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Efficient Integration in the Plasticity of Crystals with Pencil Glide and Deck Glide

A. Krawietz

A stress update algorithm is proposed based on an approximate additive decomposition of the elastic predictor strain. It yields acceptable results even if the strain increments are an order of magnitude larger than the elastic strains. Moreover, it is shown that, in the context of the models of pencil glide and deck glide, at most four nonlinear equations for the computation of the unknown increments of plastic shear are needed in the case of b.c.c. and f.c.c. crystals.

1 Introduction

We discuss large elastic-plastic deformations of single crystals in the context of the multiplicative theory. First, it is shown that a stress update algorithm may be based on an approximate additive decomposition of the elastic predictor strain. Our numerical examples demonstrate that this approximation yields results which are accurate enough even if the strain increments are an order of magnitude larger than the elastic strains. Special attention is given to the models of pencil glide and deck glide, discussed by Krawietz (1981) in the context of the multiplicative theory under the names "Bündelstruktur" (bundle structure) and "Schichtenstruktur" (layered structure). When applied to b.c.c. and f.c.c. crystals, respectively, these models allow at most four active sliding mechanisms and hence only four unknown increments of plastic shear. However, the planes of sliding or the directions of sliding, respectively, seem to constitute additional unknowns. Fortunately, we succeed to prove that these are not independent but are determined by the values of the increments of plastic shear.

2 Multiplicative Plasticity

We base our description of rate-independent plasticity on the multiplicative decomposition

$$\mathbf{F} = \mathbf{F}_e \mathbf{F}_p \tag{1}$$

of the local transplacement $\mathbf{F}$ into an elastic and a plastic part. We define the right Cauchy-Green tensor by

$$\mathbf{C} = \mathbf{F}^T \mathbf{F} \tag{2}$$

and denote the actual mass density by ϱ and the Cauchy stress by $\mathbf{T}$. The elastic right Cauchy-Green tensor $\mathbf{C}_e$, Green's elastic strain tensor $\mathbf{E}_e$, and the modified lattice stress — stress over density — $\mathbf{Z}_e$ are defined by

$$\mathbf{C}_e = \mathbf{1} + 2\mathbf{E}_e = \mathbf{F}_e^T \mathbf{F}_e = \mathbf{F}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1} \tag{3}$$

$$\mathbf{Z}_e = \mathbf{F}_e^{-1} \frac{\mathbf{T}}{\varrho} \mathbf{F}_e^{-T} \tag{4}$$

The linear elastic behavior of the lattice is characterized by

$$\mathbf{Z}_e = \mathcal{C} : \mathbf{E}_e \tag{5}$$

The plastic deformation of a crystal occurs by sliding on discrete planes in the form

$$\dot{\mathbf{F}}_p \mathbf{F}_p^{-1} = \sum_j \kappa_j \mathbf{m}_j \otimes \mathbf{n}_j \tag{6}$$

where κ_j denotes the velocity of shearing and $\mathbf{n}_j$ and $\mathbf{m}_j$ are unit vectors normal to the plane of sliding and in the direction of sliding, respectively, both measured in the (stress free) reference placement of the lattice. The power of dissipation is given by

$$\delta = \mathbf{C}_e\mathbf{Z}_e : \dot{\mathbf{F}}_p\mathbf{F}_p^{-1} = \sum_j \kappa_j \bar{\tau}_j \tag{7}$$

with the abbreviation

$$\bar{\tau}_j = \mathbf{m}_j\mathbf{C}_e\mathbf{Z}_e\mathbf{n}_j \approx \mathbf{m}_j\mathbf{Z}_e'\mathbf{n}_j \tag{8}$$

The last simplification is admissible if the elastic strain $\mathbf{E}_e$ is small compared with the unit tensor. Then the expression $\bar{\tau}_j$ depends only on the deviatoric part $\mathbf{Z}_e'$ of $\mathbf{Z}_e$ and shall be termed modified Schmid stress.

