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PLASTICITY OF CRYSTALS WITH INTERACTING SLIP SYSTEMS(1)

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A new, non-conventional approach to the analysis of crystalline lattice rotations caused by large plastic strains of crystals is presented. Only rigid-ideally plastic crystals are considered. Contrary to the theory based on the Schmid law, the proposed model assumes that a yield initiation depends on stress states of all slip systems, i.e. interactions between slip systems are taken into account. In the paper an interaction rule, founded on microscopic observations, is governed by one integer constant n. For $n = 1$, the crystals satisfy the Mises criterion with a quadratic yield surface. For $n \to \infty$, the crystals are described by smooth (with rounded-off corners) yield surfaces tending to those generated by the Schmid law. For a fixed n, the interaction rule determines constitutive relations in terms of the strain rate tensor, the plastic spin tensor and the stress tensor. Three additional constitutive equations for the plastic spin components lead to an explicit descriptions of lattice reorientations. A generalized plastic potential for the strain rate and the plastic spin is introduced. A smooth yield condition generated by this potential enables to formulate a complete system of equations for the model, what considerably simplifies the numerical analysis. The f.c.c. crystals in tension and compression are examined in detail. The presented strain paths demonstrate a predominant influence of interactions between slip systems on the lattice reorientations.

1. Introduction

The plasticity of crystals formulated by HILL and RICE [8] (an extended review is given in ASARO [11]) is based on the Schmid law and the constitutive relations between slip rates and the resolved stress rates. According to the Schmid law, apperance of a slip in a certain slip system depends only on

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the value of the shear stress component in that system. Influence of stress states in other slip systems is not taken into account. One can say that the theory assumed a model of a crystal with *independent slip systems* (with respect to the plastic yield onset).

The independence of slip systems leads to the ambiguity of the crystal kinematics – various combinations of slip rates give the same strain rate of the crystal. The proper choice of active slip systems needs to satisfy an additional criterion – the minimum slip rate (TAYLOR [3]) or the maximum plastic work (BISHOP and HILL [4]). Because the number of uknowns of the model exceeds the number of formulated equations, the theory is not represented by a complete system of equations. An analysis of real crystals based on searching of active slip systems is very complex. On the other hand, experimental data for f.c.c. and b.c.c. crystals indicate some deviations from the Schmid law. Paper by DIEHL [5] on copper has shown that values of the critical shear stress are higher than the expected ones when similar values of the resolved shear stress appear on several slip systems. It indicates, that interactions between slip systems take place.

The aim of the paper is to formulate a model of a rigid-ideally plastic crystal at large strains, which takes into account interactions of a various degree between slip systems. Particularly, if the interactions are sufficiently weak, the model should give the results close to those obtained from the Hill and Rice theory for the case of rigid-ideally plastic crystals.

In the next section, a short summary on kinematics of crystals at finite strains and large lattice rotation is given. Later, an interaction rule for slip systems will be introduced. It will be shown that the constitutive behaviour of crystals is fully determined by this rule.

2. BASIC KINEMATICAL CONCEPTS

Crystal deformed by slip only are considered. Slips may appear on some crystallographical planes with normal versors $\mathbf{n}^{(r)}$ and some crystallographical directions $\mathbf{m}^{(r)} (r = 1, ..., M)$. A pair composed of a family of parallel slip planes and one slip direction creates a slip system. Formally, a slip system may be defined as a dyad $\mathbf{m}^{(r)} \otimes \mathbf{n}^{(r)}$. A set of all slip systems of a crystal $\{\mathbf{m}^{(r)} \otimes \mathbf{n}^{(r)}; r = 1, ..., M\}$ forms a system of slip systems.

To describe the lattice orientation, one can choose a certain crystallographic plane with a normal $\mathbf{a}_1$ and a crystallographic direction $\mathbf{a}_2$ lying on this plane. Let $\mathbf{a}_3$ be a vector-product of $\mathbf{a}_1$ and $\mathbf{a}_2$. A triad of orthonormal vectors $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ will be called a lattice frame. An orientation of the frame $\{\mathbf{a}_\alpha\}$ with respect to the fixed system of coordinates $\{\mathbf{e}_i\}$, is given by the orthogonal matrix $R_{\alpha i}$ (expressed by three Euler angles ϕ_m)

$$\mathbf{a}_\alpha = R_{\alpha i}(\phi_m)\, \mathbf{e}_i \, . \tag{2.1}$$

Consider *a lattice motion* during a deformation process. For crystals deformed by slip only, elastic strains of a lattice are neglected. Then, a lattice motion is described by a rotation of its frame. A rotation rate is the same at each point $\mathbf{x}$ from the space occupied by the crystal

$$\dot{\mathbf{a}}_\alpha(t) = \omega^L_{\alpha\beta} \mathbf{a}_\beta \,(t) \, , \tag{2.2}$$

where

$$\omega^L_{ij} = \dot{R}_{i\alpha} R_{j\alpha} \tag{2.3}$$

are components of the lattice spin.

During the crystal motion, the system of slip systems is rigidly connected with the lattice frame. Then, for $r = 1, ..., M$

$$\mathbf{m}^{(r)}(t) = \hat{m}^{(r)}_\alpha \, \mathbf{a}_\alpha(t) \, , \tag{2.4}$$

$$\mathbf{n}^{(r)}(t) = \hat{n}^{(r)}_\alpha \, \mathbf{a}_\alpha(t) \, , \tag{2.5}$$

where $\hat{m}^{(r)}_\alpha$ and $\hat{n}^{(r)}_\alpha$ are constants describing the geometry of the lattice. Note that for r, $s = 1, ..., M$

$$m^{(r)}_{(i} n^{(r)}_{j)} \; m^{(s)}_{(i} n^{(s)}_{j)} = \hat{m}^{(r)}_{(\alpha} \hat{m}^{(r)}_{\beta)} \; \hat{m}^{(s)}_{(\alpha} \hat{n}^{(s)}_{\beta)} \, , \tag{2.6}$$

where (i, j) denotes symmetrization with respect to i and j.

It means that the left side of Eq.(2.6) does not depend on the lattice orientation.

Time derivative of Eqs.(2.4) – (2.5) and the rule (2.2) lead to the relations

$$\dot{m}_i(t) = \omega^L_{ij}(t)\, m_j(t) \, , \tag{2.7}$$

$$\dot{n}_i(t) = \omega^L_{ij}(t)\, n_j(t) \, . \tag{2.8}$$

The motion of a material element of the crystal, in vicinity of a point $\mathbf{x}$, is a superposition of a rigid body motion with the spin $\omega^L_{ij}(t)$ (the same for all material elements) and simple shears (on motionless slip systems) with rates $\dot{\gamma}^{(r)}(\mathbf{x}, \, \mathbf{t})$. Observe that such a motion is isochoric.

