The energy approach to rate-independent plasticity of metal single crystals

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Abstract

In the modelling of metal single crystals in the framework of rate-independent plasticity, there are known difficulties caused by non-uniqueness in selection of active slip-systems. A related challenge is to predict emergence of non-uniform deformation patterns and the formation and evolution of experimentally observed microstructures. A new constitutive algorithm is presented that tackles those problems using the energy approach. It is based on asymptotically exact formulation of the set of constitutive equations and inequalities as a minimum problem for the incremental work expressed by a quadratic function of non-negative crystallographic slips. The calculated examples of deformation banding patterns and of reduction of multiplicity of active slip-systems in fcc single crystals are compared with the experimental observations.

Keywords: crystal plasticity, slip-systems selection, incremental energy minimization

1. Introduction

There is a long-standing difficulty in the rate-independent crystal plasticity, in the framework of the rigorous theory established by Hill and Rice [1], related to non-uniqueness (or ambiguity) in selection of active slip-systems [2]. The common way to circumvent that problem in calculations is to apply a viscoplastic model where slip-rates are given functions of state and therefore uniquely defined [3]. However, uniqueness of solutions in crystal viscoplasticity may be accompanied by a strong sensitivity to initial imperfections, thus replacing the problem of non-uniqueness by a kind of hidden instability. In the absence of an explicit stability criterion, there are also difficulties in predicting experimentally observed instability phenomena like spontaneous emergence of deformation bands and microstructures.

2. Incremental work minimization problem

It is thus of interest to examine single crystal behaviour within the general framework of stability in materials with rate-independent dissipation [4]. In the presentation, attention is restricted to spatially discretized single crystals without strain-gradient effects. Instability is meant in the extended sense applicable to quasi-static deformation processes (paths), assuming that instability of equilibrium does not occur if the loading device is sufficiently rigid.

Path instabilities either of constitutive origin or with respect to formation of deformation patterns can be addressed in a unified manner using the energy criterion of path instability [4]. This requires the incremental (or rate) problem to be of potential type, which is not true in general in rate-independent plasticity of single crystals deformed by multislip. Recently, the selective symmetrization of the slip-system interaction moduli matrix has been proposed [5], restricted to active slip-systems. It was shown [6] that this makes the energy approach applicable because it admits an asymptotically exact formulation of the set of constitutive equations and inequalities for a crystal as a minimization problem for the incremental work.

3. Algorithm

The incremental work minimization algorithm for rate-independent plasticity of single crystals is presented in detail in [7]. It is based on iterative minimization of the incremental work expressed by a quadratic function of non-negative crystallographic slips. The constrained minimization problem was converted to a smooth unconstrained using the augmented Lagrangian method. The advantage of the incremental work minimization is that it eliminates the solution paths, expected to be of less physical interest, that do not satisfy the energy criterion of path stability. This way the algorithm deals with the long-standing difficulties mentioned in Introduction. Suitability of the algorithm for simulations of large plastic deformation of fcc crystals and polycrystals with multiple changes of active slip-systems was examined by a number of examples.

