Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 295 (2015) 396–413
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Explicit incorporation of deformation twins into crystal plasticity finite element models

Milan Ardeljan[a], Rodney J. McCabe[b], Irene J. Beyerlein[c], Marko Knezevic[a,*]

[a] *Department of Mechanical Engineering, University of New Hampshire, Durham, NH 03824, USA*
[b] *Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[c] *Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

Received 21 March 2015; received in revised form 22 June 2015; accepted 6 July 2015
Available online 14 July 2015

Highlights

- Morphology and crystallography of deformation twinning are implemented in crystal plasticity finite element models.
- Intrinsic twinning transformation shear strain is enforced to correspond to the plastic strain accommodated by the twin lamella.
- Heterogeneities in spatial mechanical fields are correlated with microstructural changes during twin formation and thickening.
- Multiple thin twin lamellae are predicted to be more favorable than a single thick twin lamella in uranium.

Abstract

Deformation twinning is a subgrain mechanism that strongly influences the mechanical response and microstructural evolution of metals especially those with low symmetry crystal structure. In this work, we present an approach to modeling the morphological and crystallographic reorientation associated with the formation and thickening of a twin lamella within a crystal plasticity finite element (CPFE) framework. The CPFE model is modified for the first time to include the shear transformation strain associated with deformation twinning. Using this model, we study the stress–strain fields and relative activities of the active deformation modes before and after the formation of a twin and during thickening within the twin, and in the parent grain close to the twin and away from the twin boundaries. These calculations are carried out in cast uranium (U), which has an orthorhombic crystal structure and twins predominantly on the {130} $<3\bar{1}0>$ systems under ambient conditions. The results show that the resolved shear stresses on a given twin system on the twin–parent grain interface and in the parent are highly inhomogeneous. We use the calculated mechanical fields to determine whether the twin evolution occurs via thickening of the existing twin lamella or formation of a second twin lamella. The analysis suggests that the driving force for thickening the existing twin lamella is low and that formation of multiple twin lamellae is energetically more favorable. The overall modeling framework and insight into why twins in U tend to be thin are described and discussed in this paper.

Keywords: Crystal plasticity finite element models; Stress fields; Deformation twinning; Twin formation; Twin thickening

* Correspondence to: University of New Hampshire, Department of Mechanical Engineering, 33 Academic Way, Kingsbury Hall, W119, Durham, NH 03824, USA. Tel.: +1 603 862 5179; fax: +1 603 862 1865.
E-mail address: marko.knezevic@unh.edu (M. Knezevic).

http://dx.doi.org/10.1016/j.cma.2015.07.003
0045-7825/

1. Introduction

Deformation twinning plays a significant role in the deformation response of many metals and their alloys, particularly those with low symmetry crystal structures, such as hexagonal close packed Mg, Zr, Be, Ti and orthorhombic uranium (U). To accommodate a general deformation state, these polycrystalline metals activate both dislocation slip and twinning [1–9]. The relative resistance and contributions of these two modes can evolve differently with strain and strain direction [4,10–12]. As a result, these metals exhibit a highly anisotropic mechanical response. Understanding the interplay of slip and twinning at the microscopic level and its influence on the macroscopic response are premier challenges in constitutive modeling of low symmetry materials. Additionally, there are fundamental questions regarding how and where twinning initiates, why a single lamella would thicken in one case while multiple lamellae would form in another, and when twinning saturates.

In the past, many studies have used materials models to link polycrystalline flow stress and hardening to slip and twinning within the individual crystals. Reproducing the effects of deformation twinning is usually more demanding and challenging than for slip. Deformation twins affect the microstructure in two ways: they reorient the lattice in a finite domain within a grain, and they introduce a twin–matrix boundary between the original parent grain and the twin domain [3,13]. Current models incorporating twins include analytical models [14], polycrystalline mean-field schemes such as Taylor [15–23] and self-consistent models [24,25], and spatially resolved techniques, such as crystal plasticity finite element (CPFE) [26–34] and Green's function fast Fourier transform (FFT) [35,36] models. Typically, polycrystalline mean-field models account for the shear produced by twinning by modeling it as a pseudo-slip process [37,38]. At the same time, they consider the reorientation effect in one of several ways, either via: (i) the predominant twin reorientation (PTR) method [38], (ii) the volume fraction transfer (VFT) scheme [12], (iii) the total Lagrangian approach [17,30], or (iv) the composite grain (CG) method [11]. While successful in capturing the macroscopic stress–strain response and bulk texture evolution [39,40], these schemes do not capture the dynamic and spatially heterogeneous nature of twinning. A particularly important limitation is their inability to account for the resolved shear stress at the twin–parent grain interface responsible for thickening of an existing twin.

Spatial full-field techniques can explicitly incorporate the characteristic twin shear and corresponding grain reorientation and, therefore, better capture fields associated with subsequent twin thickening. To understand the local stress distribution as a consequence of twin formation, phenomenological finite element modeling has been utilized to model a twin in Zr [41,42]. A cuboidal inclusion representing a parent grain that develops a twin was embedded in an isotropic medium. As such, the effects of morphology and local grain structure on the fields were not taken into account. Moreover plastic anisotropy of the inclusion was accounted for using a macroscopic Hill's yield criterion [43]. The study correlated the stress states that are energetically favorable for twinning with twin volume fraction and morphology. More recently, a full-field, elasto-viscoplastic formulation based on the Green's function FFT method was used to study distributions of local stress states around a twin in Mg [36]. The study revealed the variation in the shear stress profile on the twin planes consistent with the lenticular shape of twins. However, modeling of twin thickening and the associated evolution of the mechanical fields have not been modeled using the FFT technique.

Explicit incorporation of deformation twinning in CPFE has not been attempted thus far. With CPFE, a polycrystal is discretized into finite elements and a crystal plasticity constitutive law operates at each FE integration point. Both stress equilibrium and strain compatibility are satisfied providing better predictions of local and overall material behavior and microstructure evolution. In CPFE, one of the main difficulties is related to FE mesh manipulation. Remeshing of every grain containing one twin or multiple twins must be performed at the initial twin formation stage and every step during twin thickening. These mesh alterations computationally intensify the already intensive calculations involved in CPFE codes.

The main objective of this work is to develop a numerical procedure for explicit 3D modeling of the formation and thickening of twin lamellae under imposed plastic deformation conditions into the CPFE framework. The novel procedure explicitly models twin transformation, i.e., the characteristic twin shear and crystallographic reorientation of the twinned domains. Moreover, the effect of both the twin transformation shear and neighboring grain shape in 3D on the local stress distribution are modeled. In addition to twin formation and thickening, the model captures grain-to-grain interactions and their effect on the mechanical fields. To showcase this capability, we apply the newly developed twin-CPFE model to study twinning in U. Specifically, we treat the case of twin lamellae formation and thickening within a grain in U favorably oriented for twinning, which is surrounded by other grains that are not favorably oriented for twinning. The analysis aims to demonstrate how the technique can provide unique insights into the changes