# Simple shear and torsion of a perfectly plastic single crystal in finite transformations

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THE TWO-DIMENSIONAL plane behaviour of a single crystal is investigated under large deformations and rotations. Attention is restricted to the rigid plastic case with or without isotropic hardening. After recalling the basic equations, the conditions under which a single crystal can be treated as two-dimensional is discussed; this results in two plane single crystal models. One of them is then considered, and a general geometrical method is presented to investigate its behaviour under prescribed stress or strain conditions. This is then applied to simple shear and sample torsion. Particular attention is devoted to the rotation of the lattice and its asymptotic behaviour. In particular, it is shown that in both cases this orientation stabilizes to some values which are characterized. As a conclusion, the implications of these results for phenomenological models of anisotropic plasticity in large deformations are discussed.

W pracy analizuje się zachowanie tzw. płaskich pojedynczych kryształów w zakresie dużych deformacji i obrotów. Rozważany jest sztywno-plastyczny model materiału ze wzmocnieniem izotropowym lub bez. Po przypomnieniu podstawowych równań dyskutuje się warunki, które muszą zostać spełnione by pojedynczy kryształ mógł być traktowany jako płaski. Prowadzi to do dwóch płaskich modeli pojedynczego kryształu. W dalszej części tylko jeden z tych modeli jest rozważany. Przedstawiono ogólną metodę geometryczną do badania zachowania się płaskiego kryształu przy danych warunkach naprężeniowych lub odkształceniowych. Następnie zastoso wano ją do prostego ścinania i do analizy asymptotycznego zachowania się kryształu. W szczególności wykazano, że w obu rozważanych przypadkach orientacja sieci stabilizuje się osiągając pewne wartości, które zostały opisane w pracy. Na zakończenie przedstawiono wnioski, które anizotropowych w zakresie dużych odkształceń.

В работе анализируется поведение т. наз. плоских единичных кристаллов в области больших деформаций и вращений. Рассматривается жестко-пластическая модель материала с изотропным упрочнением и без упрочнения. После приведения основных уравнений, обсуждаются условия, которые должны быть удовлетворены, чтобы единичный кристалл можно трактовать как плоский. Это приводит к двум плоским моделям единичного кристалла. В дальнейшей части рассматривается только одна из этих моделей. Представлен общий геометрический метод для исследования поведения плоского кристалла, при заданных напряженных или деформационных условиях. Затем он применен к простому сдвигу и к анализу асимптотического поведения кристалла. В частности показано, что в обоих рассматриваемых случаях, ориентировка решетки стабилизируется, достигая некоторых значений, которые были описаны в работе. В заключении представлены следствия, которые следует учитывать при формулировке феноменологических моделей для пластически анизотропных сред в области больших деформаций.

### 1. Introduction

LARGE STRAIN anisotropic plasticity is a controversial subject. Kinematic hardening has been extensively investigated and many propositions have been made about the objective derivative to be used [1-5]. Initial anisotropy can be treated in the same way introducing a rotating frame formalism [6-8] and similar results are obtained. For instance, use of the corotational frame results in an oscillatory behaviour in simple shear, which can be elim-

2 Arch. Mech. Stos. 5-6/88

inated by using, for instance, the proper rotating frame. In [8] these oscillations have been shown as essentially related to the asymptotic behaviour of the rotating frame for increasing shear: a regularly increasing rotation (as in the case of the corotational frame) results in an oscillatory behaviour, while a bounded rotation stabilizing to a fixed position results in a stabilized behaviour.

The definition of the rotating frame in which the anisotropic constitutive equations are to be written therefore appears as a constitutive assumption, the only one in fact to be specific of large strain, because all the other components of the model are already present in the small strain case [8]. Whenever possible, this phenomenological assumption must rely on some microstructural information resulting from the microscopic origin of anisotropy. In metals the basic anisotropy is the crystal structure and much information about phenomenological plasticity can be gained from single crystal analysis.

The mechanics of a single crystal, however, is not so simple [9] and many problems are still to be settled in connection, in particular, with slip indetermination. Moreover, even if the plasticity of single crystals is naturally formulated in large strain [10], very few simulations have been performed in situations involving the large rotations which are necessary to settle the issues discussed above. A step towards that direction has been made in [11] which proved that in case of a f.c.c. "viscous" single crystal, the corotational frame was to be used and that an oscillatory behaviour was in that case actually obtained. But the extension of these results to the plastic or viscoplastic case is not available.

The purpose of the present work is to analyze a plastic f.c.c. single crystal in simple shear and torsion. Elasticity will be neglected and hardening will not be taken into account, but it will be shown that the main results remain true for most hardening cases.

### 2. The basic mechanical framework

The kinematics of a rigid plastic single crystal is described, as in Fig. 1, by the decomposition

(2.1) 
$$\mathbf{F} = \mathbf{R}^t \mathbf{P}, \quad \dot{\mathbf{P}} \mathbf{P}^{-1} = \Sigma \dot{\gamma}^s \overline{\mathbf{M}}^s, \quad \overline{\mathbf{M}}^s = \bar{g}^s \otimes \bar{n}^s$$

for the deformation gradient F [10]. In this relation  $\mathbf{R}^{l}$  denotes the rotation of the crystal lattice while **P** is the "plastic" contribution to **F** resulting from dislocation motions. Each



FIG. 1. Large strain of the rigid plastic single crystal.

slip system is characterized by the unit normal to the slip plane  $\bar{n}^s$  and the gliding direction  $\bar{g}^s$ . These vectors are fixed in the isoclinic configuration  $\bar{C}(t)$  while the corresponding Eulerian vectors  $g^s$  and  $n^s$  are rotated by  $\mathbf{R}^t$ .

