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An efficient parallel-operational explicit algorithm for Taylor-type model of rate dependent crystal plasticity

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ABSTRACT

Low computational efficiency and instability remain the greatest obstacle for crystal plasticity model applied to industrial practice. Herein, an explicit algorithm was deduced by introducing Taylor series expansion to recast the high-order nonlinear equation (for shear strain rate of slip systems) of rate dependent crystal plasticity into a set of linear equations. By virtue of a new approach to perform constitutive update in the crystallographic system, the linear model was so built with unknowns of the increments of stress and deformation resistance of slip systems. It was then solved directly by the complete pivot Gaussian elimination method within a two-level solving procedure. Full-strain-constraints (FC) Taylor model and crystal plasticity finite element method (CPFEM) model were utilized to verify the reliability, efficiency and stability of the presented algorithm. Then, texture evolution in two typical forming processes, in-plane shear and ideal plane-strain compression, was analyzed through pole figures and orientation distribution functions (ODF). The results achieved indicated that the presented algorithm was of high efficiency, especially in parallel operation with multiple CPUs, together with acceptable accuracy in the prediction of stress–strain response and texture evolution.

1. Introduction

Elastic–plastic anisotropy and texture evolution are the typical characters in metal forming, which are the primary objectives for constitutive modeling trying to capture. Comparing with the empirical models accounting for anisotropic yield in industrial practice, the prevalence of the crystal plasticity finite element method (CPFEM) in basic research is due to its physical basis and the incorporation of texture changes. However, the major drawback of the crystal plasticity approaches is the long calculation time [1]. To overcome this drawback, most improvements have been done in two aspects. One is to develop efficient numerical algorithm for constitutive calculation of single crystal, and the other is to modify polycrystal framework. Additionally, modifications on polycrystal framework are usually not only for computational efficiency issue but also for prediction precision of texture evolution.

In the developments of numerical algorithm, implicit iterations and explicit algorithms are two salient approaches. In rate independent crystal plasticity (RICP) modeling, implicit iterations are utilized to identify active slip systems [2] and to determine their shearing rates [3]. While, implicit algorithms were applied to solve the high-order nonlinear equation to determine shearing rates of slip systems in rate dependent crystal plasticity (RDCP). Among them, Newton–Raphson iteration method was the most popular procedure adopted by scholars [4–6]. Of course, several modified methods on Newton-type iteration can also be found in [7–9]. Although these algorithms were proved with good stability, they involved iterations both at the local level to update the stress and globally to enforce equilibrium, requiring thus much computational effort [7]. So, it is too expensive to apply crystal plasticity in industrial practice. Therefore, explicit algorithms without iterations are expected as an effective way to speed up the calculation of crystal plasticity model. Rate-tangent method [10] and Euler forward method [11] are the typical representatives of the explicit algorithms. They increased the computational efficiency of crystal plasticity model remarkably (more than 50 times than implicit algorithms [12]). However, they were proved very rigid needing very small step length (rate-tangent method and Euler forward method) and not self-starting (rate-tangent method) [13].

On the other hand, polycrystal framework has been modified for texture prediction as well as computational efficiency. Two simple mechanical homogenization models were proposed by Sachs [14] and Taylor [15]. The Sachs model represents a lower-bound result for the stress of a mechanically loaded polycrystalline sample since it is a no-strain-constraints (NC) model only accounting for stress equilibrium. While, the Taylor model is a full-strain-constraints (FC) approach in which the external strains are equally valid for each single grain. Since the Taylor model neglects stress equilib-