States are only admissible if they lie within the elastic range characterized by the restrictions

$$\bar{\tau}_j \leq y(\zeta_j) \tag{9}$$

where ζ_j denotes a hardening parameter, and sliding of the mechanism j is possible, if the yield condition

$$\bar{\tau}_j = y(\zeta_j) \tag{10}$$

is valid.

Remark: The yield condition is formulated with the modified Schmid stress — lattice stress over mass density (which is influenced by an elastic volume change of the lattice) — and not with the classical (Cauchy) Schmid stress in order to meet the principle of maximum dissipation according to von Mises, discussed in Krawietz (1981, 1999).

The hardening laws are assumed to be of the type

$$\dot{\zeta}_j = (1-q)\kappa_j + q\sum_k \kappa_k \tag{11}$$

The sliding directions $\mathbf{m}_j$ of a body-centered cubic crystal are the four space diagonals which include equal angles with the three crystal axes. Actually there is a finite number of corresponding planes of sliding. In place of that, the model of pencil glide, proposed by Taylor, assumes that every plane which contains a space diagonal may be a plane of sliding. The modified Schmid stress on such a plane with unit normal $\mathbf{n}_j$ is given by

$$\bar{\tau}_j = \mathbf{m}_j\mathbf{Z}_e'\mathbf{n}_j = \mathbf{m}_j\mathbf{Z}_e'(\mathbf{1} - \mathbf{m}_j \otimes \mathbf{m}_j)\mathbf{n}_j = \mathbf{s}_j \cdot \mathbf{n}_j \tag{12}$$

where

$$\mathbf{s}_j = \mathbf{m}_j\mathbf{Z}_e'(\mathbf{1} - \mathbf{m}_j \otimes \mathbf{m}_j) \tag{13}$$

denotes the modified shear stress vector on the plane which is perpendicular to the sliding direction $\mathbf{m}_j$. The modified Schmid stress takes its maximal value

$$\bar{\tau}_j = |\mathbf{s}_j| \tag{14}$$

on the plane with the unit normal

$$\mathbf{n}_j = \frac{\mathbf{s}_j}{|\mathbf{s}_j|} = \frac{\mathbf{m}_j\mathbf{Z}_e'(\mathbf{1} - \mathbf{m}_j \otimes \mathbf{m}_j)}{|\mathbf{m}_j\mathbf{Z}_e'(\mathbf{1} - \mathbf{m}_j \otimes \mathbf{m}_j)|} \tag{15}$$

If we assume that the critical value $y(\zeta_j)$ is the same for all the planes containing the same sliding direction $\mathbf{m}_j$, then sliding can only be activated on that plane with the maximum modified Schmid stress.

3 An Implicit Integration Algorithm

We assume that, during the finite time increment $(t_0,\, t_0 + \Delta t)$, the ratios of the shearing velocities κ_j remain constant. In the case of pencil glide, we additionally assume the constancy of the unit vectors $\mathbf{n}_j$ of the planes of sliding. Thus we set

$$\kappa_j = \dot{k}(t)\Delta\gamma_j \qquad \text{with} \qquad k(t_0) = 0, \quad k(t_0 + \Delta t) = 1 \tag{16}$$

and hence

$$\dot{\mathbf{F}}_p\mathbf{F}_p^{-1} = \sum_j \kappa_j \mathbf{m}_j \otimes \mathbf{n}_j = \dot{k}(t)\,\mathbf{K} \qquad \text{with} \qquad \mathbf{K} = \sum_j \Delta\gamma_j \mathbf{m}_j \otimes \mathbf{n}_j \tag{17}$$

Since the tensor $\mathbf{K}$ is constant according to our assumptions, the solution of this differential equation can be written down:

$$\mathbf{F}_p(t) = e^{k(t)\mathbf{K}}\,\mathbf{F}_p(t_0) \qquad \Longrightarrow \qquad \mathbf{F}_p(t_0 + \Delta t) = e^{\mathbf{K}}\,\mathbf{F}_p(t_0) \tag{18}$$