The classical decomposition follows from the relations (2.1) for the velocity gradient L, the rate of deformation  $D = L^s$  and the spin  $W = L^A$ 

(2.2) 
$$\mathbf{L} = \mathbf{\Omega}^{l} + \mathbf{R}^{l} \dot{\mathbf{P}} \mathbf{P}^{-1} \mathbf{R}^{lT}, \quad \mathbf{\Omega}^{l} = \dot{\mathbf{R}}^{l} \mathbf{R}^{lT}, \\ \mathbf{D} = \mathbf{R}^{l} (\dot{\mathbf{P}} \mathbf{P}^{-1})^{s} \mathbf{R}^{lT}, \quad \mathbf{w} = \mathbf{\Omega}^{l} + \mathbf{R}^{l} (\dot{\mathbf{P}} \mathbf{P}^{-1})^{4} \mathbf{R}^{lT},$$

but it is more convenient to rotate these tensors in C(t)

(2.3) 
$$\overline{\mathbf{D}} = \mathbf{R}^{lT} \mathbf{D} \mathbf{R}^{l} = (\mathbf{P} \mathbf{P}^{-1})^{s} = \Sigma \dot{\gamma}^{s} \overline{\mathbf{M}}^{ss},$$

(2.4) 
$$\mathbf{R}^{lT}\mathbf{w}\mathbf{R}^{l} = \overline{\mathbf{\Omega}}^{l} + \Sigma \dot{\gamma}^{s} \overline{\mathbf{M}}^{sA}, \quad \overline{\mathbf{\Omega}}^{l} = \mathbf{R}^{lT} \dot{\mathbf{R}}^{l}$$

The behaviour of the single crystal follows from the slip law which relates the slip rate  $\dot{\gamma}^s$  on each system to the resolved shear stress

(2.5) 
$$\tau^{s} = g^{s} \mathbf{T} n^{s} = \mathbf{T} : \mathbf{M}^{s} = \mathbf{\overline{T}} : \mathbf{\overline{M}}^{s}, \quad \mathbf{T} = \mathbf{R}^{l} \mathbf{\overline{T}} \mathbf{R}^{lT}.$$

In the following, attention will be focussed on perfect plasticity

(2.6)  
$$\begin{aligned} \dot{\gamma}^s \ge 0 \quad \text{if} \quad \tau^s = \tau_0, \\ \dot{\gamma}^s = 0 \quad \text{if} \quad -\tau_0 \leqslant \tau^s \leqslant \tau_0, \\ \dot{\gamma}^s \leqslant 0 \quad \text{if} \quad \tau^s = -\tau_0, \end{aligned}$$

with a constant critical shear stress  $\tau_0$ . The constitutive equation then results from the elimination of the slip rates  $\dot{\gamma}^s$  (s = 1, ..., N) from the relations (2.2) and (2.6). More precisely, for an imposed kinematics **L** (tr **L** = 0), the relations (2.2) and (2.6) provide 8+N equations for 8+N unknowns (N slip rates  $\dot{\gamma}^s$ , 5 components of the deviatoric part **T**<sup>D</sup> of **T** and 3 components of  $\Omega^t$ ).

However, these equations can be treated in two steps: at first, the relations (2.3) and (2.6) provide N+5 equations for  $\overline{\mathbf{T}}$  and  $\dot{\gamma}^s$ , and after this system has been solved, the lattice spin  $\Omega^l$  is directly obtained from Eq. (2.4). The essential part, therefore, is the determination of  $\dot{\gamma}^s$  and  $\overline{\mathbf{T}}$  from  $\overline{\mathbf{D}}$  and this is exactly the usual algebraic small strain problem [9] with the well-known slip indetermination. As mentioned in the introduction, the large strain analysis of single crystals is simply obtained by complementing the usual small strain analysis by the rotation description and evolution equation (2.4). In other words, and using the terminology introduced in [8], the constitutive model is the usual small strain single crystal written in the isoclinic rotating frame defined by  $\overline{\mathbf{Q}} = \mathbf{R}^t$  and can be followed by Eq. (2.4) which is obviously a special case of the general form discussed in [8].

In the viscous case ( $\tau^s = \mu \dot{\gamma}^s$ ) this equation can be explicitly derived and in the case of a f.c.c. single crystal, it has been obtained as  $\Omega^l = W$  [11]. Unfortunately, such an explicit form cannot be obtained in the plastic case and our purpose in the following will be to analyze this evolution in some simple situations involving large rotations: simple shear and torsion.

## 3. The F.C.C.P2 single crystal

System	n		g	
1	(111) [110]	$1/\sqrt{3}(1, 0, \sqrt{2})$	( 0, 1, 0)	
2	(111) [101]	$1/\sqrt{3}(1, 0, \sqrt{2})$	$\frac{1}{2}(-\sqrt{2}, 1, 1)$	
3	(111) [011]	$1/\sqrt{3}(1, 0, \sqrt{2})$	$\frac{1}{2}(-\sqrt{2},-1,1)$	
4	(111) [101]	$1/\sqrt{3}(-1, 0, \sqrt{2})$	$\frac{1}{2}(\sqrt{2}, 1, 1)$	
5	(111) [110]	$1/\sqrt{3}(-1, 0, \sqrt{2})$	( 0, 1, 0)	
6	(111) [011]	$1/\sqrt{3}(-1, 0, \sqrt{2})$	$\frac{1}{2}(\sqrt{2}, -1, 1)$	
7	(111) [101]	$1/\sqrt{3}(1, \sqrt{2}, 0)$	$\frac{1}{2}(-\sqrt{2}, 1, 1)$	
8	(111) [011]	$1/\sqrt{3}(1, \sqrt{2}, 0)$	$\frac{1}{2}(\sqrt{2}, -1, 1)$	
9	(111) [110]	$1/\sqrt{3}(1, \sqrt{2}, 0)$	( 0, 0, 1)	
10	(111) [011]	$1/\sqrt{3}(1, -\sqrt{2}, 0)$	$\frac{1}{2}(-\sqrt{2}, -1, 1)$	
11	(111) [110]	$1/\sqrt{3}(1, -\sqrt{2}, 0)$	( 0, 0, 1)	
12	(111) [101]	$1/\sqrt{3}(1, -\sqrt{2}, 0)$	$\frac{1}{2}(\sqrt{2}, 1, 1)$	

We shall now consider a f.c.c. single crystal in which the 12 slip systems are associated to the planes  $\{111\}$  and directions  $\langle 110 \rangle$ . They will be denoted according to Table 1.

Table 1. The 12 slip systems.

