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Multi-scale modeling and experimental study of twin inception and propagation in hexagonal close-packed materials using a crystal plasticity finite element approach—Part I: Average behavior

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ABSTRACT

A Crystal Plasticity Finite Element (CPFE) code is used to study the effect of grain boundary geometry and texture on twin inception and propagation. Three dimensional grains with random shapes are generated using Voronoi tessellation and used for simulations. The results are compared with previously published Electron Backscattered Diffraction (EBSD) studies carried out on zirconium and magnesium. It is shown here that the majority of phenomena observed experimentally regarding the average (statistical) behavior of twins can be captured by considering the grain boundary geometry. It is observed that twins are prone to initiate at grain boundaries and specifically at the conjunction of more than two grains. The various stress conditions and concentrations at grain boundaries also result in selection of different twin variants.

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1. Introduction

Plastic deformation in polycrystalline materials can generally be explained by movement of dislocations in the slip plane in a slip direction where under static loading, plastic slip is accompanied by gradual changes in the crystallographic orientation of grains (Taylor and Elam, 1923; Hill, 1966; Hill and Rice, 1972; Asaro, 1983). Due to lack of easy-slip systems, on the other hand, materials with Hexagonal Close-Packed (HCP) crystals often accommodate imposed deformation by a rapid change in the crystallographic orientation which is known as twinning (Hull, 1961; Griffiths and Cottrell, 1967; Tenckhoff, 2005). The whole twinning process can be divided into four stages. In the first stage, which will be called nucleation here, twinning related dislocations accumulate in a location where the twin zone can be considered an embryo that may or may not lead to a successful twin (Beyerlein and Tome′, 2010). In the second stage, or the inception stage, the dislocations related to twinning reach a critical state that can trigger an actual twin to first form; in the third stage twins form with a needle shape, typically crossing an entire grain, and in the fourth stage, called propagation, the twin thickens. Texture, the distribution of crystallographic orientation of grains with respect to an external coordinate, of an HCP material can change drastically during plastic deformation due to twinning which can alter mechanical behavior of the material. Hence, in order to have a better understanding of deformation mechanisms in HCP materials it is necessary to study parameters that can influence twinning.

Deformation twinning has been studied at different length scales by several experimental and numerical procedures. At a macroscopic length scale, the average behavior of families of twins has been experimentally studied using in-situ neutron diffraction tests (Agnew et al., 2003). Some fundamental questions about mechanisms involved in texture

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devolvement (Xu et al., 2009; Ma et al., 2012), interaction between twins and parent grains or other twins (Salem et al., 2005), twinning and detwinning (Proust et al., 2009), as well as the stress state inside twins at inception (Clausen et al., 2008) have been investigated. The effects of local parameters on twins, e.g. grain boundary geometry or stress fluctuations within a given grain, are some of the major missing parameters in such experiments. Two major numerical approaches, i.e., Self Consistent (SC) and Crystal Plasticity Finite Element (CPFE), have been implemented to rationalize behavior of materials under these experiments (Lebensohn and Tome′, 1993; Roters et al., 2010). In the SC approach, a grain has an ellipsoidal shape with homogenous stress and is embedded in a homogenous medium that represents the average response of all of the other grains (Eshelby, 1957). Hence, in conventional SC modeling the effect of grain boundary and stress heterogeneity inside each grain are simply neglected. Nevertheless, a short simulation-time, in comparison to CPFE models, has empowered SC models to provide a significant contribution in explaining physics behind twinning induced by plastic deformation (Wang et al., 2010a,2010b; Mareau and Daymond, 2011). On the other hand, although grain boundaries are not discernable in a neutron diffraction experiment, in terms of modeling, different grain shapes, e.g. cube or more realistic can be used, and many Integration Point (IP) can be assigned to each grain in a CPFE simulation hence capturing stress and rotation variation inside each grain (Staroselsky and Anand, 1998,2003; Myagchilov and Dawson, 1999; Quey et al., 2011).

