Available online at www.sciencedirect.com

ScienceDirect

Acta Materialia 93 (2015) 12–23

Acta MATERIALIA

www.elsevier.com/locate/actamat

Crystal plasticity simulations using nearest neighbor orientation correlation function

V. Sundararaghavan,[a,*] A. Kumar[b] and S. Sun[c]

[a]*Aerospace Engineering, University of Michigan, Ann Arbor, MI, USA*
[b]*Oak Ridge National Lab, Oak Ridge, TN, USA*
[c]*Exmar Offshore, Houston, TX, USA*

Received 6 February 2015; revised 10 April 2015; accepted 10 April 2015
Available online 27 April 2015

Abstract—A probabilistic scheme is presented for simulating evolution of polycrystalline microstructures during deformation. Microstructure images are described using a compact descriptor called the nearest-neighbor conditional orientation correlation function, defined as the probability density of occurrence of a crystal orientation at one pixel distance from a known orientation. The neighborhood information obtained from this function is used to correct a Taylor-based formulation of crystal plasticity. A finite differencing scheme is developed to capture equilibrium of each orientation in an average sense. The predictions of textures and stresses using our approach are compared against crystal plasticity finite element model of a planar polycrystalline microstructure. We find that the new descriptor is able to capture texture components that are otherwise missed by the Taylor model and provides consistent improvements in the prediction of reorientation and stresses. The simulation speed is significantly faster than crystal plasticity finite element method and is more comparable to that of Taylor models.

Keywords: Plastic deformation; Texture; Finite element analysis; Simulation; Theory

1. Introduction

Integrated Computational Materials Engineering (ICME) [1] paradigm for metal-forming processes proposes stronger tie-in of microstructural models to engineering simulations. The microstructural model of choice for polycrystalline alloys is the crystal plasticity finite element method (CPFE) [2–6]. Here, mechanical properties of aggregates of grains are analyzed by discretizing the grains into finite elements and modeling texture development using crystal plasticity constitutive models. There are two primary issues when dealing with such an approach. Firstly, multiscale simulations that use finite element representation of the underlying microstructure are computationally prohibitive. Secondly, polycrystalline microstructures vary as a function of location in the raw material and compact representations are needed to model this variability.

An alternate class of schemes developed in recent years allow compact representation of microstructures using probabilistic descriptors. The simplest of these descriptors is the one-point probability measure, the orientation distribution function (ODF), which quantifies the volume fractions of crystals in the orientation space. Under an applied deformation, texturing is simulated by numerically evolving the ODF using conservation laws [7]. Conventional solution schemes are based upon representation of the ODF using a series of harmonics [8–10] or finite elements [11–13]. The ODF representation is extremely compact in comparison to discretized microstructures used in CPFE, leading to significant speed up in microstructure analysis. However, ODF representation does not contain information about the local neighborhood of crystals. Thus, equilibrium across grain boundaries cannot be captured and a Taylor assumption ([14], where all crystals deform identically) is used. Such a constraint leads to a stiff upper bound stress response, textures that are sharper than measured and texture components that cannot be captured [15].

The next level of descriptors, the two–point orientation correlation function (OCF), $\mathcal{F}(\boldsymbol{g}', \boldsymbol{g}, \boldsymbol{r})$, gives the probability density of finding orientations $\boldsymbol{g}'$ and $\boldsymbol{g}$ at the end points of a randomly placed vector $\boldsymbol{r}$ within the microstructure. This descriptor contains neighborhood information and holds the promise of modeling grain equilibrium, thereby relaxing the Taylor assumption. Representations of the OCF in the form of global approximations (exponentially decaying functions based on the Corson's model [16,17] and Fourier space representations [18]) and local approximations (based on finite elements, [19]) have been studied

