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Deformation and strain localization in polycrystals with plastically heterogeneous grains

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ABSTRACT

A model of a polycrystalline material is studied, where each grain consists of several zones with different plastic properties. The size and configuration of the zones as well as their properties are mimicking the situation inside the crystals of artificially aged Al alloys with precipitate free zones (PFZs). The properties of the different zones are conjectured based on micromechanical models and experimental observations of the AA6000 series of Al alloys. A periodic patch of such a composite material, subjected to plane-strain tension, is modelled using the finite element method. The material behaviour is described by a single crystal plasticity model. The results of the simulations show a number of characteristic features emerging in composite material systems, including sliding and distortion of grain boundaries and shear band formation at grain boundary triple points. The assumptions made about the properties of the different zones in the crystals are evaluated. The distributions of plastic strain and deviatoric and hydrostatic stresses in the composite crystalline systems are discussed.

1. Introduction

Metallic materials are usually treated as homogeneous in practical applications, and criteria for yielding, strain localization and fracture are formulated in terms of mechanical fields acting on a homogeneous material subjected to certain boundary conditions. Any details of the microstructure are not considered explicitly and the material properties are derived from the results of macroscopic mechanical tests and some basic assumptions about the material behaviour (e.g. yielding, work-hardening and rate sensitivity). This approach produces useful results, but its scope is limited. If the knowledge of the material comes only from macroscopic mechanical tests, predictions of the material behaviour outside the domain of these tests will be just extrapolations. The accuracy of these extrapolations will depend on the accuracy of the basic assumptions. On the other hand, if a connection can be established between the material's microstructure and its macroscopic properties, more accurate predictions can be made, relying more on the underlying physical mechanisms than on mechanical tests and assumptions. The problem with this approach lies in the complexity and variety of the microstructural features encountered in real materials at small scales. An Al alloy is an aggregate of crystalline grains with different orientations and morphologies

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divided by grain boundaries. Inside the grains the material includes particles of various composition, strength, shape and size. The interfaces between all the constituent parts are an important class of microstructural features with complex behaviour as well. The lattice of the crystal includes defects, such as dislocations and their substructures (e.g. dislocation cells and dislocation pile-ups) and vacancies. If a model aims to accurately predict the properties of such a material, it should include enough of these features to be representative and at the same time be detailed and precise in their description — this is usually not possible in practice; neither analytically nor numerically.

Nevertheless, in some cases, a microstructural feature may be so prominent and important that even including some simplified representation of it in the material model may already markedly improve the model's prediction accuracy and reduce the reliance on mechanical testing. One example of such a microstructural feature could be the crystallographic texture that plays a central role in defining the plastic anisotropy of a polycrystalline material. If the crystallographic texture is measured and represented by a statistical set of orientations, the plastic anisotropy of the material may be predicted using this set in a crystal plasticity framework (Saai et al., 2011; Dumoulin et al., 2012; Khadyko et al., 2014; Zhang et al., 2014; Zhang et al., 2015, 2016; Khadyko et al., 2016a).

Another example is the Kocks-Mecking model of work-hardening. It is based on the analysis performed by Taylor (1934) on a simplified dislocation structure, which resulted in an equation that connects the dislocation density and the global shear stress necessary to start the dislocation movement (i.e., to produce plastic strain). A rule for the dislocation density evolution was added by Kocks (1976) and Mecking and Kocks (1981) to complete the work-hardening model of a metallic material. The physical nature of the model combined with its simplicity and possibilities for modifications made it very broadly used. The works that modify and enhance the basic model include Lee et al. (2010), Hamelin et al. (2011), Shanthraj and Zikry (2011), Engels et al. (2012), Bertin et al. (2013), Fan et al. (2013), Knezevic et al. (2013b) and Li et al. (2014). The problems studied with versions of Kocks-Mecking model include the influence of grain size and grain boundaries on the properties of the polycrystals (Lim et al., 2011; Li and Soh, 2012; Resende et al., 2013), changing loading paths and latent hardening (Barlat et al., 2013; Knezevic et al., 2013a,b; Bertin et al., 2014), thin film deformation (Liu et al., 2011; Lemoine et al., 2016), void growth and interaction (Lecarme et al., 2011; Shanthraj and Zikry, 2012) and multiphase alloys (Ardeljan et al., 2014).