Consider a motion of an infinitesimal fiber of a crystal, parallel to a vector $d\mathbf{x}$, with the origin at a point $\mathbf{x}$. An increment of a velocity vector along this fiber is the following:

$$dv_i(\mathbf{x},t) = \omega^L_{ij}(t)\, dx_j + \left[\sum_{r=1}^{M} \dot\gamma^{(r)}(\mathbf{x},t)\, m_i^{(r)}(t)\, n_j^{(r)}(t)\right] dx_j\,. \tag{2.9}$$

A tensor field

$$\mathbf{L}^P(\mathbf{x},t) = \sum_{r=1}^{M} \dot\gamma^{(r)}(\mathbf{x},t)\, \mathbf{m}^{(r)}(t) \otimes \mathbf{n}^{(r)}(t) \tag{2.10}$$

is a plastic part of a velocity gradient field and plays an essential role in further considerations.

Components of the tensor $\mathbf{L}^P$ may be decomposed into the plastic strain rate and the plastic spin ones

$$d^P_{ij} = \frac{1}{2}\sum_{r=1}^{M} \dot\gamma^{(r)} \left(m_i^{(r)} n_j^{(r)} + m_j^{(r)} n_i^{(r)}\right), \tag{2.11}$$

$$\omega^P_{ij} = \frac{1}{2}\sum_{r=1}^{M} \dot\gamma^{(r)} \left(m_i^{(r)} n_j^{(r)} - m_j^{(r)} n_i^{(r)}\right). \tag{2.12}$$

Equations (2.9) and (2.11) – (2.12) yield the following decomposition of the total velocity gradient field

$$v_{ij}(\mathbf{x},t) = \omega^L_{ij}(t) + d^P_{ij}(\mathbf{x},t) + \omega^P_{ij}(\mathbf{x},t)\,. \tag{2.13}$$

In the above, $\omega^L_{ij}(t)$ is expressed by three Euler angles $\phi_m(t)$ describing the actual lattice orientation. Observe that three components $\omega^L_{ij}(t)$ may be found from Eq.(2.13) if the total velocity gradient and its plastic part are known. Then, for a given velocity field, six constitutive equations for the plastic strain rate components d^P_{ij} and three additional constitutive equations for the plastic spin components ω^P_{ij} should be prescribed.

If the velocity gradient field

$$L_{ij}(\mathbf{x},t) = v_{i,j}(\mathbf{x},t) \tag{2.14}$$

is given, then the compatibility equations should be satisfied

$$L_{ij,k}\,\epsilon_{jkm} = 0\,, \tag{2.15}$$

where ϵ_{jkm} is the antisymmetric permutational symbol.

3. An interaction rule for slip systems

Looking for a rule describing interactions between slip systems the following empirical relation (Hull [9]) should be considered:

$$\frac{v}{v_0} = \left(\frac{\tau}{\tau_0}\right)^k , \tag{3.1}$$

where v is the mean velocity of dislocations moving on a certain slip plane, τ is the shear stress on that plane, and τ_0 is the shear stress producing the velocity v_0 (usually 1 cm/s). Parameter k is a material constant; for the materials tested, k has varied from 1 (Cu) to 35 (Fe-3%Si) (see Fig.1).

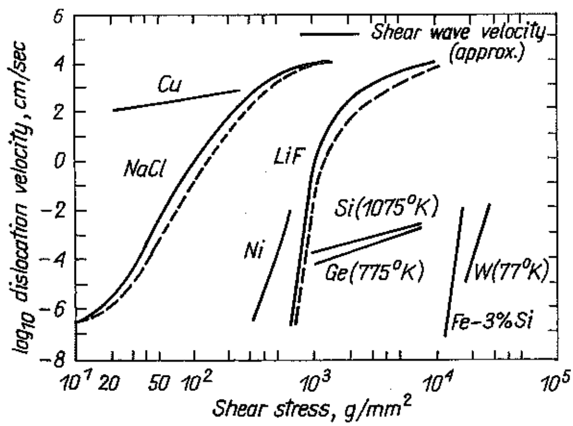

Fig. 1. Some typical data showing the dependence of dislocation velocities on applied shear stress (after Gilman [7]).

In the relation (3.1), values of v should be positive and smaller than the shear wave velocity $v_{\max}$. The above rule remains valid for

$$-v_{\max} < v < v_{\max} , \tag{3.2}$$

if v and τ are of the same sign. It is possible when

$$k = 2n - 1 , \quad \text{for} \quad n = 1, 2, 3, \ldots . \tag{3.3}$$

Let σ_{ij} be the Cauchy stress tensor, and

$$\tau^{(r)} = \sigma_{ij} m_i^{(r)} n_j^{(r)} \tag{3.4}$$

will be a resolved shear stress acting on the r-th slip system. If $\tau_0^{(r)}$ produces the mean velocity of dislocations v_0, then $\tau^{(r)}$ leads to

$$(3.5)\qquad v^{(r)} = v_0 \left(\frac{\tau^{(r)}}{\tau_0^{(r)}}\right)^{2n-1}, \quad \text{for} \quad n = 1,2,3,\dots .$$

The quantity $v^{(r)}$ is connected with the slip rate on the r-th slip system $\dot{\gamma}^{(r)}$ by the relation (HULL [9])

$$(3.6)\qquad \dot{\gamma}^{(r)} = b^{(r)} N^{(r)} v^{(r)} ,$$

where $b^{(r)}$ is the Burgers vector modulus, and $N^{(r)}$ is the number of moving dislocations on the slip system considered.

Let $k_c^{(r)}$ will be the critical shear stress on the r-th slip system. Let us make two additional assumptions: a) $\tau_0^{(r)}$ is proportional to $k_c^{(r)}$, b) for a fixed plastic strain, $b^{(r)}N^{(r)}$ is inversely proportional to $k_c^{(r)}$.

Taking into account the above assumptions, the Eqs.(3.5) – (3.6) lead to the relation

$$(3.7)\qquad \dot{\gamma}^{(r)} = \lambda \frac{1}{k_c^{(r)}} \left(\frac{\tau^{(r)}}{k_c^{(r)}}\right)^{2n-1},$$

where λ is a positive function (proportional to the number of moving dislocations), the same for all slip systems.

