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Spectral methods for capturing crystallographic texture evolution during large plastic strains in metals

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Abstract

About two decades ago, Bunge and Esling [Scripta Metall 1984; 18: 191–5] put forth a novel concept for capturing and simulating crystallographic texture evolution during large plastic strains on metals using an efficient spectral representation of the orientation distribution function. Although this methodology indicated promise, it was never evaluated critically by these authors, possibly because of the high demands it placed on computational resources. In this paper, the Bunge and Esling concept is revisited and evaluated critically for the first time for a range of deformation processes and starting textures. It is demonstrated that this technique is indeed potentially capable of providing good predictions, especially when the higher order terms in the Fourier expansion are included in the analysis.

Keywords: Texture evolution; Crystal plasticity; Spectral method; Rolling textures; Orientation distribution function

1. Introduction

The Taylor model and its extensions are widely used in the current literature for modeling crystallographic texture evolution during large plastic strains, and have been demonstrated to provide good predictions in single phase, medium to high stacking fault energy, cubic metals [2–11]. Although the Taylor model and the associated crystal plasticity theories have enjoyed major successes in their ability to predict plastic behavior of metals at various length scales, they are not yet widely used in the engineering design enterprise. The main factor hindering the much wider use of these models is the high computational cost associated with them; the requirement for high computational resources persists in spite of the successful development and implementation of very efficient numerical schemes for these calculations. Consequently, there are several ongoing efforts in current literature to develop novel techniques that would possess the predictive capabilities of the Taylor-type model, but would require significantly less computational resource [12–15]. In many of these approaches, the underlying physics governing the evolution of the crystallographic texture in deformation processes continues to be provided by the Taylor-type model (actually the proposed methods are often calibrated with the Taylor-type model to ensure good agreements). The goal of these efforts is to capture the results of the Taylor-type model in efficient databases that might require a one-time high computational cost, but once these are accomplished, the actual predictions can then be obtained with minimal computational cost.

This paper focuses on the concept proposed originally by Bunge and Esling [1], which uses spectral representation of crystallographic texture. In this method, the

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texture in the sample is represented as a probability density function, commonly referred to as the orientation distribution function (ODF) [16]:

$$\frac{dN}{N} = f(g)dg. \tag{1}$$

In Eq. (1), $f(g)$ represents the ODF, g denotes the crystal orientation (often expressed by a set of three Euler angles called Bunge's Euler angles [16]; $g = [\phi_1, \Phi, \phi_2]$), and dN/N represents the probability of finding an orientation in a small neighborhood of g, characterized by dg, in a random trial. Note that the definition of ODF is normalized such that $\oint f(g)dg = 1.0$. Since $f(g)$ is a continuous function, it can be represented in a Fourier series [16]:

$$f(g) = \sum_{l=0}^{\infty} \sum_{\mu=1}^{M(l)} \sum_{\nu=-l}^{N(l)} F_l^{\mu\nu} \dddot{T}_l^{\mu\nu}(g). \tag{2}$$

In Eq. (2), $F_l^{\mu\nu}$ represent the Fourier coefficients and $\dddot{T}_l^{\mu\nu}(g)$ denote a complete set of orthonormal basis functions (also referred to as generalized spherical harmonics) that automatically reflect the associated crystal and sample symmetries. In particular, the three dots on the spherical harmonic functions shown here imply cubic crystal symmetry (e.g., face-centered cubic, body-centered cubic metals) and orthorhombic sample symmetry (e.g., deformation processes such as rolling, cross-rolling, simple compression, simple tension). The functions $M(l)$ and $N(l)$ denote the number of terms needed in the enumeration of indices μ and ν; these numbers are a function of the index l and are determined by material and sample symmetries [16]. In order to keep things simple in this first comprehensive investigation into the validity of the Bunge–Esling approach [1], we have restricted the present study to considerations of only those deformation processes that inherently retain orthorhombic sample symmetry. The extension of this method to other deformation processes (e.g., rotations, shear deformation modes) requires the use of cubic-triclinic functions, $\dot{T}_l^{\mu\nu}(g)$, in place of the cubic-orthorhombic functions, $\dddot{T}_l^{\mu\nu}(g)$, used in the present study.