If no yield would occur ($\mathbf{K} = 0$), then the elastic deformation at the end of the increment would be given by the elastic predictor strain — cf. equation (3) —

$$\mathbf{E}_e^{\text{pre}} = \tfrac{1}{2}\left(\mathbf{F}_p(t_0)^{-T}\mathbf{C}(t_0 + \Delta t)\,\mathbf{F}_p(t_0)^{-1} - \mathbf{1}\right) \tag{19}$$

The actual elastic strain at the end of the increment, however, is

$$\begin{aligned} \mathbf{E}_e(t_0 + \Delta t) &= \tfrac{1}{2}\left(e^{-\mathbf{K}^T}\mathbf{F}_p(t_0)^{-T}\mathbf{C}(t_0 + \Delta t)\,\mathbf{F}_p(t_0)^{-1}e^{-\mathbf{K}} - \mathbf{1}\right) \\ &= \tfrac{1}{2}\left(e^{-\mathbf{K}^T}\left(\mathbf{1} + 2\mathbf{E}_e^{\text{pre}}\right)e^{-\mathbf{K}} - \mathbf{1}\right) \end{aligned} \tag{20}$$

If the total strain increment is moderate, then both the elastic predictor strain and the plastic strain increment cannot be large, and hence we replace the exponential function by a Taylor polynomial and neglect higher powers of $\mathbf{K}$ as well as products of $\mathbf{K}$ and $\mathbf{E}_e^{\text{pre}}$, thus finding

$$\begin{aligned} \mathbf{E}_e(t_0 + \Delta t) &= \tfrac{1}{2}\left(\left(\mathbf{1} - \mathbf{K}^T + \ldots\right)\left(\mathbf{1} + 2\mathbf{E}_e^{\text{pre}}\right)\left(\mathbf{1} - \mathbf{K} + \ldots\right) - \mathbf{1}\right) \\ &\approx \mathbf{E}_e^{\text{pre}} - \operatorname{sym}\mathbf{K} \end{aligned} \tag{21}$$

The elastic strain is thus represented as the difference of the elastic predictor strain and a plastic strain increment. Note that such an additive decomposition is restricted to the incremental level and does not hold for finite values of the strain.

The modified lattice stress at the end of the increment becomes

$$\mathbf{Z}_e(t_0 + \Delta t) = \mathcal{C} : \left(\mathbf{E}_e^{\text{pre}} - \operatorname{sym}\mathbf{K}\right) = \mathcal{C} : \left(\mathbf{E}_e^{\text{pre}} - \sum_j \Delta\gamma_j \operatorname{sym}\left(\mathbf{m}_j \otimes \mathbf{n}_j\right)\right) \tag{22}$$

The increments of the hardening parameters are obtained by integration of the hardening laws (11)

$$\Delta\zeta_j = (1 - q)\Delta\gamma_j + q\sum_k \Delta\gamma_k \tag{23}$$

Let there be m active sliding mechanisms and let A denote the set of their numbers, then there are m unknown increments of plastic shear $\Delta\gamma_j$ $(j \in A)$. These have to be obtained from the m yield conditions — cf. equations (8) and (10) —

$$
\begin{aligned}
&\operatorname{sym}(\mathbf{m}_j \otimes \mathbf{n}_j) : \mathcal{C} : \left(\mathbf{E}_e^{\mathrm{pre}} - \sum_{k \in A} \Delta\gamma_k \operatorname{sym}(\mathbf{m}_k \otimes \mathbf{n}_k) \right) \\
&= y\left(\zeta_j(t_0) + (1-q)\Delta\gamma_j + q \sum_{k \in A} \Delta\gamma_k \right) \qquad \text{for all } j \in A
\end{aligned} \tag{24}
$$

The selection of the active set A is done correctly if the inequalities

$$
\Delta\gamma_j \geq 0 \qquad \text{for all } j \in A \tag{25}
$$

are valid and the inequality

$$
\bar{\tau}_j \leq y(\zeta_j) \tag{26}
$$

holds for any inactive mechanism.

The m equalities (24) are nonlinear but become linear in the special case of linear hardening. Under special states of stress and hardening, it may happen that the number m of active mechanisms is high, and the solution of the equations is not unique. In this case, regularization techniques have to be applied or rules have to be postulated which select one of the solutions — cf. Miehe and Schröder (2001).

