International Journal of Plasticity xxx (2016) 1–25

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

Coupling elasto-plastic self-consistent crystal plasticity and implicit finite elements: Applications to compression, cyclic tension-compression, and bending to large strains

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ARTICLE INFO

Article history:
Received 5 May 2016
Received in revised form 27 July 2016
Available online xxx

Keywords:
A. Dislocations
A. Twinning
B. Constitutive behavior
C. Finite elements
FE-EPSC

ABSTRACT

In this work, we describe a finite element (FE) implementation of an elasto-plastic self-consistent (EPSC) polycrystal plasticity model termed FE-EPSC, which is intended for simulations of metal forming. To this end, we present an analytical Jacobian, which is necessary for the implicit coupling and ensuring a fast convergence. Every FE integration point is a material point that can be represented either by a single crystal or a polycrystalline material. The constituent crystal can deform by a combination of anisotropic elasticity, crystallographic slip, and deformation twinning. The model is validated and applied to a suite of tests, including monotonic compression, cyclic forward loading, unloading and reverse loading and non-monotonic four-point bending, and materials, such as different alloy compositions, crystal structures, and initial microstructures. The same FE-EPSC framework is applied for all these cases with the main differences pertaining to intrinsic properties, such as the available slip and twinning deformation modes, and the material parameters for activating and hardening of these modes. Full characterization for these parameters for high-purity α-Ti is presented here for the first time. Through these examples we show that, in addition to being predictive with great accuracy, the key advantage of this model lies in its versatility. It accounts for the development of backstress aided dislocation glide, thermally activated storage of dislocations, elastic anisotropy, crystallographic slip and deformation twinning via multiple modes, and de-twinning as well as multi-level homogenizations.

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1. Introduction

In metal forming techniques, metals are deformed to large strains, develop non-uniform strain fields, and experience strain path changes involving sequences of loading, unloading, and reloading in the opposite sense or other directions (Barlat et al., 2003; Hosford and Caddell, 2011; Wagoner et al., 2013; Zecevic et al., 2016e). It is well known that although the motions of dislocations (crystallographic slip) and, in some metals, slip and twinning, accommodate

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http://dx.doi.org/10.1016/j.ijplas.2016.07.016
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Please cite this article in press as: Zecevic, M., et al., Coupling elasto-plastic self-consistent crystal plasticity and implicit finite elements: Applications to compression, cyclic tension-compression, and bending to large strains, International Journal of Plasticity (2016), http://dx.doi.org/10.1016/j.ijplas.2016.07.016

most of the strains, intra- and inter-granular elastic deformation fields can play an important role in activating slip and twinning and in this way contribute to the overall deformation process. Their influence have been related to the observation of the Bauschinger effect (BE) in cyclic loading or strain reversals, or to the local stress concentrations responsible for the onset of deformation twins, de-twinning, internal stresses in two-phase metals, or the slope of the unloading response (Bauschinger, 1886; Kadkhodapour et al., 2011; Knezevic et al., 2013a; Pavlina et al., 2015; Yoshida et al., 2002).

