number	1	2	3	4	5	6
name	B4	B2	B5	D4	D1	D6
plane	(111)	(111)	(111)	$(1\bar{1}1)$	$(1\bar{1}1)$	$(1\bar{1}1)$
direction	$[\bar{1}01]$	$[0\bar{1}1]$	$[\bar{1}10]$	$[\bar{1}01]$	[011]	[110]
number	7	8	9	10	11	12
name	A2	A6	A3	C5	C3	C1
plane	$(\bar{1}11)$	$(\bar{1}11)$	$(\bar{1}11)$	$(11\bar{1})$	$(11\bar{1})$	$(11\bar{1})$
direction	$[0\bar{1}1]$	[110]	[101]	$[\bar{1}10]$	[101]	[011]

Table 1: List and names of the 12 slip systems of FCC single crystals.

Simple shear of a FCC single crystal

In this problem, we consider the deformation of a FCC single crystal subjected to shear loading conditions in the 1-2 plane represented in figure 1. The orientation of the single crystal with respect to the axes of the coordinate system is characterised by the angle θ, as indicated in the same figure.

The problem of simple shear is addressed within the small strains and small rotations framework in sections 1 and 2. An excursion towards large deformations is made in section 3.

The considered single crystal has the face centered cubic crystallographic structure (FCC). It is characterised by the 12 slip systems of table 1. The plastic behaviour of the crystal is described by the Schmid law. No hardening is considered in this problem.

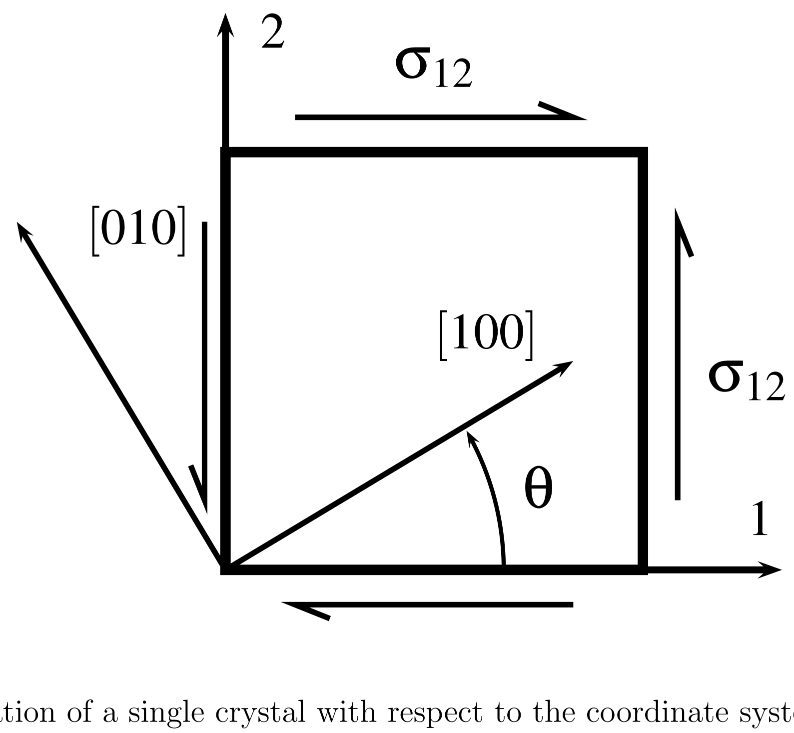

Figure 1: Orientation of a single crystal with respect to the coordinate system of the loading.

