FACULTÉ DES SCIENCES ET TECHNOLOGIES
Département Physique

Université de Lille

# Imperfections – deformation and microstructures in polycrystals

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# 5- Elementary mechanisms

# Objectives

How do textures develop in a polycrystal?

- Plasticity in a single crystal
  - Slip systems
  - Schmid law
  - Critical Resolved Shear Stress (CRSS)
  - Crystal rotation
- Examples on fcc metals
- Von Mises compatibility criterion
- Other orientation mechanisms

# Random questions

What is a mrd?

What is an ODF?

What is the ODF value for a random polycrystal?

What is the ODF value for a textured polycrystal?

What is the ODF value for a single-crystal?

What is the texture index? What is its value for random polycrystal, a textured polycrystal, a single-crystal?

Can you see the full texture on a pole figure?

When shall you use inverse pole figures?

# 5- Elementary mechanisms
## *a*- Slip systems



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Based on experiments

- At ambient T, most of plastic deformation is accommodated through dislocation movements
- Slip always
  - Occurs on a particular set of crystallographic planes, known as *slip planes*,
  - Takes place along a consistent set of directions within these planes – these are called *slip directions*.
- The crystal structure is not altered by plastic deformation.
- Plastic deformation always occurs at constant volume.

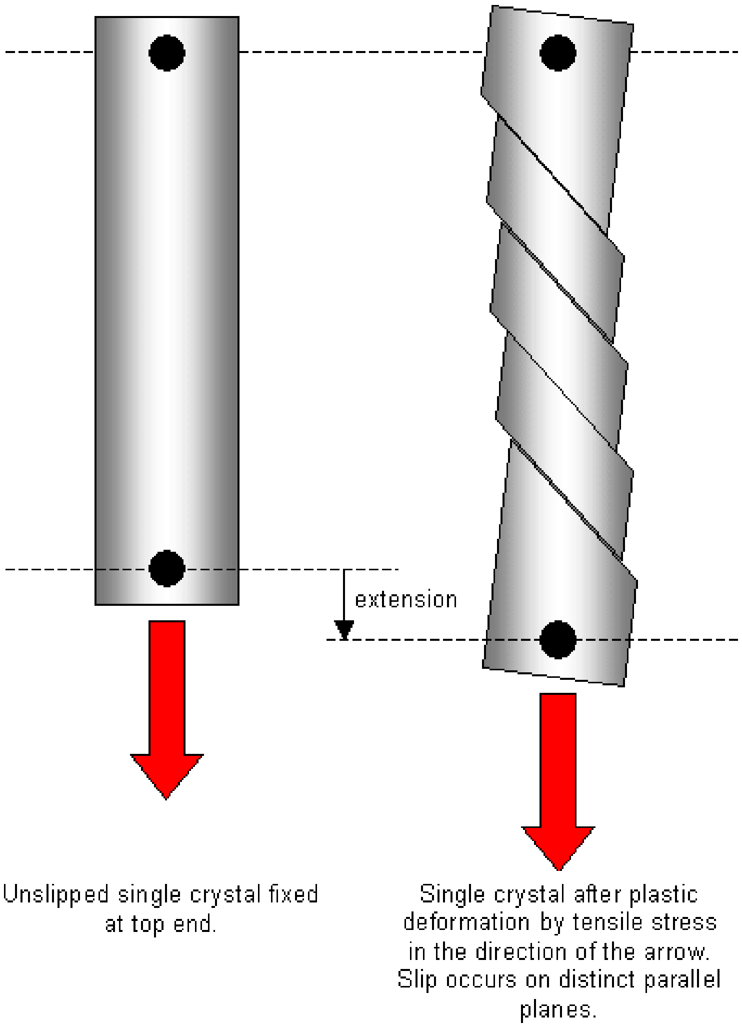
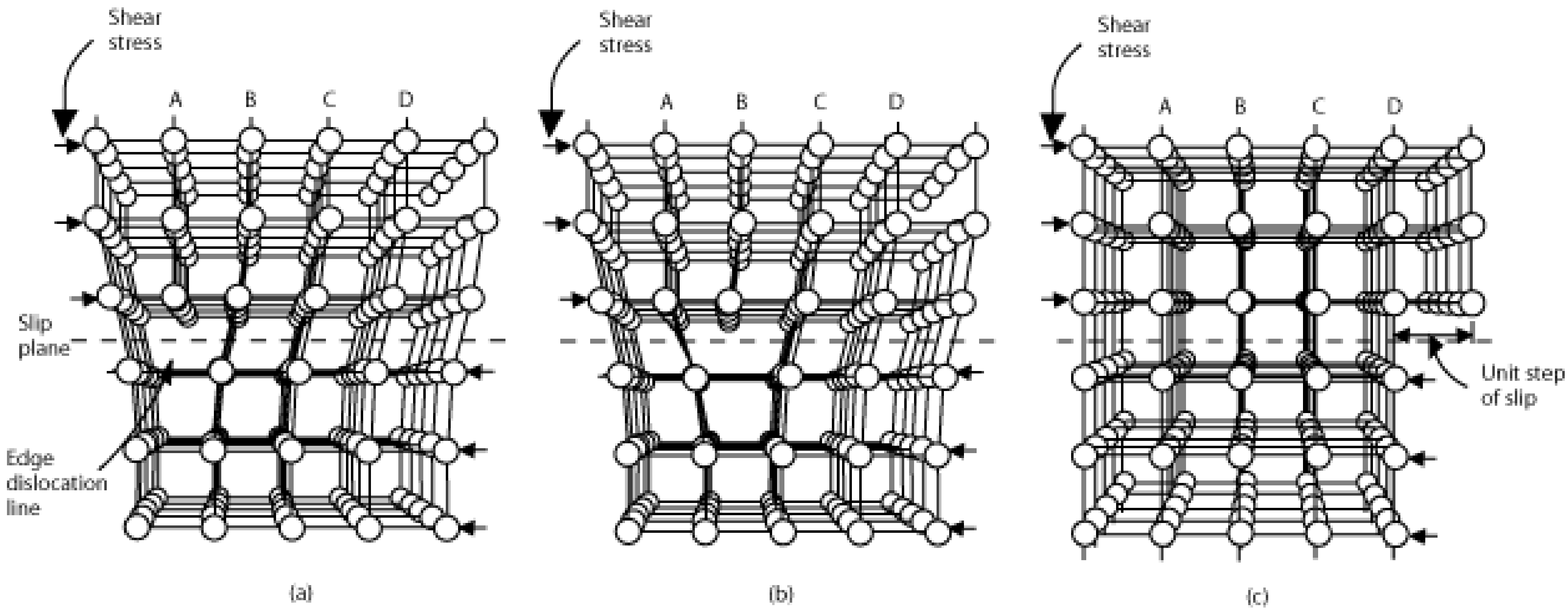