* Corresponding author. Tel.: +1 734 615 7242; e-mail: veeras@umich.edu

http://dx.doi.org/10.1016/j.actamat.2015.04.016
1359-6462/

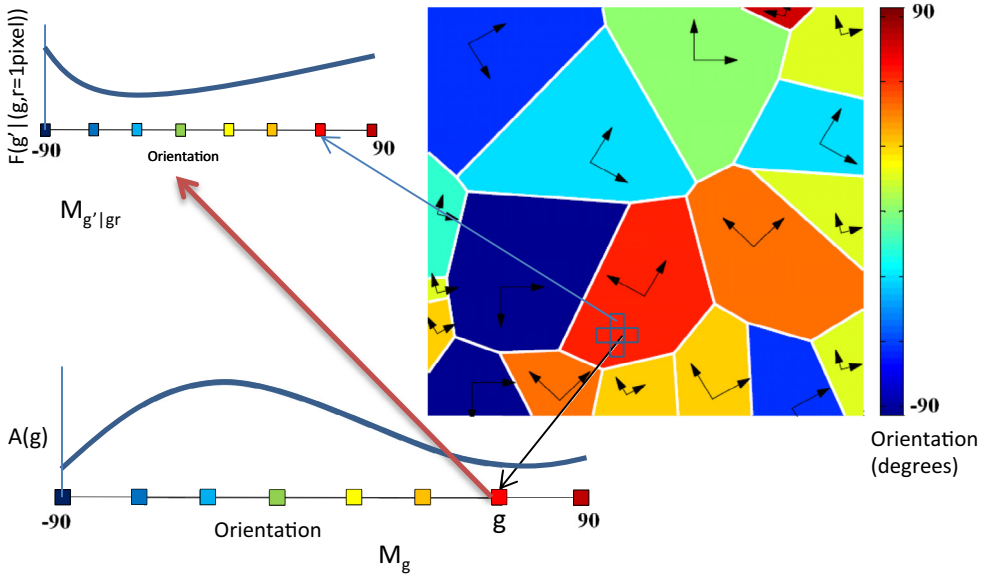

Fig. 1. NNOCF sampling from a microstructure (color coded based on grain orientation). The finite element mesh M_g represents the volume density of each orientation (color). The NNOCF mesh $M_{g'|gr}$ attached to a node g in mesh M_g represents orientation distribution for the nearest neighbor pixels of g. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

in the past. However, the two-point measure is high dimensional (e.g. OCF for a 3D FCC polycrystal is nine dimensional) and there is still a significant need for reduced representations.

Considerable improvements in OCF representation can be realized by including the physics of deformation processes. For example, in viscoplastic self consistent (VPSC) schemes, Green's function models the interaction between crystals [20,21]. The function decays with distance and can be used to estimate a cut-off radius beyond which correlation information is redundant [19]. However, this radius may encompass several grains and storage requirements are still significant. In this paper, we recognize that the nearest neighbor pixels (situated near the singularity of the Green's function) carry most of the grain interaction information. We explore the use of a conditional OCF ($\mathcal{F}(\boldsymbol{g}'|\boldsymbol{g},\boldsymbol{r})$) truncated to the nearest neighbors, hereafter called the nearest neighbor conditional orientation correlation function (NNOCF). The descriptor is extremely compact and we show that it can be used to locally enforce equilibrium (in an average sense) for each orientation using a novel finite differencing scheme. The present model significantly enhances the scope of our previous probabilistic model published in this journal [13], through addition of crystal neighborhood effects on texture development. The model is explained in Section 2. To show the relevance of this work to the material community, we have performed comparison of our new approach to verified crystal plasticity finite element codes of Refs. [13,22] in Section 3 and show testable predictions in cases where Taylor models fail and the use of two–point correlations resolves the problem. The discussion and conclusions are presented in Section 4.

2. Probabilistic representation

The complete orientation space of a polycrystal can be reduced to a smaller subset, called the fundamental region, as a consequence of crystal symmetries. Within the fundamental region, each crystal orientation is represented uniquely by a coordinate $\boldsymbol{g}$, the parametrization for the rotation (eg. Euler angles, Rodrigues vector [23]). The ODF, represented by $\mathcal{A}(\boldsymbol{g})$, describes the local density of crystals over the fundamental region. Consider a region R_δ which is a ball of radius δ centered at orientation $\boldsymbol{g}$ in the fundamental region. Let $v_f(R_\delta)$ be the volume fraction of crystals that have orientations that occur within volume R_δ. The ODF at an orientation $\boldsymbol{g}$ is defined as:

$$\mathcal{A}(\boldsymbol{g}) = \lim_{\delta\to 0} \frac{v_f(R_\delta)}{\int_{R_\delta} d\boldsymbol{g}} \tag{1}$$

The ODF is represented in this work over a finite element mesh (M_g) of the fundamental region. The ODF at any given orientation can be obtained by interpolating the nodal values of the element containing that orientation.

The nearest-neighbor conditional orientation correlation function (NNOCF), $\mathcal{F}(\boldsymbol{g}'|(\boldsymbol{g},\boldsymbol{r}))$, gives the probability density of occurrence of an orientation $\boldsymbol{g}'$ at the end point of a vector $\boldsymbol{r}$ (of one pixel length) emanating from a given orientation $\boldsymbol{g}$ (Fig. 1). The NNOCF is also represented in the FE discretized fundamental region (called mesh $M_{g'|gr}$, Fig. 1). In a 2D model of the microstructure (Fig. 1), four such meshes are needed at every node point in M_g corresponding to the four nearest neighbor pixels. The NNOCF satisfies the following conservation equations at all times during deformation[1]:

$$\begin{aligned} &\int \mathcal{F}(\boldsymbol{g}'|(\boldsymbol{g},\boldsymbol{r}))d\boldsymbol{g}' = 1, \mathcal{F}(\boldsymbol{g}'|(\boldsymbol{g},\boldsymbol{r})) \geqslant 0 \\ &\int \mathcal{A}(\boldsymbol{g}')d\boldsymbol{g}' = 1, \mathcal{A}(\boldsymbol{g}') \geqslant 0 \end{aligned} \tag{2}$$

In addition to the above constraints, the orientation space corresponding to all possible $\boldsymbol{g}$'s must satisfy the crystallographic symmetries of the chosen system (FCC,

[1] The OCF also satisfies the r-interdependence equation as described in [19]. However, due to lack of information beyond the nearest neighbors, such a constraint cannot be enforced in this work.