DESCRIPTION OF FINITE PLASTIC DEFORMATIONS IN SINGLE CRYSTALS BY MATERIAL ISOMORPHISMS

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1. Introduction

Most theories within plasticity are based on the notion of an *unstressed configuration* that is taken as a reference configuration for the elastic law which determines the stresses. The method of introducing this configuration, however, has been controversially discussed for more than 20 years. There were the suggestions by Green and Naghdi [8, 9] of an additive decomposition of the right Cauchy-Green tensor, and by Lee [11] of a multiplicative decomposition of the deformation gradient. Of course, in all of these theories the decomposition is a constitutive assumption which has strong consequences on the range of applicability of such theories. Unfortunately, these consequences are not easy to investigate, as there is still no general framework available within which all these different theories can be imbedded and thereafter compared.

The aim of the present paper is to construct such a general framework (see [2, 5, 6, 7, 10]) that is based on some assumptions which are clearly stated and commonly used in most of the theories in plasticity. The first assumption concerns the existence of elastic ranges which have a copy in the configuration space and in the stress space. The relation between the two is given by an elastic law that is introduced without any restriction. It can be isotropic or anisotropic, linear or nonlinear, hyperelastic or not, etc. The second assumption states that all these elastic laws are equal, if the variables are transformed in an appropriate way.

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The underlying concepts of the present theory are well-known from finite elasticity and a brief recapitulation will be given in the following section. By means of these concepts, we are able to state precisely our two assumptions. As a result, the concept of the *inelastic transformation* is derived, which contains all information about the influence of plastic deformations on the behaviour within the elastic ranges. This enables us to compare different decompositions and other concepts that are discussed in the field of finite plasticity.

As all of our constitutive equations are formulated by means of intrinsic concepts (see [3, 10, 13]) which are invariant under Euclidean transformations, they identically fulfil the requirement of objectivity under change of observer or superimposed rigid body motions.

If applied to crystal plasticity, the rather abstract concepts of the general theory can be specified and interpreted using crystallographical ideas. Taylor's theory on crystal glide mechanisms can be easily implemented within this context and gives an example of a non-symmetric inelastic transformation. Numerical results confirm Taylor and Elam's [14] experimental findings related to lattice rotations within single crystals. Other numerical investigations show the behaviour of f.c.c. single crystals under large shear strains.

2. Notations and Concepts from Finite Elasticity

The intrinsic description of stresses and strains is based on the geometrical concept of the tangent space $T_X B$ at a material point X to the body manifold B. The three-dimensional Euclidean point space is denoted by E and its associated vector space of the Euclidean shifters by V being endowed with the Euclidean metric or inner product $\mathbf{E}$. We will denote the dual to a mapping or a space by a superposed star. So, $\mathbf{E}$ can be considered as a symmetric ($\mathbf{E} = \mathbf{E}^*$) and positive-definite linear mapping from V onto V^*. A (local) placement $\mathbf{K}$ of the tangent space in the Euclidean space is a linear and invertible mapping from $T_X B$ on V, being the differential at X of the global placement of the body in E. The intrinsic (local) configuration is defined as the pull-back of the Euclidean metric $\mathbf{G} := \mathbf{K}^* \, \mathbf{E} \, \mathbf{K}$ to the tangent space $T_X B$ evaluated at X. If $\mathbf{T}$ denotes the Cauchy stress tensor, its pull-back to the tangent space $\mathbf{S} := \mathbf{K}^{-1} \, \mathbf{T} \, \mathbf{K}^{-*}$ defines the intrinsic stress tensor, a symmetric linear mapping from $T_X{}^*B$ to $T_X B$. The intrinsic stresses and configurations are power-conjugate variables, such that the specific power equals $l = (2\rho)^{-1} \, tr(\mathbf{S} \, \mathbf{G}^{\cdot})$.

As **S** and **G** are invariant under Euclidean transformations, any relation between **S** and **G** identically fulfils the requirement of material objectivity. Thus any objective simple elastic material can be described by a constitutive equation $\mathbf{S} = h(\mathbf{G})$. An example is the linear law

$$\mathbf{S} = \mathcal{C}[\Delta\mathbf{G}]\,\mathbf{G}_u^{-1} \tag{1}$$

where $\mathcal{C}$ is the fourth rank elasticity tensor and $\Delta\mathbf{G} := (2\rho)^{-1}\,\mathbf{G}_u^{-1}(\mathbf{G} - \mathbf{G}_u)$ is the change of configuration relative to $\mathbf{G}_u$, a material constant.

