Small strain crystal plasticity based on the primal-dual interior point method

Lisa Scheunemann¹,* , Paulo S.B. Nigro¹, Jörg Schröder¹, and Paulo M. Pimenta²
¹ University Duisburg-Essen, Institute of Mechanics, Universitätsstraße 15, 45141 Essen, Germany
² University of São Paulo, Structural and Geotechnical Engineering, São Paulo, Brazil

The paper presents a novel approach for rate-independent single crystal plasticity based on the Infeasible Primal-Dual Interior Point Method in a small strain framework. Therein, the principle of maximum dissipation together with the yield functions on the slip systems in the crystal are considered as the constrained optimization problem. The constraint conditions adapted using slack variables and a Lagrangian is formulated using barrier functions. The equations are linearized and solved using Newton’s method. Numerical examples are presented for slip on the individual slip systems in a single crystal under global rotation.

© 2019 The Authors Proceedings in Applied Mathematics & Mechanics published by Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim

1 Introduction

Single crystal plasticity, which plays a major role in the analysis of material anisotropy and texture evolution, treats each crystalline grain, having a distinct orientation, individually. The polycrystalline material response is obtained upon considering a structure consisting of various individual grains, often also considering interface effects at the grain boundaries. On the individual grain level, single crystal plasticity can be treated in the mathematical framework of multisurface plasticity, leading to a constrained optimization problem wherein multiple constraints are defined as yield criteria on the different slip systems.

Different approaches have been established in this field, see, e.g., [2], [3]. In rate-independent models, the set of active slip systems in the grain is possibly nonunique and is identified in, e.g., an active set search. Rate dependent approaches are based on power-type creep laws which do not differentiate into active or inactive slip systems. However, the constitutive equations of these formulations are often very stiff and require a small time increment.

Here, a new algorithm for the solution of the constrained optimization problem based on the primal dual interior point method (PDIPM), [1], involving slack variables is presented for the framework of small strain single crystal plasticity. The use of slack variables therein stabilizes the conventional method and allows for a temporary violation of the constraint during the optimization. The optimization is solved using a Lagrange functional, wherein the nonlinear system of equations resulting from the derivation of the Lagrange functional is linearized using Taylor expansion and solved by a Newton Raphson scheme. All slip systems are considered simultaneously, omitting an iterative active set search. PDIPM has been found to lead to very efficient algorithms and better convergence rates than barrier or penalty methods. The stability of the algorithm would be especially beneficial in complex material models, such as a multiscale description of polycrystalline materials. Numerical examples for a face-centered cubic single crystal are presented.

2 Theoretical framework

A classical constitutive framework for single crystal plasticity considering small strains the basis of the formulation. With the classical assumption of the linear strain tensor \( \varepsilon = \text{sym}[\nabla u] \) as the symmetric part of the displacement gradient and further its additive decomposition \( \varepsilon = \varepsilon^c + \varepsilon^p \) into an elastic part and a plastic part, we assume an associative framework with a decoupled free energy \( \psi(\varepsilon^c, \gamma^c) = \psi^d(\varepsilon^c) + \psi^p(\gamma^c) \) \( \forall \alpha \) and an associated structure of crystal plasticity for the modelling of hardening phenomena, \( g^\alpha = \partial \psi^p / \partial \gamma^\alpha \). The reduced dissipation inequality is then given by

\[ D_{\text{red}} = \sum_{\alpha} (P^\alpha : C^\alpha : \varepsilon - \sum_{\beta} P^\beta : C^\beta : P^\beta \gamma^\beta - g^\alpha ) \gamma^\alpha \geq 0. \]  

(1)

with the classical Kuhn-Tucker conditions \( \dot{\gamma}^\alpha \geq 0 \), \( \Phi^\alpha \leq 0 \), \( \Phi^\alpha \dot{\gamma}^\alpha = 0 \) where \( \Phi^\alpha(\sigma, g^\alpha) = \tau^\alpha - g^\alpha \) for \( \alpha = 1, 2, ..., m \). The nonlinear constrained optimization problem is then defined by

\[ \max D_{\text{red}} \quad \text{subject to} \quad \Phi^\alpha \leq 0, \quad \dot{\gamma}^\alpha \geq 0 \quad \forall \quad \alpha = 1, 2, ..., m \]

