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A virtual laboratory using high resolution crystal plasticity simulations to determine the initial yield surface for sheet metal forming operations

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ABSTRACT

We present a virtual laboratory to investigate the anisotropic yield behavior of polycrystalline materials by using high resolution crystal plasticity simulations. Employing a fast spectral method solver enables us to conduct a large number of full-field virtual experiments with different stress states to accurately identify the yield surface of the probed materials. Based on the simulated yield stress points, the parameters for many commonly used yield functions are acquired simultaneously with a nonlinear least square fitting procedure. Exemplarily, the parameters of four yield functions frequently used in sheet metal forming, namely Yld91, Yld2000-2D, Yld2004-18p, and Yld2004-27p are adjusted to accurately describe the yield behavior of an AA3014 aluminum alloy at two material states, namely with a recrystallization texture and a cold rolling texture. The comparison to experimental results proves that the methodology presented, combining accuracy with efficiency, is a promising micromechanics-based tool for probing the mechanical anisotropy of polycrystalline metals and for identifying the parameters of advanced yield functions.

1. Introduction

Because of their complex thermo-mechanical treatments, polycrystalline metals are generally crystallographically textured, and therefore their mechanical properties are anisotropic. The directionality of the mechanical properties must be taken into account when modeling metal forming operations. The anisotropy induced by plastic strain during forming operations is small compared to that induced by the thermo-mechanical treatment and negligible for most applications (Yoon et al., 2006). Crystal plasticity (CP) models which use the crystallographic texture and the intrinsic single crystalline anisotropy as input can accurately describe the anisotropic behavior of polycrystalline materials and naturally consider the stress and strain partitioning among different phases, grains, and subgrains (Roters et al., 2010). However, the long computation times required to integrate the underlying constitutive equations render their use infeasible for engineering simulations of large scale components. Due to their high efficiency and straightforward implementation, analytical yield functions are thus used instead of full-field CP simulations at the engineering scale to describe the anisotropy of materials.

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Starting with the first anisotropic yield function proposed by von Mises (1928), various yield functions have been established to describe the flow behavior of different material classes. The quadratic anisotropic yield function developed by Hill (1948) was validated by numerous experiments and is well suited for body centered cubic (bcc) materials, especially for steels (Hill, 1990). However, it can not accurately describe the yield behavior of face centered cubic (fcc) metals, *e.g.,* aluminum alloys (Hosford, 1988), as only higher order ansatz functions are capable of predicting the rather angular form of yield surfaces and the so-called "anomalous behavior" (Darrieulat and Piot, 1996), *i.e.,* the experimental observation that the equi-biaxial yield stress is higher than the uniaxial yield stress while the *r*-value is below 1.0 (Woodthorpe and Pearce, 1970). To overcome these limitations, Hill (1979) and Hosford (1985) proposed non-quadratic anisotropic yield functions. Later, Barlat and Lian (1989), Barlat et al. (1991, 1997, 2003, 2005), Karafillis and Boyce (1993), Banabic et al. (2003), Bron and Besson (2004) introduced further improved formulations, where linear transformations of the stress tensor are used to describe the anisotropy (Barlat et al., 2007).

For material models used in a commercial context, it is preferable that only a small set of simple and low-cost tests, *e.g.,* uniaxial tensile tests, are necessary for calibration (Lademo et al., 1999). The ability of advanced yield functions to describe the mechanical anisotropy of various material classes, however, comes at the price of requiring many parameters. Improved flexibility and accuracy therefore makes the parameter identification process more challenging as more experimental results are needed. These experiments are expensive, time consuming, and sometimes very difficult to perform, *e.g.,* when out-of-plane properties of sheet metals are required. Additionally, since no standards are defined for most of these experiments, evaluation of a parameter set requires an in-depth knowledge about the details of the fitting procedure that was employed to retrieve it.

