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Grain interaction mechanisms leading to intragranular orientation spread in tensile deformed bulk grains of interstitial-free steel

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The spatially resolved intragranular orientation spread in two representative bulk grains of interstitial-free steel deformed to 9% tension has been investigated. A three-dimensional X-ray diffraction microscopy experiment revealed that the two similarly oriented grains are both embedded in local environments representing the bulk texture, yet their deformation-induced rotations are very different. The ALAMEL model is employed to analyse the grain interaction mechanisms. Predictions of this model qualitatively agree with the directionality and magnitude of the experimental orientation spread. However, quantitative agreement requires fine-tuning of the boundary conditions. The majority of the modelled slip is accounted for by four slip systems also predicted to be active by the classical Taylor model in uniaxial tension, and most of the orientation spread along the grain boundaries is caused by relative variations in the activities of these. Although limited to two grains, the findings prove that shear at the grain boundaries as accounted for by the ALAMEL model is a dominant grain interaction mechanism.

1. Introduction

The deformation-induced evolution of crystallographic texture in metals has been a subject of research for decades due to its consequences for the properties of the metal, in particular mechanical anisotropy. By comparison of deformation textures measured by X-rays or neutrons with predictions of the earliest models of crystal plasticity by Sachs (1928) and Taylor (1938)/Bishop and Hill (1951), it became clear that these models in general produce too sharp textures. This deficiency is attributed to their basic assumptions that ignore complex interactions between the grains, which will also lead to intragranular orientation spreads.

Experimental studies of the orientation spread within individual grains observed at a surface became possible with the emergence of the technique of electron back scatter diffraction (EBSD), including in-situ deformation studies of the lattice rotations of surface grains (Allain-Bonasso et al., 2012; Chen et al., 2013; Di Gioacchino and Quinta Da Fonseca, 2015; Guery et al., 2016). Three dimensional data may be obtained by serial sectioning (Afrin et al., 2013; Lin et al., 2010), which is, however, destructive, implying that the dynamics of the grains cannot be monitored. By pressing two metal surfaces closely together during deformation, a three-dimensional environment of neighbouring grains has been mimicked while still

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enabling dynamic studies by intermittent separation and EBSD investigation of the surfaces (Bhattachayya et al., 2001; Quey et al., 2015, 2010).

By contrast, the method of three-dimensional X-ray diffraction (3DXRD) is capable of monitoring the dynamics of individual grains in their natural environment of neighbouring grains (Margulies et al., 2001; Poulsen et al., 2003). The technique can produce large maps of grain structures (Pokharel et al., 2014; Poulsen et al., 2001; Rollett et al., 2015; Schuren et al., 2015; Sørensen et al., 2012b), including crystallographic orientations and neighbour relations (Hefferan et al., 2009; Li and Suter, 2013; Schmidt et al., 2008), and also allows measurement of the elastic strain in each individual grain during deformation (Bernier et al., 2011; Oddershede et al., 2010). This gives a unique possibility of investigating the behaviour of individual grains and how they interact with their environment. Particular emphasis has been on understanding the deformation behaviour of metals by mapping intra-granular orientation gradients as a function of plastic deformation (Li et al., 2013; Lind et al., 2014; Pokharel et al., 2015; Toda et al., 2016) and measuring grain-resolved stresses associated with deformation twinning in hexagonal close packed metals (Abdolvand et al., 2015a, 2015b; Aydiner et al., 2009; Bieler et al., 2014; L. Wang et al., 2014a), but also processes such as grain nucleation (West et al., 2009), growth (Poulsen et al., 2011; Schmidt et al., 2004, 2008) and coarsening (Dake et al., 2016; Sharma et al., 2012), crack evolution (Cerrone et al., 2015; Chatterjee et al., 2015; Oddershede et al., 2012; Ozturk et al., 2016), stress relaxation (Tang et al., 2015), creep (Schuren et al., 2015) and phase transformations (Barton and Bernier, 2012; Hedström et al., 2010; Offerman et al., 2006) have been investigated using 3DXRD. For completeness applications of 3DXRD to minerals (Borthwick et al., 2012; Hall and Wright, 2015; Sørensen et al., 2012a), deep earth science (Nisr et al., 2014, 2012; Rosa et al., 2015), nuclear materials (Brown et al., 2014; X. Zhang et al., 2015a), superalloys (Sedmák et al., 2016) and ferroelectrics (Daniels et al., 2016; Majkut et al., 2016; Oddershede et al., 2015a; Varlioglu et al., 2010) should also be mentioned.