4 The Case of Pencil Glide

The problem of non-uniqueness does not occur in the case of pencil glide since there are at most four active mechanisms. So the choice of this model may be regarded as a physical method of regularization. However, the equations (24) are not applicable since the normal vectors $\mathbf{n}_j$ are not given *a priori* and hence seem to play the part of additional unknowns.

Fortunately, however, we are able to show that these normal vectors are determined by the increments of plastic shear, which therefore remain the only unknown quantities even in the case of pencil glide. In order to see this, we introduce equations (10) and (14) into (15) and find

$$
\mathbf{n}_j = \frac{\mathbf{s}_j}{|\mathbf{s}_j|} = \frac{\mathbf{m}_j \mathbf{Z}_e'(\mathbf{1} - \mathbf{m}_j \otimes \mathbf{m}_j)}{y(\zeta_j)} \tag{27}
$$

Since $\mathbf{n}_j$ was assumed to be constant during the increment, we have to evaluate the right-hand side expression with fixed values of $\mathbf{Z}_e'$ and ζ_j, and we do it with the values at the end of the increment. With the fourth-order tensors $\mathcal{I}$ and $\mathcal{I}'$ — identical mappings on the spaces of symmetric and of symmetric deviatoric tensors, respectively — and

$$
\mathcal{C}' = (\mathcal{I} - \tfrac{1}{3}\mathbf{1} \otimes \mathbf{1}) : \mathcal{C} \tag{28}
$$

the deviatoric part of equation (22) reads

$$
\mathbf{Z}_e'(t_0 + \Delta t) = \mathcal{C}' : \left(\mathbf{E}_e^{\mathrm{pre}} - \sum_{j \in A} \lambda_j \operatorname{sym}\left(\mathbf{m}_j \otimes \mathbf{m}_j \mathbf{Z}_e'(t_0 + \Delta t)(\mathbf{1} - \mathbf{m}_j \otimes \mathbf{m}_j) \right) \right) \tag{29}
$$

and can be rearranged to read

$$
\left(\mathcal{I}' + \sum_{j \in A} \lambda_j \mathcal{K}(\mathbf{m}_j) \right) : \mathbf{Z}_e' = \mathcal{C}' : \mathbf{E}_e^{\mathrm{pre}} = \mathbf{Z}_e^{\mathrm{pre}\,\prime} \tag{30}
$$

with the abbreviations

$$
\lambda_j = \frac{\Delta\gamma_j}{y(\zeta_j(t_0 + \Delta t))} = \frac{\Delta\gamma_j}{y\left(\zeta_j(t_0) + (1-q)\Delta\gamma_j + q \sum_{k \in A} \Delta\gamma_k \right)} \tag{31}
$$

and the fourth-order tensor $\mathcal{K}$ defined by the linear mapping

$$\mathcal{K}(\mathbf{a}) : \mathbf{B}' = \mathcal{C}' : \text{sym}\left(\mathbf{a} \otimes \mathbf{a}\,\mathbf{B}'(\mathbf{1} - \mathbf{a} \otimes \mathbf{a})\right) \tag{32}$$

We see that the parameters λ_j are determined by the increments $\Delta\gamma_k$ of plastic shear. So inversion of the deviator equation (30) — which means inverting five scalar linear equations — gives $\mathbf{Z}'_e$ as a function of these increments

$$\mathbf{Z}'_e = \left(\mathcal{I}' + \sum_{j \in A} \lambda_j\, \mathcal{K}(\mathbf{m}_j)\right)^{-1} : \mathbf{Z}_e^{\text{pre}\,'} = \mathbf{Z}'_e(\Delta\gamma_1, \Delta\gamma_2, \Delta\gamma_3, \Delta\gamma_4) \tag{33}$$

and equation (27) shows that the unit normals $\mathbf{n}_j$ of the planes of sliding are then indeed also determined by these increments.