1 Ideally oriented single crystal under simple shear

We consider in this section the special configuration $\theta = 0$ where the crystallographic axes [100] and [010] are respectively aligned with the axes 1 and 2 of the coordinate system. The crystal is subjected to homogeneous simple shear conditions

$$[\underset{\sim}{\sigma}] = \begin{bmatrix} 0 & \sigma_{12} & 0 \\ \sigma_{12} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{1}$$

in the coordinate system (1,2), as indicated in figure 1. Equivalently, we can write

$$\underset{\sim}{\sigma} = \sigma_{12}(\underline{\boldsymbol{e}}_1 \otimes \underline{\boldsymbol{e}}_2 + \underline{\boldsymbol{e}}_2 \otimes \underline{\boldsymbol{e}}_1) \tag{2}$$

1.1

Define and compute the Schmid factors for all 12 slip systems under the considered shear loading conditions. For the labelling of slip systems, please use the nomenclature of table 1.
The resolved shear stress on slip system $(\underline{\boldsymbol{\ell}}^s, \underline{\boldsymbol{n}}^s)$ is computed as:

$$\tau^s = \underset{\sim}{\sigma} : (\underline{\boldsymbol{\ell}}^s \otimes \underline{\boldsymbol{n}}^s) = \sigma_{12}((\underline{\boldsymbol{e}}_1 \cdot \underline{\boldsymbol{\ell}}^s)(\underline{\boldsymbol{e}}_2 \cdot \underline{\boldsymbol{n}}^s) + (\underline{\boldsymbol{e}}_2 \cdot \underline{\boldsymbol{\ell}}^s)(\underline{\boldsymbol{e}}_1 \cdot \underline{\boldsymbol{n}}^s)) = \sigma_{12}(l_1^s n_2^s + l_2^s n_1^s) \tag{3}$$

For each slip system a Schmid factor

$$M^s = l_1^s n_2^s + l_2^s n_1^s \tag{4}$$

can therefore be defined. The corresponding values for the 12 slip systems of table 1 are given in the following table:

name	B4	B2	B5	D4	D1	D6	A2	A6	A3	C5	C3	C1
M^s	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{6}}$	0	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	0	$\frac{1}{\sqrt{6}}$	0	$\frac{1}{\sqrt{6}}$	0	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$

1.2

Determine the yield stress σ_{12}^0 corresponding to the activation of the first slip systems, as a function of the critical resolved shear stress τ_c. The latter is assumed to be the same for all 12 slip systems. Give the corresponding numerical value when $\tau_c = 50$ MPa.

How many slip systems are simultaneously activated?

Plastic slip is activated when:

$$\tau^s = |\sigma_{12}|/\sqrt{6} = \tau_c \quad \Rightarrow \quad \sigma_{12}^0 = \sqrt{6}\tau_c \tag{5}$$

The yield stress is reached simultaneously for 8 slip systems.
We find σ_{12}^0 =122 MPa.

1.3

The total strain and rotation is split into elastic and plastic parts:

$$\underset{\sim}{\varepsilon} = \underset{\sim}{\varepsilon}^e + \underset{\sim}{\varepsilon}^p, \quad \underset{\sim}{\omega} = \underset{\sim}{\omega}^e + \underset{\sim}{\omega}^p \tag{6}$$

and the plastic deformation is the result of slip system activity according to

$$\underset{\sim}{\varepsilon}^p + \underset{\sim}{\omega}^p = \sum_{s=1}^{12} \gamma^s \underline{\boldsymbol{\ell}}^s \otimes \underline{\boldsymbol{n}}^s \tag{7}$$

where γ^s is the amount of slip for slip system s.

Give the matrix of $\underset{\sim}{\varepsilon}^p + \underset{\sim}{\omega}^p$ depending on the slip amount γ of the activated slip systems. Give then the plastic strain matrix $\underset{\sim}{\varepsilon}^p$. Assuming that the total strain reached is of the form

$$[\underset{\sim}{\varepsilon}] = \begin{bmatrix} 0 & \varepsilon_{12} & 0 \\ \varepsilon_{12} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{8}$$

give the amount of slip as a function of the total imposed shear strain ε_{12} and the material properties. The elastic behaviour of the crystal is assumed to be isotropic with shear modulus μ.

Does the crystal lattice rotate during such a shear test?