In the following we shall be concerned with plane situations where the rate of deformation and stress tensors  $\overline{\mathbf{D}}$  and  $\overline{\mathbf{T}}$  in  $\overline{C}(t)$  have the following form:

(3.1) 
$$\overline{\mathbf{T}} = \begin{bmatrix} \overline{T}_{11} & \overline{T}_{12} & 0\\ \overline{T}_{12} & \overline{T}_{22} & 0\\ 0 & 0 & 0 \end{bmatrix}, \quad \overline{\mathbf{D}} = \begin{bmatrix} \overline{D}_{11} & \overline{D}_{12} & 0\\ \overline{D}_{12} & \overline{D}_{22} & 0\\ 0 & 0 & -(\overline{D}_{11} + \overline{D}_{22}) \end{bmatrix}.$$

However, the compatibility of these two forms requires that  $x_3$  is a symmetry axis for the crystal, namely, a  $\langle 100 \rangle$  or  $\langle 110 \rangle$  direction. In this paper we shall consider the plane single crystal f.c.c.P2 which is a f.c.c. single crystal under plane stress and strain in a  $\{110\}$  plane (the f.c.c.P1 single crystal corresponds to a  $\{100\}$  plane, but it seems more difficult for our purpose). The basis vectors  $\overline{e}_1$ ,  $\overline{e}_2$ ,  $\overline{e}_3$  in the isoclinic frame  $\overline{C}(t)$  are, respectively, chosen along the [001], [110] and [110] directions. The resulting components of  $\overline{n}^s$  and  $\overline{g}^s$  are given in Table 1, and the tensors  $\overline{\mathbf{M}}^s$  and resolved shear stress  $\tau^s$  are easily obtained for all systems. Let us consider, for instance, the systems 2 and 6:

$$\overline{\mathbf{M}}^{2} = \frac{1}{2\sqrt{3}} \begin{bmatrix} -\sqrt{2} & 0 & -2\\ 1 & 0 & \sqrt{2}\\ 1 & 0 & \sqrt{2} \end{bmatrix}, \quad \overline{\mathbf{M}}^{6} = \frac{1}{2\sqrt{3}} \begin{bmatrix} -\sqrt{2} & 0 & 2\\ 1 & 0 & -\sqrt{2}\\ -1 & 0 & \sqrt{2} \end{bmatrix},$$
$$\tau^{2} = \tau^{6} = \frac{1}{2\sqrt{3}} \left(\overline{T}_{12} - \sqrt{2}\overline{T}_{11}\right).$$

The systems 2 and 6 are symmetric and it is reasonable to assume that  $\dot{\gamma}^2 = \dot{\gamma}^6$ . The contribution of these two systems to  $\dot{\mathbf{P}}\mathbf{P}^{-1}$  therefore is

$$\dot{\gamma}^{2}(\overline{\mathbf{M}}^{2}+\overline{\mathbf{M}}^{6}) = \frac{\dot{\gamma}^{2}}{\sqrt{3}} \begin{bmatrix} -\sqrt{2} & 0 & 0\\ 1 & 0 & 0\\ 0 & 0 & \sqrt{2} \end{bmatrix} = \dot{\alpha}^{2}\overline{\mathbf{N}}^{2},$$

which is a plane strain. The two systems 2 and 6 are degenerated in one single plane pseudoslip system defined by  $\overline{N}^2$ . A similar analysis can be performed on the other systems: the systems 9 and 11 disappear while the 10 remaining systems can be symmetrized into 5 plane pseudo-slip systems (Tabl. 2).

Table 2. The 5 plane pseudo-slip	systems.
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1	$\dot{\alpha}^1 = \dot{\gamma}^1 - \dot{\gamma}^5$	$\sigma^1 = \overline{T}_{12}/\sqrt{3}$	$\overline{N}^{1} = \frac{1}{2\sqrt{3}} \begin{bmatrix} 0 & 0 \\ 2 & 0 \end{bmatrix}$
2	$\dot{\alpha}^2 = \dot{\gamma}^2 + \dot{\gamma}^6$	$\sigma^2 = (\overline{T}_{12} - \sqrt{2} \overline{T}_{11})/2 \sqrt{3}$	$\overline{N}^2 = \frac{1}{2\sqrt{3}} \begin{bmatrix} -\sqrt{2} & 0\\ 1 & 0 \end{bmatrix}$
3	$\dot{\alpha}^3 = -\dot{\gamma}^3 - \dot{\gamma}^4$	$\sigma^3 = (\overline{T}_{12} + \sqrt{2} \overline{T}_{11})/2 \sqrt{3}$	$\overline{N}^{3} = \frac{1}{2\sqrt{3}} \begin{bmatrix} \sqrt{2} & 0 \\ 1 & 0 \end{bmatrix}$
4	$\dot{\alpha}^4 = -\dot{\gamma}^7 + \dot{\gamma}^8$	$\sigma^4 = \big(\overline{T}_{12} + \sqrt{2}(\overline{T}_{11} - \overline{T}_{22})\big)/2\sqrt{3}$	$\overline{N}^4 = \frac{1}{2\sqrt{3}} \begin{bmatrix} \sqrt{2} & 2\\ -1 & -\sqrt{2} \end{bmatrix}$
5	$\dot{\alpha}^5 = \dot{\gamma}^{10} - \dot{\gamma}^{12}$	$\sigma^5=\big(\overline{T}_{12}\!-\!\sqrt{2}(\overline{T}_{11}\!-\!\overline{T}_{22})\big)/2\sqrt{3}$	$\overline{N}^{5} = \frac{1}{2\sqrt{3}} \begin{bmatrix} -\sqrt{2} & 2\\ -1 & \sqrt{2} \end{bmatrix}$

With these notations, the plane single crystal f.c.c.P2 is defined by

(3.2)  $\mathbf{F} = \mathbf{R}^{l}\mathbf{P}, \quad \dot{\mathbf{P}}\mathbf{P}^{-1} = \boldsymbol{\Sigma}\dot{\boldsymbol{\alpha}}^{s}\mathbf{\overline{N}}^{s},$ 

where  $\dot{\alpha}^s$  is related to  $\sigma^s = \overline{\mathbf{T}}: \overline{\mathbf{N}}^s$  by the slip law which in the plastic case is

(3.3) 
$$\begin{aligned} \dot{\alpha}^s &\ge 0 \quad \text{if} \qquad \sigma^s = \tau_0, \\ \dot{\alpha}^s &= 0 \quad \text{if} \qquad -\tau_0 \leqslant \sigma^s \leqslant \tau_0, \\ \dot{\alpha}^s \leqslant 0 \quad \text{if} \qquad \sigma_s = -\tau_0. \end{aligned}$$

