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Procedures for reducing large datasets of crystal orientations using generalized spherical harmonics

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ABSTRACT

We present a rigorous methodology for the compaction of crystallographic texture data associated with a given material volume and show that a statistical orientation distribution function (ODF) containing any number of orientations can be compacted to a significantly smaller but representative set of orientations. This methodology is based on the spectral representation of ODFs through the use of generalized spherical harmonic functions. The Fourier coefficients of an initial full-size ODF can be matched with those of a more compact but equivalent ODF. The reduced-size ODF contains a predetermined set of representative orientations whose weights are adjusted using an algorithm for finding the closest reduced-size ODF to a given full-size ODF. To demonstrate the accuracy of the methodology, we consider three measured ODFs of two cubic metals (pure Cu and an Al alloy) and a hexagonal metal (pure Zr) and then subsequently perform plane strain and simple compression simulations with both the initial ODFs and the reduced-size ODFs. We quantitatively demonstrate that texture evolution and stress–strain response simulated with reduced-size ODFs are in excellent agreement with those simulated with initial full-size ODFs.

1. Introduction

Crystallographic texture (also called the orientation distribution function, or the ODF) is an important feature of the microstructure in polycrystalline materials known to have a strong influence on the anisotropy of various material properties (Adams and Olson, 1998; Bhattacharyya et al., 2015; Bunge, 1993; Fromm et al., 2009; Fuentes-Cobas et al., 2013; Jahedi et al., 2014; Knezevic et al., 2014a; Kocks et al., 1998). Therefore, anisotropic material models must consider the distribution of crystal orientations. In particular, modeling the anisotropy of plastic properties requires consideration of the crystal structure and orientation because of their roles in the activation of micro-scale deformation mechanisms (Taylor, 1938). A number of polycrystal plasticity material models have been developed to predict material response based on the crystallography of deformation mechanisms and the distribution of crystal orientations. These models are classified based on the homogenization scheme that links the grain scale response to the response of a polycrystalline aggregate to the mean-field models of self-consistent (Lebensohn and Tomé, 1993; Lebensohn et al., 2007) and Taylor type (Knezevic et al., 2008a; Taylor, 1938; Van Houtte et al., 2004) and the full-field models of finite-element (FE) (Kalidindi et al., 1992; Knezevic et al., 2014c; Roters et al., 2010) and Green's function fast Fourier transform (FFT) type (Lebensohn et al., 2012). Since they are physically based and able to capture the evolution of the crystallographic texture, these models are important for understanding microstructural

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processes and associated effects on plasticity (Asaro and Needleman, 1985; Roters et al., 2010). As such, they are also highly desirable for performing accurate simulations of metal forming processes. Example applications include simple compression and tension tests (Beaudoin et al., 1993; Knezevic et al., 2012b), bending (Knezevic et al., 2013c,d,e), cup-drawing (Balasubramanian, 1996; Raabe and Roters, 2004), sheet hydroforming (Beaudoin et al., 1994), and bulk forming (Jahedi et al., 2015a; Knezevic et al., 2014d; Kumar and Dawson, 1995; Zecevic et al., 2015b). However, performing complex metal forming process simulations with polycrystal plasticity is recognized as a vast computational challenge because of the need for (1) specialized Newton–Raphson iterative schemes to solve sets of highly non-linear, extremely stiff constitutive equations with poor convergence characteristics for every constituent crystal at every material point and at each trial time increment and (2) storing large sets of state variables related to texture data. For example, the computational time involved in simulating a simple compression up to a strain of 0.2 with about 1000 elements and 1000 grains at an integration point is approximately 60 h on a regular PC (Knezevic et al., 2013d). Clearly, speedups are necessary to render metal forming simulations with polycrystal plasticity constructive laws practical.