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rium, it represents an upper-bound result for the strains of polycrystals [16]. Since the FC Taylor model was found too strict, conceptual modifications of the constitutive descriptions consist essentially in the introduction of grain-interactions in strain relaxation schemes, i.e. the so called relaxed-constraints (RC) Taylor models [16,5,17,18]. Except for the CPFEM model which automatically takes grain interactions into account, early modifications of the FC Taylor model were introduced by incorporating partly strain relaxations ($\varepsilon_{13}, \varepsilon_{23}$) between neighboring grains. Then, the LAMEL model proposed by Van Houtte et al. [17] tried to capture some specific effects due to the interaction of neighboring grains (full strain relaxations) through looking at two grains simultaneously. Further, Van Houtte et al. [18] presented an advanced LAMEL (ALAMEL) model to overcome the theoretical shortcomings of the multi-grain models (including LAMEL), such as the misfit of freedom degrees between individual grain and the aggregate, the assumption of two different types of boundaries existing, and the assumption of uniformly distributed stress and strain inside each grain. Although the texture prediction obtained by RC models principally yields better results than those of the NC or FC approaches, deviations have been observed particularly in the large strain regime since the choice of relaxations in a RC model seems somewhat artificial. Also, additional calculation was added to the FC Taylor model. Besides, an excellent work to reduce calculation amount of the FC Taylor model is the texture component method proposed by Raabe and co-workers [19–21]. It enlarges the application of crystal plasticity model into industrial practice [1].

Beyond above discussion, the motivation of the present paper is to improve the computational efficiency of single crystal plasticity itself, so that simple or advanced polycrystal plasticity models may benefit from it. So, the contents in the present paper are to develop a new linear explicit algorithm of rate dependent crystal plasticity, and issues concerning computational efficiency and precision, i.e. constitutive update system and parallel operation, will also be discussed by investigating the effects of system for the update of stress and grain orientation. Then, the algorithm presented will be verified on its efficiency and precision in stress–strain responses and texture prediction, by adopting the FC Taylor model and the CPFEM model, which will be quantified by pole figures and orientation distribution functions (ODF).

2. Taylor-type polycrystal constitutive framework

The Taylor-type polycrystalline constitutive framework proposed by Taylor [15] is adopted here. The local deformation gradient in each grain is homogeneous and identical to the macroscopic deformation gradient $\mathbf{F}$ at the continuum material point level. The macroscopic stress response at each integral point is assumed as the volume-average of the multitude of microscopic single crystalline grains [4]. Then, with $\mathbf{T}(k)$ denoting the Cauchy stress in the kth crystal, these assumptions lead to

$$\bar{\mathbf{T}} = \sum_{k=1}^{N} \langle w_k \mathbf{T}^{(k)} \rangle, \tag{1}$$

where $\bar{\mathbf{T}}$ is the volume-averaged stress, N is the total number of grains, and w_k is the volume fraction of each single grain.

The elastic constitutive relation for the stress in each grain is taken as

$$\mathbf{T}^* = \Re : \mathbf{E}^*, \tag{2}$$

where

$$\mathbf{E}^* \equiv (1/2)(\mathbf{F}^{*\mathrm{T}}\mathbf{F}^* - \mathbf{I}) \tag{3}$$

is an elastic strain measure, $\Re$ is a fourth-order elasticity tensor, $\mathbf{I}$ is the second-order identity tensor, and

$$\mathbf{T}^* \equiv \mathbf{F}^{*-1}\{(\det \mathbf{F}^*)\mathbf{T}\}\mathbf{F}^{*-\mathrm{T}} \tag{4}$$

is the stress measure which is the elastic work conjugate to the strain measure $\mathbf{E}^*$. $\mathbf{F}^*$, the non-plastic deformation gradient, can be calculated from the multiplicative decomposition of deformation gradient as

$$\mathbf{F}^* = \mathbf{F}\mathbf{F}^{\mathrm{p}-1}, \tag{5}$$

where the plastic deformation gradient $\mathbf{F}^{\mathrm{p}}$ is in turn given by the evolution rule

$$\dot{\mathbf{F}}^{\mathrm{p}} = \mathbf{L}^{\mathrm{p}}\mathbf{F}^{\mathrm{p}}, \tag{6}$$

with the plastic part of velocity gradient

$$\mathbf{L}^{\mathrm{p}} = \sum_{\alpha} \dot{\gamma}^{\alpha}\mathbf{S}_0^{\alpha}, \quad \mathbf{S}_0^{\alpha} \equiv \mathbf{m}_0^{\alpha} \otimes \mathbf{n}_0^{\alpha}. \tag{7}$$