If, moreover, the power possesses a potential σ such that $l = \sigma^{\bullet} = tr(d\sigma/d\mathbf{G}\ \mathbf{G}^{\bullet})$, the material is hyperelastic and the stresses are given by $\mathbf{S} = 2\rho\ d\sigma/d\mathbf{G}$. But, for what follows this further assumption is not necessary.

As all the intrinsic variables are defined in terms of the tangent space at a material point X , it is not possible to compare them directly with those defined at another point Y . For this purpose an identification between the tangent spaces at the two points is needed, which is given by an invertible linear mapping **B** from $T_X B$ to $T_Y B$. By this mapping the configurations at the two points are related as

$$\mathbf{G}_X = \mathbf{B}^*\,\mathbf{G}_Y\,\mathbf{B} \tag{2}$$

and the stresses by

$$\mathbf{S}_Y = \mathbf{B}\,\mathbf{S}_X\,\mathbf{B}^*. \tag{3}$$

The elastic behaviour in these two points is isomorphic, if the elastic laws at the two points are related by

$$\mathbf{B}^{-1}\,h_Y(\mathbf{G}_Y)\,\mathbf{B}^{-1*} = h_X(\mathbf{B}^*\,\mathbf{G}_Y\,\mathbf{B}) \tag{4}$$

for all configurations within the domains. In this case, **B** is called a *material isomorphism.*

For $X \equiv Y$ this equation trivially holds for $\mathbf{B} = \mathbf{I}$, the identity. But there may also be non-trivial automorphisms **A** such that

$$\mathbf{A}^{-1}\,h(\mathbf{G})\,\mathbf{A}^{-1*} = h(\mathbf{A}^*\,\mathbf{G}\,\mathbf{A}) \tag{5}$$

holds for all possible **G** . The set of all such symmetry transformations **A** is called the *symmetry group* of the elastic law h , which specifies the crystal class of the material. If, for some (undistorted) configuration within the domain of the elastic law the symmetry group equals its orthogonal group, the material is called *isotropic*, while otherwise it is *anisotropic*. The following theory holds for both cases.

3. Elastic Ranges

The common feature of most theories in plasticity is the existence of elastic ranges.

Assumption 1. The material is at any instant in some elastic range.

That means that at any time t there exists a connected subset $\mathscr{E}_t$ of the configuration space together with an elastic law h_t such that the following holds:
(i) the configuration $\mathbf{G}(t)$ is in $\mathscr{E}_t$;
(ii) for any configuration process that starts from $\mathbf{G}(t)$ and remains entirely in $\mathscr{E}_t$ the stresses at the end are given by its final configuration $\mathbf{G}$ through $\mathbf{S} = h_t(\mathbf{G})$.

We do not restrict the shape of the elastic ranges. Thus it may also consist of a singleton as a degenerate case. If the elastic law is invertible, the elastic range in the configuration space has a unique correspondence in the stress space. That means that the yield limit, which determines the shape of the elastic range, can be expressed equivalently in terms of **S**, **G**, or any combination of them.

If the current stresses of the material, however, hit such a yield limit, then yielding can occur. This means, that the elastic range as well as the elastic law changes continuously. Of course, it is a material property, how this elastic law varies during yielding. But it is not just a question of convenience, but also substantiated by microphysics for many materials, that the elastic laws are isomorphic. This assumption is made in most plasticity theories, at least in their applications and examples. This saves us the identification work for an infinite number of elastic laws.

Assumption 2. All elastic ranges of the material are isomorphic.

That means, that between two elastic ranges $\mathscr{E}_1$ and $\mathscr{E}_2$ there exists a material isomorphism such that for the elastic laws of the two ranges

$$\mathbf{B}^{-1}\, h_2(\mathbf{G})\, \mathbf{B}^{-1*} = h_1(\mathbf{B}^*\, \mathbf{G}\, \mathbf{B}) \tag{6}$$

holds for all configurations within their ranges.

