ELSEVIER

Computational Materials Science 26 (2003) 154–158

COMPUTATIONAL MATERIALS SCIENCE

www.elsevier.com/locate/commatsci

A rate independent approach to crystal plasticity with a power law

M. Schurig *, A. Bertram

Institut für Mechanik, Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany

Abstract

The ambiguity problem in rate independent multisurface theory of plastic flow in crystals can be solved by usage of a rate dependent theory. Here, a proposal presented similarly by Gambin and Barlat [Int. J. Plast. 13 (1997) 75] is used that is rate independent but unique without need for a generalized inversion technique. Some other useful properties can be shown. Applications to f.c.c. single and polycrystals are demonstrated.

PACS: 46.35.+z
Keywords: Crystal plasticity; Rate independence; Rounded yield locus; Uniqueness of slip

1. Introduction

For the description of plastic deformations of crystals by dislocation movement along glide planes, the multisurface theory of plasticity has been well established. It uses a flow rule based on the kinematics of crystallographic slip. In its symmetric and antisymmetric parts it contains both the plastic strain as well as the plastic spin.

In a rate independent theory, the determination of the respective slip rates is an inverse problem. As the decomposition of an arbitrary volume preserving deformation into a number of shear modes is in general not unique, this problem can be ill posed. A solution can be found by use of a generalized inverse, as in [1,7,9].

In a rate dependent theory, a constitutive law for the slip rates is assumed, usually by means of a power law. It resolves the ambiguity and reproduces the fact that conjugate slip systems are active before reaching the critical resolved shear stress. It is often used to approximate rate-insensitive behaviour [2,8,10].

Here we try to take advantage of both theories at once. An ansatz function for the slip rates is inserted into a single condition of consistency for the rounded crystallite yield locus that has been proposed similarly by Gambin and Barlat [6].

The result is a non-associated flow rule, rate-independent without the ambiguity of the classical multisurface plasticity. The ratios of the slip rates and the nonlinear creep are as in the physically well established rate dependend theory. However, in certain special cases it coincides with multisurface theory.

* Corresponding author. Tel.: +49-391-67-12592; fax: +49-391-67-12863.
E-mail address: schurig@mb.uni-magdeburg.de (M. Schurig).

0927-0256/02/$ - see front matter
PII: S0927-0256(02)00413-5

Shear deformation of a single and polycrystal are computed as simple examples.

2. Basic equations

In the context of elastoplastic materials with isomorphic elastic ranges [3], we use an elastic reference law in the undistorted state for the Kirchhoff stress tensor $J\mathbf{T}$ and the right Cauchy–Green tensor $\mathbf{C} = \mathbf{F}^{\top}\mathbf{F}$, $J = \sqrt{\det \mathbf{C}}$, where $\mathbf{F}$ is the deformation gradient, $\widetilde{\mathbb{K}}$ is a constant fourth-order tensor containing the single crystal constants,

$$J\mathbf{T} = \mathbf{FP}\widetilde{\mathbb{K}}\left[\frac{1}{2}(\mathbf{P}^{\top}\mathbf{CP} - \mathbf{1})\right](\mathbf{FP})^{\top}. \qquad (1)$$

The unimodular inelastic transformation $\mathbf{P}$ contains plastic effects and enters the elastic reference law only through the elastic transformation $\widetilde{\mathbf{F}} := \mathbf{FP}$. There exists an imbedding into theories based on multiplicative decomposition of the deformation gradient $\mathbf{F}$ since the identity

$$\mathbf{F} = \widetilde{\mathbf{F}}\mathbf{P}^{-1} \qquad (2)$$

holds.