Formally these relations are identical with the three-dimensional case of Sect. 2, but they are much simpler. In particular, the lattice rotation  $\mathbf{R}^{l}$  is a plane rotation

(3.4) 
$$\mathbf{R}^{l} = \begin{bmatrix} \cos\theta & \sin\theta & 0\\ -\sin\theta & \cos\theta & 0\\ 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{\Omega}^{l} = \begin{bmatrix} 0 & \dot{\theta} & 0\\ -\dot{\theta} & 0 & 0\\ 0 & 0 & 0 \end{bmatrix}$$

so that the spin equation (2.4) becomes a scalar relation

(3.5) 
$$w = \dot{\theta} + \omega^{p}, \quad \omega^{p} = \frac{1}{4\sqrt{3}} (3\dot{\alpha}^{4} + 3\dot{\alpha}^{5} - 2\dot{\alpha}^{1} - \dot{\alpha}^{2} - \dot{\alpha}^{3}),$$

where  $w = w_{12}$  is the total spin. Similarly, the relation (2.3) becomes

(3.6)  
$$\overline{D}_{11} = \frac{1}{\sqrt{6}} (\dot{\alpha}^3 + \dot{\alpha}^4 - \dot{\alpha}^5 - \dot{\alpha}^2), \quad \overline{D}_{22} = \frac{1}{\sqrt{6}} (\dot{\alpha}^5 - \dot{\alpha}^4),$$
$$\overline{D}_{12} = \frac{1}{4\sqrt{3}} (2\dot{\alpha}^1 + \dot{\alpha}^2 + \dot{\alpha}^3 + \dot{\alpha}^4 + \dot{\alpha}^5).$$

For given kinematics, we then have to solve Eqs. (3.3) and (3.6) for the 8 unknowns  $\dot{\alpha}^s$  and  $\overline{\mathbf{T}}$  while the lattice spin  $\dot{\theta}$  is obtained afterwards from the relation (3.5). Of course it is not possible to obtain the  $5\dot{\alpha}^s$  from the 3 equations (3.6). However, it will be convenient to solve these three equations in the form

$$\dot{\alpha}^{1} = \frac{\sqrt{3}}{2} (3\overline{D}_{12} - \omega^{p} - \xi),$$
(3.7) 
$$\dot{\alpha}^{2} = \frac{\sqrt{3}}{2} [\xi - \sqrt{2}(\overline{D}_{11} + \overline{D}_{22})], \quad \dot{\alpha}^{3} = \frac{\sqrt{3}}{2} [\xi + \sqrt{2}(\overline{D}_{11} + \overline{D}_{22})],$$

$$\dot{\alpha}^{4} = \frac{\sqrt{3}}{2} (\overline{D}_{12} + \omega^{p} - \sqrt{2}\overline{D}_{22}), \quad \dot{\alpha}^{5} = \frac{\sqrt{3}}{2} (\overline{D}_{12} + \omega^{p} + \sqrt{2}\overline{D}_{22}),$$

which gives  $\dot{\alpha}^s$  in terms of **D** and two indeterminate quantities  $\xi$  and  $\omega^p$ .

### 4. Strain rate space representation

A geometrical representation will prove most convenient to describe the constitutive relation between  $\overline{T}$  and  $\overline{D}$ . These tensors are therefore considered as points in three-dimensional vector spaces. An orthogonal basis is introduced in both spaces:

$$\begin{aligned} X_1 &= \overline{T}_{11}, \quad X_2 &= \overline{T}_{22}, \quad X_3 &= \sqrt{2}\,\overline{T}_{12}, \\ Y_1 &= \overline{D}_{11}, \quad Y_2 &= \overline{D}_{22}, \quad Y_3 &= \sqrt{2}\,\overline{D}_{12}. \end{aligned}$$

In the stress space X, the constitutive relation is represented by the plasticity surface which is the boundary of the plastic convex  $|\tau^s| \leq \tau_0$ . These 5 conditions are easily expressed through Table 2 and the corresponding domain is a decahedron which is represented in Fig. 2. Each face corresponds to the activity of one slip system. For instance, on the face  $1^+ = CDEF$  we have  $\tau^1 = +\tau_0$  and  $\dot{\alpha}^1 \geq 0$ . The corresponding strain rate is normal to this face and represented in the strain rate space by the direction  $Y_3 > 0$ ,  $Y_1 = Y_2 = 0$ .



FIG. 2. Plasticity surface in the stress space.

More generally, because of rate insensitivity, the strain rate space may be considered as the two-dimensional space of all (oriented) directions in the vector space Y. A plane representation is obtained by defining a direction by its intersection with two parallel planes. In the following, we shall represent the strain space in the planes  $Y_3 = \pm 1$ . Of course the directions which are parallel to these planes are rejected at infinity, but this is easily dealt with in projective geometry. The construction proceeds as follows (Fig. 3) from the decahedron in the X-space.



FIG. 3. System activity in the strain rate space.

a) On each face of the decahedron, the strain rate direction is normal to this face resulting in a point in the  $Y_3 = \pm 1$  planes. The 10 points are easily obtained either from this normality condition or directly from the relations (3.6) with the only non-vanishing  $\dot{\alpha}^s$ .

b) An edge such as  $CF = 1^{+}4^{+}$  is the intersection of two faces  $\sigma^{1} = +\tau_{0}$ ,  $\sigma^{4} = +\tau_{0}$ . The corresponding strain rate is defined from the relations (3.6) with  $\dot{\alpha}^{1} \ge 0$ ,  $\dot{\alpha}^{4} \ge 0$  $(\dot{\alpha}^{2} = \dot{\alpha}^{3} = \dot{\alpha}^{5} = 0)$ . Straightforward calculations show that the corresponding point in the  $Y_{3} = +1$  plane lies on the segment  $1^{+}4^{+}$  and that  $\dot{\alpha}^{1}$  and  $\dot{\alpha}^{4}$  are proportional to the barycentric coordinates of this point with respect to  $1^{+}$  and  $4^{+}$ . For an edge such as AB = $= 3^{+}2^{-}$ , this works in a similar way, although some complications arise from the fact that the corresponding segment  $3^{+}2^{-}$  goes through infinity. This can be avoided by using different planes,  $Y_{1} = \pm 1$  for instance, but this will not be necessary.