The practical procedure will be as follows. We take as a reference an arbitrary elastic law h_0 such as the initial one. At any instant there exists a material isomorphism $\mathbf{B}_t$, which we call *inelastic transformation*, such that the elastic law of the current elastic range is given by

$$h_t(\mathbf{G}) = \mathbf{B}_t\, h_0(\mathbf{B}_t^{\,*}\ \mathbf{G}\ \mathbf{B}_t)\ \mathbf{B}_t^{\,*}. \tag{7}$$

Clearly, we can identify $\mathbf{B}_t$ with the identity if the two elastic ranges coincide. $\mathbf{B}_t$ remains constant during periods when no yielding occurs. Otherwise its change must be determined by some evolution equation or *flow rule* such as

$$\mathbf{B}_t^{\bullet} = g(\mathbf{B}_t, \mathbf{G}, \mathbf{G}^{\bullet})\ . \tag{8}$$

In this general form the evolution equation could consist of (i) the yield limit, (ii) the flow rule, (iii) the hardening rules, if applied to classical plasticity schemes. Examples such as the plastic potential will be given later. If such a flow rule is rate-independent, the material is called *plastic*. If it is rate-dependent, however, we obtain a special class of *viscoplasticity* with elastic ranges, such as the BINGHAM model. If the elastic range is, as a degenerate case, just a singleton, then we could as well describe finite viscoelastic behaviour such as the MAXWELL model. It should be emphasized that the inelastic transformation is not introduced as a deformation or configuration, but as a (non-symmetric) rearrangement of the tangent space. Moreover, no constitutive decomposition of the deformation into elastic and plastic parts is needed. Instead, **G** is always meant to be the (entire) current configuration.

4. Inelastic Transformation and Material Symmetry

Up to this point, the existence of the inelastic transformation is assured by the assumption of isomorphic elastic ranges. But nothing has yet been said about its uniqueness. It turns out that this question is closely related to the symmetry properties of the elastic laws within these ranges. So let $\mathscr{E}_i$ be an elastic range with elastic law h_i and Γ_i its symmetry group. The following theorems specify the relation between material isomorphy and material symmetry. Their proofs can be found in [5].

Theorem 1: Let $\mathscr{E}_{1,2}$ be elastic ranges with symmetry groups $\Gamma_{1,2}$ and **B** an inelastic transformation from $\mathscr{E}_1$ to $\mathscr{E}_2$. Then $\Gamma_2 = \mathbf{B}\ \Gamma_1\ \mathbf{B}^{-1}$ holds.

Theorem 2: Let $\mathscr{E}_{1,2}$ be elastic ranges with symmetry groups $\Gamma_{1,2}$ and **B** an inelastic transformation from $\mathscr{E}_1$ to $\mathscr{E}_2$, then $\mathbf{A}_2\ \mathbf{B}\ \mathbf{A}_1$ also is an inelastic transformation from $\mathscr{E}_1$ to $\mathscr{E}_2$ for all $\mathbf{A}_1 \in \Gamma_1$ and all $\mathbf{A}_2 \in \Gamma_2$.

The inelastic transformation, which describes the influence of the yielding on the elastic behaviour, is thus only determined up to symmetry transformations from both sides. The converse, however, also holds. If two elastic ranges are transformed by different inelastic transformations, then their differences are nothing but symmetry transformations of the respective elastic law.

Theorem 3: Let $\mathscr{E}_{1,2}$ be elastic ranges with symmetry groups $\Gamma_{1,2}$ and let $\mathbf{B}$ and $\underline{\mathbf{B}}$ be inelastic transformations from $\mathscr{E}_1$ to $\mathscr{E}_2$, then $\mathbf{B}^{-1}\,\underline{\mathbf{B}}$ is in Γ_1 and $\underline{\mathbf{B}}\,\mathbf{B}^{-1}$ is in Γ_2.

5. Relation to the Concept of Intermediate Configurations

Many authors in the field of finite plasticity use the concept of intermediate, unloaded, or isoclinic configurations or placements. The common conception of all these approaches is the following: At any instant it is possible to completely unload the material point, at least in a local sense. The deformation of the current configuration with respect to the unloaded one is the "elastic deformation" which determines the stresses by an elastic law. The constitutive assumption on the decomposition of the elastic and plastic deformation, which is given in different ways, for example as multiplicative or additive decomposition, is fundamental for the resulting theory.

In the present theory such an assumption is not necessary, nor is the existence of an unloaded configuration within each elastic range. But in as far as these authors also assume the existence of isomorphic elastic ranges - and most of them do so -, these theories must fit into our concept of inelastic transformations.