The ratio $|\tau_\alpha/\tau_\alpha^c|$ indicates whether or not a certain slip system is active. τ_α are the resolved shear stresses and τ_α^c their critical values. A pull-back operation by $\widetilde{\mathbf{F}}$ leads to $\widetilde{\mathbf{C}} = \widetilde{\mathbf{F}}^{\top}\widetilde{\mathbf{F}}$, $\widetilde{\mathbf{S}} = \widetilde{\mathbf{F}}^{-1}\mathbf{T}\widetilde{\mathbf{F}}^{-\top}$, and

$$\tau_\alpha = J\widetilde{\mathbf{C}}\widetilde{\mathbf{S}} \cdot \widetilde{\mathbf{M}}_\alpha, \qquad (3)$$

while $\widetilde{\mathbf{M}}_\alpha = \tilde{\mathbf{d}}_\alpha \otimes \tilde{\mathbf{n}}^\alpha$ is the (constant) Schmid tensor with slip direction and slip plane normal fixed to the crystal lattice.

Based on the kinematics of crystallographic slip, we use the flow rule

$$\widetilde{\mathbf{L}}_p := -\mathbf{P}^{-1}\dot{\mathbf{P}} = \sum_\alpha |\dot{\gamma}_\alpha| \operatorname{sign}\tau_\alpha \widetilde{\mathbf{M}}_\alpha \qquad (4)$$

and the hardening rule (using the hardening moduli $h_{\alpha\beta}$ that may depend on the process)

$$\dot{\tau}_\alpha^c = \sum_\beta h_{\alpha\beta}|\dot{\gamma}_\beta|. \qquad (5)$$

For the slip rates we make an ansatz that is similar to the constitutive law used in the rate dependent theory, namely

$$\dot{\gamma}_\alpha = \lambda\left|\frac{\tau_\alpha}{\tau_\alpha^c}\right|^n \operatorname{sign}\tau_\alpha, \quad \lambda > 0. \qquad (6)$$

However, λ is not a process parameter but a plastic multiplier independent of α.

The condition of consistency for the determination of λ uses a rounded yield locus (as found similar in [6])

$$\Phi = \left(\sum_\alpha \left|\frac{\tau_\alpha}{\tau_\alpha^c}\right|^{n+1}\right) - 1 = 0. \qquad (7)$$

By taking the time derivative

$$\left|\frac{\tau_\alpha}{\tau_\alpha^c}\right|^{\cdot} = \sum_\beta m_{\alpha\beta}|\dot{\gamma}_\beta| - c_\alpha, \qquad (8)$$

where the coefficients

$$m_{\alpha\beta} = \frac{J}{\tau_\alpha^c}\Bigg((\widetilde{\mathbf{M}}_\beta\widetilde{\mathbf{C}} + \widetilde{\mathbf{C}}\widetilde{\mathbf{M}}_\beta)\widetilde{\mathbf{S}} + \frac{1}{2}\widetilde{\mathbf{C}}\widetilde{\mathbb{K}}[\widetilde{\mathbf{M}}_\beta\widetilde{\mathbf{C}} + \widetilde{\mathbf{C}}\widetilde{\mathbf{M}}_\beta]\Bigg) \cdot \widetilde{\mathbf{M}}_\alpha \operatorname{sign}\tau_\alpha \operatorname{sign}\tau_\beta + \frac{J}{\tau_\alpha^c}\left|\frac{\tau_\alpha}{\tau_\alpha^c}h_{\alpha\beta}\right|, \qquad (9)$$

$$c_\alpha = \frac{J}{\tau_\alpha^c}\Bigg(\mathbf{P}^{\top}\dot{\mathbf{C}}\mathbf{P}\widetilde{\mathbf{S}} + \frac{1}{2}\widetilde{\mathbf{C}}\widetilde{\mathbb{K}}[\mathbf{P}^{\top}\dot{\mathbf{C}}\mathbf{P}] + \frac{1}{\tau_\alpha^c}\frac{\dot{J}}{J}\widetilde{\mathbf{C}}\widetilde{\mathbf{S}}\Bigg) \cdot \widetilde{\mathbf{M}}_\alpha \operatorname{sign}\tau_\alpha \qquad (10)$$

have been introduced for brevity, we get by the chain rule a single condition of consistency, namely

$$\dot{\Phi} = (n+1)\sum_\alpha \left|\frac{\tau_\alpha}{\tau_\alpha^c}\right|^n \left(\sum_\beta m_{\alpha\beta}|\dot{\gamma}_\beta| - c_\alpha\right) = 0. \qquad (11)$$

