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Modeling and simulation of deformation behavior, orientation gradient development and heterogeneous hardening in thin sheets with coarse texture

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ABSTRACT

The purpose of this work is the modeling of the deformation behavior and orientation gradient development in a highly anisotropic thin metal sheet and comparison with experiment. This sheet consists of a single layer of "large" Fe-3%Si grains exhibiting a coarse texture. Since such materials are highly heterogeneous, they are modeled by combining single-crystal plasticity for each grain with the finite-element method for the grain morphology and specimen as a whole. The single-crystal model is rate-dependent, accounts for (local) dissipative hardening effects, and has been identified with the help of single-crystal data. In previous work Klusemann et al. (2012b), model predictions for the evolution of the specimen geometry and grain morphology during tension loading to large deformation have been shown to agree reasonably well with the corresponding experimental results of Henning and Vehoff (2005). In the current work, model predictions for the development of orientation gradients in the specimen under different modeling assumptions (e.g., active glide-system family) are compared with EBSD-based experimental results of Henning and Vehoff (2005). Model predictions for the development of geometrically necessary dislocations are also discussed. As well, additional measures of local orientation evolution such as reorientation are examined and compared with the orientation gradient picture. In addition, we examine the effect of additional grain boundary strengthening related to grain boundary misorientation and grain size and the effect of additional GND-based kinematic hardening.

1. Introduction

A topic of past and on-going interest in material science and material mechanics is the investigation of the relations between the microstructure, material properties and material behavior at various length- and timescales (e.g., McPherson, 1981; Fu et al., 2001; Kalidindi et al., 2003; Wyss et al., 2004; Greer et al., 2005; Fülöp et al., 2006; Pierard et al., 2007; Janssen et al., 2008; Li and O'Dowd, 2011; Resende et al., 2013). One reason for continued interest here has to do with the increasing availability, application and further development of advanced material characterizations methods facilitating further insight; besides traditional methods like TEM, these include methods such as electron backscatter diffraction (EBSD),

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electron channel contrast imaging (ECCI) (see for description and explanation of these methods, e.g.,Henning and Vehoff, 2005; Welsch et al., 2007; Gutierrez-Urrutia et al., 2009, 2010; Gardner et al., 2010; Henning and Vehoff, 2010; Wilkinson et al., 2010). Another reason for this is the trend toward "micro- and nanomization" of many technological systems. Among other things, this results in a significant increase in the degree of material heterogeneity in these systems, related for example to the increasing dominance of boundaries and interfaces as the size of the system decreases. From the point of view of the material behavior, increasing heterogeneity invariably results in a corresponding increasing discrepancy between the global system and the local material behavior. Hence the increasing importance of local characterization methods such as micro- and nano-indentation (e.g., Berke et al., 2009; Mordehai et al., 2011; Saito et al., 2012; Kim et al., 2012).

This state of affairs has and continues to offer a number of challenges for the modeling of such systems. The mechanical behavior of a given microstructure can be modeled in different ways. A common approach is based on statistical or averaging theories. The associated homogenization can be performed on basis of a representative volume element (RVE). This concept is based on the assumption of scale separation between the microstructural and macrostructural lengthscale. If the characteristic size of the system (e.g., sheet thickness) approaches that of the microstructure (e.g., grain size), however, such scale separation is no longer given and one must resort to other means of representing the effect of microstructural heterogeneity on the system behavior. One possibility in this regard is based on distribution functions (e.g., orientation distribution functions, e.g., Böhlke et al., 2009, 2010) and averaging. As the macrostructural lengthscale approaches the microstructural one, the degree of material heterogeneity increases, and the local microstructural behavior may deviate significantly from the average macrostructural behavior (e.g., Kalidindi et al., 2003; Pierard et al., 2007). In this case, the model has to account for the microstructural details such as orientation details of the grain structure (e.g., Schneider et al., 2010) or phase distribution (e.g., Klusemann et al., 2012a). In the extreme case, the microstructural and macrostructural lengthscales are of the same order of magnitude, and one must resort to numerical modeling of the microstructure with the help of, e.g., the finite-element method (e.g., Evers et al., 2004b; Zhao et al., 2008; Roters et al., 2010; Klusemann et al., 2012b). In the case of polycrystalline materials, for example, such finite-element models are often constructed with the help of e.g., optical and/ or EBSD data on the grain morphology. In specimens with more than one grain over the thickness, the common method of projecting the two-dimensional EBSD information uniformly in the third dimension will generally lead to incorrect results (e.g., Wiederkehr et al., 2010). If the specimen is one grain thick, however, such an optical-/SEM-/EBSD-based approach should be reasonable. For such a specimen a number of size effects are expected to influence its mechanical properties. These effects have been known for years and are still the subject of active research (e.g., Fu et al., 2001; Engel and Eckstein, 2002; Greer et al., 2005; Fülöp et al., 2006; Geers et al., 2006; Janssen et al., 2006, 2008; Bargmann et al., 2010; Greer and De Hosson, 2011; Klusemann and Yalcinkaya, 2013).