Over the years, crystal plasticity based models have been developed for simulating stress–strain response and texture evolution during small-scale monotonic loading tests. These include upper bound full-constraint Taylor-type or mean-field visco-plastic self-consistent (VPSC) homogenization schemes (Knezevic et al., 2016c; Lebensohn and Tomé, 1993; Lebensohn et al., 2016; Taylor, 1938; Van Houtte, 1982). Agreement with mechanical stress–strain data and texture evolution is commonly managed with some elasticity-driven physical phenomena in mind with the aid of underlying phenomenological models (Beyerlein and Tomé, 2007; Carpenter et al., 2015; Kitayama et al., 2013; Knezevic et al., 2013b, 2014d, 2015a, 2015b; Zecevic et al., 2016b). To facilitate simulations of non-monotonic boundary conditions, Taylor-type and VPSC techniques have been embedded into finite element (FE) methods and used in a number of studies (Ardeljan et al., 2016a; Kalidindi et al., 1992; Knezevic et al., 2016a, 2014c, 2013d; Segurado et al., 2012; Zecevic et al., 2016a, 2016c). In the case of FE-VPSC, the elastic portion of the total strain at each material point is treated separately from the polycrystal model. Thus the elastic strains are not based on the crystal-scale response. Models like elasto-plastic self-consistent (EPSC) (Turner and Tomé, 1994) and elasto–visco–plastic self-consistent (EVPSC) (Wang et al., 2010) account for granular elasticity. In stand-alone (SA) form, these models also do not account for the heterogeneity in the mechanical fields that can develop across the sample during metal forming. Crystal plasticity finite element or crystal plasticity fast Fourier transform (FFT) models can calculate the spatially resolved mechanical fields in 3D (Ardeljan et al., 2015a, 2016b; Kalidindi et al., 2006; Knezevic et al., 2014b; Lebensohn et al., 2012; Zecevic et al., 2015b) but are computationally intensive for deformation sequences involving large strains and multiple paths in series. Therefore, these models are typically used for modeling a representative volume element of a given material rather than a forming process. Efforts have begun towards the development of computationally efficient methods (Al-Harbi et al., 2010; Knezevic et al., 2008; Knezevic and Landry, 2015; Zecevic et al., 2015c) as well as the utilization of specialized hardware (Knezevic and Savage, 2014; Savage and Knezevic, 2015) for achieving computationally tractable simulations of forming processes using such crystal plasticity constitutive models. Modeling deformation twins within these techniques is possible but formation and growth can still be challenging (Ardeljan et al., 2015b; Knezevic et al., 2016b; Kumar et al., 2015).

In this work, we develop a multi-scale FE-EPSC model, where every material point is a single crystal or a polycrystal that deforms by elasticity, crystallographic slip and twinning. Most generically, it accounts for the development of intra-granular backstresses, backstress aided dislocation glide, thermally activated storage of dislocations, elastic anisotropy, inter-granular stresses, crystallographic slip and deformation twinning via multiple modes, and de-twinning. We derive a fully analytical Jacobian to facilitate implicit coupling within ABAQUS Standard and fast convergence. The model is applied to simulate the response of several metals under different mechanical test conditions. The tests include monotonic loading, cyclic forward loading, unloading, and reverse loading for model validation and non-monotonic four-point beam bending for model application. We simulate these tests for pure Cu, DP 590 steel, AA-6022-T4, and high-purity α-Ti featuring body-centered cubic (BCC), face-centered cubic (FCC), and hexagonal close-packed (HCP) crystal structures, and different initial microstructures. Since the materials vary in crystal structure, they will vary in their underlying number and types of deformation mechanisms. We demonstrate that the FE-EPSC developed here can be used as a simulation tool for simulating metal forming of anisotropic metals and, in particular, processes where granular elasticity is important to be taken into account, such as in capturing springback effects.

2. The FE-EPSC model

2.1. EPSC, a polycrystal plasticity model

We use the elasto-plastic self-consistent (EPSC) model for the constitutive response at each material point. This model relates the deformation of each crystal to the deformation of the polycrystal. The homogenization scheme used in EPSC was originally developed in Neil et al. (2010) and Turner and Tomé (1994). The polycrystal is represented by a collection of single crystals each having a specific orientation, an ellipsoidal shape, and a volume fraction. The mechanical fields of each crystal are determined by modeling it as an elasto-plastic inclusion in the homogeneous equivalent medium (HEM). The HEM has properties of the polycrystal and hence why the homogenization scheme is called 'self-consistent'. We refer the reader (Lentz et al., 2015a, 2015b; Neil et al., 2010; Turner and Tomé, 1994; Zecevic and Knezevic, 2015) for a description of the formulation and applications to simulate different phenomena in materials. In this section, we describe the EPSC User MATerial (UMAT) model termed the FE-EPSC model. In what follows, we will use "$\cdot$" and "$\otimes$" to denote a dot product and a tensor product, respectively.

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