Note that (8) is the condition of consistency for the classical multisurface theory of crystal plasticity, and (11) is a weighted average of it. Inserting (6) into (11) we find a solution for the plastic multiplier λ:

$$\lambda = \frac{\sum_\alpha \left|\frac{\tau_\alpha}{\tau_\alpha^c}\right|^n c_\alpha}{\sum_\alpha \sum_\beta \left|\frac{\tau_\alpha}{\tau_\alpha^c}\right|^n m_{\alpha\beta}\left|\frac{\tau_\beta}{\tau_\beta^c}\right|^n}. \qquad (12)$$

If it yields a negative value, the loading condition is violated and $\lambda = 0$ has to be taken instead. From (10), a flowrule can be found, which is positive homogeneous of degree 1 in $\dot{\mathbf{C}}$, assuring rate-independence.

In addition, in proportional processes a corner stress state means that $|\tau_\alpha/\tau_\alpha^c|^n = 1$ for several α simultaneously, while the others have a negligible value. As the Schmid tensors for the active slip systems differ by symmetry transformations of the lattice only, the coefficients in (8) for the active slip systems are equal. In this case our approach and the multisurface theory coincide. Another coincidence is given for single slip.

The behaviour between those two limit processes can be seen in Fig. 1 in comparison with Schmid-law. The direction of plastic flow is indicated by the small strokes. The rule of normality is obeyed to for the case of equal hardening states, as found from comparison of $\widetilde{\mathbf{L}}_p$ and

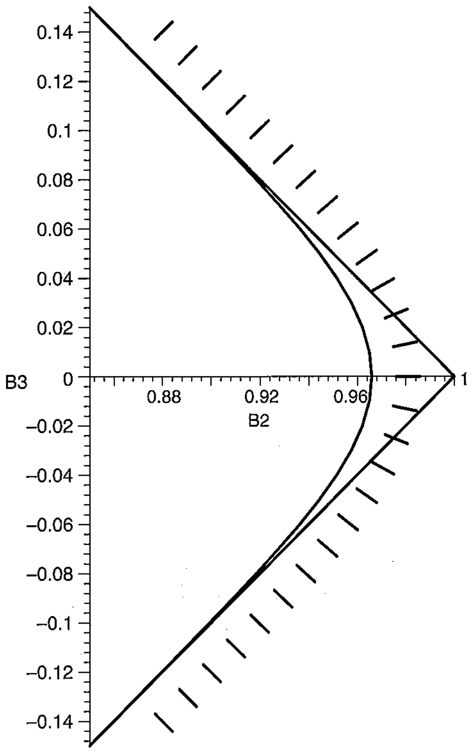

Fig. 1. Vertex of the 2D crystallite rounded yield locus, and according Schmid laws. Shear vs. direct stress.

$$\frac{\mathrm{d}}{\mathrm{d}(J\widetilde{\mathbf{C}}\widetilde{\mathbf{S}})}\Phi = \sum_\alpha \widetilde{\mathbf{M}}_\alpha \frac{\operatorname{sign}\tau_\alpha}{\tau_\alpha^c}\left|\frac{\tau_\alpha}{\tau_\alpha^c}\right|^n. \tag{13}$$

A yield criterion can be established by multiplying λ by the Heaviside jump function $\lambda \mathrm{u}(\Phi) = \lim_{n\to\infty} \lambda \sum_\alpha |\tau_\alpha/\tau_\alpha^c|^n$ in the range $|\tau_\alpha/\tau_\alpha^c| \in [0,1]$. To get the same smooth activation behaviour as in the rate dependent approach, we can choose $n < \infty$, or as inspection of (12) shows, by computing λ for a stress state proportionally scaled to $\Phi = 0$,

$$\sum_\alpha \left|\frac{a\tau_\alpha}{\tau_\alpha^c}\right|^n = 1 \Rightarrow a = \frac{1}{\sqrt[n]{\Phi+1}} \Rightarrow \lambda \to \sum_\alpha \left|\frac{\tau_\alpha}{\tau_\alpha^c}\right|^n \lambda. \tag{14}$$