It means that a slip rate on the s-th slip system is connected with a slip rate on the r-th slip system by the relation

$$(3.8)\qquad \dot{\gamma}^{(s)} = \dot{\gamma}^{(r)} \left(\frac{k_c^{(r)}}{k_c^{(s)}}\right) \left(\frac{\bar{\tau}^{(s)}}{\bar{\tau}^{(r)}}\right)^{2n-1},$$

where

$$(3.9)\qquad \bar{\tau}^{(r)} = \frac{\tau^{(r)}}{k_c^{(r)}} \neq 0 .$$

According the above rule, all slip systems are active from the beginning of plastic yielding. The distribution of slip rates between slip systems is governed by the parameter n. For n large enough, $\dot{\gamma}^{(s)}(s = 1, \dots, M;\ s \neq r)$ are negligibly small in comparison with $\dot{\gamma}^{(r)}$, and the slip distribution is close to that predicted by the single slip theory. Then, the parameter n describes *the slip systems independence degree.*

Concluding, one can introduce the following

DEFINITION. *A crystal will be called a crystal with interacting slip systems of the n-th independence degree* ($n = 1, 2, 3, ..$), *if*

$$\frac{\dot{\gamma}^{(1)} k_c^{(1)}}{[\bar{\tau}^{(1)}]^{2n-1}} = \ldots = \frac{\dot{\gamma}^{(M)} k_c^{(M)}}{[\bar{\tau}^{(M)}]^{2n-1}} = \lambda \geq 0\,. \tag{3.10}$$

The relation (3.10) is the interaction rule sought for. It will be treated as a phenomenological assumption, disregarding the previous physical motivations.

Assuming that λ is a material constant we have to do with rate-dependent materials. For further considerations λ will be regarded as a function of the loading process, which follows from the assumed yield condition. It means, that crystals with interacting slip systems will be considered as a class of ideally plastic, rate-independent materials.

4. CONSTITUTIVE RELATIONS AND A GENERALIZED PLASTIC POTENTIAL

Multiplying both sides of Eq.(3.7) by a dyad $m_i^{(r)} n_j^{(r)}$ and summing up for $r = 1, ..., M$, one obtains

$$\sum_{r=1}^{M} \dot{\gamma}^{(r)}\, m_i^{(r)} n_j^{(r)} = \lambda \sum_{r=1}^{M} \frac{1}{k_c^{(r)}} \left[\frac{\tau^{(r)}}{k_c^{(r)}}\right]^{2n-1} m_i^{(r)} n_j^{(r)}\,. \tag{4.1}$$

The left-hand side of Eq.(4.1) is the plastic part of the velocity gradient, and the right-hand one may be expressed by the Cauchy stress tensor. Then, the following constitutive relations yield from Eq. (3.7)

$$L_{ij}^P = \lambda \sum_{r=1}^{M} \frac{1}{k_c^{(r)}} \left[\frac{m_k^{(r)} \sigma_{kl}\, n_l^{(r)}}{k_c^{(r)}}\right]^{2n-1} m_i^{(r)} n_j^{(r)}\,, \tag{4.2}$$

where λ is a non-negative, scalar function.

Nine equations (4.2) can be divided into two groups:

a) six equations for the plastic strain rate

$$d_{ij}^P = \lambda \sum_{r=1}^{M} \frac{1}{2k_c^{(r)}} \left[\frac{m_k^{(r)} \sigma_{kl}\, n_l^{(r)}}{k_c^{(r)}}\right]^{2n-1} \left[m_i^{(r)} n_j^{(r)} + m_j^{(r)} n_i^{(r)}\right]\,, \tag{4.3}$$

b) three additional equations for the plastic spin

$$\omega_{ij}^P = \lambda \sum_{r=1}^{M} \frac{1}{2k_c^{(r)}} \left[\frac{m_k^{(r)} \sigma_{kl}\, n_l^{(r)}}{k_c^{(r)}}\right]^{2n-1} \left[m_i^{(r)} n_j^{(r)} - m_j^{(r)} n_i^{(r)}\right]\,. \tag{4.4}$$

The above approach to the constitutive description of crystals has been introduced in my previous paper (GAMBIN [12]) as a practical realization of the theoretical proposal of MANDEL [6].

Similarly to the classical theory of plasticity, one can introduce potentials for the strain rate and the plastic spin. Note that $\mathbf{m}^{(r)}$ and $\mathbf{n}^{(r)}$ depend on three Euler angles ϕ_m. Then, the components L^P_{ij}, d^P_{ij} and ω^P_{ij} may be regarded as three-parameter functions of the stress state. The following three-parameter function of nine stress components

$$(4.5)\qquad F_n(\sigma_{ij};\phi_m) = \frac{1}{2n}\left\{\sum_{r=1}^{M}\left[\frac{m_i^{(r)}\sigma_{ij}\,n_j^{(r)}}{k_c^{(r)}}\right]^{2n} - m\right\},$$

will be called the *generalized plastic potential.* The quantity m in Eq.(4.5) depends on n only, and it will be determined later. One can see that

$$(4.6)\qquad L^P_{ij} = \lambda\frac{\partial F_n}{\partial\sigma_{ij}},$$

$$(4.7)\qquad d^P_{ij} = \lambda\frac{1}{2}\left(\frac{\partial F_n}{\partial\sigma_{ij}}+\frac{\partial F_n}{\partial\sigma_{ji}}\right),$$

$$(4.8)\qquad \omega^P_{ij} = \lambda\frac{1}{2}\left(\frac{\partial F_n}{\partial\sigma_{ij}}-\frac{\partial F_n}{\partial\sigma_{ji}}\right).$$

Introduce now a *smooth* yield condition

$$(4.9)\qquad f_n(\sigma_{ij};\phi_m) = F_n\left(\frac{\sigma_{ij}+\sigma_{ji}}{2};\phi_m\right) = 0,$$

associated with the flow rule (4.3).

The case $n = 1$. For cubic crystals (k_c is the same for all slip systems) the interaction rule takes the form

$$(4.10)\qquad \frac{\dot\gamma^{(1)}}{\tau^{(1)}} = \ldots = \frac{\dot\gamma^{(M)}}{\tau^{(M)}} = \frac{\lambda}{M},$$

where λ is a non-negative, scalar function. The considered case has been examined in my previous papers (GAMBIN [13, 14, 15]). The constitutive equations and a smooth, quadratic yield criterion take the form

$$(4.11)\qquad L^P_{ij} = \lambda\, H_{ijkl}\sigma_{kl},$$

$$(4.12)\qquad \sigma_{ij}\, H_{ijkl}\sigma_{kl} = m,$$

where

$$H_{ijkl} = \frac{1}{M} \sum_{r=1}^{M} m_i^{(r)} n_j^{(r)} m_k^{(r)} n_l^{(r)} , \tag{4.13}$$

and m is a material constant. Here, the components of H_{ijkl} are fully determined by the lattice geometry and its orientation.

A general form of the quadratic yield criterion for crystals has been proposed and examined by MISES [2].

