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Study of large strain behavior of OFHC copper: The role of polycrystal plasticity model

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ABSTRACT

The large strain behavior of single-phase OFHC copper under different deformation processes are studied based on various polycrystal plasticity models including the classic Taylor-type model and various popular self-consistent models. The models are evaluated by comparing the predictions for the evolution of crystallographic texture and the stress–strain response in uniaxial compression and tension, plane strain compression, and simple shear against corresponding experiments. It is found that while the Taylor-type model is in reasonable first-order agreement with the experiments for the evolution of texture and the overall stress–strain response, the self-consistent models with grain interaction stiffness halfway between those of the limiting secant (stiff) and tangent (compliant) approximations give better results.

1. Introduction

A polycrystal comprises many single crystals with different orientations. Constitutive modeling of crystalline materials starts with developing a single crystal model to describe elastic and plastic deformation at the grain level. However, predicting the mechanical behavior of polycrystalline materials from the responses of their single crystals has been a tremendous challenge for a long time. The reason for this is that it is very difficult to mathematically solve a boundary value problem with extremely high degrees of freedom due to interactions between grains. Therefore, the response of a polycrystal, consisting of many grains, is usually calculated by introducing some averaging/homogenization assumptions.

To predict the global response of the polycrystal, the transition from the microscopic response of the individual grains to the macroscopic response of the polycrystalline aggregate, various polycrystal plasticity models have been developed. The classic Taylor model (Taylor, 1938) assumes that all grains must accommodate the same plastic strain equal to the macroscopically imposed strain (see also Asaro and Needleman, 1985). It has been generally accepted that the Taylor assumption is reasonable for materials that show a mildly anisotropic plastic response and which are comprised of crystals with many slip systems of comparable strength. Consequently, the Taylor model works quite well for face centered cubic (FCC) and body centered cubic (BCC) materials having high crystallographic symmetries. Therefore, the Taylor model has played an important role in the field of modeling of forming of aluminum and steel sheets (see e.g. Wu et al., 1997; Dawson et al., 2003; Eyckens et al., 2009). However, the use of the Taylor model in other situations may lead to predictions of excessively high stresses, incorrect texture evolutions, or both (Lebensohn et al., 2003). The modeling of polycrystals with a hexagonal close packed (HCP) crystallographic structure is consistent with these trends. MacEwen et al. (1989) have shown that the Taylor-type approach does not work well for the prediction of residual grain-interaction stresses in zirconium alloys. Generally speaking, for metals like HCP polycrystals with low crystallographic symmetry, stress and strain variations from grain to grain and interactions among grains in a polycrystalline aggregate are significant and cannot be neglected in an attempt to accurately describe deformation behavior. Consequently, polycrystal plasticity models based on the self-consistent approach originally proposed by Kröner (1958) for the elastic case, and later extended to the elasto-plastic (Hill, 1965) and viscoplastic (Hutchinson, 1976), have been becoming more popular than the Taylor model when modeling HCP polycrystals.

In general, self-consistent models allow for a different strain response in each grain, depending on the relative stiffness between the grain and a surrounding homogeneous equivalent medium (HEM). The consistency conditions require that the averaged behavior over all the grains must be the same as the macroscopically imposed one. The viscoplastic self-consistent (VPSC)

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model, proposed by Molinari et al. (1987) and Lebensohn and Tomé (1993), has been successfully applied to simulate large strain behavior and texture evolution of HCP polycrystalline materials under various deformations (see e.g. Agnew and Duygulu, 2005; Xu et al., 2008). Recently, Wang et al. (2010a) have developed a finite strain elastic-viscoplastic self-consistent (EVPSC) model for polycrystalline materials. The EVPSC model is a completely general elastic-viscoplastic, fully anisotropic, self-consistent polycrystal model, applicable at large strains and to any crystal symmetry. It has been demonstrated that at large monotonic strains elasticity saturates and the EVPSC model gives results very close to the VPSC model. For deformations involving elasto-plastic transients associated with unloading and strain path changes, EVPSC predicts clear and gradual transitions, while VPSC gives stress discontinuities due to the lack of elastic deformation. It has been also shown that the EVPSC model can capture some important experimental features which cannot be simulated using the VPSC model (Wang et al., 2010a, 2012a, 2012b, 2013a, 2013b, 2013c; Guo et al., 2013; Lee et al., 2014; Wu et al., 2014; Qiao et al., 2015; Wang et al., 2016a; Wang et al., 2016b; Wang et al., 2016c). Furthermore, it has been found that numerical results based on the VPSC and EVPSC models are extremely sensitive to the stiffness of the grain–matrix interaction associated with the various self-consistent schemes (SCSs). Therefore, Wang and his co-workers have carried out a series of assessments of the predictive capability of the VPSC/EVPSC model with various SCSs including the secant, affine, tangent and effective interaction meff (Wang et al., 2010b, 2010c, and 2011). For HCP materials, it has been concluded that, among the examined models, those with an interaction stiffness halfway between the secant (stiff) and tangent (compliant) give the best results. In particular, no model gives a better overall performance than the affine self-consistent approach (Wang et al., 2010b).

