The Incorporation of Discrete Deformation Twins in a Crystal Plasticity Finite Element Framework

Matthew Kasemer and Paul Dawson

Abstract

The most prevalent twinning models homogenize the local deformation response by considering twins as "pseudoslip" systems, obscuring the physical differences between slip and twinning—namely the discrete nature of twinning. Presented is a computational approach designed to consider discrete deformation twinning in a crystal plasticity finite element framework. A polycrystalline domain is pre-discretized at the sub-grain scale into lamellar regions dependent on the geometry of the twin systems, which facilitates a finite element mesh that is attendant to this geometry. A twin is activated in a lamellar region by applying essential velocities to its nodes and rapidly mapping their locations to their expected twinned positions. The rest of the body deforms by crystallographic slip to enforce mechanical equilibrium. Results indicate stress relaxation in the parent grain and regions of large stress concentrations in neighboring grains. These trends are discussed in light of global and local energetic observations.

Keywords

Crystal plasticity • Finite element method • Twinning

Extended Abstract

Hexagonal materials are used in demanding structural applications due to (broadly) their high strength, low density, resistance to corrosion, and other desirable properties. Metallic alloys tend to exhibit elastic and plastic single crystal anisotropy. Magnesium, for example, tends to exhibit a fair degree of plastic anisotropy [1]. This tends to lead to complex deformation behavior, namely the development of heterogeneous plasticity both intra-grain and globally [2]. Mathematical models aid in the understanding of the relationship between the crystal response and the macroscopic response of a sample. The crystal plasticity finite element method (CPFEM) represents perhaps the most sophisticated tool in predicting the deformation response of polycrystals [3].

Typically, crystal plasticity finite element models consider crystallographic slip as their only mode of plastic deformation. Deformation twinning, however, may play a large role in the development of plasticity across a polycrystal composed of crystals exhibiting hexagonal symmetry. Various models have been developed to consider the deformation response due to twinning. The most popular choice—due to its simplicity, relative ease in implementation, and low marginal computational cost—is the so-called pseudo-slip model [4], in which the deformation response due to slip and twinning is homogenized locally, considering a variable "volume fraction" of material deforming by either slip or twinning. This model, while adept at predicting texture evolution and bulk response, ignores the discrete nature of twinning and obscures the relative rate disparities between slip and twinning, thus hampering the precise prediction of local stress fields.

Recent modeling efforts [5] have instead focused on attempting to model discrete deformation twins to better predict the complex local heterogeneity in the stress fields due to twinning. In this study, a discrete deformation twinning framework is proposed [6]. Broadly, this framework considers the deformation response of discrete regions, twinned at a relatively rapid rate—upholding the main physical differences between slip and twinning. The framework relies on the pre-discretization of a polycrystalline aggregate at the sub-grain scale into lamellar regions (a single crystal is illustrated for simplicity in Fig. 1). Lamellar regions are included by means of a novel multi-level tessellation algorithm, in which the polycrystal domain is first discretized into grains (via a Voronoi or Laguerre

M. Kasemer (✉)
Department of Mechanical Engineering, The University of Alabama, Tuscaloosa, USA
e-mail: mkasemer@eng.ua.edu

P. Dawson
Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, USA

J. B. Jordon et al. (eds.), *Magnesium Technology 2020*, The Minerals, Metals & Materials Series, https://doi.org/10.1007/978-3-030-36647-6_24

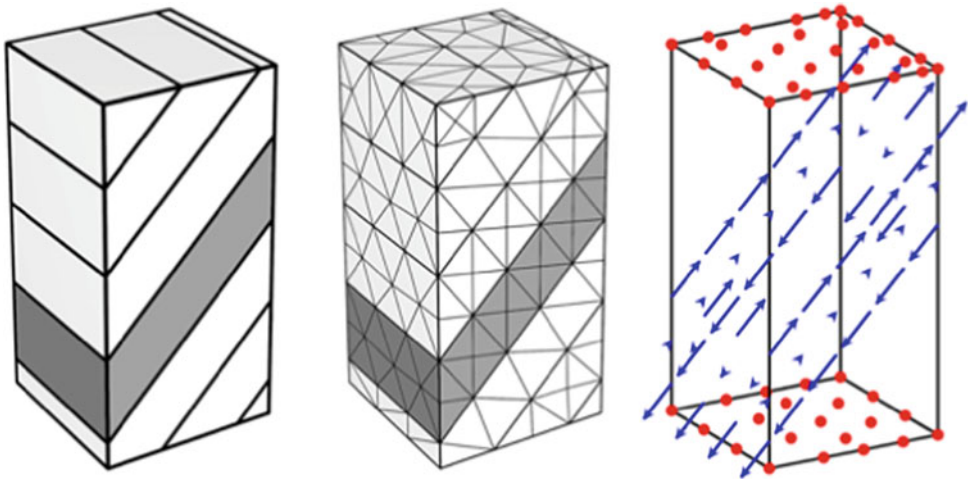

Fig. 1 Single crystal discretized into lamellar regions, along with its mesh, and twin velocity field (reproduced from [6])

