Assessment of plastic heterogeneity in grain interaction models using crystal plasticity finite element method

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ABSTRACT

Micromechanical models aimed at simulating deformation textures and resulting plastic anisotropy need to incorporate local plastic strain heterogeneities arising from grain interactions for better predictions. The ALAMEL model [Van Houtte, P., Li, S., Seefeldt, M., Delannay, L. 2005. Deformation texture prediction: from the Taylor model to the advanced Lamel model. Int. J. Plasticity 21, 589–624], is one of the models in which the heterogeneous nature of plastic deformation in metals is introduced by accounting for the influence of a grain boundary on the cooperative deformation of adjacent grains. This is achieved by assuming that neighbouring grains undergo heterogeneous shear rates parallel to the grain boundary. The present article focuses on understanding the plastic deformation fields near the grain boundaries and the influence of grain interaction on intra-grain deformations. Crystal Plasticity Finite Element Method (CPFEM) is employed on a periodic unit cell consisting of four grains discretised into a large number of elements. A refined study of the local variation of strain rates, both along and perpendicular to the grain boundaries permits an assessment of the assumptions made in the ALAMEL model. It is shown that the ALAMEL model imbibes the nature of plastic deformation at the grain boundaries very well. However, near triple junctions, the influence of a third grain induces severe oscillations of the stress tensor, reflecting a singularity. According to CPFEM, such singularity can lead to grain subdivision by the formation of new boundaries originating at the triple junction.

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1. Introduction

The response of the microstructure of a material to an externally applied (plastic) deformation is not fully understood. A better understanding is a requisite to enable the prediction of the macroscopic mechanical behaviour in a more accurate way. Mechanical properties at the macroscale are influenced by the material behaviour at the microstructural scale. Micromechanical models adapted to polycrystalline aggregates are either used as stand alone programs to predict the plastic anisotropy and texture evolution (Van Houtte et al., 2005, 2006) or embedded into commercial finite element (FE) software. Such FE software can then be used to study material behaviour both at microstructural scale (e.g. Becker and Panchanadeeswaran 1995; Barbe et al., 2001; Diard et al., 2005; Van Houtte et al., 2006; Zhao et al., 2008; Bieler et al., 2009) and sample scale (e.g. Dawson et al., 2003; Delannay et al., 2005; Zamiri et al., 2007). The Crystal Plasticity Finite Element Method (CPFEM) has now become a regular tool for studying microscopic heterogeneity associated with plastic deformation in metals.

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Experimentally, it is difficult to track the evolution of the heterogeneous strain field throughout a plastically deforming microstructure. Many microscopy techniques can only reveal the footprint of already applied deformation (Bhattacharyya et al., 2001). Only a few recent techniques allow probing microscopic deformation fields, in-situ, both at the surface (Schroeter and McDowell, 2003; Musienko et al., 2007) and in the bulk (Poulsen et al., 2003) of the sample being deformed.

Various CPFEM studies were conducted in tandem with experimental investigations. Kalidindi et al. (2004) and Erieau and Rey (2004) compared the local lattice rotations observed experimentally with those predicted by CPFEM. They succeeded in predicting the overall texture of the sample, however, failing to correctly predict the orientation patterns observed inside certain grains. Also using CPFEM, Mika and Dawson (1999), Delannay et al. (2003) and Zhao et al. (2008) managed to reproduce in-grain orientation spreads only in a statistical sense. Similar conclusions were drawn recently by relying on fast Fourier transforms (FFT) in replacement of CPFEM (Lebensohn et al., 2008).