Whereas the material-behavior-based size effects discussed above have been investigated in detail in the literature, (unwanted) size effects due to sample preparation have not. An exception here is the work of Janssen et al. (2008), who reported for example that machining-induced damage to crystals just below a newly created surface cannot be neglected for grain sizes of the same order-of-magnitude as the specimen size. The overall mechanical response is strongly influenced by the orientation of the individual grains if the number of grains over the thickness is fairly small (Fülöp et al., 2006). In the case of thin sheets the mechanical properties in a given cross section are increasingly dominated by each individual grain as reported in Henning and Vehoff (2005). Due to the different orientations of the grains located in the sheet plane, the deformation is no longer uniform even under homogeneous loading conditions. This heterogeneity and the size-dependence of deformation give rise to size effects (e.g., Henning and Vehoff, 2010). Different mechanisms can occur at different stages of deformation. The initial yield stress is influenced by grain size, grain orientation and elastic anisotropy (Hall, 1951; Petch, 1953; Prohászka and Dobránszky, 2003). With ongoing deformation strain hardening occurs which may be related to geometrically necessary dislocations (GNDs) (e.g., Nye, 1953; Ashby, 1970; Evers et al., 2004a,b; Ma et al., 2006). The grain size dependent mechanical response in a polycrystal is modeled by Evers et al. (2002) using a local strain gradient dependent crystal plasticity model accounting for GNDs. Various interesting viewpoints concerning the modeling and experimental concept of GNDs can be found in El-Dasher et al. (2003), Gao and Huang (2003) and Kubin and Mortensen (2003). To understand and predict the behavior correctly, simulation and experiment have to be compared *locally*, e.g., within individual grains in a polycrystalline specimen. For this purpose, detailed local experimental information is necessary (Henning and Vehoff, 2005). The measurement of local dislocation densities and their evolution during the deformation process via methods such as, e.g., TEM (e.g., Wang et al., 2012), is very time-consuming. Thus there is a need for the development of additional methods for quantitative local characterizations of the microstructure. Henning and Vehoff (2005) for example used EBSD data to determine orientation gradients locally in the specimen which can be understood as measure of local hardening. More recently, additional methods such as ECCI (e.g., Welsch et al., 2007; Gutierrez-Urrutia et al., 2009, 2010) show promise in this regard.

The purpose of the current work is the modeling of the large-deformation behavior of a bcc Fe-3%Si sheet metal sample (of about 1 mm thickness) with coarse texture subject to tension loading. This sample has been investigated experimentally by Henning and Vehoff (2005) (see also Henning and Vehoff, 2010). These samples are grown in such a way that there is only one grain over the thickness, and grain boundaries are perpendicular to the sample surface. The modeling is carried out with the help of crystal–plasticity and the finite-element method (CPFEM: e.g., Raabe et al., 2001; Fülöp et al., 2006; Roters et al., 2010). In the literature, specimens consisting of one or more coarse-textured layers over their thickness are sometimes referred to as oligocrystals. In this sense, related previous work includes for example that of Sachtleber et al. (2002), who investigated grain interaction in an Al oligocrystal with columnar grains subject to plane strain channel die extrusion. In addition,