There are at most four unknown increments of plastic shear and — noting equations (10), (13), (14) — we may obtain them from the equations

$$\left|\mathbf{m}_j \mathbf{Z}'_e(\Delta\gamma_1, \Delta\gamma_2, \Delta\gamma_3, \Delta\gamma_4)(\mathbf{1} - \mathbf{m}_j \otimes \mathbf{m}_j)\right| = y\left(\zeta_j(t_0) + (1-q)\Delta\gamma_j + q \sum_{k \in A} \Delta\gamma_k\right) \quad \text{for all } j \in A \tag{34}$$

The right-hand side of these equations becomes linear in the special case of linear hardening but the left-hand side is essentialy nonlinear in the unknowns.

When the equations are solved, we obtain the tensor $\mathbf{Z}'_e$, the vectors $\mathbf{n}_j$, the tensor $\mathbf{K}$, and the updated tensor $\mathbf{F}_p$ successively from equations (33), (15), (17), and (18). Since $\mathbf{K}$ is deviatoric, the determinant of $\exp(\mathbf{K})$ is equal to 1, which ensures that the plastic deformation is volume-preserving. In order to retain this property, a rather accurate evaluation of the exponential of a non-symmetric tensor is needed. A representation with an error of the determinant of the order of $|\mathbf{K}|^5$ is given by the (2,2) Padé formula

$$e^{\mathbf{K}} \approx \mathbf{1} + \mathbf{K}\left(\mathbf{1} - \tfrac{1}{2}\mathbf{K} + \tfrac{1}{12}\mathbf{K}^2\right)^{-1} \tag{35}$$

In Krawietz (1999, equations (28) to (30)), a different integration scheme was proposed, which made use of 12 unknowns (the eight components of the deviatoric tensor $\mathbf{K}$ and the four increments of plastic shear $\Delta\gamma_j$). The new algorithm, proposed above, reduces the number of unknowns and of nonlinear equations to at most four and is thus obviously more efficient.

5 Accuracy Assessment

Two numerical examples shall prove the usefulness of our approach. The elastic constants of the b.c.c. crystal are taken from α-Fe (E = 134 000 N/mm^2, G = 118 000 N/mm^2, ν = 0.367). For simplicity, we assume linear hardening ($y(\zeta) = (140 + 100\zeta)$ N/mm^2) and choose the parameter of alternate hardening to be $q = 1$. The initial orientation is chosen to be

$$\mathbf{F}_p(t=0) = 2\mathbf{n} \otimes \mathbf{n} - \mathbf{1} \qquad \text{with} \qquad \mathbf{n} = 0.668\,(\mathbf{e}_1 + \mathbf{e}_2) + 0.327\,\mathbf{e}_3 \tag{36}$$

First we simulate a compression test by applying the deformation

$$\mathbf{F}(t) = e^{-t}\,\mathbf{e}_1 \otimes \mathbf{e}_1 + e^{t/2}\left(\mathbf{e}_2 \otimes \mathbf{e}_2 + \mathbf{e}_3 \otimes \mathbf{e}_3\right) \tag{37}$$