Within these theories, three different (local) placements are used: (i) the current placement $\mathbf{K}$, (ii) the reference placement $\mathbf{K}_R$ which is time-independent, observer-independent and arbitrary, and (iii) a time-dependent intermediate placement $\mathbf{K}_Z$, which is usually assumed to be stress-free. If we arbitrarily choose $\mathbf{K}_R$, the deformation gradient is $\mathbf{F} := \mathbf{K}\,\mathbf{K}_R^{-1}$ and the right Cauchy-Green tensor is $\mathbf{C} := \mathbf{F}^*\,\mathbf{E}\,\mathbf{F}$. We define

$$\mathbf{K}_Z := \mathbf{K}_R\,\mathbf{B}^{-1} \tag{9}$$

and the local displacement from the reference to the intermediate placement as

$$\mathbf{F}_p := \mathbf{K}_Z\,\mathbf{K}_R^{-1} = \mathbf{K}_R\,\mathbf{B}^{-1}\,\mathbf{K}_R^{-1} \tag{10}$$

and from the intermediate to the current one as

$$\mathbf{F}_e := \mathbf{K}\,\mathbf{K}_Z^{-1} = \mathbf{F}\,\mathbf{F}_p^{-1} = \mathbf{K}\,\mathbf{B}\,\mathbf{K}_R^{-1}\,. \tag{11}$$

Then the multiplicative decomposition of the deformation gradient

$$\mathbf{F} = \mathbf{F}_e\,\mathbf{F}_p \tag{12}$$

holds. Note, that neither of these parts is a gradient. This decomposition is not unique, as the reference placement is arbitrary. By use of these notions it is possible to derive a representation for the Cauchy stresses

$$\mathbf{T} = \rho/\rho_0\,\mathbf{F}_e\,p_0(\mathbf{C}_e)\,\mathbf{F}_e^{-1*}\,, \tag{13}$$

where

$$\mathbf{C}_e := \mathbf{F}_e^{*}\,\mathbf{E}\,\mathbf{F}_e = \mathbf{K}_R^{-1*}\,\mathbf{B}^{*}\,\mathbf{G}\,\mathbf{B}\,\mathbf{K}_R^{-1} \tag{14}$$

plays the role of an elastic deformation, and

$$p_0(\mathbf{C}_e) := \rho_0/\rho\,\mathbf{K}_R\,h_0(\mathbf{K}_R^{*}\,\mathbf{C}_e\,\mathbf{K}_R)\,\mathbf{K}_R^{*} \tag{15}$$

is the elastic law with respect to the reference placement. Equation (13) is essentially Equation (18) of Lee [11]. Note that we did not make use of the assumption that $\mathbf{K}_Z$ is stress free.

Another approach is that of an additive decomposition of the right Cauchy-Green tensor $\mathbf{C}$ into its plastic part

$$\mathbf{C}_p := \mathbf{F}_p^{*}\,\mathbf{E}\,\mathbf{F}_p \tag{16}$$

and its elastic part

$$\hat{\mathbf{C}} := \mathbf{C} - \mathbf{C}_p\,, \tag{17}$$

which does not equal $\mathbf{C}_e$ in Equation (14). In this case one obtains the form

$$\mathbf{T}^{p} = \mathbf{F}_p^{-1}\,p_0(\mathbf{E} + \mathbf{F}_p^{-1*}\,\hat{\mathbf{C}}\,\mathbf{F}_p^{-1})\,\mathbf{F}_p^{-1*} = q(\hat{\mathbf{C}}, \mathbf{F}_p^{-1}) \tag{18}$$

for the second Piola-Kirchhoff stress $\mathbf{T}^p$. The difference from Green and Naghdi's Equation (5.4) in the isothermal case is that they use $\mathbf{F}_p^{\mathrm{T}}\,\mathbf{F}_p$ as argument instead of $\mathbf{F}_p$ or its inverse. This is, however, only important in the anisotropic case.

6. Crystal Plasticity

As an example we will now consider a face-centred cubic (f.c.c.) single crystal subject to glide mechanisms within crystallographic slip systems according to Taylor's theory. The behaviour remains purely elastic if all Schmid stresses are below a critical one. If one or several Schmid stresses hit this limit, yielding can occur as shearing in the activated slip systems (see [1]).

