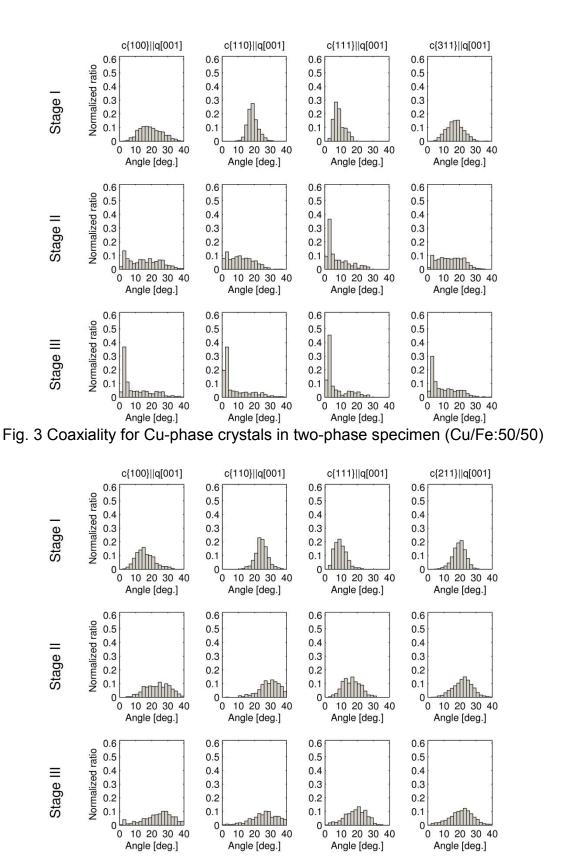


Fig. 3 Coaxiality for Fe-phase crystals in two-phase specimen (Cu/Fe:50/50)

As can be noted in Fig. 1, there are three stages based on yielding of phases. In Stage I, both phases are in elastic regime. After the yielding of the weaker (Cu) phase and before the yielding of the stronger (Fe) phase, the regime is denoted as Stage II. Finally, both phases are under plastic flow in Stage III. The change of slope in the macro-scale stress-strain response which specifies the boundary between the stages can be observed.

Coaxiality for Cu-phase and Fe-phase crystals in two-phase material with equal volume fraction is shown in Figs. 2 and 3, respectively. Coaxiality for particular crystal orientations aligned with the loading direction (fibers) is presented. Crystals on each fiber has the same characteristics, e.g., same angular distance between the loading direction and the closest SCYS vertex direction. It is clear from Fig. 2 that the weaker phase crystal stresses tend to move toward the SCYS vertex since the coaxiality values are reduced to zero as the plasticity develops. However, in Fig. 3, the stronger phase crystal stresses do not move toward the SCYS vertex, and sometimes move away from the SCYS vertex. Although not shown here, the stronger phase crystal stresses tend to move toward the SCYS vertices after yielding of the weaker phase crystal stresses are already near the SCYS vertices after yielding of the weaker pase, which relieves the requirement of coaxiality for the stronger phase since the complex compatibility can be obtained by the crystal stress state of the weaker phase.

3. CONCLUSIONS

The effect of phase interaction within two-phase polycrystalline solid was investigated using the parameter coaxiality between crystal stresses and SCYS vertices from finite element simulations. From the analysis, it was found that the crystal stresses in a stronger phase do not move toward the SCYS vertices since the weaker phase crystal stresses are already at the SCYS vertices and provide enough freedom to satisfy the deformation compatibility among crystals.

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REFERENCES

- Han, T.-S. Chung, S.-Y. and Lee B. (2013), "Crystal stress distribution evolution of elastoplastically deforming polycrystals over crystal orientation space," *Comput. Mater. Sci.*, **75**, 9-17.
- Marin, E.B. and Dawson, P.R. (1998), "Elastoplastic finite element analyses of metal formations using polycrystal constitutive models", *Comput. Methods Appl. Mech. Eng.*, **165**, 23-41.