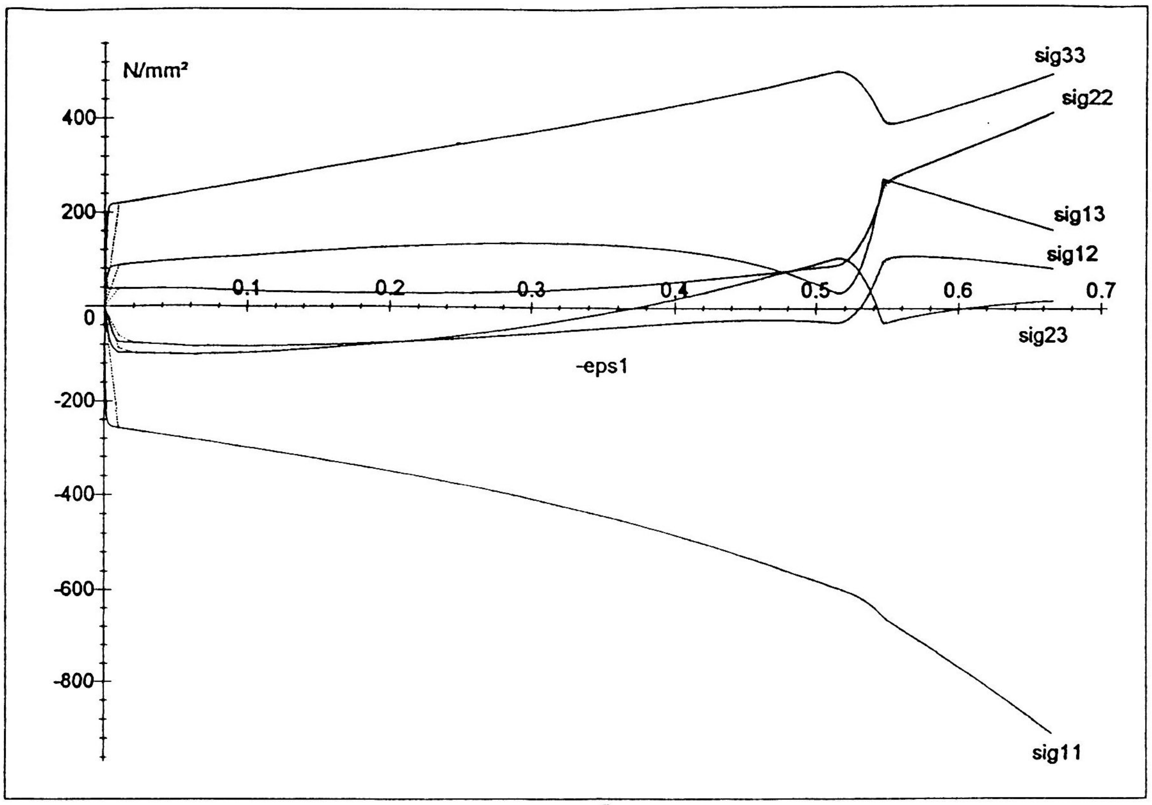

Figure 1. Compression of a crystal in the 1-direction which does not coincide with a crystal axis. Integration with small (——) and large (- - - -) time step

Figure 1 shows the evolution of the components of the Cauchy stress tensor as functions of the engineering strain in the 1-direction. During the first part of the process (after about $\epsilon_1 = -0.07$), three of the four possible sliding mechanisms are active. At about $\epsilon_1 = -0.52$, one of these three mechanisms stops sliding, so that a rearrangement of the stress pattern takes place. At about $\epsilon_1 = -0.55$, however, the remaining one of the four mechanisms is activated, so that there are again three active mechanisms during the rest of the process.

The calculation was done with a small time increment of 0.001 (solid lines) as well as with a moderate one of 0.01 (dashed lines). In the first case the total strain increment is of the order of the elastic strain while in the second case it is ten times larger. The equations (34) were solved by Newton's method.

The average number of iterations was two in the case of the small time increment and three in the case of the larger one. We notice that the results of the two calculations, which are based on the linearization according to equation (21), do not differ remarkably. So we learn that it is admissible and efficient to use strain increments that are an order of magnitude larger than the elastic strain.

However, our process was one of constant direction. It is sometimes pointed out, that errors become intolerable if large steps are used after a change of the direction of the deformation increment. Indeed, the stresses and hence the shearing velocities will rapidly change after such a kink in the deformation path so that the basic assumption (16) of our integration scheme cannot be realistic in the case of large steps.

Fortunately, the following second example shows that the situation is not necessarily dramatic. The applied deformation is

$$\mathbf{F}(t) = e^{-0.00122}\, \mathbf{e}_1 \otimes \mathbf{e}_1 + e^{0.00122/2-t}\, \mathbf{e}_2 \otimes \mathbf{e}_2 + e^{0.00122/2+t}\, \mathbf{e}_3 \otimes \mathbf{e}_3 \qquad (38)$$

Hence, a purely elastic compression in the 1-direction is followed by a compression in the 2-direction during which the strain in the 1-direction is kept constant. Figures 2a and 2b show the evolution of the normal stress and shear stress components, respectively, of the Cauchy stress tensor as functions of the engineering strain in the 2-direction.