We add the orientation matrices of the 8 activated slip systems taking care of the sign of the resolved shear stress in each case:

$$\begin{aligned} &- \begin{bmatrix} \bar{1} & \bar{1} & \bar{1} \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 \\ \bar{1} & \bar{1} & \bar{1} \\ 1 & 1 & 1 \end{bmatrix} + \begin{bmatrix} \bar{1} & 1 & \bar{1} \\ 0 & 0 & 0 \\ 1 & \bar{1} & 1 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 1 & \bar{1} & 1 \\ 1 & \bar{1} & 1 \end{bmatrix} \\ &+ \begin{bmatrix} 0 & 0 & 0 \\ 1 & \bar{1} & \bar{1} \\ \bar{1} & 1 & 1 \end{bmatrix} + \begin{bmatrix} \bar{1} & 1 & 1 \\ 0 & 0 & 0 \\ \bar{1} & 1 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 1 & \bar{1} \\ 0 & 0 & 0 \\ 1 & 1 & \bar{1} \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 1 & 1 & \bar{1} \\ 1 & 1 & \bar{1} \end{bmatrix} \end{aligned} \tag{9}$$

The plastic strain tensor therefore is

$$[\underset{\sim}{\varepsilon}^p] = \frac{\gamma}{\sqrt{6}} \begin{bmatrix} 0 & 4 & 0 \\ 4 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{10}$$

The elastic strain tensor is:

$$[\underset{\sim}{\varepsilon}^e] = \begin{bmatrix} 0 & \sigma_{12}/2\mu & 0 \\ \sigma_{12}/2\mu & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{11}$$

Noting that $\sigma_{12} = \sqrt{6}\tau_c$, it follows that

$$\varepsilon_{12} = \frac{4\gamma}{\sqrt{6}} + \frac{\sqrt{6}\tau_c}{2\mu} \quad \Longrightarrow \gamma = \frac{\sqrt{6}}{4}\varepsilon_{12} - \frac{3\tau_c}{4\mu} \tag{12}$$

From (9), we find that $\underset{\sim}{\omega}^p = 0$. The lattice rotation is therefore equal to the material rotation, $\underset{\sim}{\omega} = 0$.

2 Inclined single crystal under shear

The initial orientation of the crystal is now considered as $\theta \neq 0$ according to figure 1. The question of plastic slip activity under simple shear is reconsidered in this case.

2.1

The applied stress tensor is still of the form given by equation (1).
Provide the matrix of the components of the stress tensor in the crystal coordinate system.
We have

$$\underline{e}_1 = \cos\theta\,[100] - \sin\theta\,[010], \quad \underline{e}_2 = \sin\theta\,[100] + \cos\theta\,[010] \tag{13}$$

so that the components of the stress tensor in the lattice based coordinate system is

$$\sigma_{12}\,[\underline{e}_1 \otimes \underline{e}_2 + \underline{e}_2 \otimes \underline{e}_1] = \sigma_{12} \begin{bmatrix} \sin 2\theta & \cos 2\theta & 0 \\ \cos 2\theta & -\sin 2\theta & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{14}$$

2.2

Give the 12 Schmid factors for the previous loading condition.

Discuss the number of simultaneously activated slip systems depending on the angle θ.

Double contracting the matrix (1) with the twelve orientation tensors $\underline{\ell}^s \otimes \underline{n}^s$ of table 1 yields the following list of Schmid factors:

B4	B2	B5	D4
$-(\sin 2\theta + \cos 2\theta)/\sqrt{6}$	$(\sin 2\theta - \cos 2\theta)/\sqrt{6}$	$-2\sin 2\theta/\sqrt{6}$	$(\cos 2\theta - \sin 2\theta)/\sqrt{6}$
D1	D6	A2	A6
$(\sin 2\theta + \cos 2\theta)/\sqrt{6}$	$2\sin 2\theta/\sqrt{6}$	$(\sin 2\theta + \cos 2\theta)/\sqrt{6}$	$-2\sin 2\theta/\sqrt{6}$
A3	C5	C3	C1
$(\cos 2\theta - \sin 2\theta)/\sqrt{6}$	$-2\sin 2\theta/\sqrt{6}$	$(\cos 2\theta + \sin 2\theta)/\sqrt{6}$	$(\cos 2\theta - \sin 2\theta)/\sqrt{6}$