As the elastic deformations for most metals are small, we will use a linear elastic law (1) where the stiffness tensor depends on the lattice direction indicated by the lattice-vector base $\{ \mathbf{e}_i \} \subset T_X B$ and its dual $\{ \mathbf{e}^k \} \subset T_X^* B$. For an f.c.c. crystal the stiffness tensor can always be represented as a linear combination of three projection tensors (see [4])

$$\mathbb{C} = \Sigma_i \, \alpha_i \, P_i \tag{19}$$

with

$$P_1(\mathbf{e}_i) := \tfrac{1}{3} \, (\Sigma_k \, \mathbf{e}_k \circ \mathbf{e}^k) \circ (\Sigma_j \, \mathbf{e}^j \circ \mathbf{e}_j)$$

$$P_2(\mathbf{e}_i) := (\Sigma_k \, \mathbf{e}_k \circ \mathbf{e}^k \circ \mathbf{e}^k \circ \mathbf{e}_k) - P_1(\mathbf{e}_i) \tag{20}$$

$$P_3(\mathbf{e}_i) := (\Sigma_{k,j} \, \mathbf{e}_k \circ \mathbf{e}^j \circ \mathbf{e}^k \circ \mathbf{e}_j) - P_1(\mathbf{e}_i) - P_2(\mathbf{e}_i) \, .$$

$\circ$ denotes the tensor product. By the isomorphy condition (4) we find, that the lattice vectors of the elastic law between two elastic ranges are transformed by the inelastic transformation

$$\mathbb{C}_t \, [\Delta \mathbf{G}] = \mathbf{B}_t \, \mathbb{C}_0 \, [\mathbf{B}_t^{-1} \, \Delta \mathbf{G} \, \mathbf{B}_t] \, \mathbf{B}_t^{-1} \tag{21}$$

$$\Rightarrow \quad \mathbb{C}_t = \Sigma_i \, \alpha_i \, P_i(\mathbf{e}_{ti}) = \Sigma_i \, \alpha_i \, P_i\{\mathbf{B}_t(\mathbf{e}_{0i})\}. \tag{22}$$

A slip system (with index i) consists of a pair $\{ \mathbf{n}^i, \mathbf{d}_i \}$, where $\mathbf{n}^i \in T_X^* B$ is the normal to the slip plane and $\mathbf{d}_i \in T_X B$ indicates the slip direction, such that $\langle \mathbf{d}_i, \mathbf{n}^i \rangle = 0$ holds. The slip systems are transformed by the inelastic transformation between the reference range and the current one

$$\mathbf{B}_t(\mathbf{d}_{0i}) = \mathbf{d}_{ti} \, ; \quad \mathbf{B}_t^{-1*}(\mathbf{n}_0^{\,i}) = \mathbf{n}_t^{\,i}. \tag{23}$$

The resolved shear stress in such a system is

$$\tau_i := |\langle \mathbf{n}^i, \mathbf{S} \, \mathbf{G}(\mathbf{d}_i) \rangle| \, . \tag{24}$$

If it reaches a critical value in one or several slip systems, then crystal gliding can occur as a superposed shear

$$\mathbf{B}_t^{\bullet} = \Sigma_i \mathbf{B}_i^{\bullet} = \Sigma_i (- \mu_i^{\bullet} \mathbf{d}_{ti} \circ \mathbf{n}_0^i) = - \Sigma_i \mu_i^{\bullet} \mathbf{d}_{ti} \circ \mathbf{B}_t^{*}(\mathbf{n}_t^i) \tag{25}$$

or

$$\mathbf{B}_t^{\bullet} \ \mathbf{B}_t^{-1} = \Sigma_i \mathbf{B}_i^{\bullet} \ \mathbf{B}_t^{-1} = \Sigma_i (- \mu_i^{\bullet} \mathbf{d}_{ti} \circ \mathbf{n}_t^i) \tag{26}$$

where the sum runs over all active shear systems. Here, μ_i is the shear in the i-th slip system. Note that $\mathbf{B}_t^{\bullet}$ is a differential if only one slip system has been active. Otherwise, it is path-dependent.

7. Computational Results

The described constitutive model has been implemented into an FEM-code to compute finite inelastic deformations of single crystals. Special attention has been given to effects of lattice rotations. On the slip system level, dry friction and linear viscous elements have been used in parallel, such that the material is elastic-viscoplastic. Kinematic hardening is considered by reducing the resolved shear stress by the back stress. Isotropic hardening increases the critical stress of the dry friction element. The hardening rates are allowed to depend on the slip rates in all active slip systems via a linear interaction model. This includes both, self and latent hardening.