At a microscopic length scale, statistical studies of twins have been experimentally carried out via Electron BackScattered Diffraction as well as micro x-ray diffraction (Capolungo et al., 2009; Beyerlein et al., 2010; Aydiner et al., 2009). Effects of a wide variety of parameters such as mis-orientation between two neighboring grains and grain diameter or volume on nucleation of twins or twin variant selection are studied. In terms of modeling, the assumption of having homogenous stress distribution within each grain or ellipsoidal shaped-grain, where stress concentration due to grain boundary geometry are basically ignored, in SC models results in missing local effect on twin inception and consequently difficulty in interpreting experimental data. Recently, by introducing new parameters which are chosen with the aid of atomistic models, modification has been applied to the current existing SC models to take in to account the probability of having some susceptible/probable twinning sites in a grain boundary. For instance, Beyerlein and Tome′ (2010) introduced new parameters to virtually create susceptible sites for twinning in their SC model. Also, virtual fluctuations were induced on the Resolved Shear Stress (RSS) of each twin variant to generate deviations from the average RSS calculated from the homogenous stress of the grain; reflecting in reality both the variation in RSS within the parent grain and the potential for variation in RSS required for twin inception due to grain boundary type. With these considerations, it was shown that grains with both high and low tendency to twin can twin, where the probability of having twins increases with grain tendency to twin based on Schmid factor. More recently, the modified code was connected to an atomistic model (Wang et al., 2010c) to calculate a statistical distribution of grain boundary defects. Effects of these statistical defects in grain boundaries as well as local stresses on twin inception are studied in Beyerlein et al. (2011). At a lower length scale, effects of various parameters on twin formation have been studied within an atomistic modeling framework. To name some key observations from this area, following the work conducted by Yoo (1981), Serra and Bacon (1996) showed that plastic slip is not transferred from one crystal to the other with a residual dislocation left at the interface; instead, the matrix dislocation decomposes into interfacial defects. Hence matrix slip dislocations can become a new source of twinning dislocations; these then produce twin growth when the appropriate stress is applied to the crystal. Also, the interaction observed at the twin boundary depends on the type of dislocation and twin interface. For instance, it is shown by the same authors (Serra and Bacon, 1995) that screw dislocations cross the $\{10\bar{1}2\}$ twin interface by cross slip, but a $\{10\bar{1}1\}$ boundary usually absorbs the screws. Studies of nucleation mechanisms of deformation twins within an atomistic simulation framework showed that, in HCP metals, a stable twin nucleus consists of multiple atomic layers (Wang et al., 2009a, 2009b). Also, a molecular dynamic study by Wang et al. (2010c) showed that low angle tilt boundaries contain a uniform array of large misfit grain boundary dislocations that when exposed to a local stress concentration, the grain boundary dislocations dissociate into small number of twin partial dislocations which then coalesce into a single twin nucleus. In comparison with the range of work using SC models and atomistic simulations, little attention has been paid to the statistical study of twins using CPFE approaches.

In the current study, grains with random shape are mapped into a FE solver to study the effects of texture variation, grain boundary geometry, and stress fluctuation within grains on twin inception and propagation. Twins are allowed to incept anywhere in a grain, but it is shown that they are prone to incept at the grain boundaries. The CPFE results are compared against previously published experimental EBSD data on zirconium (Capolungo et al., 2009). The question that is tried to tackle here is to what extent conventional crystal plasticity FE models can rationalize the statistically observed data—given that such models do not include atomistic information about grain boundary character, but only the impact of grain shape and stress concentration. In Part II of the current study (Abdolvand and Daymond, this issue), grains with actual measured shapes are studied and local effects on twin inception and propagation are investigated.

2. CPFE description

2.1. General mathematical formulation

In this section, the general formulation and assumptions of the code is explained; details of the code are described in Abdolvand et al. (2011). For a general solid mechanics problem, fifteen equations are required to be solved simultaneously:

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