Only three functions of θ arise in the previous list, each associated with 4 slip systems:

$$f_1(\theta) = |\sin 2\theta - \cos 2\theta|/\sqrt{6}, \quad f_2(\theta) = |\sin 2\theta + \cos 2\theta|/\sqrt{6}, \quad f_3(\theta) = 2|\sin 2\theta|/\sqrt{6} \tag{15}$$

They are plotted on figure 2. The maximum of these functions is also plotted showing that generally 4 slip systems are simultaneously activated except at the intersections of two upper curves where 8 systems are activated.

3 Large elastic deformations of a single crystal under simple glide

In this section, we consider the single glide test characterised by the following form of the deformation gradient:

$$[\underset{\sim}{F}] = \begin{bmatrix} 1 & \Gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{16}$$

where $\Gamma(t)$ is the prescribed time–dependent glide. In this section, we work within the large deformation framework.

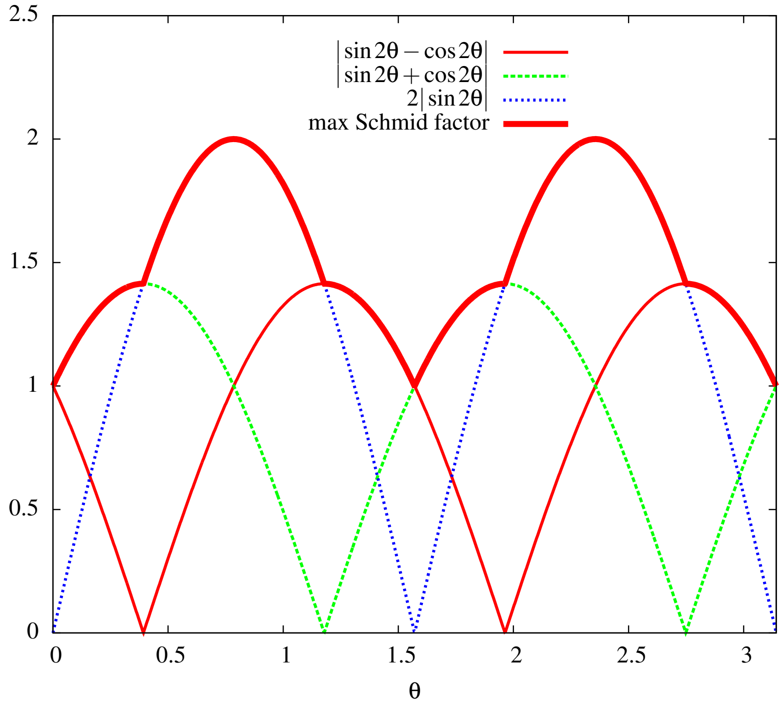

Figure 2: Schmid factors for the simple shear of a single crystal as a function of the θ orientation angle.

3.1 Velocity gradient

Compute the velocity gradient $\underset{\sim}{\boldsymbol{L}} = \dot{\underset{\sim}{\boldsymbol{F}}} \cdot \underset{\sim}{\boldsymbol{F}}^{-1}$, the strain rate tensor $\underset{\sim}{\boldsymbol{D}}$ and the spin tensor $\underset{\sim}{\boldsymbol{W}}$.