The case $n \to \infty$. For increasing values of parameter n the degree of interactions between slip system decreases. In the limiting case one can state only that, for $r = 1, ..., M$, $\dot{\gamma}^{(r)}$ and $\bar{\tau}^{(r)}$ are of the same sign, i.e.

$$\frac{\dot{\gamma}^{(r)}}{\bar{\tau}_{(r)}} = \lambda^{(r)} , \tag{4.14}$$

where independent functions $\lambda^{(r)}$ take non-negative values. This is the case of *independent slip systems.*

The relations (4.14) lead to the following constitutive equations

$$L_{ij}^P = \sum_{r=1}^{M} \lambda^{(r)} \bar{\tau}^{(r)} m_i^{(r)} n_j^{(r)} , \tag{4.15}$$

where functions $\lambda^{(r)}$ remain undetermined.

Symmetrization of Eq.(4.15) yields the following flow rule:

$$d_{ij}^P = \frac{1}{2} \sum_{r=1}^{M} \lambda^{(r)} \bar{\tau}^{(r)} \left[m_i^{(r)} n_j^{(r)} + m_j^{(r)} n_i^{(r)} \right] . \tag{4.16}$$

For a single slip on the r-th slip system,

$$d_{ij}^P = \lambda^{(r)} \frac{\partial f^{(r)}}{\partial \sigma_{ij}} , \tag{4.17}$$

where

$$f^{(r)} = \left[\bar{\tau}^{(r)} \right]^2 - 1 . \tag{4.18}$$

In the stress space, the equation

$$f^{(r)} = 0 \tag{4.19}$$

describes a pair of parallel hyperplanes. The strain rate vector is orthogonal to each of them. A set of such hyperplanes, for $r = 1, ..., M$, is a boundary of the domain described by the system of inequalities

$$|\tau^{(r)}| \le k_c^{(r)} , \qquad \text{for } r = 1, \dots , M . \tag{4.20}$$

Then, the crystals with independent slip systems, which obey the orthogonality principle, satisfy the Schmid law. On the other hand, these crystals may be regarded as a limiting case of crystals with interacting slip systems.

Concluding, the model of crystals with interacting slip systems may be used as an approximation of the model based on the Schmid law. The above observation will enable a determination of the parameter m in the definition (4.5).

5. A smooth approximation of the Schmid yield condition

A smooth previously introduced yield condition can be obtained in a purely phenomenological way. For this purpose let us observe that the square shown in Fig.2a and described by the equation

$$\max_{x,y} (|x|, |y|) = 1 , \tag{5.1}$$

may be approximated by the sequence of curves (Fig.2b)

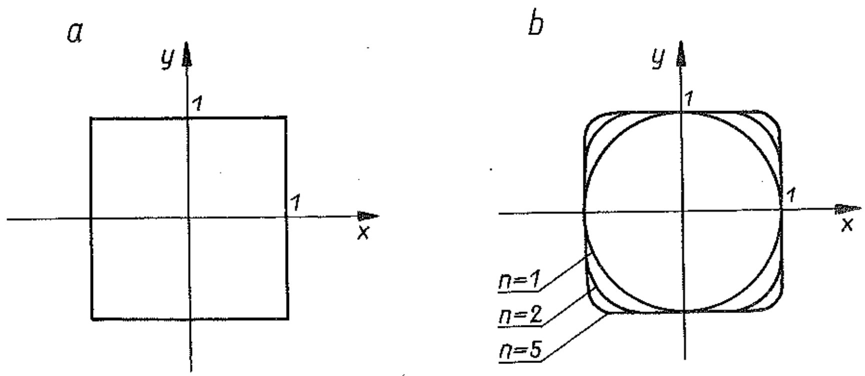

FIG. 2. A smooth approximation of the square: a) the original figure, b) its approximations for $n = 1, 2, 5$.

$$x^{2n} + y^{2n} = 1 , \qquad \text{for} \quad n = 1, 2, 3, \ldots . \tag{5.2}$$

In the similar way, one can approximate a multi-plane yield surface. Consider a classical Tresca yield condition

$$\max_{\tau_1, \tau_2, \tau_3} \left(\frac{|\tau_1|}{k_0}, \frac{|\tau_2|}{k_0}, \frac{|\tau_3|}{k_0} \right) = 1 , \tag{5.3}$$

where τ_1, τ_2, τ_3 are the maximum shear stresses, and k_0 is their critical value. Denoting by $\sigma_1, \sigma_2, \sigma_3$ the principal stresses, and by σ_0 their critical value, the Tresca yield surface is described by the equation

$$\max_{\sigma_1,\sigma_2,\sigma_3} \left(\frac{|\sigma_1 - \sigma_2|}{\sigma_0}, \frac{|\sigma_2 - \sigma_3|}{\sigma_0}, \frac{|\sigma_3 - \sigma_1|}{\sigma_0} \right) = 1 . \tag{5.4}$$

The multi-plane surface (5.4) may be approximated (with accuracy to a scale parameter m) by the sequence of the smooth surfaces

$$(\sigma_1 - \sigma_2)^{2n} + (\sigma_2 - \sigma_3)^{2n} + (\sigma_3 - \sigma_1)^{2n} = m\sigma_0^{2n} . \tag{5.5}$$

Assuming that in the simple tension test ($\sigma_1 = \sigma_0$, $\sigma_2 = \sigma_3 = 0$) both conditions (5.4) and (5.5) are satisfied, one can obtain

$$m = 2 . \tag{5.6}$$

For $n = 1$, the quadratic Huber - Mises yield surface is obtained. When $n \to \infty$, the Tresca yield surface appears.

Similarly the yield surfaces for crystals may be considered. The Schmid yield condition can be written in the form

$$\max_{r=1,\dots,M} \frac{|\tau^{(r)}|}{k_c^{(r)}} = 1 , \tag{5.7}$$

or in the form

$$\max_{r=1,\dots,M} \frac{|\sigma_{ij} m_i^{(r)} n_j^{(r)}|}{k_c^{(r)}} = 1 . \tag{5.8}$$

For a fixed lattice orientation, the equation (5.8) describes a convex, multi-plane yield surface. With an accuracy to a scale parameter m, this surface may be approximated by the sequence of smooth surfaces

$$\sum_{r=1}^{M} \left[\frac{\sigma_{ij} m_i^{(r)} n_j^{(r)}}{k_c^{(r)}} \right]^{2n} = m , \qquad \text{for} \quad n = 1, 2, 3, \dots . \tag{5.9}$$

Looking for such a value of m which gives the best approximation of Eq.(5.8), assume that for the pure shear on the s-th slip system both the conditions (5.8) and (5.9) are satisfied. It is possible for the following stress state

$$\sigma_{ij}^* = k_c^{(s)} \left[m_i^{(s)} n_j^{(s)} + m_j^{(s)} n_i^{(s)} \right] . \tag{5.10}$$

Introducing Eq.(5.10) into Eq.(5.9), one obtains the following value of m (denoted temporarily by m^*)

$$(5.11)\qquad m^* = \sum_{r=1}^{M} \left[2\,\frac{k_c^{(s)}}{k_c^{(r)}}\, m_{(i}^{(s)} n_{j)}^{(s)}\, m_{(i}^{(r)} n_{j)}^{(r)} \right]^{2n}.$$

Taking the mean value of m^* over all the slip systems, we have

$$(5.12)\qquad m = \frac{1}{M} \sum_{s=1}^{M} \sum_{r=1}^{M} \left[2\,\frac{k_c^{(s)}}{k_c^{(r)}}\, m_{(i}^{(s)} n_{j)}^{(s)}\, m_{(i}^{(r)} n_{j)}^{(r)} \right]^{2n}.$$

According to Eq.(2.6), the quantity m does not depend on the lattice orientation.