Other studies involved comparing the experimentally observed local strain fields to the ones obtained by CPFEM. Delaire et al. (2000) and Raabe et al. (2002) conducted mechanical tests and mapped the strain field inside individual grains along free surfaces of the sample. Also see Héripré et al. (2007) and St-Pierre et al. (2008) wherein they present the coupling between the experimentally measured local strain fields and those obtained by implementing material constitutive behaviour in a realistic microstructural mesh mapped from the OIM data. CPFEM captured the trends in the local strain heterogeneity in a rather convincing way. Zaefferer et al. (2003) studied the role of grain boundaries on the local heterogeneity of strain and concluded that the lattice orientations of individual grains play a more important role than the lattice disorientations across grain boundaries.

The previous paragraphs refer to CPFEM studies which rely on conventional crystal plasticity. This theory is based on time and volume averages of the dislocation slip activity and hence overlook the discrete nature of dislocation slip. It is well established nowadays that the intra-granular heterogeneity of plastic strain is influenced by physical phenomena that are captured only if the crystal constitutive law is enriched, e.g. by introducing physical length scales or by accounting for the relative permeability of grain boundaries to dislocation glide (Ashmawi and Zikry, 2003; Ma et al., 2006; Acharya et al., 2008). Nevertheless, the objectives of the present study have been met by relying on conventional crystal plasticity. The motivation of this is that this approach allows the identification of features that can be predicted from conventional crystal plasticity, and those that cannot. Expected outcomes of the eventual implementation of a more advanced constitutive law are discussed in Section 4.

CPFEM is used here in order to assess simplified modelling assumptions about the interaction of neighbouring grains and the resulting strain heterogeneity. Most micromechanical models used in metal forming simulations rely on a crude estimate of the microscopic strain field, and clearly fail to fulfil the equilibrium equations at every position throughout the polycrystalline aggregate. Even though it satisfies the equilibrium equations only in the weak sense (e.g. Beaudoin et al., 1995), CPFEM provides realistic predictions of local strain fields on the condition that the mesh is sufficiently refined.

A typical simplification of the microstructure representation is the assumption that grains are separated by planar grain boundaries. It is adopted by various crystal plasticity models (Van Houtte et al., 2002, 2005; Lee et al., 2002; Evers et al., 2002; Engler et al., 2005; Al-Fadhalah et al., 2005; Mahesh 2009). Considering that grain boundaries (GB) are perfect, i.e. excluding damage and grain boundary sliding, the following condition must hold across the planar interface separating the two grains (labelled a and b):

$$L_{ij}^a = L_{ij}^b \quad \text{for} \quad i = 1, 2, 3 \quad \text{and} \quad j = 1, 3$$
$$\sigma_{i2}^a = \sigma_{i2}^b \tag{1}$$

in which X_2 is the normal to the plane interface. Hence the components corresponding to surface traction on the interface need to be equal (in the current case, these are 12, 22, and 32) besides, the components for the corresponding velocity gradient can be free. In these equalities, the local velocity gradient tensor, L, and the local stress tensor, σ, are both expressed in a reference frame attached to the GB, with direction 2 perpendicular to the interface (Fig. 1).
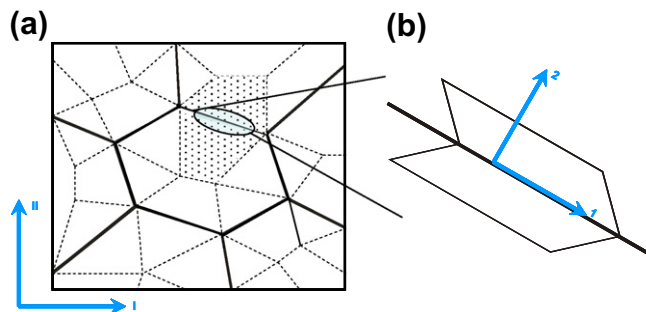
Fig. 1. (a) Schematic of microstructure and its representation in the ALAMEL model. Dark lines indicate grain boundaries. Lighter dashed lines indicate regions of heterogeneous deformation in a grain. The shaded region corresponds to pair of regions as those used in the ALAMEL model. (b) Reference frame attached to a grain boundary segment and complementary shear relaxations.