Illustration: © DoITPoMS, University of Cambridge

# Effect of slip

Dislocation movement:

- One half of the crystal moves relative to the other half
- Movement in *shear*, that give rise to *deformation in shear*.



# Resolved stress

- Effect of geometry on slip
- Resolved stress: applied force, projected in the direction of slip, divided by the surface of application
- Applied force, projected in the direction of slip

  $F \cos \lambda$
- Surface of application

  $A / \cos \Phi$
- Resolved stress

  $\tau = F \cos \lambda / (A / \cos \Phi)$

  $\tau = \sigma \cos \lambda \cos \Phi$

  $\tau = \sigma m$ ;
- $m = \cos \lambda \cos \Phi$ is called the Schmid factor

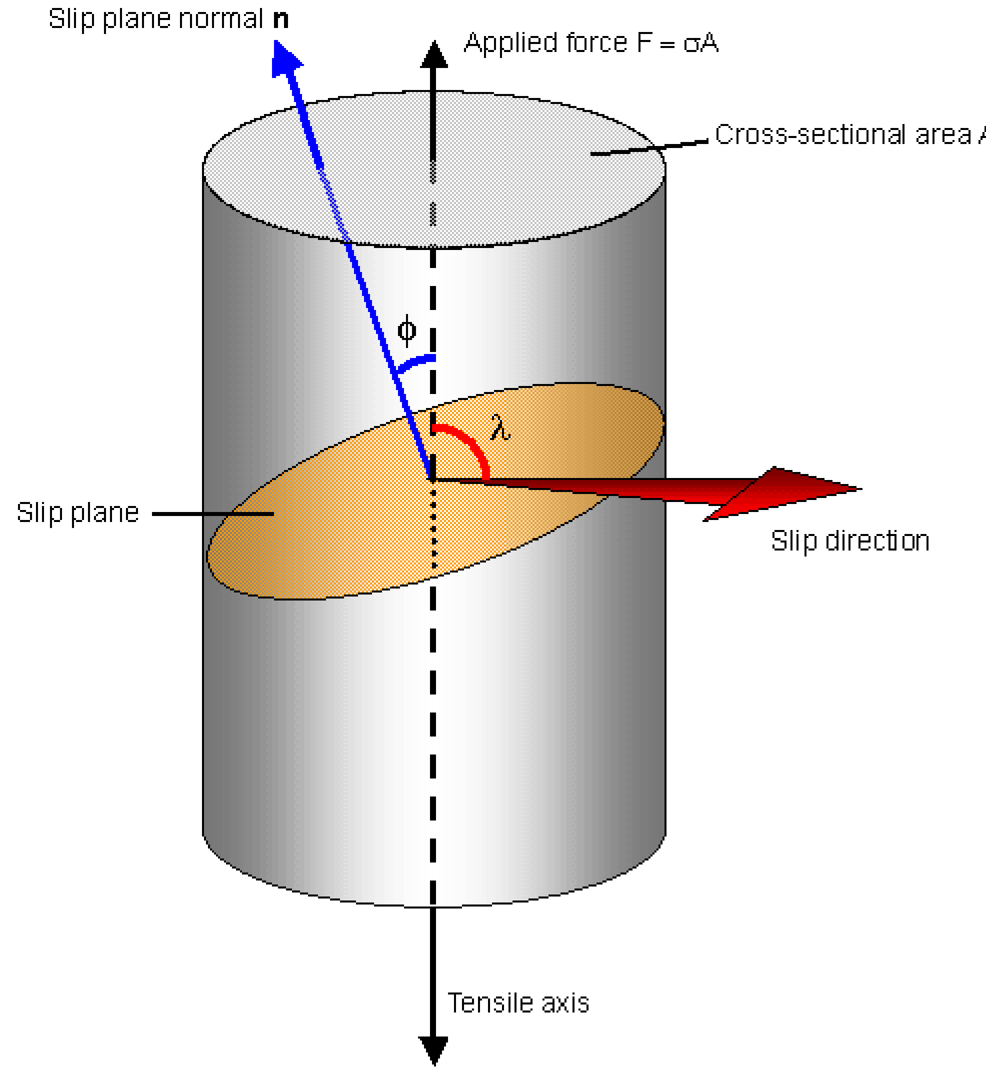



Illustration: © DoITPoMS, University of Cambridge

# Schmid law

Schmid law:

- In a single crystal, the flow stress depends on the orientation of the crystal relative to the deformation direction
- Plastic flow begins when the resolved stress on a given slip system reaches a threshold.
- This threshold stress is independent of other stresses applied on the slip plane.
- It is called the "*Critical Resolved Shear Stress*" : the *CRSS*.

E. Schmid & W. Boas (1950), *Plasticity of Crystals*, Hughes & Co., London

# CRSS: illustration

Slip system with

- CRSS of 1 GPa ($\tau_c$ = 1 GPa)
- $\lambda$ = 60°, $\Phi$ = 45°

Schmid factor

- $m = \cos\lambda \cos\Phi = \sqrt{2}/4 \simeq$ 0?35

Resolved stress

- $\tau = \sigma\, m$

CRSS

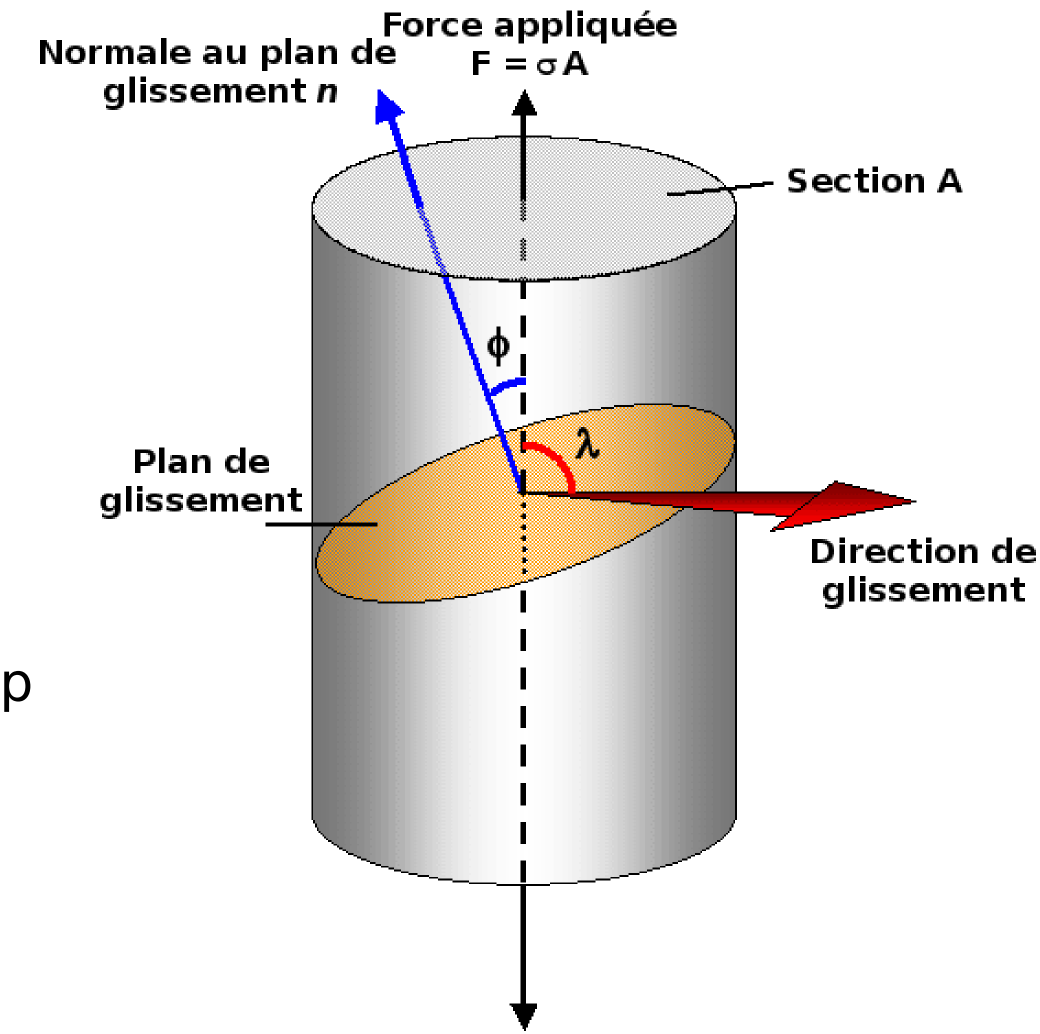
- $\tau < \tau_c$: no slip,
- $\tau = \tau_c$: slip system activated,
- $\tau > \tau_c$: should not happen, the slip system is activated when $\tau = \tau_c$.