Fig. 2 Von Mises stress field prior to and post-twin activation (reproduced from [6])

tessellation), and each grain is subsequently considered as a domain for further (lamellar) discretization. The spatial normals of these lamellar regions are calculated based on the crystallographic orientation of the grain and the twin system under consideration. Each lamellar region is assigned the same orientation as the parent crystal. Lamellar boundaries are not explicitly modeled as grain boundaries, and thus, a collection of lamella that forms a grain is considered a single crystal. These lamellar regions allow for the formation of a finite element mesh that conforms to these boundaries. Figure 1 further details the attendant finite element mesh (with an example lamellar region highlighted). Note how the lamellar regions facilitate in the formation of a mesh that adheres to these boundaries. At some point in deformation when a twin is considered for activation, the elements and nodes within a lamellar region are thus readily queried.

Upon twin activation, the elemental orientations are utilized to calculate an average deformation gradient due to twinning. This deformation gradient is used to be calculated the expected nodal positions due to twinning of each node within the lamellar region. Velocities are calculated and essential velocities placed on each node. A number of small time steps are taken until the point at which the twin is mapped to its final location, and the essential velocities on the lamellar region are then relaxed. The elemental orientations are updated for each element in the lamellar region to their expected twinned orientations. The regions outside of the lamellar region accommodate this deformation via crystallographic slip, via the base CPFEM framework. At this point, the framework considers the twin region as a new grain, and deformation proceeds along the specified macroscopic deformation path.

This framework allows for the inspection of the complex stress fields that form due to twinning. Note in Fig. 2, for example, that the von Mises stress experiences a drop in the parent grain, especially in the vicinity of the twinned region, and sharp increases in neighboring grains at the twin tip. The consequences of a twinning event may be readily assessed via this framework. Most interesting is the assessment of local and global work metrics, calculated via the deformation rate/Cauchy stress conjugate, which allows for the comparison of the total, elastic, and plastic work over the course of twin activation. The framework additionally allows for the consideration of twin growth (thickening) via the successive activation of lamella neighboring the twinned region and is additionally poised to approach the problem of transformation induced plasticity, which exhibits similar modeling challenges.

Presented are results from simulations in which a single grain at the center of a polycrystalline aggregate is considered for twinning. Multiple simulations are performed in which a single lamellar region is activated at (1) various points in the deformation history, and (2) with various initial twin widths. Changes to the stress field as a function of twin width and the point of activation are discussed with respect to energetic metrics, and the comparisons are made to simulations performed considering only crystallographic slip.

References

1. I.J. Beyerlein, L. Capolungo, P.E. Marshall, R.J. McCabe, C.N. Tomé, "Statistical analyses of deformation twinning in magnesium", Philos. Mag., 90(16) (2010), pp. 2161-2190, https://doi.org/10.1080/14786431003630835
2. M.P. Echlin, J.C. Stinville, V.M. Miller, W.C. Lenthe, T.M. Pollock, "Incipient slip and long range plastic strain localization in microtextured Ti-6Al-4 V titanium", Acta Mater., 114 (2016), pp. 164-175, https://doi.org/10.1016/j.actamat.2016.04.057
3. M. Kasemer, R. Quey, P. Dawson, "The influence of mechanical constraints introduced by β annealed microstructures on the yield strength and ductility of Ti-6Al-4 V", J. Mech. Phys. Solids, 103 (2017), pp. 179-198, https://doi.org/10.1016/j.jmps.2017.03.013
4. S.R. Kalidindi, "Incorporation of deformation twinning in crystal plasticity models", J. Mech. Phys. Solids, 46(2) (1998), pp. 267-271, 273-290, https://doi.org/10.1016/s0022-5096(97)00051-3
5. M. Ardeljan, R.J. McCabe, I.J. Beyerlein, M. Knezevic, "Explicit incorporation of deformation twins into crystal plasticity finite element models", Comput. Method Appl. M., 295 (2015), pp. 396-413, https://doi.org/10.1016/j.cma.2015.07.003
6. M. Kasemer, P. Dawson "A finite element methodology to incorporate kinematic activation of discrete deformation twins in a crystal plasticity framework", Comput. Method Appl. M., In Press (2019)