The velocity gradient $\mathbf{L}$ and its symmetric and antisymmetric parts $\mathbf{D}$ and $\mathbf{W}$ are

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{\mathrm{p}}, \qquad \mathbf{D} = 1/2(\mathbf{L} + \mathbf{L}^{\mathrm{T}}), \qquad \mathbf{W} = 1/2(\mathbf{L} - \mathbf{L}^{\mathrm{T}}), \tag{8}$$

and

$$\mathbf{W} = \mathbf{W}^* + \mathbf{W}^{\mathrm{p}}, \tag{9}$$

$$\mathbf{W}^{\mathrm{p}} = \sum_{\alpha} \mathbf{w}^{\alpha}\dot{\gamma}^{\alpha}, \tag{10}$$

$$\mathbf{w}^{\alpha} = \frac{1}{2}[\mathbf{m}_0^{\alpha} \otimes \mathbf{n}_0^{\alpha} - \mathbf{n}_0^{\alpha} \otimes \mathbf{m}_0^{\alpha}] \tag{11}$$

Here, $\mathbf{W}^{\mathrm{p}}$ is the so-called plastic spin and $\mathbf{W}^*$ is the spin, $\mathbf{m}_0^{\alpha}$ and $\mathbf{n}_0^{\alpha}$ are time-independent orthonormal unit vectors which define the slip direction and slip plane normal of the slip system α in a fixed reference configuration, and $\mathbf{S}_0^{\alpha}$ is the Schmid tensor. For face-centered cubic (FCC) metal, there are 12 {111}<110 > type slip systems as listed in Table 1. $\mathbf{F}^{\mathrm{p}}$ in Eq. (6) should be normalized necessarily by dividing the computed values of each of its components by the cube root of the computed determinant to ensure det $\mathbf{F}^{\mathrm{p}} = 1$ by virtue of plastic incompressibility. The plastic shearing rate on the slip system α can be given by an exponential type law in terms of resolved shear stress (RSS) τ^{α} and deformation resistance s^{α} of the α slip system, as

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left|\frac{\tau^{\alpha}}{s^{\alpha}}\right|^{1/m} \mathrm{sign}(\tau^{\alpha}), \tag{12}$$

where $\dot{\gamma}_0$ is a reference value, m is the strain rate sensitive coefficient of material, and the symbol sign stands for getting the sign symbol of τ^{α}.In Eq. (12), RSS may be approximated by

$$\tau^{\alpha} \doteq \mathbf{T}^* : \mathbf{S}_0^{\alpha}, \tag{13}$$

and s^{α} evolves as

$$\dot{s}^{\alpha} = \sum_{\beta} h^{\alpha\beta}|\dot{\gamma}^{\beta}|, \tag{14}$$

where $h^{\alpha\beta}$ is the rate of strain hardening on slip system α due to a shearing on the slip system β, and is related to a single slip hardening rate, $h^{(\beta)}$, and the hardening matrix, $q^{\alpha\beta}$, as

Table 1
Slip systems in FCC crystal.

α	$\mathbf{m}_0^{\alpha}$	$\mathbf{n}_0^{\alpha}$	α	$\mathbf{m}_0^{\alpha}$	$\mathbf{n}_0^{\alpha}$
#1	(1 −1 0)	(1 1 1)	#7	(1 0 −1)	(1 −1 1)
#2	(1 0 −1)	(1 1 1)	#8	(0 1 1)	(1 −1 1)
#3	(0 1 −1)	(1 1 1)	#9	(1 1 0)	(1 −1 1)
#4	(1 0 1)	(−1 1 1)	#10	(1 −1 0)	(1 1 −1)
#5	(1 1 0)	(−1 1 1)	#11	(1 0 1)	(1 1 −1)
#6	(0 1 −1)	(−1 1 1)	#12	(0 1 1)	(1 1 −1)