ACTA MECHANICA SOLIDA SINICA 000 (2017) 1–13

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Simulation of plastic deformation induced texture evolution using the crystallographic homogenization finite element method☆

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ARTICLE INFO

Article history:
Received 22 June 2016
Revised 17 October 2016
Accepted 18 October 2016
Available online xxx

Keywords:
Homogenization
Local periodicity
Crystalline plasticity
Texture
Finite element

ABSTRACT

A semi-implicit elastic/crystalline viscoplastic finite element (FE) method based on a "crystallographic homogenization" approach is formulated for a multi-scale analysis. In the formulation, the asymptotic series expansion is introduced to define the displacement in the micro-continuum. This homogenization FE analysis is aimed at predicting the plastic deformation induced texture evolution of polycrystalline materials, the constituent microstructure of which is represented by an assembly of single crystal grains. The rate dependent crystal plasticity model is adopted for the description of microstructures. Their displacements are decomposed into two parts: the homogenized deformation defined in the macro-continuum and the perturbed one in the micro-continuum. This multi-scale formulation makes it possible to carry out an alternative transition from a representative micro-structure to the macro-continuum. This homogenization procedure satisfies both the compatibility and the equilibrium in the micro-structure. This developed code is applied to predict the texture evolution, and its performance is demonstrated by the numerical examples of texture evolution of FCC polycrystalline metals.

1. Introduction

Polycrystalline solid materials consisting of a multitude of individual crystallites or grains after large plastic deformation generally demonstrate a certain degree of anisotropy in material properties, which is a natural reflection of the crystallographic texture induced by the reorientation of crystal lattices towards a preferential distribution orientation. The experimental determination, interpretation [1, 2] and the numerical simulation for texture analysis have been attracting the attention of researchers in the field of materials science and applied mechanics [3]. On the one hand, recent advances in experiment techniques, such as EBSD [4], have made it possible to measure the texture more efficiently and accurately than the traditional X-ray diffraction method does; on the other hand, the rapid development of computer technology promises an unprecedented means for the large scale numerical simulation of materials deformation process and design, which is, however, essentially dependent on the constitutive model and the numerical techniques.

Polycrystal plasticity models [5–9] were employed to predict the texture evolution induced by plastic deformation and the corresponding plastic anisotropy. In these simulations, the assumption is made that the microstructure of polycrystals is represented by an aggregate of microscopic crystals, whose plastic deformation is brought about by the shearing along crystallographic planes, and whose individual responses, on

☆ Project supported by NSFC (11272129, 11472114, 51175202).
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http://dx.doi.org/10.1016/j.camss.2016.10.002
0894-9166/

Please cite this article as: Y.P. Chen, Y.Y. Cai, Simulation of plastic deformation induced texture evolution using the crystallographic homogenization finite element method, Acta Mechanica Solida Sinica (2017), http://dx.doi.org/10.1016/j.camss.2016.10.002

average, determine the overall macroscopic response of polycrystals. Two ingredients are indispensable for the establishment of these models: one is the constitutive equations used to describe the mechanical behaviors of a single crystal; the other is the mean field hypothesis or averaging schemes that relate the overall response of polycrystals to that of the constituent single crystals by a micro-macro-transition on the basis of homogenization procedures. The commonly adopted averaging schemes include the Taylor-type model, in which each crystal is assumed to experience identical macroscopic deformation and the stress of polycrystal aggregate is calculated by averaging the crystal stress, the equilibrium-based schemes require the same stress state for each grain, and the aggregate deformation is obtained by averaging the crystal deformation. In addition to these averaging procedures, Miehe [10,11] established two different homogenization schemes which attached the macro-continuum locally with a polycrystalline micro-structure made up of single crystal grains. The boundary of the micro-structure was specified by the local deformation of the macro-continuum with three alternative deformation constraints: (i) zero fluctuation in the domain (Taylor-type assumption), (ii) zero fluctuation on the boundary, and (iii) periodic fluctuation on the boundary, making improvements to the Taylor-type models. It seems that these two approaches were the first to have applied homogenization method to the prediction of texture evolution and strain localization in crystalline materials.