Applied stress to get slip

- $\sigma = \tau_c / m$

Stress to be applied to have slip

- $\sigma \simeq 1/0.35 \simeq 2.86$ GPa



# Induced rotation: tension

The slip direction rotates towards the tension direction.

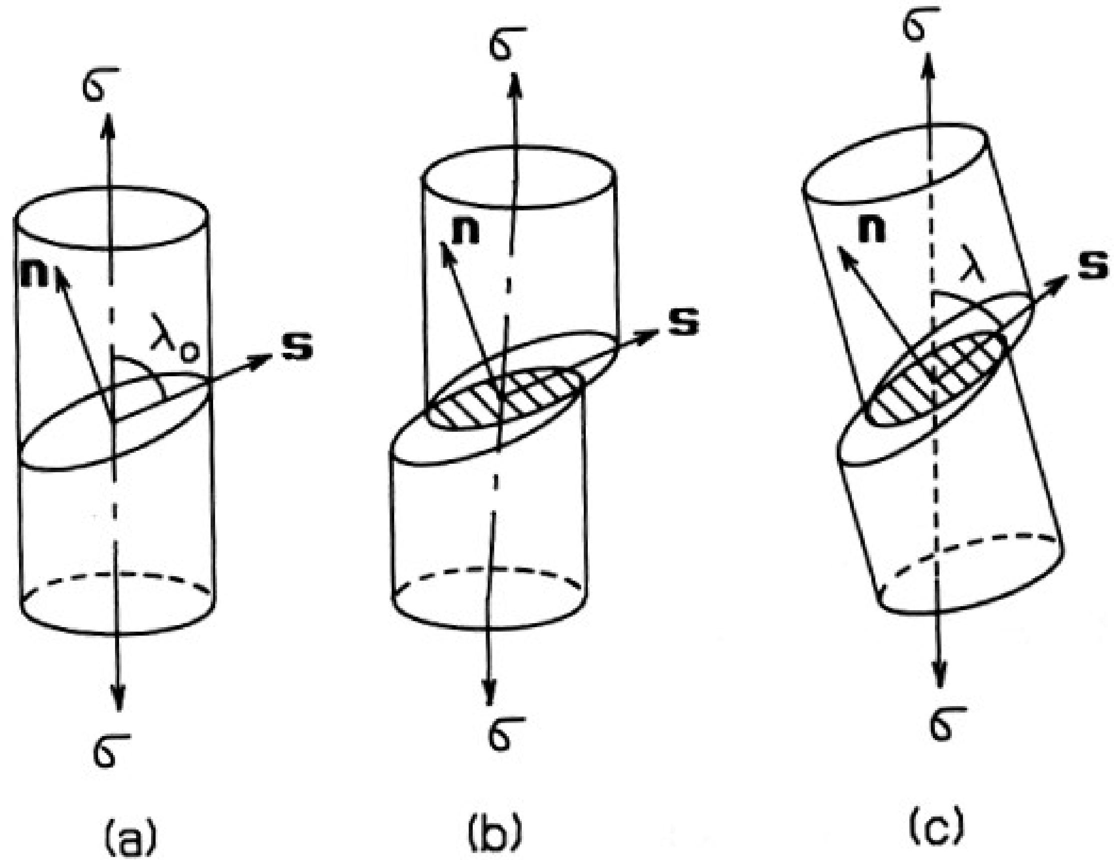



**Fig. 10.5** Rotation of crystal lattice in tension

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# Induced rotation: compression

The slip plane becomes orthogonal to the compression direction.