3. Numerical implementation

We use a first-order implicit discretization of the flow rule (4),

$$\mathbf{0} = \mathbf{P}_{k+1}\left(\mathbf{1} + \Delta t \widetilde{\mathbf{L}}_{p,k+1}\right) - \mathbf{P}_k. \tag{15}$$

By left-hand application of $\mathbf{F}_{k+1}$ and introduction of the incremental deformation gradient $\mathbf{F}_\Delta = \mathbf{F}_{k+1}\mathbf{F}_k^{-1}$, the resulting nonlinear equation is

$$\widetilde{\mathbf{F}}_{k+1}(\mathbf{1} + \Delta t \widetilde{\mathbf{L}}_{p,k+1}) - \mathbf{F}_\Delta \widetilde{\mathbf{F}}_k = \mathbf{0}. \tag{16}$$

Using the Taylor expansion of $\mathbf{F}_{k+1} = \mathbf{F}_k + \Delta t \mathbf{L}_{k+1}\mathbf{F}_{k+1} + \mathrm{O}(\Delta t^2)$ and $\mathbf{P}_k = \mathbf{P}_{k+1} - \Delta t \mathbf{P}_{k+1}\widetilde{\mathbf{L}}_{p,k+1} + \mathrm{O}(\Delta t^2)$ we find that the last term of (16) can be rewritten as

$$\mathbf{F}_\Delta \widetilde{\mathbf{F}}_k = \mathbf{F}_{k+1}\mathbf{P}_k = \widetilde{\mathbf{F}}_k + \Delta t \mathbf{L}\widetilde{\mathbf{F}}_{k+1} + \mathrm{O}(\Delta t^2). \tag{17}$$

Inserting (17) into (16) we end up with a scheme that has been shown in [4,11] to be a first-order implicit integration scheme for the evolution of $\widetilde{\mathbf{F}}$,

$$\dot{\widetilde{\mathbf{F}}} = -\widetilde{\mathbf{F}}\widetilde{\mathbf{L}}_p + \mathbf{L}\widetilde{\mathbf{F}}. \tag{18}$$

By (17) our approach is also consistent with (18) but has the advantage that it does not depend on the velocity gradient $\mathbf{L}$ but only on the incremental deformation gradient. In the evaluation of λ, we need

$$\mathbf{P}^\top \dot{\mathbf{C}} \mathbf{P} = 2\widetilde{\mathbf{F}}^\top \operatorname{sym} \frac{\mathbf{F}_\Delta - \mathbf{1}}{\Delta t}\widetilde{\mathbf{F}} + \mathrm{O}(\Delta t^2). \tag{19}$$

For the integration of (16) we use $\widetilde{\mathbf{F}}_k$ as the starting point for a Newton iteration. At each step λ is determined by the above projection onto the yield surface. The analytical computation of the terms of the Jacobian is straightforward, as the implicit dependence on $\widetilde{\mathbf{F}}$ is through $|a\tau_\alpha/\tau_\alpha^c|^n$ only, as can be seen by (4) and (12).

4. Examples

4.1. Simple shear

As an example, an f.c.c. crystal has been subjected to a simple shear deformation. Hardening has been excluded for simplicity. For this process there exists no stable orientation and the lattice gets into an continuous rotation. This is reflected in the oscillating behaviour of the elastic deformation as well as of the Cauchy stress (Fig. 2b,c).

In Fig. 2d the resolved shear stresses and the respective slip rates are compared. For this non-proportional example there are differences in the slip system activity of the multisurface theory and our approach.