We find,

$$[\underset{\sim}{\boldsymbol{F}}^{-1}] = \begin{bmatrix} 1 & -\Gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad [\dot{\underset{\sim}{\boldsymbol{F}}}] = \begin{bmatrix} 0 & \dot{\Gamma} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad [\underset{\sim}{\boldsymbol{L}}] = \begin{bmatrix} 0 & \dot{\Gamma} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{17}$$

$$[\underset{\sim}{\boldsymbol{D}}] = \begin{bmatrix} 0 & \dot{\Gamma}/2 & 0 \\ \dot{\Gamma}/2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad [\underset{\sim}{\boldsymbol{W}}] = \begin{bmatrix} 0 & \dot{\Gamma}/2 & 0 \\ -\dot{\Gamma}/2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{18}$$

3.2 Elastic response

The material is assumed to behave purely elastically with the following isotropic constitutive law:

$$\underset{\sim}{\boldsymbol{\Pi}} = \lambda \mathrm{trace}\,(\underset{\sim}{\boldsymbol{E}}^{GL})\underset{\sim}{\boldsymbol{1}} + 2\mu \underset{\sim}{\boldsymbol{E}}^{GL} \tag{19}$$

where λ, μ are elastic moduli, $\underset{\sim}{\boldsymbol{\Pi}}$ is the Piola stress tensor defined as

$$\underset{\sim}{\boldsymbol{\Pi}} = J \underset{\sim}{\boldsymbol{F}}^{-1} \cdot \underset{\sim}{\boldsymbol{\sigma}} \cdot \underset{\sim}{\boldsymbol{F}}^{-T} \tag{20}$$

and $\underset{\sim}{\boldsymbol{E}}^{GL}$ is the Green-Lagrange strain tensor:

$$\underset{\sim}{\boldsymbol{E}}^{GL} = \frac{1}{2}(\underset{\sim}{\boldsymbol{F}}^{T} \cdot \underset{\sim}{\boldsymbol{F}} - \underset{\sim}{\boldsymbol{1}}) \tag{21}$$

Compute analytically the components of the Cauchy stress tensor, $\underset{\sim}{\boldsymbol{\sigma}}$ as functions of Γ.
Comment on the various active stress components.
Discuss the differences between simple shear and simple glide.
We compute successively,

$$[\underset{\sim}{\boldsymbol{C}}] = \begin{bmatrix} 1 & \Gamma & 0 \\ \Gamma & 1+\Gamma^2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad [\underset{\sim}{\boldsymbol{E}}^{GL}] = \begin{bmatrix} 0 & \Gamma/2 & 0 \\ \Gamma/2 & \Gamma^2/2 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{22}$$

$$[\underset{\sim}{\boldsymbol{\Pi}}] = \begin{bmatrix} \lambda\Gamma^2/2 & \mu\Gamma & 0 \\ \mu\Gamma & (\lambda/2+\mu)\Gamma^2 & 0 \\ 0 & 0 & \lambda\Gamma^2/2 \end{bmatrix} \tag{23}$$

$$[\underset{\sim}{\boldsymbol{\sigma}}] = \left[\frac{1}{J}\underset{\sim}{\boldsymbol{F}}\cdot\underset{\sim}{\boldsymbol{\Pi}}\cdot\underset{\sim}{\boldsymbol{F}}^T\right] = \begin{bmatrix} \lambda\Gamma^2/2 + 2\mu\Gamma^2 + (\lambda/2+\mu)\Gamma^4 & \mu\Gamma + (\lambda/2+\mu)\Gamma^3 & 0 \\ \mu\Gamma + (\lambda/2+\mu)\Gamma^3 & (\lambda/2+\mu)\Gamma^2 & 0 \\ 0 & 0 & \lambda\Gamma^2/2 \end{bmatrix} \tag{24}$$

The linearisation of the previous expression with respect to Γ provides the usual small strain result:

$$[\underset{\sim}{\boldsymbol{\sigma}}] = \begin{bmatrix} 0 & \mu\Gamma & 0 \\ \mu\Gamma & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{25}$$

In the general case, the result shows that simple glide is different from simple shear since the components $\sigma_{11}, \sigma_{22}, \sigma_{33}$ do not vanish, even though they are small at the beginning.