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# Dynamic explicit solution for higher-order crystal plasticity theories

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ABSTRACT

Dynamic terms are included in the balance equations that govern a higher-order crystal plasticity formulation. The resulting equations are integrated in time by the central-difference explicit method. The methodology avoids solution methods based on the inversion of the associated stiffness matrices. This is a great advantage of the proposed methodology, considering that these matrices tend to be highly ill-conditioned. As the solution becomes dependent on the time-step size used in the integration, a stability study is presented. Only a rate independent constitutive law is taken into account. As examples, a crystal layer and a composite material under simple shear and the wedge indentation of a single crystal are considered. Comparisons with an implicit quasi-static solution method show the robustness of the proposed methodology, but reveal an elevated computational cost related to it.


## 1. Introduction

Numerous higher-order plasticity theories have been proposed in the last few years. The attractive aspect of this kind of formulation is the introduction of higher-order boundary conditions. For instance, it permits to capture the formation of boundary layers in grain crystals or to associate boundary conditions to the flux of dislocations. In these cases, kinematic variables linked to plasticity are considered independent variables. Depending on the formulation these variables can be plastic strains (e.g. Shu and Fleck, 1999), crystal slips (e.g. Gurtin, 2002), density of dislocations (e.g. Evers et al., 2004), etc. Balance equations are written in terms of these variables. Through the principle of virtual work, formulations amenable to implementation in a finite element framework can be built. Kinematic plastic variables can be then obtained by standard solution methods normally used in the finite element method. Basically, in the solution method, a stiffness matrix associated to the kinematic plastic variables has to be inverted in order to determine the variables. This stiffness matrix is spatially integrated in the finite elements by standard quadrature methods, for instance Gauss quadrature.

The problem in this case is that this matrix can be very ill-conditioned or even singular. Solutions by ordinary solvers used in finite element algorithms can be incorrect or unreachable, since uniqueness of the solution process can not be guaranteed. Lele and Anand (2008), Kuroda (2011) and Bittencourt, 2012 have observed unexpected behaviors and/or convergence problems considering higher-order crystal plasticity models. In general these problems have a tendency to increase when (1) multiple slip systems are activated, (2) higher-order term contribution increases and (3) deformation gradients are non-uniform. In the last case, if a rate independent formulation is used, necessarily some of the points of the domain will be plastic and others elastic. Elastic Gauss points will not contribute to the spatial integration of the plastic stiffness matrix. The result is an under-integrated stiffness matrix that can result singular. A possible solution is to add an arbitrary contribution for elastic points (De and Mülhaus, 1992; Bittencourt, 2012), but the result is a solution dependent on this arbitrary contribu-

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tion. To shift to a rate dependent formulation is not a guarantee of solution, since Gauss points with low resolved stresses will contribute with infinitely high values to the stiffness matrix, which can lead to a numerical locking, as seen in Bittencourt (2012).

An explicit solution procedure that completely eliminates inversion of stiffness matrices seems to be an appealing alternative to solve this kind of problem and it is the methodology pursued in the present work. The higher-order crystal plasticity developed by Gurtin (2002) is followed. An application of explicit solution method to nonlocal crystal plasticity can be found in Lee and Han (2012), but higher-order terms are not included. The author is not aware of other publications in this context, so the purpose of this work is mainly exploratory. Inertia effects are added in the balance equations and solution in time is done by the explicit central-difference method. Details of the crystal plasticity formulation are given in Section 2. In Section 3 details of the solution method are described. In Section 4 a stability study of the formulation is presented. Applications are regarded in Section 5. Two simple cases, where solutions are well-known, are studied: a layer and a model composite material are subjected to simple shear. Finally the wedge indentation of a single crystal is shown. Comparisons with an implicit quasi-static formulation are emphasized. Conclusions are presented in Section 6.