Besides considering experimental results, numerical models are frequently used to examine the mechanical response of polycrystalline materials. Micromechanical models based on CP theory play a significant role in understanding yielding and anisotropy of metals, as well as in evaluating yield surface models. The earliest of such approaches, proposed by Sachs (1929), uses an iso-stress approach and assumes the same resolved stress on the slip systems with the highest resolved shear stress in all grains within the polycrystalline aggregate. In contrast, the full-constraint (FC) model developed by Taylor (1938) is based on the iso-strain assumption, *i.e.,* all grains within an aggregate experience the same state of deformation. The FC Taylor model was elaborated further by Bishop and Hill (1951), and was used as the Taylor–Bishop–Hill (TBH) model by many researchers to validate yield functions (Hosford, 1972; Barlat and Lian, 1989; Barlat et al., 1997) or to generate the analytical expressions for plastic potentials and yield surfaces of anisotropic polycrystalline materials (Gambin, 1991; Van Houtte, 1994, 2001; Li et al., 2003; Van Houtte and Van Bael, 2004; Kowalczyk and Gambin, 2004; Van Houtte et al., 2009). It should be noted that the Sachs model satisfies the stress equilibrium condition across the grains but violates the compatibility condition between them, while, in contrast, the TBH model violates the stress equilibrium condition but satisfies the compatibility condition among differently oriented grains (Kocks, 1958). The deformation behavior of real polycrystals, where both, compatibility and equilibrium are fulfilled, is in-between these two extremes (Sachtleber et al., 2002). The former model therefore sets the lower bound and the latter is the upper bound of the observed behavior.

Although the Taylor model shows good performance in the prediction of deformation textures, it is not fully realistic due to the violation of stress equilibrium. Various relaxed-constraint (RC) Taylor models were developed relieving the rigid deformation constraint in Taylor's iso-strain hypothesis (Honneff and Mecking, 1981; Kocks and Chandra, 1982; Raphanel and Van Houtte, 1985; Hölscher et al., 1991, 1994; Raabe, 1995c). Also, a number of grain cluster models were introduced such as the LAMEL model, the advanced LAMEL (ALAMEL) model (Van Houtte et al., 1999, 2002, 2005), the grain interaction (GIA) model (Raabe, 1995a,b; Raabe et al., 2002b; Crumbach et al., 2006), and the relaxed grain cluster (RGC) model (Tjahjanto et al., 2010).

Another important class of homogenization schemes is based on the self consistent (SC) approach which was originally proposed by Kröner (1958) for the elastic case and later extended to the elastoplastic (Hill, 1965) and viscoplastic (Hutchinson, 1976) cases. In the SC theory, each grain within a polycrystalline aggregate is considered to be an ellipsoidal inclusion embedded in the surrounding homogeneous equivalent medium (HEM). Such models satisfy the stress equilibrium and the deformation compatibility simultaneously as they allow for different deformation responses in each grain depending on the relative stiffness between the grain and the HEM. Among the various SC models, the visco-plastic self consistent (VPSC) model developed by Molinari et al. (1987) and extended by Lebensohn and Tomé (1993, 1994) has been widely used to simulate plastic behavior and texture evolution of polycrystalline materials (Lebensohn et al., 1996, 1998; Segurado et al., 2012; Knezevic et al., 2013). Although the SC models relieve the drawbacks associated with the Taylor type models, further microstructural aspects of the deformation, such as local grain interaction and intra-grain inhomogeneities of the micromechanical fields, are not accessible to these models (Zhao et al., 2007; Lebensohn et al., 2012).

Recently, full-field CP models, which are capable of incorporating additional morphological information beyond crystallographic texture, either employing the finite element method (FEM, CPFEM) (Raabe et al., 2001; Raabe and Roters, 2004; Dawson et al., 2005; Zhao et al., 2008; Kanjarla et al., 2010; Roters et al., 2010; Van Houtte et al., 2011; Zhang et al., 2015a) or a spectral method using fast Fourier transformation (FFT) (Lebensohn et al., 2012; Kanjarla et al., 2012; Eisenlohr et al., 2013; Tasan et al., 2014a; Shanthraj et al., 2015) based solvers have become computationally feasible for the simulation of representative volume elements (RVEs). The merits of such full-field approaches include: (i) fulfillment of both, stress equilibrium and strain compatibility at grain boundaries; (ii) representation of a real grain morphology as long as the discretisation is fine enough; (iii) consideration of the local grain interactions and intra-grain inhomogeneities associated with plastic deformation. The main drawback of the full-field CPFEM is the computational cost associated with the large number of material points needed for the simulation of a sufficiently highly resolved polycrystalline RVE. Compared with their FEM counterparts,