The first example (Fig.1) reproduces the *overshooting* effect, observed by Taylor and Elam [14]. The lattice of a tensile specimen, initially oriented for single slip (region A), rotates toward the symmetry position between regions A and B. Considering only the ratio of resolved shear stress to global stress (Schmid-factor), double slip is expected for symmetric positions. In the stereographic projection, this corresponds to points on the line between the regions A and B. However, single slip may not stop at the symmetry line, thus the tensile axis is *overshooting*. This can be explained by assuming larger latent hardening than self hardening. Our simulations based on this assumption show good agreement with the results of Taylor and Elam. It should be emphasized that no material constants have been fitted.

The second example is a simulated tensile test with two single crystal specimens, demonstrating the non-uniformity of deformation and lattice rotation (Fig. 2). The initial angles φ between the tensile axis and [100]-direction are 15° and 30°. The specimens were extended by 50%, while allowing no deformation or rotation of the end planes. In

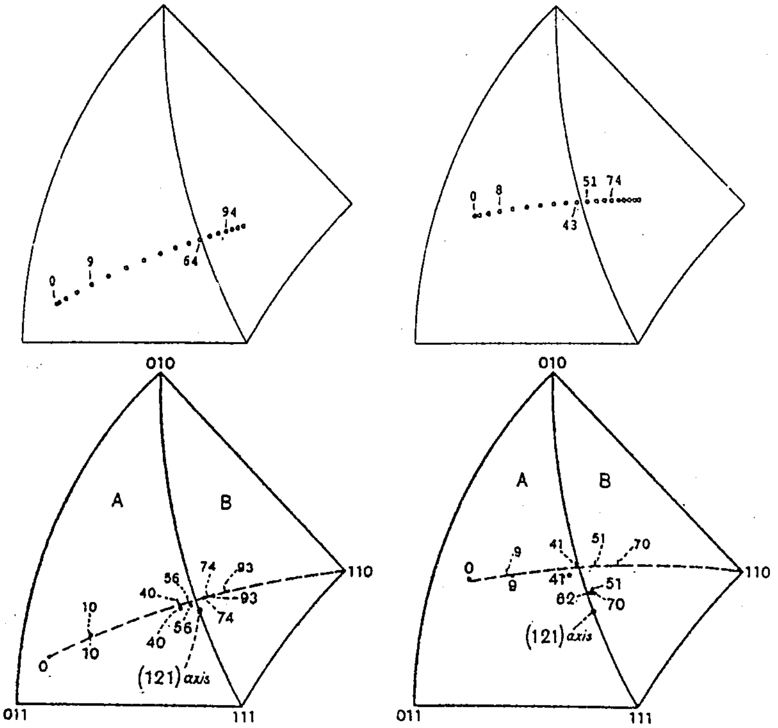

Figure 1. Overshooting: Simulation (above) and experimental result [14] (below). The stereographic projection indicates the crystallographic position of the tensile axis for different extensions (in %).

the central parts one can observe large shear strains and extensions. The lattice rotates from φ = 15° to 3° and from 30° to 12°. A particular result for the 15°-specimen is that the direction of lattice rotation is opposite to that of the cross sections. This effect is very sensitive to the initial crystal orientations. Due to the boundary conditions the deformations and lattice orientations are non-uniform.

As a last example, simple shear tests at large shear numbers are given. They are difficult to perform but easy to simulate. Fig. 3 shows four specimens of identical material but with different initial orientations.
The corresponding curves of global shear stress in units of critical shear stress τ_0 versus shear number are given in Fig. 4. Three different cases of lattice rotation behaviour depending on the initial orientation can be observed: steady rotation (c), convergence towards stationary orientation (b, d), or constant orientation (a).
As the Schmid-factors depend on the current lattice position, the global shear stress may oscillate even under steady shear. In case (c), each stress cycle corresponds to a planar rotation of 90° according to the cubic symmetry. Depending on the current orientation