From the numerical implementation point of view, several strategies have been explored to speed up the polycrystal plasticity calculations. Database approaches that store precompiled solutions in the form of spectral coefficients of the generalized spherical harmonics (GSH) basis (Kalidindi et al., 2006; Knezevic et al., 2008b; Shaffer et al., 2010; Wu et al., 2007) and the fast Fourier transform bases (Al-Harbi et al., 2010; Knezevic et al., 2009; Zecevic et al., 2015a) improved the speed for about two orders of magnitude. A process plane concept, based on proper orthogonal decomposition in Rodrigues–Frank space, has been presented in Sundararaghavan and Zabaras (2007). Other attempts to improve efficiency of the polycrystal plasticity codes rely on adaptive sampling algorithms and building a database that constantly updates itself (Barton et al., 2011, 2008). The latter methods improved the speed by about an order of magnitude. It has recently been shown that solving polycrystal plasticity using the Jacobian-Free Newton–Krylov (JFNK) technique in place of the Newton–Raphson method can yield some computational benefits (Chockalingam et al., 2013). Recently, we have successfully developed a high performance computational application of the databases approach containing discrete Fourier transforms that runs on graphic processing units (GPUs) (Mihaila et al., 2014). We have also developed an improved version that has the advantage of an efficient GPU8 algorithm for matrix–matrix multiplication (Knezevic and Savage, 2014). The latter implementation resulted in a major improvement in computational speed, exceeding three orders of magnitude over the conventional numerical schemes.

Because the computational time involved in crystal plasticity calculations scale linearly with the number of crystal orientations, the numerical schemes summarized above can further benefit from the data compaction technique aimed at minimizing the amount of state variables related to texture data. Experimental techniques for acquisition of texture data produce data sets consisting of large numbers of single crystal orientations (Jahedi et al., 2015b; Knezevic et al., 2010; Lentz et al., 2015a,b). The use of such large discrete single crystal orientations in subsequent crystal plasticity simulations is not practical, and we will show not necessary for capturing plastic anisotropy and concomitant evolution of texture. We develop a procedure for the reduction of texture data described in the form of statistical distributions (ODFs) to a level of computationally manageable but representative statistical distributions where qualitatively and quantitatively sufficient details can be recovered without losing any physical significance. The developed procedure is independent on techniques used to determine the measured full-size ODFs. The techniques for measuring ODF are broadly classified according to whether they measure macro-texture or micro-texture. The former includes X-ray diffraction (XRD) and neutron diffraction while the latter is based on electron backscattered diffraction (EBSD).

Quantitatively an ODF can be expressed by a weighted set of discrete orientations. To this end, a fundamental problem is determining a statistically significant set of discrete orientations. A number of studies for estimating the minimum number of crystal orientations representing an ODF have been conducted in the past (Baudin et al., 1995; Baudin and Penelle, 1993; Pospiech et al., 1994; Wright and Adams, 1990). The most promising methodology was based on an appropriately defined error difference between a macroscopically measured ODF and an ODF constructed from experimentally measured individual grain orientations (Baudin et al., 1995; Pospiech et al., 1994). The number of orientations in the constructed ODF was systematically increased until the error was minimized ensuring that the newly constructed ODF is statistically significant. The estimated number of orientations varied with a given ODF. Part of the reason for this variation is because weights of individual orientations were not adjusted.

The procedure developed in this paper is based on the spectral representation of ODFs using the GSH bases. A given ODF containing any number of orientations is represented by corresponding Fourier coefficients as a point in an infinite-dimensional Fourier space. We refer to this point as the target point, or the full-size target ODF. We recognize that the Fourier coefficients of the given/target full-size ODF can be matched with those of another equivalent ODF using algorithms for finding the closest reduced-size ODF to the target ODF. This key recognition led to the development of a procedure capable of reducing large datasets of crystal orientations. In our approach, the procedure starts by selecting a set of crystal orientations that cover an orientation space and delineating the complete set of all physically realizable textures using the selected orientations. The delineated space is referred to as the texture hull (Kalidindi et al., 2004; Knezevic and Kalidindi, 2007; Lyon and Adams, 2004; Wu et al., 2007) and must contain the target ODF. We then solve a linear programming problem to match the Fourier coefficients of the given ODF with those of an equivalent ODF. The methodology takes advantage of the linearity of the Fourier