Concluding, one can state that for the parameter n large enough, the yield surface

$$(5.13)\qquad \sum_{r=1}^{M} \left[\frac{\sigma_{ij} m_i^{(r)} n_j^{(r)}}{k_c^{(r)}} \right]^{2n} = \frac{1}{M} \sum_{s=1}^{M} \sum_{r=1}^{M} \left[2\,\frac{k_c^{(s)}}{k_c^{(r)}}\, \hat{m}_{(\alpha}^{(s)} \hat{n}_{\beta)}^{(s)}\, \hat{m}_{(\alpha}^{(r)} \hat{n}_{\beta)}^{(r)} \right]^{2n}$$

is arbitrarily close to the Schmid yield surface.

As an example illustrating the accuracy of the approximation consider a case of f.c.c. crystals. The Schmid yield surfaces, for three orientations of the lattice with respect to the principal stress axes, are shown in Fig.3, and their approximations – in Fig.4.

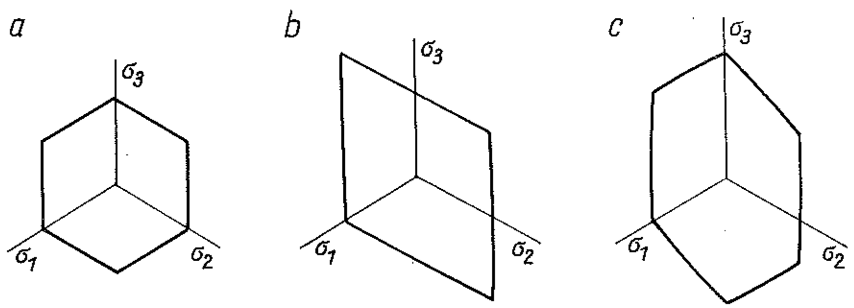

FIG. 3. Schmid yield surfaces of f.c.c. crystals for three orientations of the direction σ_3 : a) [001], b) [011], c) [111].

One can observe the rounded-off corners of the surfaces in Fig.4. Their curvature increases to infinity for increasing values of the parameter n.

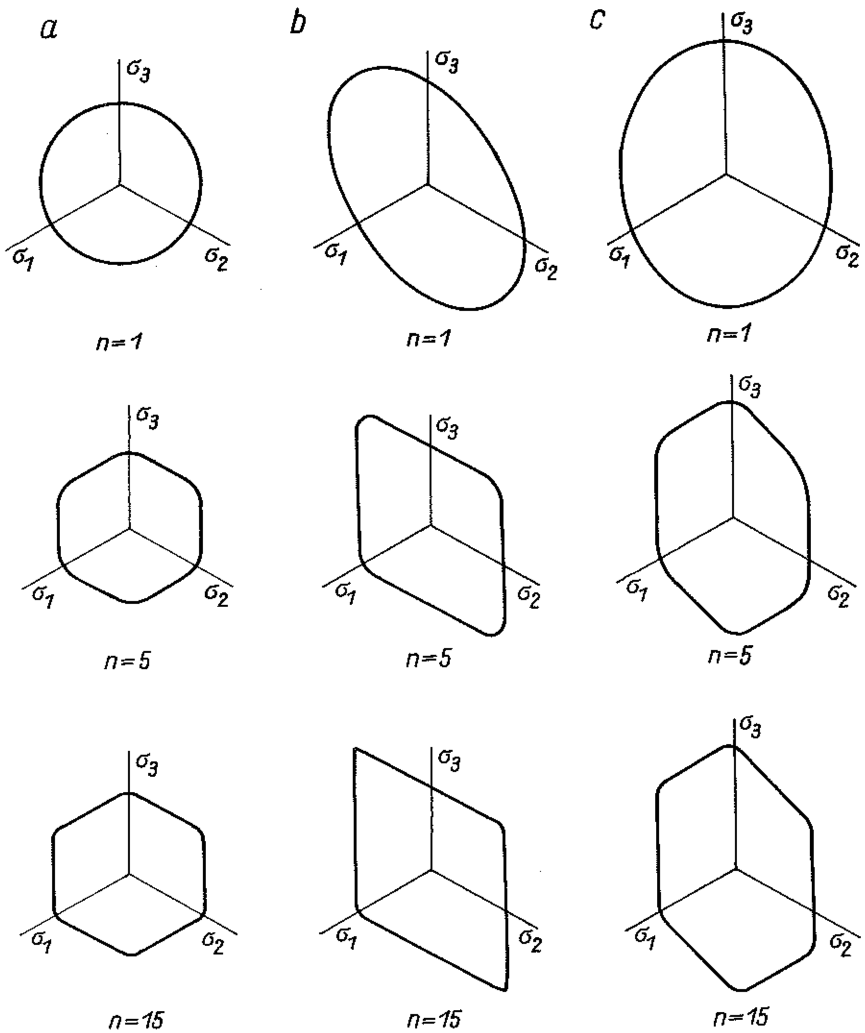

FIG. 4. Smooth yield surfaces for f.c.c crystals for three orientations of the direction σ_3 : a) [001], b) [011], c) [111].

Consider the lattice orientation shown in Fig.3a. Denote by σ_0 and σ_n the critical values of the principal stresses according to the Schmid law and its n-th approximation, respectively. Then

(5.14) $$\Delta_n = \left|\frac{\sigma_n - \sigma_0}{\sigma_0}\right|$$

will be the relative error of the approximation. A dependence of Δ_n on the parameter n is shown in Fig.5.

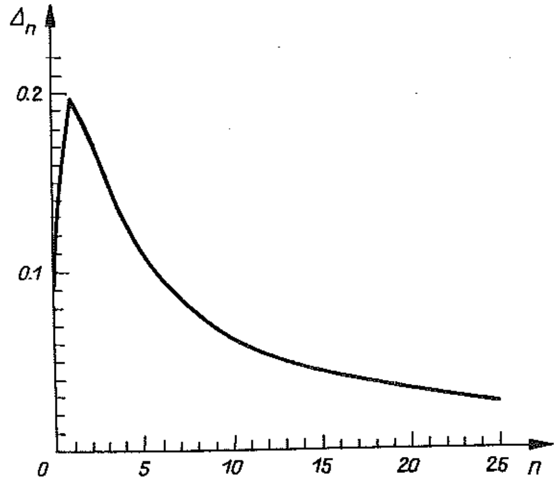

FIG. 5. A relative error of the Schmid law approximation for f.c.c. crystal, as a function of parameter n.