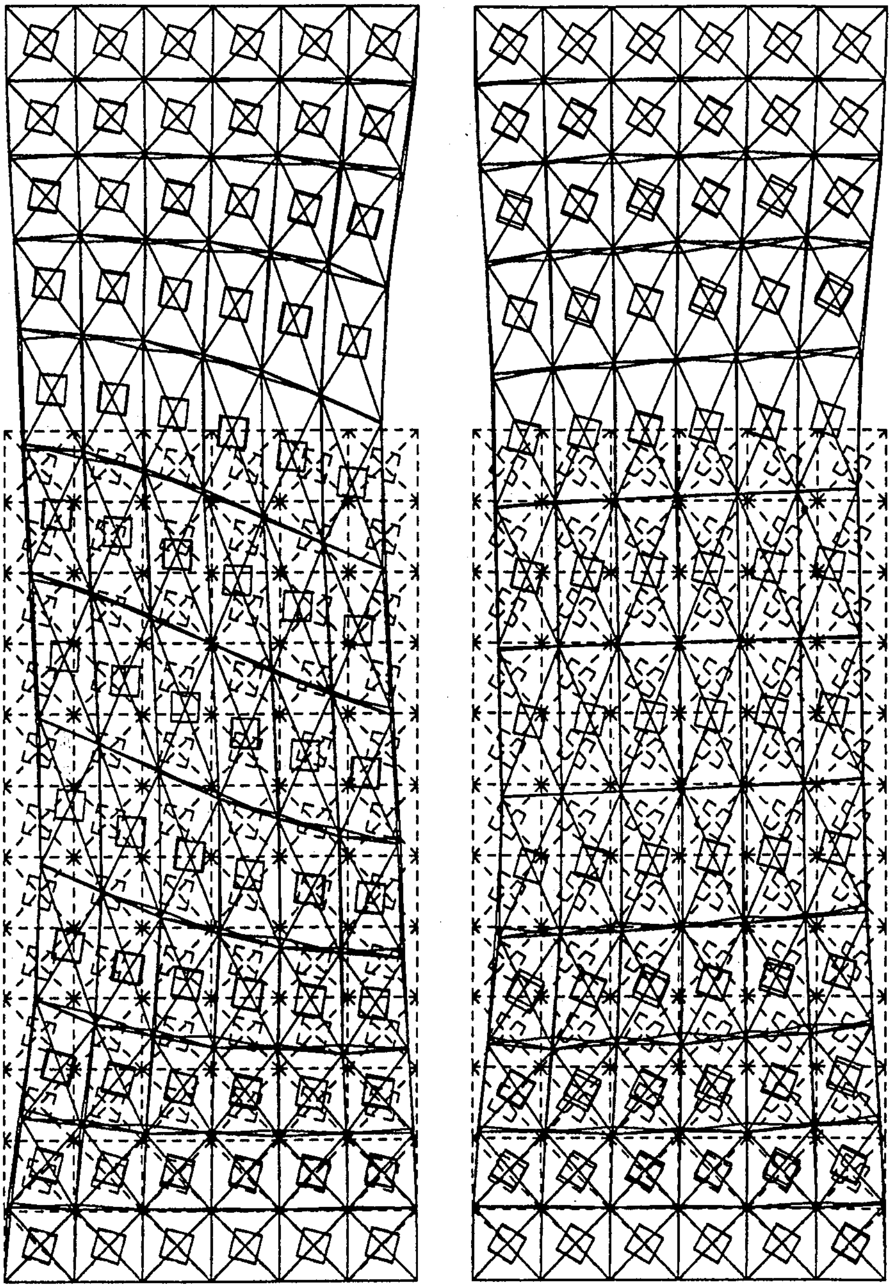

Figure 2. Simulated tensile tests (50% extension). Left: φ_0=15°, right: φ_0=30°. Initial position dashed, final position solid. Small cubes in the centre of the elements indicate their lattice orientation.