Homogenization based on the multi-scale asymptotic series expansion of field variables has been utilized as an effective numerical technique over the last three decades to describe the mechanical behaviors of real heterogeneous materials by taking into account the length scale difference between macrostructures and individual microstructure components [12,13]. The advantage of this method lies in the fact that it is a rigorous mathematical theory and is capable of characterizing equivalent mechanical properties of composite materials and at the same time determining their dependence on different constituent components. It has been employed successfully to solve the problems of both finite elasticity [14] and elasto-plasticity [15]. In the homogenization theory, it is generally assumed that the composite material is locally formed by the spatial repetition of very small microstructures, i.e. the microscopic cells, when compared with the overall macroscopic dimensions of the structure of interest. In other words, it is assumed that the materials properties are periodic functions of the microscopic variables, where the period is very small compared with the macroscopic variables. This assumption enables the computation of equivalent material properties by a limiting process when the size of microscopic cell is reduced to zero. It can also provide a reasonable solution for some problems where the experimental data are not available, or for which only bounds for the equivalent material contents can be found by other theories. The basic theory of homogenization method can be found in the papers published in 1970s and early 1980s, for instance, by Babuska [16], Sanchez-Palencia [17], Bakhvalov and Panasenko [18] and many other applied mathematicians. Guedes and Kikuchi [19] developed a new formulation of this method in a weak form and provided a guideline for numerical analysis.

The purpose of the present paper is to establish a homogenization framework based on the two-scale asymptotic expansion of field variables to simulate the texture evolution in polycrystalline materials. A recapitulation of crystalline constitutive equations for characterizing single crystal grains is first presented and then followed by the derivation of governing equations for solving homogenized macro-deformation and characteristic displacements for micro-models to evaluate the homogenized material properties, respectively, from the virtual power principle. The proposed formulation is implemented in the updated Lagrangian finite element form and the performance of the code is demonstrated by the numerical examples of texture evolution in polycrystalline materials.

2. Formulation of the problem

We consider a general infinite polycrystalline body, Ω^ε, in two dimensional space, as seen in Fig. 1. It is assumed that the material is formed by a spatial repetition of a microstructure at least locally, and therefore, the microstructure is usually called a unit cell. The region, Y, of the unit cell (microstructure) is made up of an aggregate of well defined crystal grains and is very small compared with the overall region Ω^ε by an order of $\varepsilon \ll 1$, which also represents the reciprocal order of the repetition. In order to describe the effects of heterogeneity in the microstructures, we attach ε as a superscript to all the variables in the formulation when it is essential. We also introduce both microscopic and macroscopic coordinate systems, so that physical quantities are represented by two different length scales: one is x representing the macroscopic region, Ω; and the other is $y = x/\varepsilon$ standing for the microscopic one, Y. The summation convention is used and the dot over a variable denotes material time derivative.

2.1. *Kinematics of crystal plasticity*

We recapitulate the rate-dependent crystal plasticity constitutive model to describe the elasto-plastic deformation of constituent single crystals (Fig. 2). For details, we refer to the work of Asaro and Needleman [7]. The total deformation of a crystallite is assumed to be the result of two distinct physical mechanisms: crystallographic slip due to dislocation motion on the active slip systems, and elastic lattice distortion. FCC crystals are considered to have the usual $\{111\}\langle 110\rangle$ slip systems, where the slip planes are the $\{111\}$ crystallographic planes with normals $\boldsymbol{m}$, and the $\langle 110\rangle$ directions are the shear directions with slip vectors $\boldsymbol{s}$. Plastic deformation of the crystal is understood to occur as a set of simple plastic shear along various slip systems, having the lattice and the slip systems' vectors $(\boldsymbol{s}^{(\alpha)}, \boldsymbol{m}^{(\alpha)})$ not only essentially undistorted, but also unrotated (the brackets in the superscripts (α) indicate that α is not a tensor index and ranges from one to the number of slip systems). Next, the materials and lattice are considered to deform elastically and rotate rigidly from the physically deformed state to the current configuration.

Accordingly, the decomposition for the deformation gradient tensor is

$$F_{ij} = F^*_{ik} F^p_{kj} \tag{1}$$

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