One more example of a crucial microstructural feature that may define a macroscopic property in a certain way is the precipitate particles that form in age-hardening Al alloys after heat treatment. The most important role of these particles in the alloy is to serve as additional dislocation obstacles, trapping mobile dislocations and thus increasing the yield stress. If the particles are non-shearable, geometrically necessary dislocations will accumulate around them and contribute to an increase of the work-hardening rate. Ashby (1970) and Russell and Ashby (1970) used a simplified model to analyse the generation of geometrically necessary dislocations around non-shearable particles. The results were used by Myhr et al. (2010) to estimate the stress–strain curve of the AA6000 series Al alloys with an arbitrary heat treatment.

In other cases the connection between a microstructural feature and the macroscopic behaviour is not as explicit or strong as in these examples. Nevertheless the understanding of the mechanisms operating at the microscale is necessary to improve higher scale models. Examples of this type of studies may be found in Forest and Sedláček (2003), Dahlberg and Gudmundson (2008) and Cordero et al. (2010). The inhomogeneous deformation in a crystal consisting of several different phases is studied based on a laminate model, with varying thickness and strength of the layers. Strain gradient plasticity is used to reveal the influence of the characteristic lengths and interface conditions on the global response of the laminate and the local mechanical fields. The simplicity of the laminate model allows the use of advanced material models and sometimes an analytical solution. While this laminate does not correspond directly to any physical system, the obtained results may be (with some reservations) extended to the behaviour of precipitate particles, multiphase crystals or thin films.

Other works which utilize simplified models to study complex systems include Chang et al. (2012), where the precipitates in a heat-treated crystal are modelled as a periodic cubic array of spherical particles. The crystal is also simplified to a single slip plane, so that an advanced strain gradient plasticity model could be used to study the dislocation density distribution around the particles. Shearing of a thin crystalline strip is studied by Sedláček and Werner (2004), and a soft plastic channel in a harder medium is used by Taupin et al. (2012) to represent phenomena like slip bands in crystals.

One of the prominent microstructural features, which may be found in heat-treated alloys, is the precipitate free zones (PFZs) which form at the grain boundary. During the heat treatment the grain boundary acts as a sink for solute atoms and vacancies. This leads to formation of large precipitates on the grain boundary and an adjacent zone depleted of alloying elements and vacancies. The relative purity of the material in the PFZs, i.e., lack of dislocation obstacles, leads inevitably to the assumption that this zone is softer than the rest of the crystal, which is reinforced with solute atoms of the alloying elements and precipitate particles. Nano-indentation tests in Ogura et al. (2004) confirm this hypothesis. On the other hand, one can assume that under straining dislocations will accumulate in the PFZs and work-harden these zones in the same way as any other crystal. The influence of the PFZs on the deformation and fracture of polycrystals has been studied by use of simplified models. Crystals with PFZs were represented by a regular hexahedral structure in Fourmeau et al. (2015). The width of the real PFZs may be from 100 to 10,000 times smaller than the grain diameter. This makes a direct one-to-one modelling, e.g. with the finite element method (FEM), very complex, so in Fourmeau et al. (2015) the PFZs are much wider relative to the grain diameter. The material in the PFZs is modelled with porous plasticity, following the aforementioned assumptions about its lower yield stress and high work-hardening rate. The same regular hexagonal grain geometry and broad PFZs, but with a more advanced material model, was used by Pardoen and Brechet (2004) and Scheyvaerts et al. (2004). The influence of grain shape on the behaviour of such a system was studied, among others, by Pardoen et al. (2010). The softer PFZ may be assumed to deform differently than the rest of the grain, thus producing considerable plastic strain gradients from early stages of