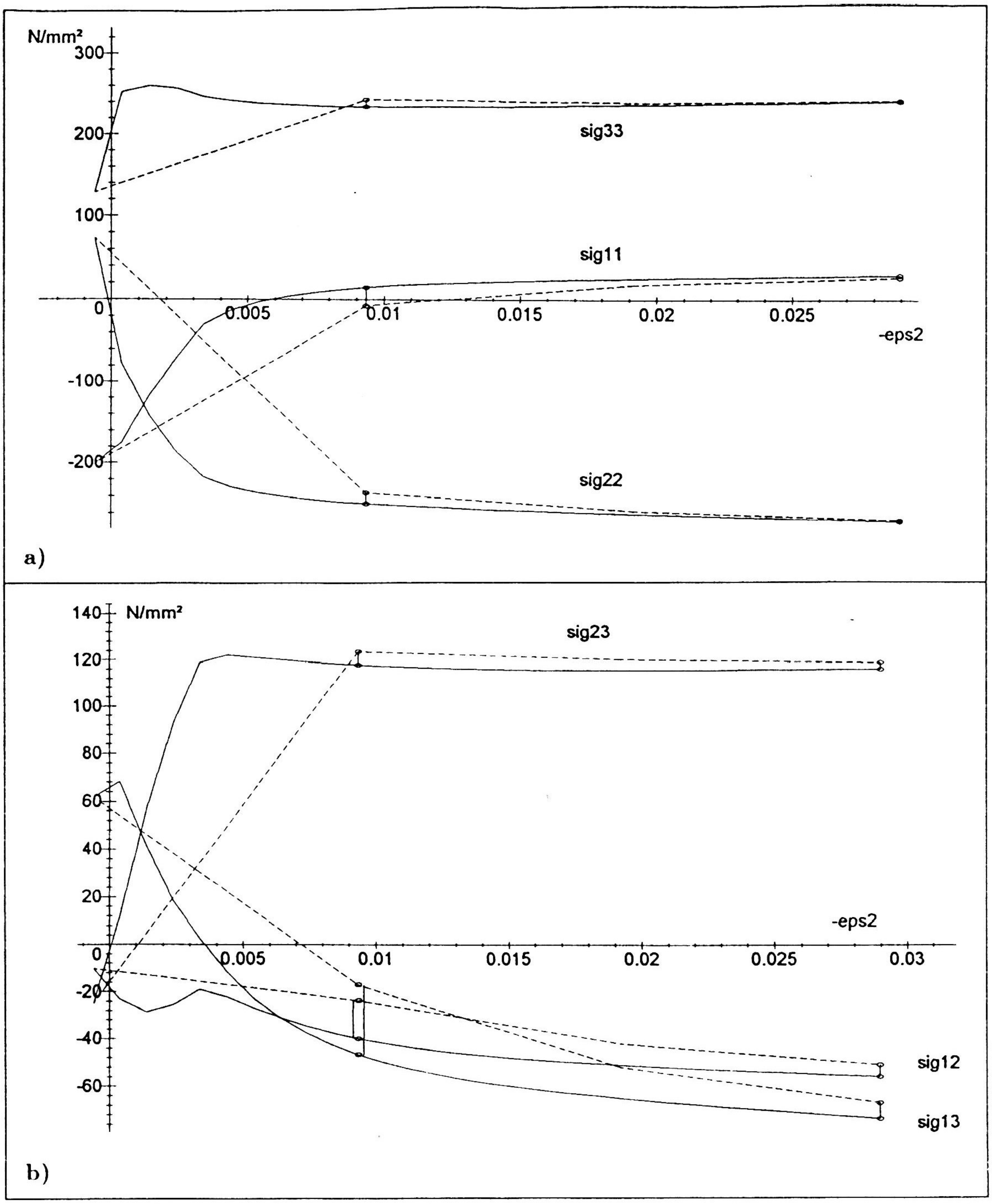

Figure 2. Elastic compression of a crystal in the 1-direction followed by a compression in the 2-direction. None of these directions coincides with a crystal axis.
Integration with small (——) and large (- - - -) time step.
a) Normal stresses, b) Shear stresses