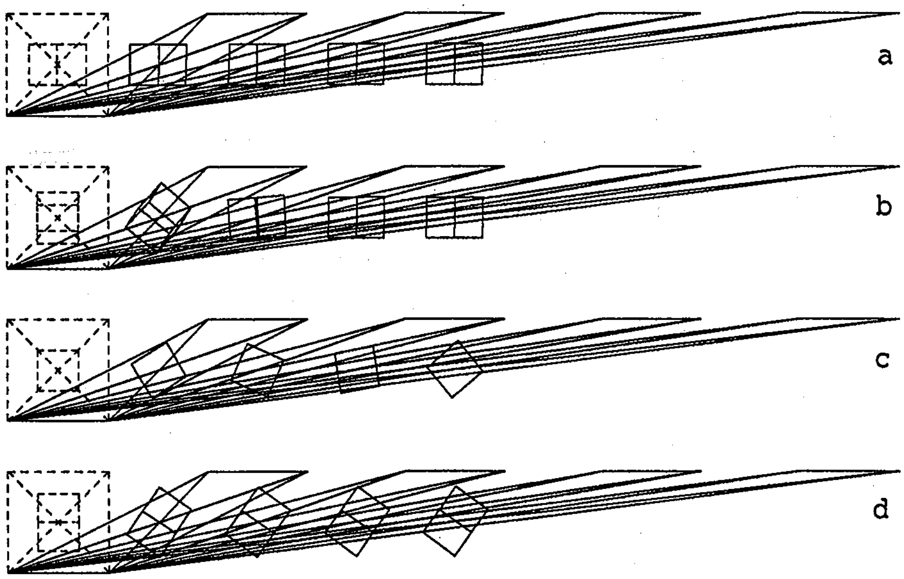

Figure. 3. Simple shear with different initial orientations. Deformation and lattice orientation for shear numbers 0, 2, 4, 6, and 8.

angle, the material will soften or harden. This is a purely geometrical effect, as no explicit hardening law has been used in this case.

The influence of different hardening rules is shown in Fig. 5. The solid curve is the shear stress for case (c) of Fig. 3 without hardening. The dashed curve corresponds to isotropic (equal self and latent) hardening. The original shape is preserved, but shifted by a value increasing with the shear number. Also, the amplitude grows with the shear number. The dotted curve was calculated using kinematic self hardening. The stress is limited, the shape is different. After a rotation of 180° the slip direction in each slip system is reversed and so is the back stress rate. Thus the back stress oscillates. Kinematic latent hardening is only feasable if the mutual orientation of the slip systems is taken into account.

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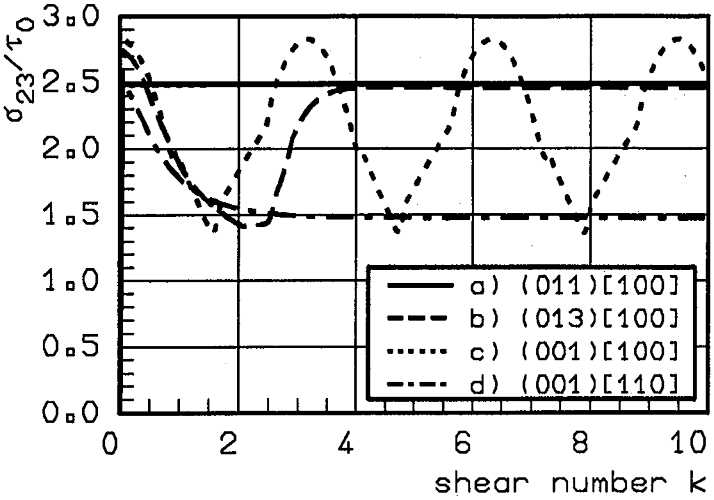

Figure 4. Shear stress, influence of different initial orientations, indicated by (global shear plane nomal)[global shear direction] corresponding to cases a, b, c and d of Fig. 3.

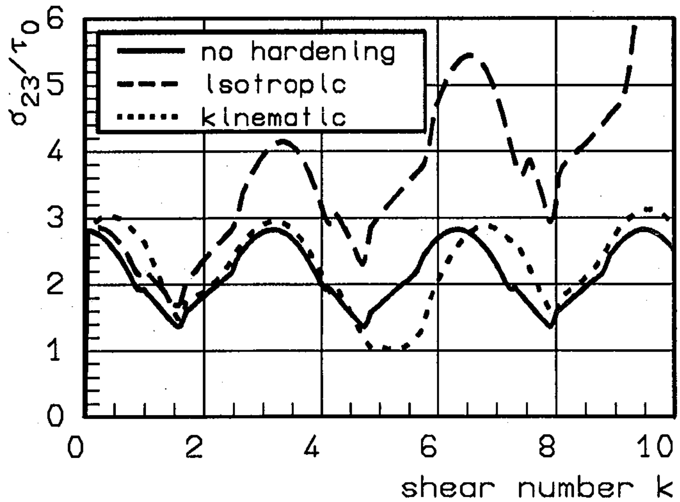

Figure 5. Shear stress (initial orientation c) - effect of different hardening rules.

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