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A virtual environment for the interrogation of 3D polycrystalline microstructures including grain size effects

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ABSTRACT

A finite element analysis of the large deformation of three-dimensional polycrystals is presented using pixel-based finite elements as well as finite elements conforming with grain boundaries. The macroscopic response is obtained through volume-averaging laws. A constitutive framework for elasto-viscoplastic response of single crystals is utilized along with a fully-implicit Lagrangian finite element algorithm for modeling microstructure evolution. The effect of grain size is included by considering a physically motivated measure of lattice incompatibility which provides an updated shearing resistance within grains. A domain decomposition approach is adopted for parallel computation to allow efficient large scale simulations. Conforming grids are adopted to simulate flexible and complex shapes of grains. The computed mechanical properties of polycrystals are shown to be consistent with experimental results for different grain sizes.

1. Introduction

Material properties of polycrystalline materials are highly dependent on the underlying microstructural features. Quantitative description of plastic flow by crystallographic slip is a long standing problem in microstructure evolution theories [1]. The thermo-mechanical description of polycrystals is usually based on analysis on the macro- and meso-scales. The macro-scale is associated with the homogenized continuum and the meso-scale is characterized by the underlying microstructure. Since rate-dependent methods are computationally intensive, recent work emphasizes the use of rate-independent models [1,2]. Taylor-type transition models have been considered extensively [3–6] by assuming that all grains are subjected to the same deformation. This assumption satisfies compatibility but fails to account for equilibrium across grain boundaries. It poses a stringent kinematic constraint on the grains and thus provides a stiff response. The anisotropic response of the grains to the deformation is not taken into account in the Taylor model. In order to correct this inaccuracy, the overall response of the microstructure at the macro-scale is derived in this work on the basis of homogenization [7], which assumes homogeneous deformation on the boundaries of the microstructure while allowing for non-uniform deformation within the microstructure [8]. This approach is further improved here to allow interrogation of complex 3D microstructures using single crystal constitutive models [9] and mechanical property calculation through volume-averaging laws.

While the homogenization method allows for heterogeneous deformation inside the microstructure, it does not include the effect of the interactions between neighboring grains. In single crystal and polycrystalline materials exposed to plastic deformation, a dominant source of resistance to deformation is the dislocation density. The evolution of dislocation density is controlled by an additive combination of an athermal hardening component and a dynamic recovery component [10]. In continuum theory of crystal plasticity [11–14], the lattice is assumed to distort only elastically though generally elastic deformation is not compatible with single-valued displacement field. Thus, lattice incompatibility is characterized by the elastic component of the deformation gradient [15]. Grain size effect is included by considering the lattice incompatibility which is closely related to the dislocation density in the grains. In recent work [15–19], a grain size effect model based on

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dislocation density was developed for mechanical response simulation. We follow a similar approach here with some distinct differences: (a) a rate-independent model is used to accelerate the computational efficiency of the methodology, (b) Voronoi tessellation techniques are implemented for modeling of realistic microstructures with finite elements that conform with grain boundaries instead of pixel elements that are assigned orientations to mimic grains, (c) we simulate varying mean sizes of grains by adjusting the number of grains in a fixed region rather than changing the size of the calculation region, and (d) this work includes the elastic component of the deformation gradient and models incompatibility effects at initial yield and the major portion of the elasto-plastic transition [17]. To allow efficient interrogation of realistic 3D polycrystalline microstructures, domain decomposition algorithms are also considered.

The structure of the paper is as follows: Section 2 introduces the homogenization method and Section 3 provides a summary of the constitutive model considered. The grain size model is reviewed in Section 4. The results obtained from the present computational framework are summarized in Section 5, where both numerical results and experimental data from the literature are used to verify the methodology. The paper concludes in Section 6 with a summary of the developments.

2. Microstructure homogenization method

The approach adopted here for interrogation of microstructures involves finite element based elasto-viscoplastic analysis of microstructures using a constitutive model derived from the continuum slip theory. In this section, the microstructure interrogation and property evaluation scheme is systematically developed using the theory of non-linear homogenization.

Let $\boldsymbol{y}:\mathscr{B}_{\text{ref}}\to\mathscr{B}$ represent the non-linear deformation map of the microstructure at time t, and $\boldsymbol{F}=\nabla_{\text{ref}}\boldsymbol{y}$ the associated tangent map (Fig. 1). $\boldsymbol{F}$ maps points $\boldsymbol{Y}\in\mathscr{B}_{\text{ref}}$ onto points $\boldsymbol{y}(\boldsymbol{Y},t)$ of the current configuration $\mathscr{B}$. The reference microstructure configuration is considered of volume $V(\mathscr{B}_{\text{ref}})$ and boundary $\partial\mathscr{B}_{\text{ref}}$ with outward normal $\boldsymbol{N}$. The microstructure at time t of volume $V(\mathscr{B})$ and boundary $\partial\mathscr{B}$ with outward normal $\boldsymbol{n}$ is attached to the material point $\boldsymbol{X}$ in the macro-continuum. Further, we use superposed bars (e.g. $\overline{\boldsymbol{F}}$) to denote homogenized quantities and angular brackets (e.g. $\langle\boldsymbol{F}\rangle$) to denote volume-averaged quantities.

