THE ENERGY APPROACH TO DETERMINING PLASTIC DEFORMATION OF METAL CRYSTALS

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1. Introduction

Non-uniqueness of active slip systems selection in the rate-independent theory of single crystal plasticity represents a well-known difficulty, and different methods have been proposed in the literature to overcome it. The method used in this paper is based on the energy criterion of path stability. The main concept is that a stable deformation path corresponds to step-by-step minimization of the incremental energy supply under prescribed kinematic constraints and under certain symmetry restrictions imposed on the constitutive law. A novel feature of the present approach is that the minimization is simultaneously performed with respect to shear increments on all slip systems and to the deformation gradient components that are left unconstrained. In particular, if only the overall deformation gradient is prescribed, either fully or partially, then the energetically preferable deformation pattern in a crystal can be nonuniform and lead to deformation banding and microstructure formation. A respective computational algorithm for large elastoplastic deformations of metal single crystals has been developed and used to simulate typical tests like uniaxial tension and channel-die compression.

2. Minimization of incremental energy supply

A general description of the incremental energy minimization approach can be found in [1]. The following minimization problem is examined

(1) $\Delta E \to \min$ subject to kinematical constraints

where ΔE is the increment in energy to be supplied from external sources to the mechanical system, consisting of the deformed body and the loading device, in order to produce quasi-statically a deformation increment. In this paper we consider either kinematic control or zero external loads, so that ΔE reduces to the increment of deformation work ΔW split into the sum of the increments in the Helmholtz free energy and virtual dissipation. For each slip system the Schmid yield condition $\tau_k = \tau_k^c$ is adopted, where τ_k is the resolved stress (projection of Kirchhoff stress $\boldsymbol{\tau}$ on k-th slip-system dyad $\mathbf{s}_k$) and τ_k^c is its current critical value. It is shown that the symmetry restriction imposed by intrinsic consistency between minimization (1) performed with accuracy to the first- and second-order terms [1] is reduced to the requirement $g_{kj} = g_{jk}$ examined below.

3. The hardening moduli and symmetry restriction

The evolution equations for critical shear stresses τ_k^c and yield functions $f_k = \tau_k - \tau_k^c$ are

$$(2) \qquad \dot{\tau}_k^c = \sum_j h_{kj}^* \dot{\gamma}_j \,, \qquad \dot{f}_k = \mathbf{\Lambda}_k \cdot \dot{\mathbf{F}} - \sum_j g_{kj} \dot{\gamma}_j \,,$$

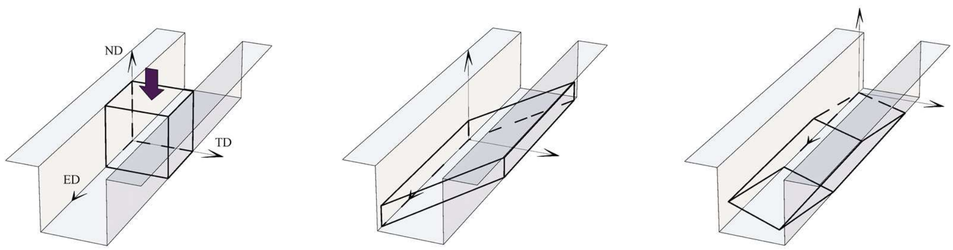
where $\dot{\gamma}_j \geq 0$ is the shear-rate on j-th slip-system, h_{kj}^* are slip-system hardening moduli, g_{kj} are slip-system interaction moduli at prescribed strain-rate, $\mathbf{F}$ is the deformation gradient, and $\mathbf{\Lambda}_k$ is a tensor orthogonal to the yield surface $f_k = 0$ in $\mathbf{F}$-space. Taking into account the plastic flow of the material relative to the crystallographic lattice, it is shown that

$$(3) \qquad g_{kj} - g_{jk} = h_{kj}^* - h_{jk}^* + \boldsymbol{\tau} \cdot (\mathbf{s}_k \mathbf{s}_j - \mathbf{s}_j \mathbf{s}_k) \,.$$

Different ways of ensuring the required symmetry $g_{kj} = g_{jk}$ by reducing to zero the right-hand expression in (3) are considered, and their quantitative effect on the material behaviour is studied.

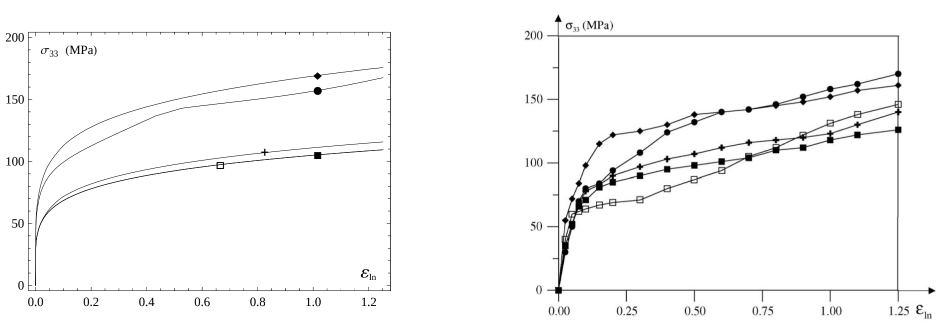
4. Example

As an example, the channel-die compression of an Al-alloy single crystal is considered. Idealized geometry of the specimen before and after deformation is shown in Fig. 1, the latter determined for two different initial orientations of the crystal. Compressive stress-strain diagrams calculated for five different crystal orientations are shown in Fig. 2a which can be compared to respective experimental data taken from reference [2] and shown in Fig. 2b. The effect of formation of deformation bands is also investigated.



(a) (b) (c)

Figure 1. Initial configuration of a sigle crystal in a channel die (a) and calculated configurations after compression to $\varepsilon_{\ln} = 1.25$ for Cube (b) and Copper (c) initial crystallographic orientations.



(a) (b)

Figure 2. Compressive stress-strain diagrams for channel-die compression of a single crystal of five different crystallographic orientations: calculated curves (a) and experimental results from ref. [2] (b).

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5. References

[1] H. Petryk (2003). Incremental energy minimization in dissipative solids, *C.R. Mecanique*, **331**, 469–474.

[2] M. Darrieulat, J.-Y. Poussardin, R.-Y. Fillit and Ch. Desrayaud (2007). Homogeneity and heterogeneity in channel-die compressed Al-1%Mn single crystals: Considerations on the activity of the slip systems, *Mat. Sci. Engng A*, **445–446**, 641-651.