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Micromechanical modelling of twinning in polycrystalline materials: Application to magnesium

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ABSTRACT

In this work, a crystal plasticity constitutive model is proposed to describe the mechanical behavior of metallic materials for which twinning plays a significant role in the deformation process. Constitutive relations are obtained from a micromechanical approach that explicitly considers the interactions between twinned and untwinned domains. Then, based on a thermodynamical analysis of the problem, a new expression for the driving force for the expansion of twinned domains is proposed. Finally, to account for the polycrystalline nature of metallic materials, the constitutive model is implemented in a FFT spectral solver.

In the second part of this paper, the model is used to study the mechanical behavior of a AZ31 magnesium alloy under compression, for which a significant amount of experimental data is available in the literature. The comparison between numerical and experimental data allows for discussion of the influence of the different deformation modes on the development of both crystallographic texture and lattice strains. The evolution of lattice strains is found to be largely influenced by the internal stress redistribution process associated with the expansion of twinned domains. Also, the polycrystalline plasticity model provides a correct description of how the morphological texture is strongly altered during the deformation process due to the important activity of twinning systems.

1. Introduction

For some metallic alloys (e.g. magnesium alloys, zirconium alloys, austenitic steels), mechanical behavior is strongly impacted by the coexistence of mechanical twinning and crystallographic slip deformation modes. While the crystal plasticity framework (Asaro and Needleman, 1985; Rashid and Nemat-Nasser, 1990; Cuitiño and Ortiz, 1992) provides a convenient way of introducing the influence of crystallographic slip in constitutive models, the incorporation of deformation twinning within such models is not trivial. Indeed, in order to include the role of deformation twinning in a consistent manner, some specific features of twinning deformation modes have to be considered:

- First, because of the abrupt crystallographic reorientation process associated with twinning, significant texture evolution is often observed during a deformation process (Vercammen et al., 2004; Brown et al., 2005; Xu et al., 2009). As a result, for

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polycrystalline aggregates, the anisotropic nature of macroscopic properties is strongly dependent on the crystallographic orientations of twinned domains.

- Second, as mentioned by Remy (1981) and Basinski et al. (1997), during a deformation process, deformation twinning results in the formation of additional boundaries that provide a significant contribution to strain hardening. The mechanical behavior of materials for which twinning plays an important role is thus governed by a strong coupling between slip and twinning deformation modes.
- Third, depending on loading conditions, twinning may contribute importantly to the plastic deformation process because the expansion of twinned domains involves the accumulation of large plastic shear strains at the grain scale. The macroscopic behavior is therefore very sensitive to the growth rate of twinned domains.
- Finally, different diffraction studies have demonstrated that twinning is accompanied by a significant redistribution of internal stresses (Clausen et al., 2008; Wu et al., 2008; Xu et al., 2009). Indeed, because the local behavior of individual crystals is influenced by their orientation, the reorientation process associated with twinning results in some complex load sharing mechanisms that affect the macroscopic behavior.

To account for these aspects of deformation twinning in constitutive relations, different strategies have been adopted. Using the self-consistent approximation, many efforts have been made to incorporate twinning in polycrystalline plasticity models. For instance, to investigate the evolution of texture in zirconium and magnesium alloys, some extensions of the viscoplastic self-consistent model of Lebensohn and Tomé (1993) have been proposed (Proust et al., 2007; Capolungo et al., 2009a; Knezevic et al., 2015). However, by construction, such models do not readily allow the evaluation of internal stresses because elastic strains are not considered. To circumvent this limitation, different elasto-(visco)plastic formulations have been developed. From a micromechanical approach considering twins as ellipsoidal inclusions, Cherkaoui (2003) proposed a set of constitutive relations to investigate the behavior of f.c.c. metals. Shiekhelsouk et al. (2009) developed a physically based model where the resistance opposed by twin interfaces to dislocation glide is explicitly considered. Clausen et al. (2008) constructed a rate-independent self-consistent model to study the development of lattice strains and texture in a magnesium alloy. Nevertheless, mostly because the interactions between twinned and untwinned domains are ignored, the approach of Clausen et al. (2008), which has been reformulated in a rate-dependent framework by Mareau and Daymond (2011), does not completely succeeds in matching the experimental observations. To better describe these interactions, Juan et al. (2014) proposed a self-consistent formulation based on a double inclusion formalism. Although this strategy allows the investigation of the competition between slip and twinning deformation modes, the moving boundary aspect of the problem of twin growth is not considered in the approach of Juan et al. (2014).

Though some efforts have been made to include the effect of stress field fluctuations on twin variant selection (Niezgoda et al., 2014; Zecevic et al., 2015), self-consistent formulations do not explicitly account for the intragranular stress and strain field gradients. To circumvent this limitation, several attempts have been made at incorporating deformation twinning within crystal plasticity based finite element models (Kalidindi, 2001; Staroselsky and Anand, 2003; Abdolvand et al., 2012; Cheng and Ghosh, 2015). In a large strain formalism, Kalidindi (2001) has developed a constitutive model that uses a simple mixture rule to include the contribution of both twinning and slip deformation modes. While this type of approach has been successful in describing texture evolution, some aspects of the development of internal stresses are not well described, mostly because the elastic strain field is assumed to be the same in the twinned and untwinned domains. Cheng and Ghosh (2015) proposed a non-local crystal plasticity model to investigate the twin nucleation process in magnesium alloys. Also, as discussed by Knezevic et al. (2016), different strategies have been employed to explicitly model discrete twinned domains (Zhang et al., 2008; Arul Kumar et al., 2015; Ardeljan et al., 2015). Indeed, Zhang et al. (2008) and Arul Kumar et al. (2015) have used either the finite element method or FFT-based techniques to investigate the internal stress field produced by an isolated deformation twin. A more complex numerical procedure has recently been proposed by Ardeljan et al. (2015) to deal with twin propagation and twin growth in crystal plasticity based finite element models. The major drawback of these approaches is that the twin morphology needs to be known a priori.

In this work, a method for considering the influence of deformation twinning in polycrystalline plasticity models is presented. The first part of this paper is dedicated to the description of the proposed model. Adopting a similar strategy as Cherkaoui (2003), the local constitutive relations are derived from a micromechanical analysis of the problem. Within a thermodynamically consistent framework, the proposed formulation provides an explicit description of the interactions between twinned and untwinned domains. To account for intragranular heterogeneities, the constitutive relations are then implemented in a spectral (FFT) solver that exploits the method originally proposed by Moulinec and Suquet (1998). In the second part, to demonstrate the relevance of the proposed constitutive relations, the model is used to investigate the behavior of an AZ31 magnesium alloy, for which an extensive experimental dataset has been obtained by Clausen et al. (2008). During the mechanical testing of a magnesium alloy sample, Clausen et al. (2008) carried out neutron diffraction measurements to study the development of lattice strains and crystallographic texture. The direct comparison of numerical results with experimental measurements thus allows for better understanding the contribution of the different deformation modes, the evolution of internal stresses, the formation of intragranular lamellar microstructures and the reorientation processes.