In parallel with advances in the experimental studies of plastically deformed metals, polycrystal plasticity models have been improved to take grain interactions into account. Self-consistent polycrystal plasticity models were developed (Lebensohn and Tomé, 1993; Molinari et al., 1987), which take into account the interaction between all grains of a specific orientation with a homogenous matrix representing all the other grains. Recently, microstructurally derived hardening laws have been incorporated in self-consistent models to study the combined effects of slip and twinning on texture evolution (Brown et al., 2012; Knezevic et al., 2013). According to the self-consistent scheme, all grains of similar orientation are assumed to behave in the same way, but they are influenced by the initial and evolving texture.

Randomised fluctuations in stress (Leffers, 1979) or strain (Ma et al., 2004) or stress fluctuations derived from the stress states of neighbouring grains (Robert et al., 2004) were introduced to create scatter in the behaviour of otherwise similar grains. In addition, relaxed constraint models were developed, in which certain strain components are enforced and others allowed to fluctuate, based on the geometry of the grains (Kocks and Chandra, 1982). Inspired by these concepts, the interaction between two grains has been modelled by the LAMEL model (Van Houtte et al., 1999) with focus on the interaction across the large faces of flat and elongated grains. This model has since been generalized to the ALAMEL model (Van Houtte et al., 2005), in which the grain boundary plane is also introduced as a variable. Whereas the LAMEL and ALAMEL models consider the interaction between two grains, the GIA model (Crumbach et al., 2001) takes into account interactions between a cluster of grains. Additional cluster-type models have also been derived (Xie et al., 2014). Common to this class of models is that grains are paired for interaction studies on a statistical basis considering the initial texture and possibly also the experimental misorientation distribution across grain boundaries (Zhang et al., 2015b).

More recently, advanced finite element (Roters et al., 2010; Zhang et al., 2016) or Fourier transformation (Eisenlohr et al., 2013; Lebensohn et al., 2012) based polycrystal plasticity models, which consider more detailed interactions, have been employed to simulate intragranular orientation spreads (Lebensohn et al., 2016; Quey et al., 2015). The grain structures used as input to these models differ in geometrical complexity, and assignment of neighbouring grains may be based on statistics or experimentally determined grain structures, either in 2D by EBSD or in 3D by synchrotron methods.

The combination of experiment and modelling has led to significant advances in our understanding of grain-scale behaviour, including effects of grain orientation (Pokharel et al., 2015; Winther et al., 2004), grain size (Allain-Bonasso et al., 2012) and shape (Delannay and Barnett, 2012), formation of grain boundary regions (Pokharel et al., 2015; Vachhani et al., 2016), directionality of intragranular orientation spread (Krog-Pedersen et al., 2009; Lebensohn et al., 2016) and the interaction of plastically soft and hard grains (Raabe et al., 2001).

The present study is a follow-up on a previous study, which characterised the intragranular orientation spread within selected grains of similar orientation in a 9% tensile deformed interstitial-free steel (Oddershede et al., 2015b) by 3DXRD and analysed this by Taylor/Bishop-Hill modelling. It was concluded that the orientation spread of the grains had the same overall directionality, which was attributed to unbalanced activation of a few slip systems. The present study adds the experimentally determined spatial distribution of the orientation spread in the deformed state as well as information about the neighbouring grains. This extension allows analysis of the grain interaction mechanisms. In particular, the aim is to investigate if co-operative shear at the grain boundaries, as assumed by the ALAMEL model, is an important and effective mechanism of grain interaction.

The ALAMEL model was originally derived as a statistical model. Subsequent comparison of the predictions of the ALAMEL model with a finite element-based crystal plasticity model, using a model microstructure of columnar grains with hexagonal cross sections, however, showed good agreement (Kanjarla et al., 2010). To the authors' knowledge, the present study is the first evaluation of the ALAMEL model by direct comparison to experimentally observed grains.