ALGORITHM FOR RATE-INDEPENDENT PLASTICITY OF SINGLE CRYSTALS BASED ON INCREMENTAL WORK MINIMIZATION

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1. Introduction

The paper addresses the long-standing difficulty in constitutive algorithms in rate-independent crystal plasticity, related to the non-uniqueness in selection of active slip systems in the Hill-Rice framework [1]. Applicability of earlier algorithms for multi-surface plasticity [2, and the references therein] is limited due to the lack of positive definiteness and symmetry of the slip-systems interaction matrix. Iterative procedures were proposed e.g. in [3] and [4] but the question remained open how to proceed if there are non-unique solutions associated with distinct active slip system sets.

The present constitutive algorithm [5] determines the active slip-system set and incremental slips by constrained minimization of the incremental work formulated as a quadratic function of non-negative crystallographic slips.

2. Incremental work minimization algorithm for a finite time step

The main concept of the algorithm for a fully kinematic control is to perform minimization of a small increment Δw of the deformation work density along a given straining path,

$$\Delta w(\Delta\mathbf{F}, \Delta\gamma^\alpha) \to \min_{\Delta\gamma^\alpha \geq 0} \qquad \text{for given } \Delta\mathbf{F}, \qquad \alpha \in \mathcal{P}, \tag{1}$$

for a known finite time step $[t_n, t_{n+1}]$ starting from a selected set $\mathcal{P}$ of potentially active slip-systems. The final set of active slip-systems $\mathcal{A} = \{\alpha \mid \Delta\gamma^\alpha > 0\} \subseteq \mathcal{P}$ is obtained at the minimum point of Δw. The search strategy for the active slip-systems set $\mathcal{A}$ is thus embedded in the incremental work minimization. When the algorithm is extended to a partially kinematic control then minimization is performed also with respect to a free complementary part of deformation gradient increment $\Delta\mathbf{F}$. The increment of deformation work density $\Delta w(\Delta\mathbf{F}, \Delta\gamma^\alpha)$ in minimization problem (1) reads

$$\Delta w = \mathbf{S}_n \cdot \Delta\mathbf{F} + \frac{1}{2}\Delta\mathbf{F} \cdot \mathbb{C}^{\mathrm{e}} \cdot \Delta\mathbf{F} - \sum_\alpha \left(f_n^\alpha + \mathbf{\Lambda}^\alpha \cdot \Delta\mathbf{F}\right)\Delta\gamma^\alpha + \frac{1}{2}\sum_{\alpha,\beta} \Delta\gamma^\alpha g^{\alpha\beta}\,\Delta\gamma^\beta\,. \tag{2}$$

It is obtained using time integration of the constitutive rate equations for the Piola stress $\mathbf{S}$ and yield function f^α for α-th slip-system. An implicit time integration algorithm is constructed where the non-incremental quantities: the elastic stiffness pseudomoduli tensor $\mathbb{C}^{\mathrm{e}}$ for work-conjugate pair $(\mathbf{S}, \mathbf{F})$, the slip-systems interaction matrix $(g^{\alpha\beta})$ under full kinematic control, and the α-th yield-surface normal $\mathbf{\Lambda}^\alpha =$ in $\mathbf{F}$-space, are updated at the end of time step.

The augmented Lagrangian method has been used to convert the constrained minimization problem (1) to smooth unconstrained one. The minimization algorithm has been implemented in *Wolfram Mathematica* environment, where the Newton method with line-search step control is employed in the *FindMinimum* function.

3. Results

Large plastic deformation of crystals causes lattice rotations and in turn multiple changes of active slip-systems set $\mathcal{A}$. It can result in strong irregularities in stress components as shown in Fig. 1(a). The algorithm enables related successive transitions between yield-surface corners, Fig. 1(b).