Compare the results obtained with the experimental data. The influence of lattice orientation on the values of critical shear stresses τ_{cr} for copper crystals subject to tension is shown Fig.6 (DIEHL [5]). Orientations towards

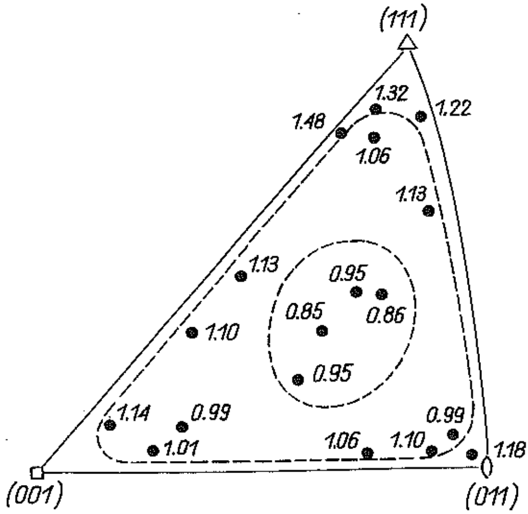

FIG. 6. Orientation dependence of τ_{cr} of copper crystals. Values in MNm^{-2} (after DIEHL) [5]).

the center of the stereographic triangle give nearly constant values of τ_{cr}, but values of τ_{cr} are much higher for orientations approaching the boundaries of the triangle. The same conclusion follows from the proposed model – the yield stresses for orientations [011] and [111] are much higher than those predicted by the Schmid law.

Note that the rule Eq.(5.14) and Fig.5 enable us to determine the parameter n for a crystal with the Schmid yield point σ_0. For the monocrystal extended in the direction [001] it is sufficient to measure the value of σ_n in the uniaxial tension test.

6. A complete system of equations for the model

Consider a rigid-ideally plastic crystal with interacting slip systems of the n-th independence degree. Properties of the crystal are prescribed by: density ρ, critical shear stresses $k_c^{(r)}$ and constants $\hat{m}_\alpha^{(r)}$, $\hat{n}_\alpha^{(r)}$ (see Eq.(2.4)), for $r = 1, ..., M$ and $\alpha = 1, 2, 3$. Denote by f_i components of a vector of body forces acting on the crystal. During the deformation process, the state of the crystal is described by: three components of the velocity field $v_i(\mathbf{x}, t)$, three Euler angles $\phi_m(t)$ and six components of the stress field $\sigma_{ij}(\mathbf{x}, t)$. To determine the above quantities and an auxiliary function $\lambda(\mathbf{x}, t)$, we have at our disposal a set of thirteen equations (including the incompressibility condition)

$$\sigma_{ij,i} + \rho f_j = \rho \dot{v}_j \,, \tag{6.1}$$

$$v_{i,j} = \lambda \sum_{r=1}^{M} \frac{1}{k_c^{(r)}} \left[\frac{\sigma_{kl} A_{kl}^{(r)}(\phi_m)}{k_c^{(r)}} \right]^{2n-1} A_{ij}^{(r)}(\phi_m) + \dot{R}_{i\alpha}(\phi_m) R_{j\alpha}(\phi_m) \,, \tag{6.2}$$

$$\sum_{r=1}^{M} \left[\frac{\sigma_{kl} A_{ij}^{(r)}(\phi_m)}{k_c^{(r)}} \right]^{2n} = \frac{1}{M} \sum_{s=1}^{M} \sum_{r=1}^{M} \left[2 \, \frac{k_c^{(s)}}{k_c^{(r)}} \, \hat{m}_{(\alpha}^{(r)} \hat{m}_{\beta)}^{(r)} \; \hat{m}_{(\alpha}^{(s)} \hat{n}_{\beta)}^{(s)} \right]^{2n} , \tag{6.3}$$

where

$$A_{ij}^{(r)} = m_i^{(r)} n_j^{(r)} . \tag{6.4}$$

In the case of non-uniform crystal deformation, its shape and initial-boundary conditions for $v_i(\mathbf{x}, t)$ and $\sigma_{ij}(\mathbf{x}, t)$ should be given. Due to the "geometrical softening effect" (see Asaro [10]) kinematical conditions will be preferred. Moreover, it is necessary to prescribe the initial conditions for the Euler angles ϕ_m .

7. The case of uniform deformations

The case of uniform deformations of crystals caused by uniform stress fields is important. Then, for quasistatical processes in absence of body forces, the equilibrium equations are satisfied identically. The remaining equations (6.2) – (6.3) may be expressed in terms of the stress deviator, the strain rate and the total spin components

$$s_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{kk}\,\delta_{ij}\,, \tag{7.1}$$

$$d_{ij} = \frac{1}{2}\left(v_{i,j} + v_{j,i}\right)\,, \tag{7.2}$$

$$\omega_{ij} = \frac{1}{2}\left(v_{i,j} - v_{j,i}\right)\,. \tag{7.3}$$

For rigid-ideally plastic crystals, the strain rate tensor $\mathbf{d}$ may be identified with the plastic one $\mathbf{d}^P$, which is described by five components d^P_{ij}.

$$d^P_{ij} = \lambda \sum_{r=1}^{M} \frac{1}{k_c^{(r)}} \left[\frac{s_{kl}A^{(r)}_{kl}(\phi_m)}{k_c^{(r)}}\right]^{2n-1} A^{(r)}_{(ij)}(\phi_m)\,, \tag{7.4}$$

$$\omega_{ij} = \lambda \sum_{r=1}^{M} \frac{1}{k_c^{(r)}} \left[\frac{s_{kl}A^{(r)}_{kl}(\phi_m)}{k_c^{(r)}}\right]^{2n-1} A^{(r)}_{<ij>}(\phi_m) + \dot{R}_{i\alpha}(\phi_m)R_{i\alpha}(\phi_m)\,, \tag{7.5}$$

$$\sum_{r=1}^{M} \left[\frac{s_{kl}A^{(r)}_{ij}(\phi_m)}{k_c^{(r)}}\right]^{2n} = \frac{1}{M}\sum_{s=1}^{M}\sum_{r=1}^{M}\left[2\,\frac{k_c^{(s)}}{k_c^{(r)}}\,\hat{m}^{(s)}_{(\alpha}\hat{n}^{(s)}_{\beta)}\,\hat{m}^{(r)}_{(\alpha}\hat{n}^{(r)}_{\beta)}\right]^{2n}, \tag{7.6}$$

where

$$A^{(r)}_{(ij)} = \frac{1}{2}\left[m_i^{(r)}n_j^{(r)} + m_j^{(r)}n_i^{(r)}\right]\,, \tag{7.7}$$

$$A^{(r)}_{<ij>} = \frac{1}{2}\left[m_i^{(r)}n_j^{(r)} - m_j^{(r)}n_i^{(r)}\right]\,, \tag{7.8}$$

for 17 unknowns: $s_{ij}, d_{ij}, \omega_{ij}, \phi_m, \lambda$.