c) An apex like C is the intersection of 3 faces  $\sigma^1 = \sigma^3 = \sigma^4 = +\tau_0$  so that  $\dot{\alpha}^1 \ge 0$ ,  $\dot{\alpha}^3 \ge 0$  and  $\dot{\alpha}^4 \ge 0$  ( $\dot{\alpha}^2 = \dot{\alpha}^5 = 0$ ). Again it is easily shown that the corresponding point lies in the triangle  $1^+4^+3^+$  and that  $\dot{\alpha}^1$ ,  $\dot{\alpha}^3$ ,  $\dot{\alpha}^4$  are determined as proportional to the barycentric coordinates of this point.

d) An apex like A is the intersection of 4 faces  $\sigma^4 = \sigma^3 = -\sigma^2 = -\sigma^5 = \tau_0$  so that  $\dot{\alpha}^3 \ge 0$ ,  $\dot{\alpha}^4 \ge 0$ ,  $\dot{\alpha}^2 \le 0$ ,  $\dot{\alpha}^5 \le 0$  and  $\dot{\alpha}^1 = 0$ . The corresponding point still lies in the quadrangle  $4^+3^+2^-5^-$ . However, the slip rates  $\dot{\alpha}^3$ ,  $\dot{\alpha}^4$ ,  $\dot{\alpha}^2$ ,  $\dot{\alpha}^5$  are no longer determined from this point, i.e. from the knowledge of  $\overline{\mathbf{D}}$ . This is the well-known slip indetermination.

This representation of the strain rate space is the basic element for the analysis of the single crystal under prescribed kinematics. For each value of  $\overline{\mathbf{D}}$  it gives the active systems, the localization of the stress point in the X plane and, when possible, the individual slip rates.

#### 5. Simple shear

Simple shear is defined in a fixed coordinate system by

(5.1) 
$$\mathbf{F} = \begin{bmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{L} = \begin{bmatrix} 0 & \Gamma & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad \mathbf{T} = \begin{bmatrix} N_1 & \tau & 0 \\ \tau & N_2 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

where the shear rate  $\Gamma = \dot{\gamma}$  is assumed constant ( $\gamma = \Gamma t$ ). The rotated strain rate **D** is

(5.2) 
$$\overline{D}_{22} = -\overline{D}_{11} = \frac{\Gamma}{2}\sin 2\theta, \quad \overline{D}_{12} = \frac{\Gamma}{2}\cos 2\theta$$

and it depends on the lattice rotation which is unknown. In the strain rate representation described above, the corresponding point is given by

(5.3) 
$$-Y_1 = Y_2 = \frac{\sqrt{2}}{2 \operatorname{tg} 2\theta} \quad \text{in} \quad Y_3 = +1 \quad \text{if} \quad \cos 2\theta \ge 0,$$
$$Y_1 = -Y_2 = \frac{\sqrt{2}}{2 \operatorname{tg} 2\theta} \quad \text{in} \quad Y_3 = -1 \quad \text{if} \quad \cos 2\theta \le 0$$

and it lies on the straight line  $Y_1 = -Y_2$  parametrized by  $\theta$  (Fig. 4). Simple shear analysis follows from the superposition of this diagram representing the prescribed kinematics with the constitutive diagram of Fig. 3 which characterizes the considered plane single crystal.



FIG. 4. Simple shear in the strain rate space.

In our special case, it follows from this superposition that when  $2\theta$  goes from 0 to  $2\pi$ , the strain rate direction successively describes the edges 1+5+4-1-5-4+1+ and that double slip occurs for almost all values of  $\theta$ ; there is no slip indetermination. More precisely the system activity is described as a function of  $\theta$  in Table 3 with  $tg 2\theta_p = 2\sqrt{2}$ .

Since double slip corresponds to an edge of the plasticity surface, the components of the stress tensor  $\overline{T}_{11}$ ,  $\overline{T}_{22}$ ,  $\overline{T}_{12}$  are not completely determined: more precisely, since we are only concerned with systems 1, 4 and 5, the expressions in Table 2 show that the activation condition will involve  $\overline{T}_{12}$  and  $(\overline{T}_{11} - \overline{T}_{22})$  only while  $\overline{T}_{11} + \overline{T}_{22}$  will remain undetermined. To be more specific, let us consider, for instance, the edge  $1^+5^+ = DE$   $(0 \le 2\theta \le 2\theta_p)$ . The activation conditions give

(5.4) 
$$\sigma^1 = \overline{T}_{12}/\sqrt{3} = \tau_0, \quad \sigma^5 = [\overline{T}_{12} + \sqrt{2}(\overline{T}_{11} - \overline{T}_{22})]/2\sqrt{3} = \tau_0$$

which can be solved

(5.5) 
$$\overline{T}_{12} = \tau_0 \sqrt{3}, \quad \overline{T}_{22} - \overline{T}_{11} = \sqrt{\frac{3}{2}} \tau_0$$

This gives the rotated stress tensor  $\overline{T}$ ; the applied normal and shear stress  $N_1$ ,  $N_2$ ,  $\tau$  are obtained through the lattice rotation as

(5.6)  
$$N_1 - N_2 = \tau_0 \sqrt{3} \left( 2\sin 2\theta - \frac{1}{\sqrt{2}} \cos 2\theta \right),$$
$$\tau = \tau_0 \sqrt{3} \left( \cos 2\theta + \frac{1}{2\sqrt{2}} \sin 2\theta \right).$$

A similar analysis can be performed for the other cases and the following results are obtained on  $5^+4^- = A'B$ :  $(2\theta_p \le 2\theta \le \pi - 2\theta_p)$ 

(5.7)  
$$N_1 - N_2 = -\tau_0 \sqrt{6} \cos 2\theta$$
$$\tau = \tau_0 \sqrt{\frac{3}{2}} \sin 2\theta$$



FIG. 5. Shear stress in simple shear.

and on  $4^-1^- = C'F'$   $(\pi - 2\theta_p \leq 2\theta \leq \pi)$ 

(5.8)  

$$N_{1}-N_{2} = \tau_{0}\sqrt{3}\left(-2\sin 2\theta - \frac{1}{\sqrt{2}}\cos 2\theta\right),$$

$$\tau = \tau_{0}\sqrt{3}\left(-\cos 2\theta + \frac{1}{2\sqrt{2}}\sin 2\theta\right).$$

The corresponding curves are given in Fig. 5. It should be noted that the stresses depend on the applied shear only through the lattice orientation  $\theta$ . This dependence results from the crystal anisotropy and it could have been analyzed in a small deformation context (Tabl. 3).