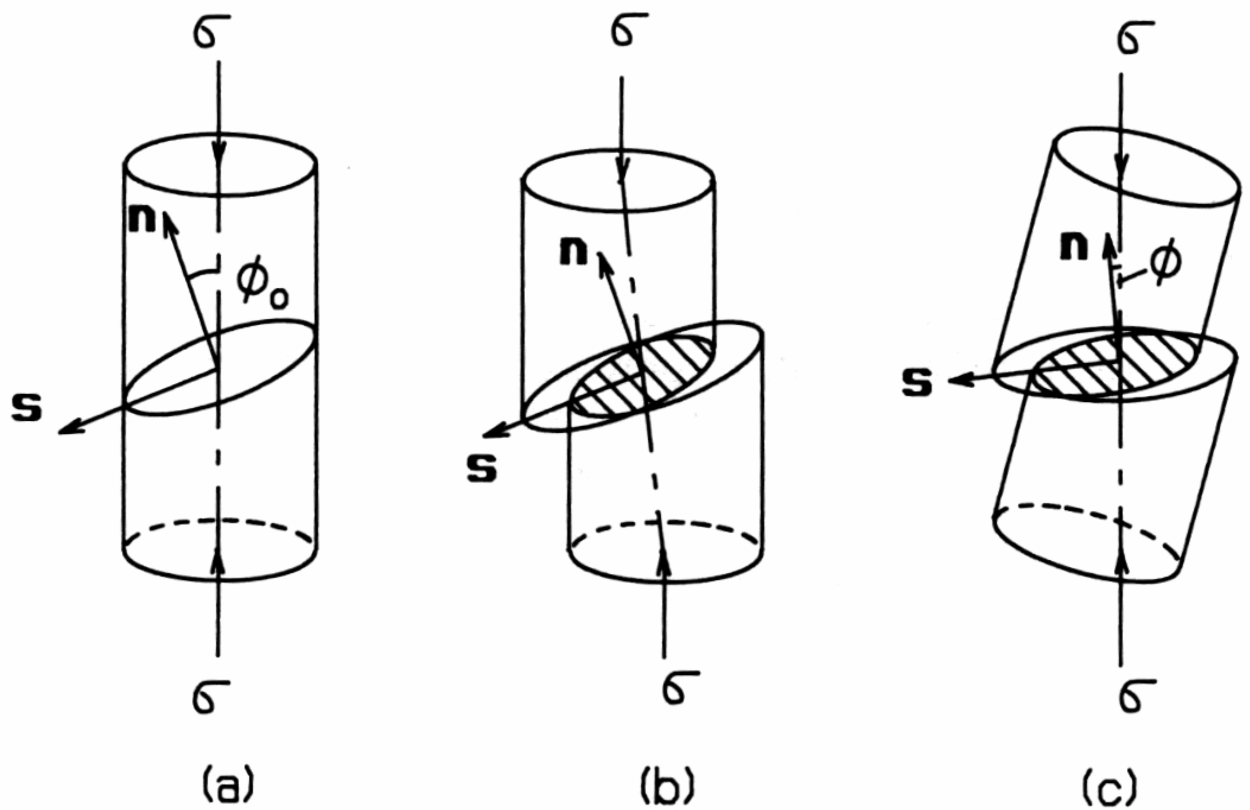


**Fig. 10.6** Rotation of crystal lattice in compression



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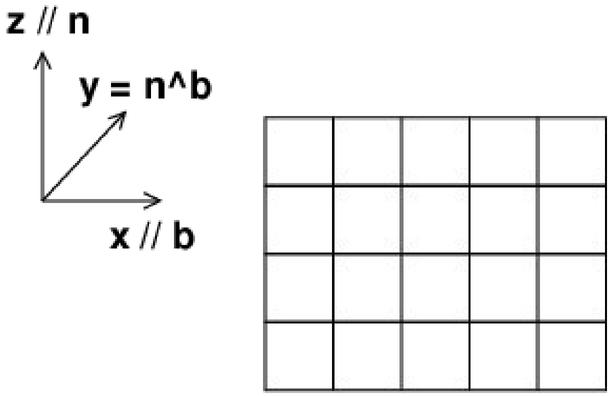
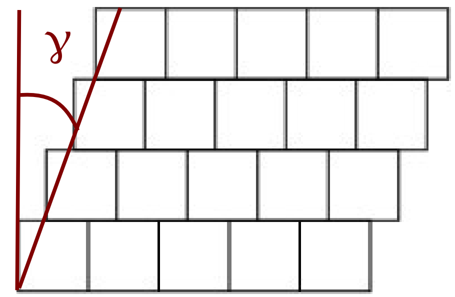



Slip // ***b***, in the plane normal to ***n***




Deformation

$$\overrightarrow{du}(x,y,z) = \begin{cases} \gamma z \\ 0 \\ 0 \end{cases}$$

Deformation gradient

$$F_{ij} = \frac{\partial du_i}{\partial x_j}$$

$$F = \begin{bmatrix} 0 & 0 & \gamma \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Kinematic analysis $F = \epsilon + \omega$

$$\epsilon = \begin{bmatrix} 0 & 0 & \gamma/2 \\ 0 & 0 & 0 \\ \gamma/2 & 0 & 0 \end{bmatrix}$$