One can assume that 5 out of the 10 components s_{ij} and d_{ij} are prescribed during the deformation process. Imposing adequate constraints on the total spin components ω_{ij}, one can obtain the 3 lacking equations. To explain this, consider two uniaxial stress states: tension and compression. One can assume the following constraints

for tension:

1a) material fibers parallel to the direction of tension $\mathbf{N}$ before deformation remain parallel to this direction during the deformation;

for compression:

1b) material planes orthogonal to the direction of compression N before deformation remain orthogonal to this direction during the deformation.

Denote by $\mathbf{N}^{(1)}$ and $\mathbf{N}^{(2)}$ two different directions orthogonal to N. Let $d\mathbf{x}, d\mathbf{x}^{(1)}, d\mathbf{x}^{(2)}$ be the infinitesimal fibers parallel to three distinguished directions, and $d\mathbf{v}, d\mathbf{v}^{(1)}$ $d\mathbf{v}^{(2)}$ – increments of velocity along these fibers. Then, the introduced constraints take the analytical form

for tension

$$N_i^{(k)}\, dv_i = 0\ , \quad \text{for} \quad k = 1,2\ ; \tag{7.9}$$

for compression

$$N_i\, dv_i^{(k)} = 0\ , \quad \text{for} \quad k = 1,2\ . \tag{7.10}$$

Introducing Eqs.(7.2) – (7.3) into Eqs.(7.9) – (7.10), two equations are obtained

for tension

$$N_i^{(k)}\ (d_{ij} + \omega_{ij})\ N_j = 0\ , \quad \text{for} \quad k = 1,2\ ; \tag{7.11}$$

for compression

$$N_i^{(k)}\ (d_{ij} - \omega_{ij})\ N_j = 0\ , \quad \text{for} \quad k = 1,2\ . \tag{7.12}$$

The last lacking equation can be obtained from the following constraint (the same for tension and compression):

2) any straight line parallel to N is not a rotation axis of the crystal.

This condition can be written in the form

$$N_i \epsilon_{ijk}\, \omega_{jk} = 0\ , \tag{7.13}$$

where ϵ_{ijk} is the antisymmetric permutational symbol.

Equations (7.11) – (7.13) complete the system (7.4) – (7.6) for the considered stress states.

In should be remembered that the lattice rotation which accompanies compression is not simply the opposite of that which occurs in tension. The reason is a difference between constrains (7.11) and (7.12) imposed on the total spin components. Moreover, it is necessary to stress that the problem of uniform deformations has been formulated as independent of a shape of the crystal.

8. Tension and compression of f.c.c. crystals

Consider a f.c.c. crystal of the n-th slip systems independence degree, with 12 slip systems $\{111\} < 110 >$ and a critical shear stress k_c. The crystal is uniformly extended (compressed) in the direction **N**. The tension (compression) is realized kinematically, i.e. the actual length (heigth) of the crystal $l(t)$ is known. The uniform stress field in the crystal

$$\sigma_{ij}(t) = \sigma(t)\, N_i(t)\, n_j(t)\,, \tag{8.1}$$

is described by an unknown loading parameter $\sigma(t)$.

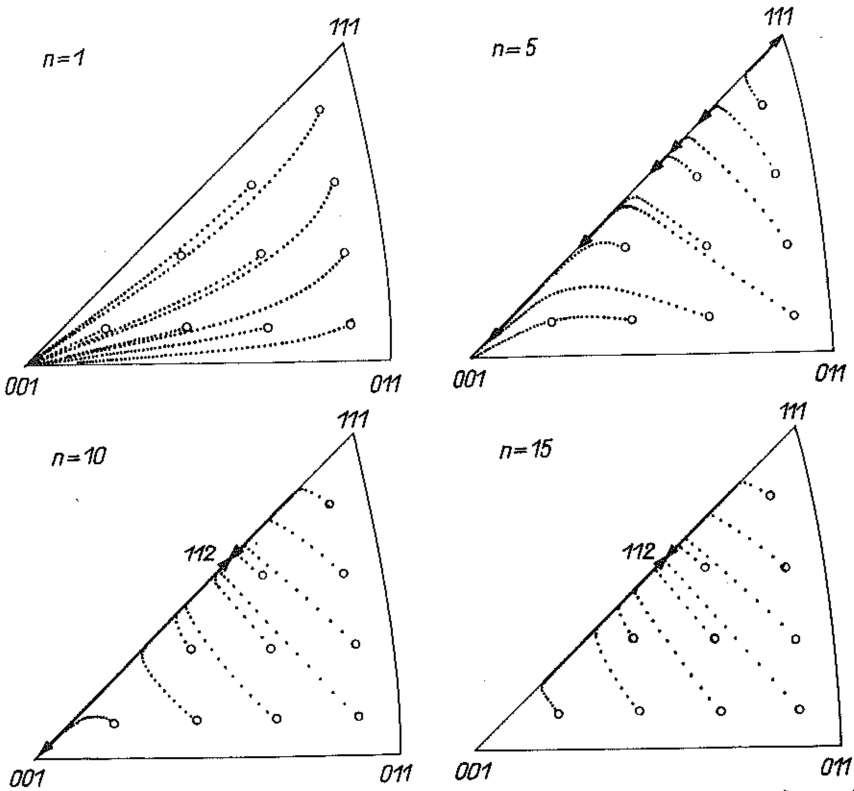

FIG. 7. Reorientations during extension of f.c.c. crystals with maximum elongation 100%, for $n = 1, 5, 10, 15$. The distance between successive dots corresponds to the strain 3.5%.

Assume that a lattice frame constitutes a fixed system of coordinates. We are going to look for the change of direction **N** during the deformation process. Since

$$\dot{\mathrm{N}}_i = \left(d_{ij} + \omega_{ij} - \frac{\dot{l}}{l}\,\delta_{ij}\right) N_j \,, \tag{8.2}$$

one can obtain from Eqs.(7.4) – (7.6)

$$\dot{\mathrm{N}}_i = \frac{\dot{l}}{l}\left\{ \frac{\sum\limits_{r=1}^{M} \left[N_k A_{kl}^{(r)} N_l\right]^{2n-1} A_{ij}^{(r)}}{\sum\limits_{r=1}^{M} \left[N_p A_{pq}^{(r)} N_q\right]^{2n}} - \delta_{ij} \right\} N_j \,. \tag{8.3}$$

It is essential to observe that the result is independent of k_c, and that k_c was assumed to be constant. It means that lattice reorientations do not depend on isotropic hardening of f.c.c. crystals.