Table	3.	System	activity	in	simple	shear
		-	-			

			Activation condition	Active systems
20	0 }— 20 ∖_	1+5+	$\tau^1 = \tau^5 = \tau_0$	$\alpha^1 \ge 0, \alpha^5 \ge 0$
	$\pi - 2\theta_{-} > -$	5+4-	$\tau^5 = -\tau^4 = \tau_0$	$\alpha^5 \ge 0, \alpha^4 \le 0$
	π >	4-1-	$\tau^4 = \tau^1 = -\tau_0$	$\alpha^4 \leqslant 0, \alpha^1 \leqslant 0$
	$\pi + 2\theta_n \rightarrow$	1-5-	$\tau^1 = \tau^5 = -\tau_0$	$\alpha^1 \leqslant 0, \alpha^5 \leqslant 0$
	$2\pi - 2\theta_n \rangle$	5-4+	$\tau^4 = -\tau^5 = \tau_0$	$\alpha^5 \leqslant 0, \alpha^4 \geqslant 0$
	2π >	4+1+	$\tau^4 = \tau^1 = \tau_0$	$\alpha^4 \ge 0, \alpha^1 \ge 0$

### 6. Evolution of the rotation

The specific aspect of large deformations is thus concentrated in the evolution equation for the rotation (3.5) which becomes

(6.1) 
$$\dot{\theta} = \frac{\Gamma}{2} - \omega^p.$$

It follows from Table 3 that the systems 2 and 3 are never activated,  $\dot{\alpha}^2 = \dot{\alpha}^3 = 0$  so that Eqs. (3.7) are reduced to  $\xi = 0$  and

(6.2)  
$$\dot{\alpha}^{1} = \frac{\sqrt{3}}{2} \left( \frac{3\Gamma}{2} \cos 2\theta - \omega^{p} \right),$$
$$\dot{\alpha}^{4} = \frac{\sqrt{3}}{2} \left( \frac{\Gamma}{2} \cos 2\theta - \frac{\sqrt{2}\Gamma}{2} \sin 2\theta + \omega^{p} \right),$$
$$\dot{\alpha}^{5} = \frac{\sqrt{3}}{2} \left( \frac{\Gamma}{2} \cos 2\theta + \frac{\sqrt{2}\Gamma}{2} \sin 2\theta + \omega^{p} \right).$$

The value of  $\omega^p$  and  $\dot{\theta}$  therefore directly follows from the active systems.

For the 1<sup>+</sup>5<sup>+</sup> zone ( $0 \le 2\theta \le 2\theta_p$ ) for instance,  $\dot{\alpha}^4 = 0$  so that  $\omega^p$ ,  $\dot{\alpha}^1$  and  $\dot{\alpha}^5$  are given by

$$\omega^{p} = \frac{\Gamma}{2} \left( \sqrt{2} \sin 2\theta - \cos 2\theta \right)$$

(6.3)

$$\dot{\alpha}^{1} = \frac{\sqrt{3}\Gamma}{4} \left(4\cos 2\theta - \sqrt{2}\sin 2\theta\right), \quad \dot{\alpha}^{5} = \frac{\sqrt{3}\Gamma}{2} 2\sqrt{2}\sin 2\theta.$$

The evolution equation (6.1) then gives  $\dot{\theta}/\Gamma = d\theta/d\gamma$  as

(6.4) 
$$\frac{d\theta}{d\gamma} = \frac{1}{2} \left( 1 + \cos 2\theta - \sqrt{2} \sin 2\theta \right), \quad 0 \le 2\theta \le 2\theta_p.$$

The other cases are analyzed in a similar way and the results are

(6.5) 
$$\frac{d\theta}{d\gamma} = \frac{1}{2} (1 - 3\cos 2\theta), \qquad \qquad 2\theta_p \leq 2\theta \leq \pi - 2\theta_p,$$

(6.6) 
$$\frac{d\theta}{d\gamma} = \frac{1}{2} \left( 1 + \cos 2\theta + \sqrt{2} \sin 2\theta \right), \qquad \pi - 2\theta_p \leq 2\theta \leq \pi$$

while Eq. (6.4) is found again for  $\pi \leq 2\theta \leq \pi + 2\theta_p$ , etc.

This function  $d\theta/d\gamma = h(\theta)$  is represented in Fig. 6. The evolution of  $\theta$  with  $\gamma$  is obtained by integration of this function:

(6.7) 
$$\int_{\theta_0}^{\theta} \frac{d\theta}{h(\theta)} = \gamma,$$



FIG. 6. Plastic spin in simple shear.

where  $\theta_0$  is the initial value of  $\theta$  for  $\gamma = 0$ . The behaviour of the rotation, which as dicussed earlier is the essential issue about large strain in a single crystal, directly results from this function  $d\theta/d\gamma = h(\theta)$ . It is a positive function vanishing for  $2\theta = 2\theta_p$ ,  $\pi$  and  $2\pi - 2\theta_p$ with a non-zero derivative. This shows that  $\theta$  is an increasing function of  $\gamma$  which tends to one of the three limit values  $2\theta_p$ ,  $\pi$  and  $2\pi - 2\theta_p$  for infinitely large  $\gamma$ . This behaviour is recapitulated in Fig. 7a.

As described in [8], the shear response,  $\tau(\gamma)$  for instance, results from the composition of two functions. The first function  $\tau(\theta)$  was constructed in Sect 5, Fig. 5, and it describes



FIG. 7. Lattice rotation in simple shear and torsion; a) simple shear, b) simple torsion.

the crystal anisotropy. The second function  $\theta(\gamma)$ , investigated here, is the basic featur of large strain behaviour of a single crystal. The asymptotic behaviour of  $\tau(\gamma)$ , in particular essentially depends on this function. Here the stress tensor **T** like  $\theta$  tends to a fixed value fo large  $\gamma$ .