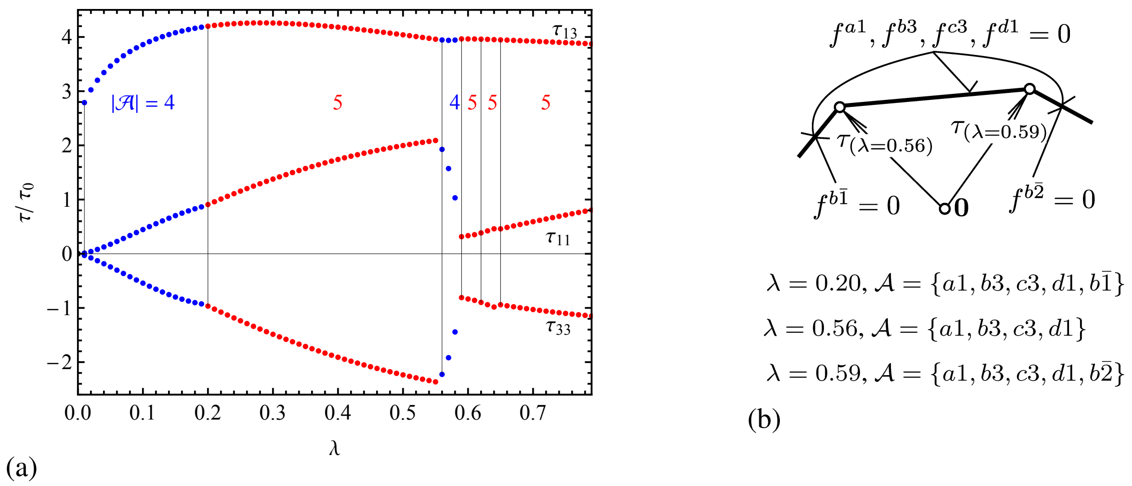

Figure 1. Uniform simple shear calculated up to shear magnitude $\lambda = 0.79$. (a) Components of Kirchhoff's stress $\boldsymbol{\tau}$ and number $|\mathcal{A}|$ of active slip-systems, and (b) the transition between yield surface corners in the stress space.

Simulation of rolling of a copper polycrystal up to 92% reduction is presented to illustrate the efficiency and robustness of the algorithm, Fig. 2. Large deformation of the polycrystal has been modeled as plane strain compression by the classical Taylor scheme for 432 randomly oriented grains.

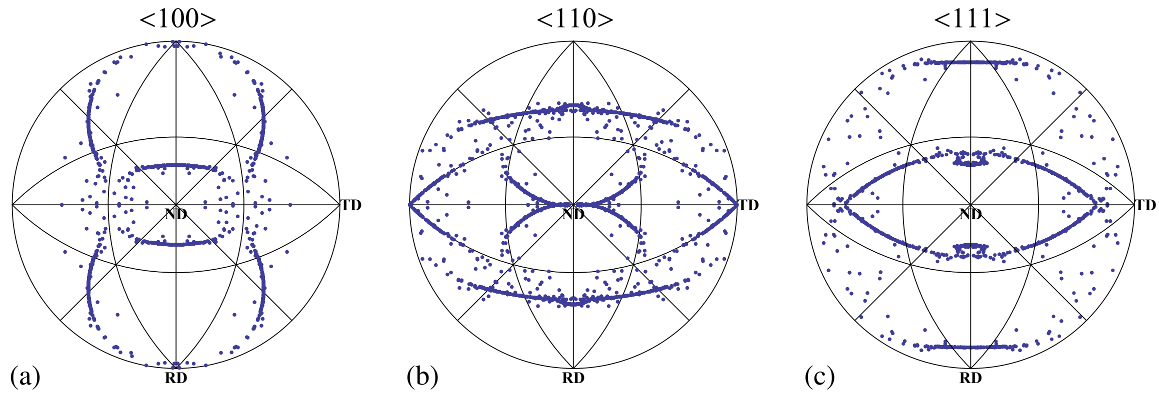

Figure 2. (a) ⟨100⟩, (b) ⟨110⟩ and (c) ⟨111⟩ pole figures of copper polycrystal rolling textures simulated by using the incremental work minimization algorithm.

4. References

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