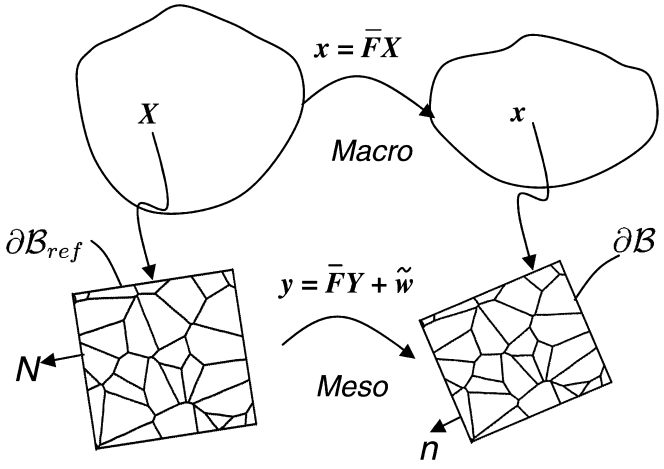

Fig. 1. The microstructure homogenization technique: each integration point in the macro-continuum is associated with an underlying microstructure. The microstructure reference configuration ($\mathscr{B}_{\text{ref}}$) and the mapping to the present microstructure configuration ($\mathscr{B}$) are shown in contrast with the homogenized macro-continuum.

The deformation gradient at the macro-scale is represented purely in terms of the motion of the exterior boundary of the microstructure [7]

$$\overline{\boldsymbol{F}}=\frac{1}{V(\mathscr{B}_{\text{ref}})}\int_{\partial\mathscr{B}_{\text{ref}}}\boldsymbol{y}\otimes\boldsymbol{N}\,\mathrm{d}A. \tag{1}$$

The deformation of the microstructure is then related to the homogenized deformation gradient in the macro-continuum based on the assumption

$$\boldsymbol{y}=\overline{\boldsymbol{F}}\boldsymbol{Y}+\tilde{\boldsymbol{w}}, \tag{2}$$

where the deformation consists of a homogeneous part $\overline{\boldsymbol{F}}\boldsymbol{Y}$ and an inhomogeneous part $\tilde{\boldsymbol{w}}$ referred to as the fluctuation field. As a consequence, we have the relationship, $\boldsymbol{F}=\overline{\boldsymbol{F}}+\tilde{\boldsymbol{F}}$ (with $\tilde{\boldsymbol{F}}=\nabla\tilde{\boldsymbol{w}}$) between the microscopic ($\boldsymbol{F}$) and the macroscopic ($\overline{\boldsymbol{F}}$) deformation gradients. From the homogenization law (Eq. (1)) and the decomposition described above, it can be shown that the superposed field $\tilde{\boldsymbol{w}}$ follows the equation:

$$\frac{1}{V(\mathscr{B}_{\text{ref}})}\int_{\partial\mathscr{B}_{\text{ref}}}\tilde{\boldsymbol{w}}\otimes\boldsymbol{N}\,\mathrm{d}A=0. \tag{3}$$

This is satisfied by homogeneous deformation on the boundaries of the microstructure while allowing for non-uniform deformations within the microstructure.

To macroscopic Cauchy stress $\overline{\boldsymbol{T}}$ is taken as a volume-averaged (in the current configuration) of the microstructural counterpart $\boldsymbol{T}$ as follows:

$$\overline{\boldsymbol{T}}=\langle\boldsymbol{T}\rangle=\frac{1}{V(\mathscr{B})}\int_{V(\mathscr{B})}\boldsymbol{T}\,\mathrm{d}V. \tag{4}$$

Alternative stress averaging laws are discussed in [8]. Finally, the equivalent stress for the microstructure in terms of the deviatoric average stress $\overline{\boldsymbol{T}}'$ is computed as

$$\bar{\sigma}_{\text{eff}}=\sqrt{\frac{3}{2}\overline{\boldsymbol{T}}'\cdot\overline{\boldsymbol{T}}'}. \tag{5}$$

A multiplicative decomposition, $\boldsymbol{F}=\boldsymbol{F}^{\text{e}}\boldsymbol{F}^{\text{p}}$, is used, where $\boldsymbol{F}^{\text{e}}$ and $\boldsymbol{F}^{\text{p}}$ are the micro-scale elastic and plastic deformation gradients, respectively. A total Lagrangian approach is utilized. An equilibrium state of the microstructure at a certain stage of the deformation process is then assumed with the equations

$$\nabla_{\text{ref}}\cdot\boldsymbol{P}=0\quad\text{in}\quad\mathscr{B}_{\text{ref}}, \tag{6}$$

$$\boldsymbol{P}^{T}N=\boldsymbol{p}\quad\text{on}\quad\partial\mathscr{B}_{\text{ref}}. \tag{7}$$

The Newton Raphson method is adopted to solve the deformation governing equation. The total Lagrangian algorithm is adopted as follows:

$$\int_{\mathscr{B}_{\text{ref}}}\mathrm{d}\boldsymbol{P}_{ik}\frac{\partial\tilde{\boldsymbol{u}}_i}{\partial\boldsymbol{X}_k}\mathrm{d}V=-\int_{\mathscr{B}_{\text{ref}}}\boldsymbol{P}_{ik}\frac{\partial\tilde{\boldsymbol{u}}_i}{\partial\boldsymbol{X}_k}\mathrm{d}V. \tag{8}$$

The tangent moduli (effectively the relation between $\mathrm{d}\boldsymbol{P}$ and $\mathrm{d}\boldsymbol{u}$) are computed from the linearization of the constitutive model. The derivation of the tangent moduli follows similar calculations as in [8].

The equivalent strain is computed with the volume-averaged of the plastic deformation rate following the constitutive laws originally developed in [9]. The plastic velocity gradient is defined as

$$\boldsymbol{L}^{\text{p}}=\dot{\boldsymbol{F}}(\boldsymbol{F}^{\text{p}}_{n})^{-1}. \tag{9}$$

The deviatoric part is

$$\boldsymbol{D}^{\text{p}}=\text{sym}(\boldsymbol{L}^{\text{p}})-\frac{1}{3}\text{tr}(\boldsymbol{L}^{\text{p}})\boldsymbol{I}. \tag{10}$$

So the average plastic rate of deformation is