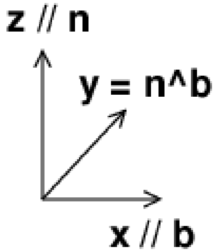
Shear

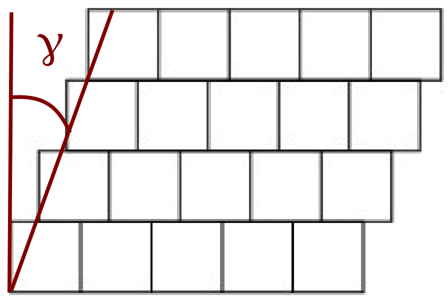
- Trace = 0
- No volume change

$$\omega = \begin{bmatrix} 0 & 0 & \gamma/2 \\ 0 & 0 & 0 \\ -\gamma/2 & 0 & 0 \end{bmatrix}$$

Rotation due to slip

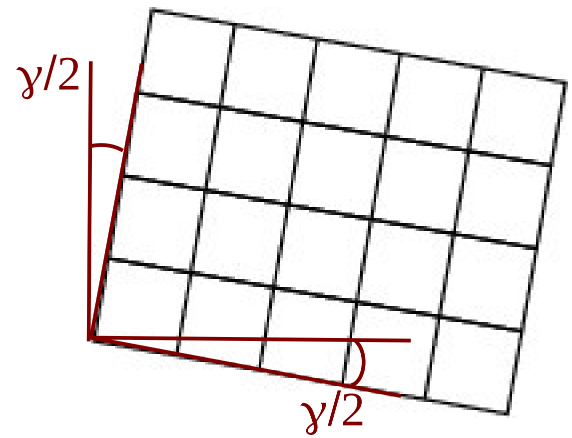
# Geometric interpretation



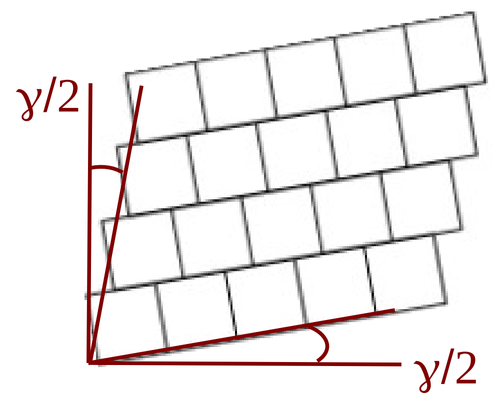

$$F = \begin{bmatrix} 0 & 0 & \gamma \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

=




$$\omega = \begin{bmatrix} 0 & 0 & \gamma/2 \\ 0 & 0 & 0 \\ -\gamma/2 & 0 & 0 \end{bmatrix}$$

+




$$\epsilon = \begin{bmatrix} 0 & 0 & \gamma/2 \\ 0 & 0 & 0 \\ \gamma/2 & 0 & 0 \end{bmatrix}$$

# General setting

- Slip system with, ***b***, burgers vector or slip direction, ***n*** normal to slip plane
- Homogeneous deformation (many dislocations uniformly distributed in the slip plane)
- Total macroscopique deformation: $\gamma$

Movement

$$\mathbf{u}(x, y, z) = \gamma\,(\mathbf{r}\cdot\mathbf{n})\,\mathbf{l}$$

$$\mathbf{l} = \mathbf{b}/\|\mathbf{b}\|$$

$$\mathbf{r} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Infinitesimal deformation

$$\epsilon_{ij} = \frac{1}{2}\gamma\,(n_j l_i + n_i l_j)$$

Infinitesimal rotation

$$\omega_{ij} = \frac{1}{2}\gamma\,(n_j l_i - n_i l_j)$$

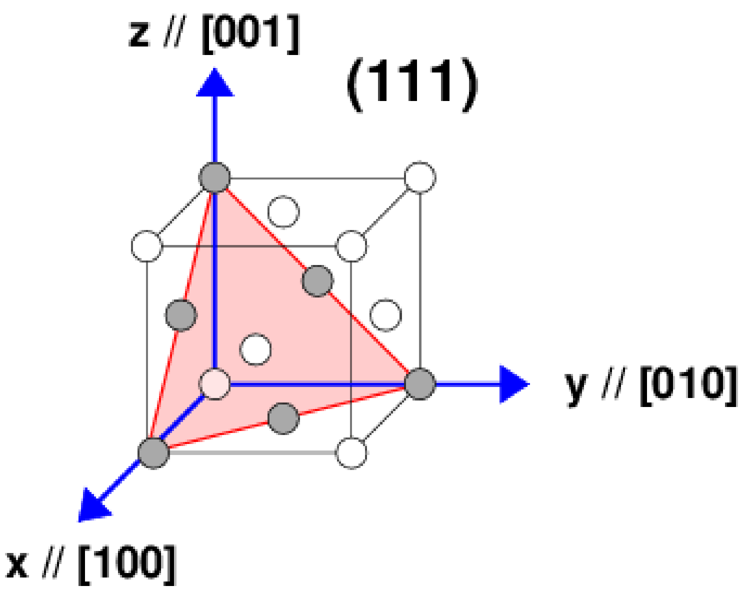
# 5- Elementary mechanisms
# *b*- Face-centered-cubic metals