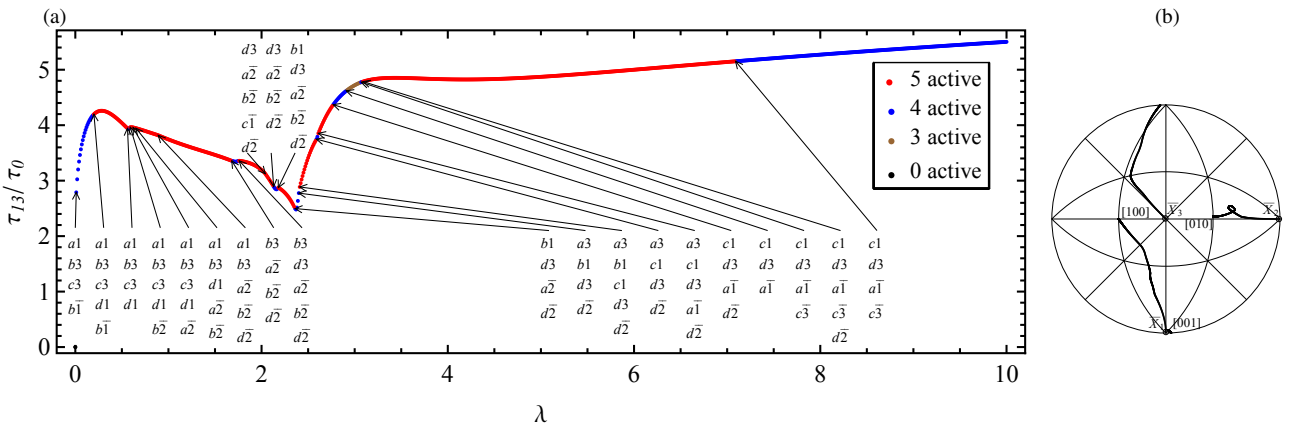

Figure 1: (a) Shear stress vs shear strain for uniform simple shear of an fcc single crystal, (b) changes in the orientation of crystallographic axes [7]

4. Results

The algorithm allows for numerical simulations of large plastic deformation of single crystals with the automatic crossing of constitutive branching points. Fig. 1 shows an example of uniform simple shear of an fcc crystal with latent-to-self hardening ratio of 1.4, for a kinematically controlled deformation gradient $\mathbf{F}(\lambda) = \mathbf{1} + \lambda\, \mathbf{B} \otimes \mathbf{A}$ starting from $\mathbf{B} \leftrightarrow [100]$ and $\mathbf{A} \leftrightarrow (001)$ at $\lambda = 0$ up to $\lambda = 10$. As indicated in the figure, unstable solutions with more that 5 active slip-systems were eliminated.

For a partially restricted deformation gradient, the number of locally active slip-systems can be much smaller, as illustrated in Fig. 3 for uniaxial tension in the high-symmetry direction with a symmetry-breaking response. Another illustration is shown in Fig. 2 where the energetically preferable pattern of deformation banding was calculated for another fcc crystal subjected to tension with two components of the macroscopic deformation gradient left free. The dependence of the deformation pattern on the loading direction is in qualitative agreement with experimental observations.

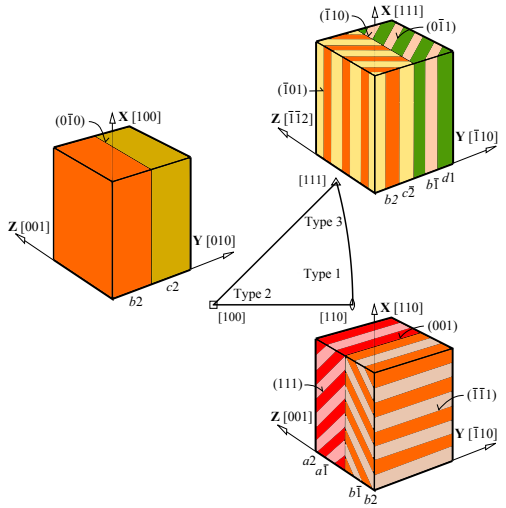

Figure 2: Simulations of uniaxial tension of fcc crystal: deformation banding in tension in different directions [6]

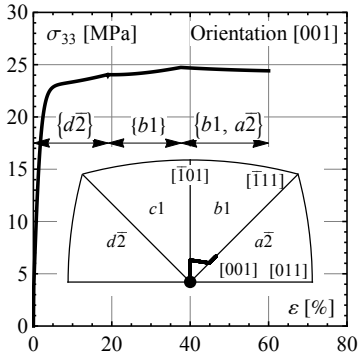

Figure 3: Simulations of uniaxial tension of fcc crystal: slip-system selection, stress-strain diagram and changes of crystallographic orientation of the tensile axis [7]

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