## 7. Simple torsion

Another similar situation is obtained in simple torsion with controlled  $\gamma = \Gamma t$ :

(7.1) 
$$\mathbf{F} = \begin{bmatrix} e^{\mathbf{e}_1} & e^{\mathbf{e}_1} \gamma & 0\\ 0 & e^{\mathbf{e}_2} & 0\\ 0 & 0 & e^{-(\mathbf{e}_1 + \mathbf{e}_2)} \end{bmatrix}, \quad \mathbf{T} = \begin{bmatrix} 0 & \tau & 0\\ \tau & 0 & 0\\ 0 & 0 & 0 \end{bmatrix}.$$

This is for instance what happens in the torsion of a thin tube [12]. For a single crystal of course, this is a rather academic problem, but it will allow us to investigate anothe situation frequently analyzed in large strain plasticity. The tensors D and W are

(7.2)  
$$D_{11} = \dot{\varepsilon}_1, \quad D_{22} = \dot{\varepsilon}_2, \quad D_{12} = \frac{1}{2} e^{\epsilon_1 - \epsilon_2} \Gamma,$$
$$w = w_{12} = \frac{1}{2} e^{\epsilon_1 - \epsilon_2} \Gamma \quad (\gamma = \Gamma t).$$

The situation in this case is somewhat simpler: starting from the Cauchy stress tensor T the rotated stress  $\overline{T}$  and resolved shear stress  $\sigma^s$  are computed

(7.3)  

$$-T_{11} = T_{22} = \tau \sin 2\theta, \quad T_{12} = \tau \cos 2\theta,$$

$$\sigma^{1} = 2\tau \cos 2\theta/2\sqrt{3},$$

$$\sigma^{2} = \tau (\cos 2\theta + 2\sin 2\theta)/2\sqrt{3},$$

$$\sigma^{3} = \tau (\cos 2\theta - 2\sin 2\theta)/2\sqrt{3},$$

$$\sigma^{4} = \tau (\cos 2\theta - 2\sqrt{2}\sin 2\theta)/2\sqrt{3},$$

$$\sigma^{5} = \tau (\cos 2\theta + 2\sqrt{2}\sin 2\theta)/2\sqrt{3}.$$

For a given  $\theta$  there will usually be one active system corresponding to the maximum absolute value of these 5 quantities. The value of  $\tau$  then follows from setting this value to the critical shear  $\tau_0$ . A direct analysis of this maximum as a function of  $\theta$  leads to Table 4 and the corresponding function  $\tau(\theta)$  is represented in Fig. 8.



Table 4. System activity in torsion.

FIG. 8. Shear stress in torsion.

Knowing the active system, the kinematical analysis directly proceeds from the relations (3.6) and (3.5). Let us, for instance, consider the case  $\dot{\alpha}^1 > 0$  ( $|2\theta| < \pi/2 - 2\theta_p$ ). It then follows from the relations (3.6)

(7.5) 
$$\overline{D}_{11} = \overline{D}_{22} = 0, \quad \overline{D}_{12} = \frac{\dot{\alpha}^1}{2\sqrt{3}}.$$

Coming back to **D** through the lattice rotation  $\theta$  and identifying with the tensors (7.2), there comes

$$D_{12} = \frac{1}{2} e^{\epsilon_1 - \epsilon_2} \Gamma = \frac{\dot{\alpha}^1}{2\sqrt{3}} \cos 2\theta,$$

which gives  $\dot{\alpha}^1$  from the prescribed  $\Gamma$ 

(7.6) 
$$\dot{\alpha}^1 = \frac{\sqrt{3} e^{\epsilon_1 - \epsilon_2} \Gamma}{\cos 2\theta}.$$

The time derivatives  $\dot{\epsilon}_1$ ,  $\dot{\epsilon}_2$  and  $\dot{\theta}$  are then easily obtained from the relations (7.2), (3.6) and (3.5). This provides a nonlinear differential system which, by integration, gives  $\epsilon_1$ ,  $\epsilon_2$  and  $\theta$  as a function of  $\gamma = \Gamma t$ . We shall not develop this further but for the rotation  $\theta$  which is our main interest here.

### 8. Rotation in torsion

We shall now restrict our attention to the evolution equation (3.5) for  $\dot{\theta}$ . Using the tensors (7.2) and the nonactivation of the systems 2 and 3 (Table 4), this gives

(8.1) 
$$\dot{\theta} = \frac{1}{2} e^{\epsilon_1 - \epsilon_2} \Gamma - \frac{1}{4\sqrt{3}} (3\dot{\alpha}^4 + 3\dot{\alpha}^5 - 2\dot{\alpha}^1)$$

while the non-vanishing slip rate is obtained from the tensors (7.2) and (3.6)

(8.2)  
$$\overline{D}_{22} = -\overline{D}_{11} = \frac{1}{\sqrt{6}} (\dot{a}^5 - \dot{a}^4), \quad \overline{D}_{12} = \frac{1}{4\sqrt{3}} (2\dot{a}^1 + \dot{a}^4 + \dot{a}^5),$$
$$D_{12} = \frac{1}{2} e^{\epsilon_1 - \epsilon_2} \Gamma = \overline{D}_{12} \cos 2\theta + \overline{D}_{22} \sin 2\theta.$$

If the active system is the system 1 then, as described above, Eqs. (8.2) give  $\dot{\alpha}^1$  by Eq. (7.6) and  $\dot{\theta}$  is obtained by Eq. (7.5) as

(8.3) 
$$e^{\epsilon_2-\epsilon_1}\Gamma\dot{\theta}=\frac{1}{2}\left(1+\frac{1}{\cos 2\theta}\right), \quad -\frac{\pi}{2}+2\theta_p\leqslant 2\theta\leqslant \frac{\pi}{2}-2\theta_p.$$

Similarly, when the active system is the system 4,

(8.4)  

$$\overline{D}_{22} = -\frac{1}{\sqrt{6}} \dot{\alpha}^{4}, \quad \overline{D}_{12} = \frac{1}{4\sqrt{3}} \dot{\alpha}^{4}, \quad \overline{D}_{12} = \frac{\dot{\alpha}^{4}}{4\sqrt{3}} (\cos 2\theta - 2\sqrt{2} \sin 2\theta), \\
\dot{\alpha}^{4} = \frac{2\sqrt{3}}{\cos 2\theta - 2\sqrt{2}} \frac{e^{\epsilon_{1} - \epsilon_{2}}\Gamma}{\sin 2\theta}, \\
(8.5) \qquad e^{\epsilon_{2} - \epsilon_{1}}\Gamma\dot{\theta} = \frac{1}{2} \left( 1 - \frac{3}{\cos 2\theta - 2\sqrt{2}} \frac{1}{\sin 2\theta} \right)$$

and when the active system is the system 5,

(8.6) 
$$e^{\epsilon_2-\epsilon_1}\Gamma\dot{\theta} = \frac{1}{2}\left(1-\frac{3}{\cos 2\theta+2\sqrt{2}\sin 2\theta}\right).$$