(2)

and treated in an Infeasible Primal-Dual Interior Point Method, leading to the Lagrangian

\[ L = -D_{\text{red}} + \sum_{\alpha} \lambda^\alpha [\Phi^\alpha + s^\alpha] - \mu \sum_{\alpha} \ln(s^\alpha) - \mu \sum_{\alpha} \ln(\dot{\gamma}^\alpha) \]

(3)

* Corresponding author: e-mail lisa.scheunemann@uni-due.de, phone +49 201 183 3603, fax +49 201 183 2680
with the logarithmic barrier functions, Lagrange multipliers \( \lambda^\alpha \) and the slack variables \( s^\alpha \). The stationary point is found from the derivation with respect to the plastic slip variables \( \gamma^\alpha \), the lagrange multipliers \( \lambda^\alpha \) and the slack variables \( s^\alpha \). The Taylor series expansion of the equations is linearized and solved using Newton’s method. Classically, a line-search algorithm is applied in the numerical algorithm.

### 3 Single crystal under simple shear

Based on the presented algorithm, a face-centered cubic (fcc) single crystal structure is simulated under global rotation using Euler angles. Fig.1a shows the octahedral arrangement of the slip systems in the fcc crystal and the table in Fig.1b defines the numbering of slip systems according to their slip normals and slip directions. The results are compared to results from the literature in order to measure the quality of results compared to other algorithms for single crystal plasticity. The elastically isotropic crystal considered here has a bulk modulus of \( \kappa = 228,888.80 \text{N/mm}^2 \) and the shear modulus is given by \( \mu = 76,296.30 \text{N/mm}^2 \). A critical resolved shear stress of \( \tau_0 = 10.0 \text{N/mm}^2 \) is considered on all slip systems, whereas the crystal is initially stress free. The rotation angles (Euler angles) are given by \( \theta_1 = -18^\circ \) about the z-axis and \( \theta_2 = -54^\circ \) about the resulting new y axis. The simple shear problem is considered in a deformation driven process where \( \varepsilon_{12} = \varepsilon_{21} = 0.01 \) is applied within 100 equal increments on a hexahedral 27-noded finite element in a plane strain setting. The activated slip systems are shown in Fig.2b.

![Fig. 1: a) Octahedral arrangement of slip planes in a fcc crystal unitcell. b) Summary of slip systems of face centered cubic unitcell with numbering given by \( \alpha \) and slip normal- and slip direction vector given by \( n^\alpha \) and \( m^\alpha \), respectively.](image1)

![Fig. 2: Orientation 10: a) Equivalent plastic strain \( A \) and b) accumulated plastic slip \( \{ \gamma^\alpha | \alpha = 2, 3, 4, 6, 7, 9, 11, 12 \} \) versus strain \( \varepsilon_{xy} \).](image2)

The results are compared to a single crystal analysis in the literature, cf. [4]. The accumulated slip \( A \) shown in Fig. 2a agrees well. Fig.2b shows that the slip is not activated at the same time on all slip systems and does not evolve uniformly.

### References

[1] El Bakry, A.S., Tapia, R.A., Tsuchiya, T. and Zhan, Y.: On the formulation and Theory of the Newton Interior Point Method for Nonlinear Programming. Journal of Optimization Theory and Applications, 89 (1996), 507-541.

[2] Cuitino, A.M. and Ortiz, M.: Computational modelling of single crystals. Modelling and Simulation in Materials Science and Engineering, 1 (1992), 225-263.

[3] Peirce, D., Asaro, R.J. and Needleman, A.: An analysis of nonlinear and localized deformation in ductile single crystals. Acta Metallographica, 30 (1982), 1087-1119.

[4] Miehe, C. and Schröder, J.: A comparative study of stress update algorithms for rate independent and rate dependent crystal plasticity. International Journal for Numerical Methods in Engineering, 50 (2001), 273–298.