In a strict elastic–plastic multisurface theory, slip systems that are only slightly below critical resolved shear stress, are inactive. In contradiction to this, experiments in a dual slip setting have stated [2] that the conjugate systems get active before reaching the critical point. This behaviour is better reflected by our approach than by the classical multisurface theory.

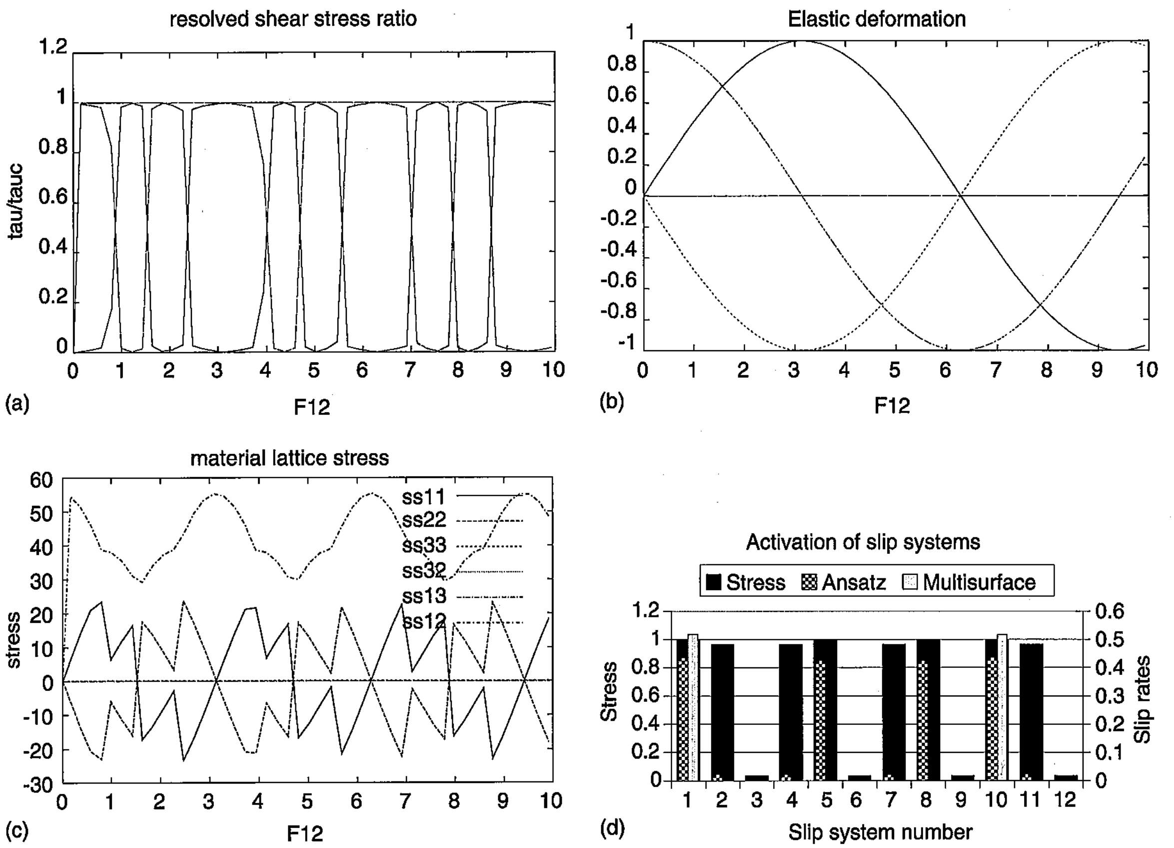

Fig. 2. Simple shear test. (a) Resolved shear stress ratio $|\tau|/\tau_c$, (b) elastic deformation $\widetilde{\mathbf{F}}$, (c) Cauchy stress $\mathbf{T}$ and (d) slip system activity.