Utilizing the representations described above together with a framework proposed by Clement and Coulomb [17] for representation of crystal lattice rotations as a vector flow field in an Eulerian angle space, Bunge and Esling [1] derived the following simple relation to represent the evolution of texture in a given deformation process (with a prescribed macroscopically imposed velocity gradient tensor):

$$\frac{dF_l^{\mu\nu}}{d\eta} = \sum_{\lambda=0}^{\infty} \sum_{\sigma=1}^{M(\lambda)} \sum_{\rho=1}^{N(\lambda)} \tilde{A}_{l\lambda}^{\mu\nu\sigma\rho} F_{\lambda}^{\sigma\rho}. \tag{3}$$

In Eq. (3), η is an appropriate metric of the deformation process (for example, for rolling η could represent the compressive strain), and the coefficients $\tilde{A}_{l\lambda}^{\mu\nu\sigma\rho}$ are constant for a given deformation process independent of the crystal lattice orientation. Following the original derivation of Eq. (3) by Bunge and Esling [1], one can recognize that the coefficients $\tilde{A}_{l\lambda}^{\mu\nu\sigma\rho}$ are essentially Fourier coefficients in the spectral representation of the texture flow field in the orientation space for a given deformation process. As with any spectral representation, one can indeed write an analytical expression for these coefficients. However, as remarked by Bunge and Esling [1], the derivation of an analytical expression for $\tilde{A}_{l\lambda}^{\mu\nu\sigma\rho}$ requires the use of tedious calculus involving field theory and Clebsch–Gordon coefficients. To circumvent this challenge, Bunge and Esling [1] suggest that the coefficients $\tilde{A}_{l\lambda}^{\mu\nu\sigma\rho}$ be established numerically for a specified deformation process by calibrating Eq. (3) with predictions from a Taylor-type model for a large number of single crystal orientations. The calibration procedure suggested by these authors is essentially a linear regression analysis to find the coefficients $\tilde{A}_{l\lambda}^{\mu\nu\sigma\rho}$ by minimizing the error in Eq. (3) for a very large number of single crystal orientations, for a given deformation process. Although they describe this numerical approach for the computation of $\tilde{A}_{l\lambda}^{\mu\nu\sigma\rho}$ in detail, they actually do not report performing such a calculation or any results of such a calculation. They specifically cite that for expansions of the Fourier series to include terms up to $l = 22$ (see Eq. (2)), one would need to handle 185 $F_l^{\mu\nu}$ terms[1] and 34,225 (=185^2) independent $\tilde{A}_{l\lambda}^{\mu\nu\sigma\rho}$ terms. This is because the number of $\tilde{A}_{l\lambda}^{\mu\nu\sigma\rho}$ coefficients in Eq. (3) increases as the square of the number of $F_l^{\mu\nu}$ terms desired in the representation of texture. Implicitly, if one was to establish the numerical values of 34,225 $\tilde{A}_{l\lambda}^{\mu\nu\sigma\rho}$ coefficients (note that these are fully coupled through Eq. (3)) using regression analysis, one would have to invert a $34{,}225 \times 34{,}225$ square matrix – a formidable task even for today's computers.

In this paper, we report for the first time a critical evaluation of the Bunge and Esling concept. Here, we have included the terms in the Fourier expansion up to $l = 17$, resulting in 83 independent $F_l^{\mu\nu}$ terms and 6972 (=83^2) independent $\tilde{A}_{l\lambda}^{\mu\nu\sigma\rho}$ terms. It should be noted that there are substantial differences between this work and the recent work of Li et al. [13], who have also addressed this problem by extending the original approach described by Bunge and Esling [1]. Our two groups have enjoyed a long history of collaboration, and in this research we have adopted two different approaches. The main differences between our two approaches are:

[1] Because of crystal and sample symmetries, certain of the $F_l^{\mu\nu}$ coefficients are always zero. So these can be skipped, reducing the number of non-zero terms that need to be handled in these calculations.