This  $e^{\epsilon_2 - \epsilon_1} I \dot{\theta} = e^{\epsilon_2 - \epsilon_1} d\theta / d\gamma = h(\theta)$  is represented in Fig. 9 and again the evolution of the rotation follows from this function. The situation is, however, more complex that in simple shear, and different situations may be found according to the initial value  $\theta_0$  of  $\theta$ .



FIG. 9. Plastic spin in torsion.

If  $|2\theta_0| < \pi/2 - 2\theta_p$ , then  $d\theta/d\gamma$  is positive and  $2\theta$  increases until it reaches, in a finite time since  $h(\theta) > 1$ , the limit value  $\pi/2 - 2\theta_p$ . Then it can neither decrease because  $d\theta/d\gamma > 0$  for  $2\theta < \pi/2 - 2\theta_p$ , nor increase because  $d\theta/d\gamma < 0$  for  $2\theta > \pi/2 - 2\theta_p$ . It must therefore remain stationary at this value with a double slip situation ( $\dot{\alpha}^1 \ge 0$ ,  $\dot{\alpha}^5 \ge 0$ ). To analyze it further, we start from Eqs. (8.1) and (8.2) written for  $2\theta = \pi/2 - 2\theta_p$  (cos  $2\theta = 2\sqrt{2}/3$ , sin  $2\theta = 1/3$ )

$$\frac{1}{2} e^{e_1 - e_2} \Gamma = \frac{1}{4\sqrt{3}} (2\dot{\alpha}^1 + \dot{\alpha}^5) \frac{2\sqrt{2}}{3} + \frac{\dot{\alpha}^5}{\sqrt{6}} \frac{1}{3} = \frac{2(\dot{\alpha}^1 + \dot{\alpha}^5)}{3\sqrt{6}},$$
$$\dot{\theta} = \frac{2(\dot{\alpha}^1 + \dot{\alpha}^5)}{3\sqrt{6}} - \frac{3\dot{\alpha}^5 - 2\dot{\alpha}^1}{4\sqrt{3}} = 0$$

and the slip rates  $\dot{\alpha}^1$  and  $\dot{\alpha}^5$  are obtained from these two equations

(8.7) 
$$\dot{\alpha}^{1} = \frac{3e^{\epsilon_{1}-\epsilon_{2}}\Gamma}{20\sqrt{2}} (9-4\sqrt{2}), \quad \dot{\alpha}^{5} = \frac{3e^{\epsilon_{1}-\epsilon_{2}}\Gamma}{20\sqrt{2}} (6+4\sqrt{2})$$

If  $\pi/2 - 2\theta_p \leq 2\theta_0 \leq 2\theta_p$ , then  $d\theta/d\gamma$  is negative and  $2\theta$  decreases to the same limiting value  $\pi/2 - 2\theta_p$  and double slip situation (8.7).

If  $2\theta_p \leq 2\theta_0 \leq \pi/2$ , then  $d\theta/d\gamma$  is negative and  $2\theta$  decreases towards the limiting value  $2\theta_p$  where  $d\theta/d\gamma = 0$  and which is reached in an infinite time.

The other cases are analyzed in the same way and the results are summarized in Fig. 7b. The situation is quite different from simple shear, Fig. 7a: the 3 limiting values  $2\theta_p$ ,  $\pi$  and  $2\pi - 2\theta_p$  still exist but their attraction zone is much more limited and they are reached through different asymptotic behaviour ( $\theta - \theta_{\infty} \sim e^{-\kappa t}$  in simple shear, A/t in torsion) and three new limit values  $\pi/2 - 2\theta_p$ ,  $\pi/2 + 2\theta_p$  and  $3\pi/2$  appear which are reached in finite time.

### 9. Conclusion

Our main objective was the evolution of lattice rotation in simple shear or torsion in a single crystal. In the special case investigated, this analysis has been fully completed and the results are summarized in Fig. 7. Different situations may be encountered, according to the initial value  $2\theta_0$  of the lattice orientation, but in any case this lattice rotation always stabilizes to a fixed value resulting in a stabilized behaviour for the crystal. The plastic behaviour, therefore, is entirely different from the viscous one [11] where an ever increasing rotation and oscillatory behaviour was found. Coming back to phenomenological large strain plasticity which was our starting point, this is an indication that in the plastic case the rotating frame must be chosen in such a way that it stabilizes under simple shear.

This analysis was performed in a restricted case: perfect plasticity of a special plane single crystal. Among these restrictions one is not essential: most of the results obtained about the rotation will remain true under reasonable assumptions about hardening. First, in the case of isotropic hardening (the critical shear stress  $\tau_0$  increases but remains the same for all systems, Taylor's assumption), the stress response as described in Figs. 5 or 8 will be modified by a scale factor but nothing will be changed as regards system activity and the resulting lattice rotation.

Under more general hardening conditions (different critical shear stress on the 5 systems) a more refined analysis is required. In simple shear our analysis is purely kinematical except for the construction of the strain rate space (Fig. 3) which directly follows from the plasticity surface (Fig. 2). Changing the critical shear stress  $\tau$  will change the position of the different faces. But as long as this plasticity surface keeps the same topography, the basic diagram in Fig. 3 and the resulting rotation analysis (Figs. 6 and 7a) does not change. Differences will only occur if one of the involved edges, *ED* or *A'B* for instance, disappears, but this will require a very drastic hardening. In torsion the active systems resulting from the relations (7.4) will be changed, but under reasonable hardening this may change the extent of the different regimes in Table 4, but not their nature, so that Fig. 7b will remain qualitatively valid but with modified boundaries.

The other assumptions are more essential. A similar analysis can be performed for a viscoplastic single crystal or for another single crystal; this still remains to be done.

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