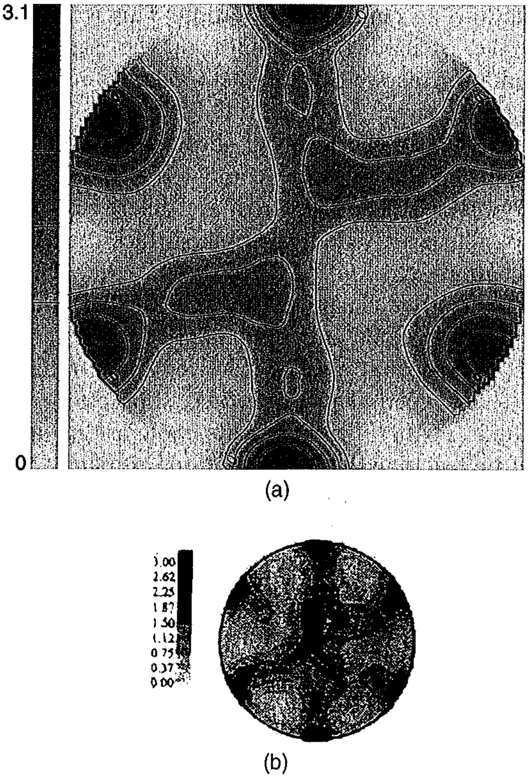

Fig. 3. Shear textures at shear number 1.5. (a) Computed and (b) experimental [5].

4.2. Shear texture of a polycrystal

The shear texture of a 256-grain copper polycrystal at a shear number of 1.5 has been calculated. Here, hardening was included. In Fig. 3 the resulting [1 1 1] pole figure is compared with experiments from [5]. Both figures look similar.

5. Conclusion

A rate independent theory of crystallographic slip has been presented that avoids the ambiguity as known from the multisurface plasticity theory. Instead an ansatz similar to the rate dependent theory has been used. No special solution technique like singular value decomposition is necessary. The result is rate independent, but shows a more realistic smooth activation behaviour of the slip systems and a unique solution. This approach has been shown to coincide with the multisurface theory for special cases. The numerical implementation is not a difficult task. An integration based on a implicit Euler scheme has been shown to yield stable, reasonable results.

References

[1] L. Anand, M. Kothari, A computational procedure for rate-independent crystal plasticity, J. Mech. Phys. Solids 44 (4) (1996) 525–558.

[2] R.J. Asaro, Micromechanics of crystals and polycrystals, Adv. Appl. Mech. 23 (1983).

[3] A. Bertram, An alternative approach to finite plasticity based on material isomorphisms, Int. J. Plast. 15 (1999) 353–374.

[4] T. Böhlke, Crystallographic texture evolution and elastic anisotropy, Ph.D. thesis, Otto-von-Guericke-Universität Magdeburg, 2001, ISBN 3-8265-8758-8, Shaker Verlag Aachen.

[5] C.A. Bronkhorst, S.R. Kalidindi, L. Anand, Polycrystal plasticity and the evolution of crystallographic texture in face centered cubic metals, Phil. Trans. R. Soc. Lond. A 341 (1992) 443–477.

[6] W. Gambin, F. Barlat, Modeling of deformation texture development based on rate independent crystal plasticity, Int. J. Plast. 13 (1997) 75–85.

[7] R. Knockaert, Y. Chastel, E. Massoni, Rate-independent crystalline and polycrystalline plasticity, application to fcc materials, Int. J. Plast. 16 (2000) 179–198.

[8] U.F. Kocks, C.N. Tomé, H.R. Wenk (Eds.), Texture and Anisotropy, Cambridge University Press, Cambridge, 1998.

[9] C. Miehe, J. Schröder, J. Schotte, Computational homogenization analysis in finite plasticity simulation of texture development in polycrystalline materials, Comput. Methods Appl. Mech. Eng. 171 (1999) 387–418.

[10] D. Peirce, R.J. Asaro, A. Needleman, Material rate dependence and localized deformation in crystalline solids, Acta Metall. 31 (1983) 1951–1976.

[11] G. Sarma, Th. Zacharia, Integration algorithm for modeling the elasto-viscoplastic response of polycrystalline materials, J. Mech. Phys. Solids 47 (1999) 1219–1238.