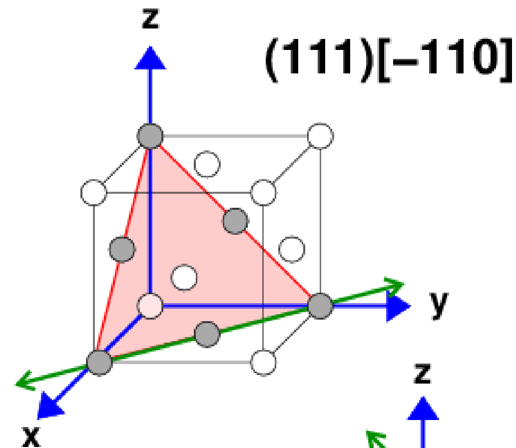
# Fcc – slip systems

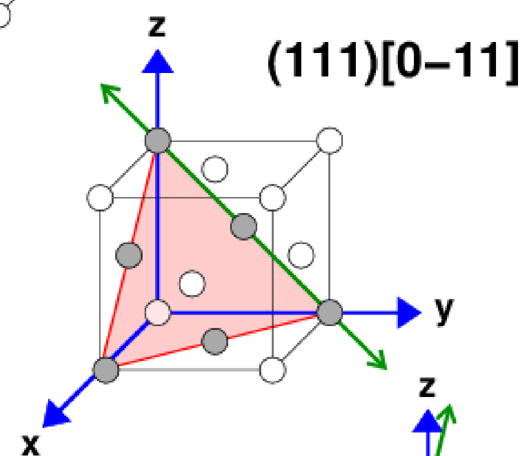
Slip systems in the fcc structure:

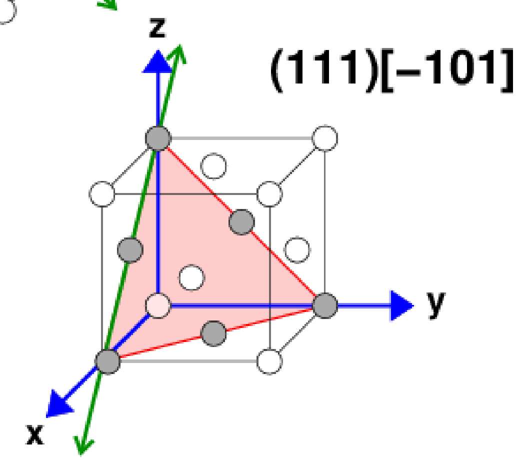
- Slip direction: <110>
- Slip plane: {111}

Slip system: (111)[-110]



# Fcc – slip systems

- 4 {111} planes: (111), $(\bar{1}11)$, $(1\bar{1}1)$, $(11\bar{1})$ ;
- For each: 3 directions <110> ;
- 12 slip systems, each can operate in 2 directions (+ ou -).

| Number | a1 | a2 | a3 | b1 | b2 | b3 |
|---|---|---|---|---|---|---|
| Plane | (111) | (111) | (111) | $(\overline{11}1)$ | $(\overline{11}1)$ | $(\overline{11}1)$ |
| Direction | $[0\bar{1}1]$ | $[10\bar{1}]$ | $[\bar{1}10]$ | [011] | [101] | $[1\bar{1}0]$ |

| Number | c1 | c2 | c3 | d1 | d2 | d3 |
|---|---|---|---|---|---|---|
| Plane | $(\bar{1}11)$ | $(\bar{1}11)$ | $(\bar{1}11)$ | $(1\bar{1}1)$ | $(1\bar{1}1)$ | $(1\bar{1}1)$ |
| Direction | $[0\bar{1}1]$ | $[\bar{1}0\bar{1}]$ | [110] | [011] | $[10\bar{1}]$ | $[\overline{11}0]$ |

# Practice 1

Let's consider a fcc crystal with stress applied parallel to [001]:

- Evaluate the Schmid factor for all 12 slip systems,
- How many will be activated?