## 2. Cristal plasticity formulation

The gradient of the displacement vector, $u_{i,j}$, is written as the sum of an elastic $u^e_{ij}$ and a plastic $u^p_{ij}$ part. The plastic part occurs by crystallographic slip on a set of slip planes. With $s^{(\beta)}_i$ and $m^{(\beta)}_i$ unit vectors specifying the slip direction and the slip plane normal, respectively, for slip on a system $\beta$, the plastic part of the displacement gradient is given by

$$u^p_{ij} = \sum_\beta \gamma^{(\beta)} s^{(\beta)}_i m^{(\beta)}_j, \tag{1}$$

with $\gamma^{(\beta)}$ the total slip on the system $\beta$. Attention is confined to plane strain. Elastic strains are considered isotropic. Greek superscripts, with no summation convention, are used to label the slip systems. Slip system directions are fixed throughout calculations.

Resolved stress $\tau^{(\beta)}$ on slip system $\beta$ can be calculated from Cauchy stresses $\sigma_{ij}$ as:

$$\tau^{(\beta)} = P^{(\beta)}_{ij}\sigma_{ij}, \quad P^{(\beta)}_{ij} = \frac{1}{2}\left(s^{(\beta)}_i m^{(\beta)}_j + s^{(\beta)}_j m^{(\beta)}_i\right). \tag{2}$$

The stress $\sigma_{ij}$ is given in the rate form

$$\dot{\sigma}_{ij} = C_{ijkl}\dot{u}_{k,l} - C_{ijkl}\sum_\alpha \dot{\gamma}^{(\alpha)} P^{(\alpha)}_{kl}, \tag{3}$$

with $(\dot{\ }) = \partial()/\partial t$, where $t$ is time. $C_{ijkl}$ is the elasticity tensor.

Attention is focused on rate independent material behavior and cases where the statistically distributed dislocations are the only to affect the dissipative hardening. Then the state of this hardening can be defined by,

$$\pi^{(\beta)} = \sigma^{(\beta)}\mathrm{sgn}\dot{\gamma}^{(\beta)}, \tag{4}$$

with $\sigma^{(\beta)}$ having the initial value $\sigma_0$ for all $\beta$ and the corresponding $\pi^{(\beta)}$ having the initial value $\pi_0$. $\sigma^{(\beta)}$ evolves as

$$\dot{\sigma}^{(\beta)} = \sum_\alpha h^{(\beta\alpha)}|\dot{\gamma}^{(\alpha)}|, \quad h^{(\alpha\beta)} = qH_0 + (1-q)H_0\delta_{\alpha\beta}, \tag{5}$$

where $H_0$ is a prescribed constant and $q$ is the latent hardening ratio. The relation (4) applies only when there is flow on slip system $\beta$, i.e. when $\dot{\gamma}^{(\beta)} \neq 0$.

A defect stress $T_{ij}$ is also present due to geometrically necessary dislocations. Gurtin (2002) proposed that it is a function of the tensor $G_{ij}$, the density of geometrically necessary dislocation, as follows:

$$T_{ji} = \ell^2 \pi_0 G_{ij}, \tag{6}$$

where $\ell$ is a material length parameter, and,

$$G_{ij} = \epsilon_{irs}\frac{\partial u^p_{js}}{\partial x_r}. \tag{7}$$

$\epsilon_{ipq}$ is the alternating tensor.

The defect stress $T_{ij}$ produces "microstresses" $\xi^{(\beta)}_i$ on the slip system given by

$$\xi^{(\beta)}_i = \epsilon_{ipq} m^{(\beta)}_p T_{rq} s^{(\beta)}_r. \tag{8}$$

Confining attention to plain strain deformation, assuming that $s^\beta_3 = m^\beta_3 = 0$, the microstress can be rewritten as (details can be found in Bittencourt et al. (2003)):

$$\xi^{(\beta)}_i = \ell^2 \pi_0 s^{(\beta)}_i \sum_\kappa s^{(\beta)}_j s^{(\kappa)}_j \gamma^{(\kappa)}_{,l} s^{(\kappa)}_l. \tag{9}$$