The calculation is again done with the time increments 0.001 (solid lines) and 0.01 (dashed lines). After the first large step, the results differ markedly from those of the small step calculation (the latter are almost exact as they do not change much if the step is further decreased). The relative error, defined by

$$r = \frac{|\mathbf{T}_{0.01} - \mathbf{T}_{0.001}|}{|\mathbf{T}_{0.001}|} \tag{39}$$

— $|.|$: Euclidean norm of a tensor — turns out to be 14% which seems to be hardly acceptable.

One may, however, look on this result from a different point of view. There is obviously a rearrangement of the stress pattern during the first stage of the plastic deformation, which can only be clarified by a small step calculation. That a large step calculation cannot resolve phenomena which occur on a smaller time scale is a much more serious statement than the fact that the results at only one single point of time during this rearrangement are not exactly reproduced. The user must decide whether this loss of information is acceptable to him. If it is, then he may be comforted by the observation that the relative error is not conserved during the rest of the process under consideration but declines to 3% during the next two large steps.

6 The Case of Deck Glide

Our results are easily transferred to the case of deck glide, which may, e.g., be used to simplify the description of the plastic behavior of face-centered cubic crystals. The unit normals $\mathbf{n}_j$ of the primary planes of sliding of such crystals are the four space diagonals which include equal angles with the three crystal axes. Actually there is a finite number of directions of sliding in each of these planes. In place of that, the model of deck glide assumes that every direction within such a plane may be a direction of sliding. The modified Schmid stress is given by

$$\bar{\tau}_j = \mathbf{m}_j \mathbf{Z}'_e \mathbf{n}_j = \mathbf{m}_j (\mathbf{1} - \mathbf{n}_j \otimes \mathbf{n}_j) \, \mathbf{Z}'_e \mathbf{n}_j = \mathbf{m}_j \cdot \mathbf{s}_j \tag{40}$$

where

$$\mathbf{s}_j = (\mathbf{1} - \mathbf{n}_j \otimes \mathbf{n}_j) \, \mathbf{Z}'_e \mathbf{n}_j = \mathbf{n}_j \mathbf{Z}'_e (\mathbf{1} - \mathbf{n}_j \otimes \mathbf{n}_j) \tag{41}$$

denotes the modified shear stress vector on the plane of sliding. The modified Schmid stress takes its maximal value

$$\bar{\tau}_j = |\mathbf{s}_j| \tag{42}$$

if the direction of sliding coincides with the direction of this stress vector:

$$\mathbf{m}_j = \frac{\mathbf{s}_j}{|\mathbf{s}_j|} = \frac{\mathbf{n}_j \mathbf{Z}'_e (\mathbf{1} - \mathbf{n}_j \otimes \mathbf{n}_j)}{|\mathbf{n}_j \mathbf{Z}'_e (\mathbf{1} - \mathbf{n}_j \otimes \mathbf{n}_j)|} \tag{43}$$

A comparison with the formulae of pencil glide shows that the vectors $\mathbf{m}_j$ and $\mathbf{n}_j$ have interchanged their roles. This means, that the tensor $\mathbf{K}$ according to equation (17) is replaced by its transpose. Nevertheless, the update of the modified lattice stress $\mathbf{Z}_e$ is exactly the same in both cases since only the symmetric part of $\mathbf{K}$ enters our approximate equations (21), (22). Note, however, that the update of the plastic part $\mathbf{F}_p$ of the transplacement according to equation (18) depends on the skew part of $\mathbf{K}$, too, and hence the texture evolution is different.

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Address: Prof. Dr.-Ing. Arnold Krawietz, Technische Fachhochschule Berlin, Fachbereich Maschinenbau, Verfahrens- und Umwelttechnik, Luxemburger Str. 10, D-13353 Berlin, E-mail: krawietz@t-online.de