In summary, it is believed by many researchers that while a self-consistent approach is more suitable than the Taylor approach for constitutive modeling of HCP polycrystals, the Taylor model is in reasonable first-order agreement with the experiments for the texture formation and also the overall stress–strain response of single-phase FCC and BCC polycrystalline materials. However, it has been also noticed that recent efforts on the development/assessment of self-consistent polycrystal plasticity models have been mainly motivated by the need to more accurately describe elastic–plastic deformation of HCP polycrystalline materials like magnesium and its alloys. The question then arises: is a self-consistent approach also more suitable than the Taylor approach for constitutive modeling of FCC and BCC polycrystals? To the best of our knowledge, an assessment for various polycrystal plasticity models has not been systematically carried out for FCC and BCC polycrystals.

The purpose of the present paper is to evaluate the predictive capability of polycrystal plasticity models for the constitutive modeling of FCC polycrystals. It is very important to point out that such an evaluation is meaningful only if the number of experiments employed is large enough to cover various different deformation processes for a given material. We believe that the experiments performed on an initially isotropic copper by Bronkhorst et al. (1992) and Anand and Kalidindi (1994) represent the most extensive sets of currently available experimental data which document both the stress and strain response and the evolution of crystallographic texture for an FCC polycrystal. The experimental data provided by Bronkhorst et al. (1992) and Anand and Kalidindi (1994) include: (1) uniaxial compression and uniaxial tension, (2) plane strain compression, and (3) simple shear. It is noted that the material experimentally studied by Bronkhorst et al. (1992) and Anand and Kalidindi (1994) is an initially isotropic OFHC copper.

It is worth to mention that crystal plasticity based finite element (CPFE) approach has been also used to study large strain behavior of polycrystalline materials (see e.g. Abdolvand and Daymond, 2012, 2013; Al-Harbi and Kalidindi, 2014; Anahid and Ghosh, 2013; Ardeljan et al., 2014; Choi et al., 2011; Fernandez et al., 2011; Ghosh and Anahid, 2013; Gonzalez et al., 2014; Hama and Takuda, 2011; Hama et al., 2014; Herrera-Solaz et al., 2014; Knezevic et al., 2014; Lim et al., 2014; Wu et al., 2004; Zhang et al., 2015). In CPFE simulations an element of the finite element mesh represents either a single crystal or a part of a single crystal, and the constitutive response at an integration point is described by the single crystal constitutive model. This CPFE approach enforces both equilibrium and compatibility throughout the polycrystalline aggregate in the weak finite element sense (Bronkhorst et al., 1992; Anand and Kalidindi, 1994). Furthermore, this CPFE approach facilitates consideration of grain morphology and the modeling of deformation inhomogeneity within individual grains (Wu and Lloyd, 2004; Wu et al., 2007; Kanjaria et al., 2010). However, the main purpose of the present paper is to assess the predictive capability of polycrystal plasticity models. Furthermore, such a CPFE simulation is computationally much more intensive than the corresponding self-consistent polycrystal calculation.

It is also worth mentioning that we are aware that mechanical behavior of copper under various deformation processes have been recently widely studied, both experimentally and numerically (see e.g. Baig et al., 2013; Balasundar et al., 2013; Gao and Zhang, 2012; Gérard et al., 2013; Hsu and Wang, 2014; Park et al., 2013). However, as we pointed out previously, the experiments performed on an initially isotropic copper by Bronkhorst et al. (1992) and Anand and Kalidindi (1994) represent the most extensive sets of currently available experimental data for an FCC polycrystal. We believe that the predictive capability of polycrystal plasticity models could be most efficiently assessed by using the experimental data from Bronkhorst et al. (1992) and Anand and Kalidindi (1994).

In addition, it is interesting to point out that although the full-constraints Taylor model is believed to be in reasonable first-order agreement with the experiments for the texture formation and the overall stress–strain response of single-phase FCC and BCC polycrystalline materials, the relaxed-constraints Taylor-type models, including those developed by Van Houtte and his co-workers (see e.g., Liu et al., 2002; Van Houtte et al., 2005), have demonstrated to be more suitable than the full-constraints Taylor model in some cases. However, these models were almost all restricted to some special applications such as predicting texture evolution under cold rolling, where the imposed macroscopic strain paths were assumed to be known. Our purpose is, however, to answer the question: which polycrystal plasticity model is suitable for applying in a real forming process, where the straining path of material elements is usually not known with any certainty?

The plan of the paper is as follows. In Section 2, we briefly review the constitutive models examined in the present paper. We begin Section 3 by estimating values of the material parameters by curve-fitting numerical simulations of uniaxial compression using the Taylor model and the EVPSC models with various SCSs to corresponding experimental data. These values of the material parameters are then used to predict large strain behavior of the material under uniaxial tension, plane strain compression and simple shear. Differences between the models in predictions as well as the differences between predicted behavior and experimental observations are emphasized. An assessment of the predictive capability of the polycrystal plasticity models is made based on comparisons of the predicted and experimental results. The conclusions are presented in Section 4.

2. Polycrystal plasticity models

In all the polycrystal plasticity models examined in the present paper, the deformation mechanisms of twinning, diffusion and