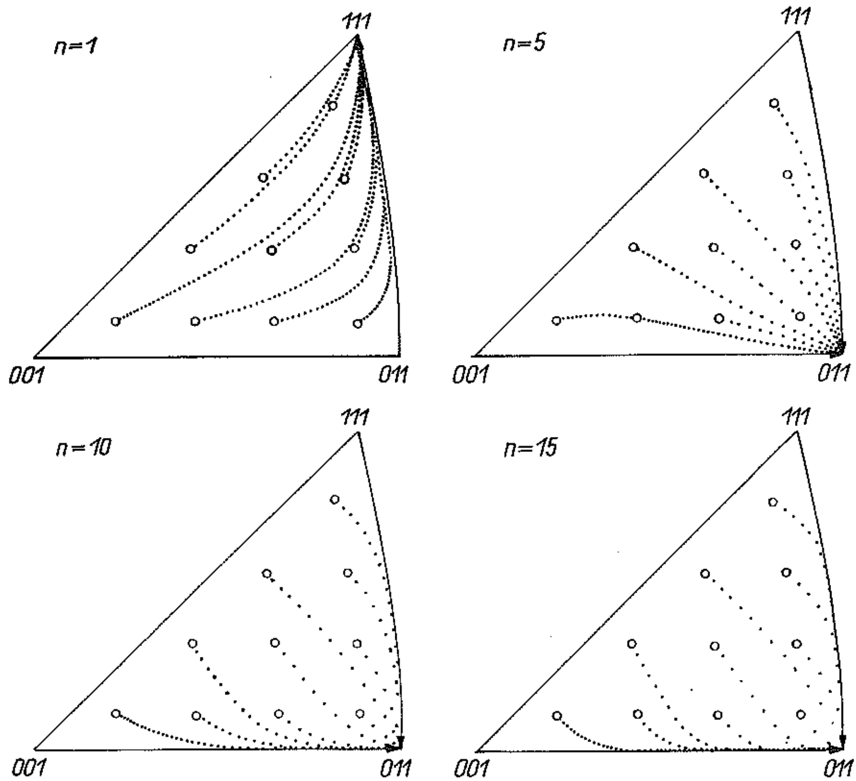

FIG. 8. Reorientations during compression of f.c.c. crystals with maximum length reduction 90%, for $n = 1, 5, 10, 15$. The dostance between successive dots corresponds to the strain 3.5%.

One can apply the above considerations to the problem of a drawing of single crystals. The stress state during this process is a superposition of an uniaxial tension with a hydrostatic pressure. Since the hydrostatic pressure does not influence the plastic yielding, one can investigate large extensions of the crystal under the stress field (8.1). Results may be shown on the inverse pole figures. Reorientations during extensions reaching up to 100%, for various values of the parameter n, are given in Fig.7.

Analogous results for compressed crystals with a thickness reduced up to 90% are presented in the Fig.8.

Note that, except for the case $n = 1$, axes of compression of the crystals tend to the direction [011], as predicted by the Schmid law.

For crystals subject to tension, the situation is more complicated. When n is greater than 10, most of the longitudinal axes move towards the direction [112], as predicted by the Schmid law. However, when n takes smaller values, additional directions [001] and [111] appear.

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STRESZCZENIE

PLASTYCZNOŚĆ KRYSZTAŁÓW ZE WZAJEMNIE ODDZIAŁYWUJĄCYMI SYSTEMAMI POŚLIZGÓW

Przedstawiono nowe, niekonwencjonalne podejście do analizy obrotów sieci krystalicznej spowodowanych dużymi odkształceniami plastycznymi kryształów. W przeciwieństwie do teorii opierającej się na prawie Schmida, w proponowanym modelu przyjmuje się, że początek plastycznego płynięcia zależy od stanów naprężenia na wszystkich systemach poślizgu, tzn. uwzględnia się oddziaływanie między systemami poślizgów. Przyjęte w pracy prawo oddziaływania, uzasadnione obserwacjami mikroskopowymi zależy od jednej stałej całkowitej n. Dla $n = 1$, kryształy zachowują się zgodnie z kryterium Misesa o kwadratowej powierzchni płynięcia. Dla $n \to \infty$, kryształy opisane są przez gładkie (z zaokrąglonymi narożami) powierzchnie płynięcia dążące do tych, które generuje prawo Schmida. Dla ustalonego n, prawo oddziaływania determinuje związki konstytutywne wiążące tensor prędkości odkształceń i spin plastyczny z tensorem naprężenia. Trzy dodatkowe równania konstytutywne dla składowych spinu plastycznego umożliwiają jawny opis reorientacji sieci. Wprowadzono uogólniony potencjał plastyczny dla prędkości odkształceń i spinu plastycznego. Gładki warunek plastyczności generowany przez ten potencjał umożliwia sformułowanie kompletnego układu równań modelu, co znacznie upraszcza analizę numeryczną. Szczegółowo zbadano rozciąganie i ściskanie kryształów typu A1. Przedstawione na odwrotnych figurach biegunowych drogi odkształceń wskazują na duży wpływ oddziaływań między systemami poślizgu na reorientacje sieci.

РЕЗЮМЕ

ПЛАСТИЧНОСТЬ КРИСТАЛЛОВ СО ВЗАИМОДЕЙСТВУЮЩИМИ СИСТЕМИАМИ СКОЛЬЖЕНИЙ

Представлен новый, неконвенциональный подход к анализу вращений кристаллической решетки, вызванных большими пластическими деформациями кристаллов. В противовес к теории, базирующей на законе Шмида, в предложенной модели принимается, что начало пластического течения зависит от состояний напряжения во всех системах скольжения, т.зн. учитивается взаимодействия между системами скольжений. Принятый в работе закон взаимодействия, обоснованный микроскопическими наблюдениями, зависит от одной натуральной постоянной n. Для $n = 1$, кристаллы ведутся согласно критерию Мизеса о квадратной

поверхности течения. Для $n \to \infty$, кристаллы описываются гладкими (с закругленными вершинами) поверхностями течения, стремящемися к этим, которые генерирует закон Шмида. Для установленного n, закон взаимодействия предопределяет определяюшие соотношения, связывающие тензор скорости деформаций и пластический спин с тензором напряжения. Три дополнительных определяющие уравнения для составляющих пластического спина дают возможность явным образом описать реориентировку решетки. Введен обобщенный пластический потенциал для скорости деформаций и пластического спина. Гладкое условие пластичности, генерированное этим потенциалом, дает возможность сформулировать полную систему уравнений модели, что значительно упрощает численный анализ. Подробно исследованы растяжение и сжатие кристаллов типа A1. Представленные на обратных полярах пути деформаций указывают на большое влияне взаимодействий между системами скольжения на реориентировку решетки.

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