| Number | a1 | a2 | a3 | b1 | b2 | b3 |
|---|---|---|---|---|---|---|
| Plane | (111) | (111) | (111) | $(\bar{1}\bar{1}1)$ | $(\bar{1}\bar{1}1)$ | $(\bar{1}\bar{1}1)$ |
| Direction | $[0\bar{1}1]$ | $[10\bar{1}]$ | $[\bar{1}10]$ | [011] | [101] | $[1\bar{1}0]$ |

a1 system

- Stress direction: $\boldsymbol{s}$ = (0;0;1)
- Slip direction: $\boldsymbol{l}$ = 1/√2 (0;-1;1)
- Normal to slip plane: $\boldsymbol{n}$ = 1/√3 (1;1;1)
- Schmid factor: m = cos λ cos Φ
- m = $\boldsymbol{s}\cdot\boldsymbol{l}\ \boldsymbol{s}\cdot\boldsymbol{n}$
- m = 1/√6

Let's consider a fcc crystal with stress applied parallel to [001]:

- Evaluate the Schmid factor for all 12 slip systems,
- How many will be activated?

| Number | a1 | a2 | a3 | b1 | b2 | b3 |
|---|---|---|---|---|---|---|
| Plane | $(111)$ | $(111)$ | $(111)$ | $(\bar{1}\bar{1}1)$ | $(\bar{1}\bar{1}1)$ | $(\bar{1}\bar{1}1)$ |
| Direction | $[0\bar{1}1]$ | $[10\bar{1}]$ | $[\bar{1}10]$ | $[011]$ | $[101]$ | $[1\bar{1}0]$ |
| Schmid F. | $1/\sqrt{6}$ | $-1/\sqrt{6}$ | 0 | $1/\sqrt{6}$ | $1/\sqrt{6}$ | 0 |

| Number | c1 | c2 | c3 | d1 | d2 | d3 |
|---|---|---|---|---|---|---|
| Plane | $(\bar{1}11)$ | $(\bar{1}11)$ | $(\bar{1}11)$ | $(1\bar{1}1)$ | $(1\bar{1}1)$ | $(1\bar{1}1)$ |
| Direction | $[0\bar{1}1]$ | $[\bar{1}0\bar{1}]$ | $[110]$ | $[011]$ | $[10\bar{1}]$ | $[\bar{1}\bar{1}0]$ |
| Schmid F. | $1/\sqrt{6}$ | $-1/\sqrt{6}$ | 0 | $1/\sqrt{6}$ | $-1/\sqrt{6}$ | 0 |

8 systems activated



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# Practice 2

Let's consider a fcc crystal with stress applied parallel to [011]:

- Same questions…

| Number | a1 | a2 | a3 | b1 | b2 | b3 |
|---|---|---|---|---|---|---|
| Plane | (111) | (111) | (111) | $(\bar{1}\bar{1}1)$ | $(\bar{1}\bar{1}1)$ | $(\bar{1}\bar{1}1)$ |
| Direction | $[0\bar{1}1]$ | $[10\bar{1}]$ | $[\bar{1}10]$ | [011] | [101] | $[1\bar{1}0]$ |

| Number | c1 | c2 | c3 | d1 | d2 | d3 |
|---|---|---|---|---|---|---|
| Plane | $(\bar{1}11)$ | $(\bar{1}11)$ | $(\bar{1}11)$ | $(1\bar{1}1)$ | $(1\bar{1}1)$ | $(1\bar{1}1)$ |
| Direction | $[0\bar{1}1]$ | $[\bar{1}0\bar{1}]$ | [110] | [011] | $[10\bar{1}]$ | $[\bar{1}\bar{1}0]$ |

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Let's consider a fcc crystal with stress applied parallel to [011]:

- Same questions…

| Number | a1 | a2 | a3 | b1 | b2 | b3 |
|---|---|---|---|---|---|---|
| Plane | (111) | (111) | (111) | $(\overline{11}1)$ | $(\overline{11}1)$ | $(\overline{11}1)$ |
| Direction | $[0\bar{1}1]$ | $[10\bar{1}]$ | $[\bar{1}10]$ | [011] | [101] | $[1\bar{1}0]$ |
| Schmid F. | 0 | $-1/\sqrt{6}$ | $1/\sqrt{6}$ | 0 | 0 | 0 |

| Number | c1 | c2 | c3 | d1 | d2 | d3 |
|---|---|---|---|---|---|---|
| Plane | $(\bar{1}11)$ | $(\bar{1}11)$ | $(\bar{1}11)$ | $(1\bar{1}1)$ | $(1\bar{1}1)$ | $(1\bar{1}1)$ |
| Direction | $[0\bar{1}1]$ | $[\bar{1}0\bar{1}]$ | [110] | [011] | $[10\bar{1}]$ | $[\overline{11}0]$ |
| Schmid F. | 0 | $-1/\sqrt{6}$ | $1/\sqrt{6}$ | 0 | 0 | 0 |

4 systems activated

# Choice of slip system for fcc metals
# Graphical representation

Active slip system in fcc, as a function of the direction of applied stress

– signs above slip system numbers:
→ opposite direction relative to that of the table
→ for instance [-1-10] instead of [110].

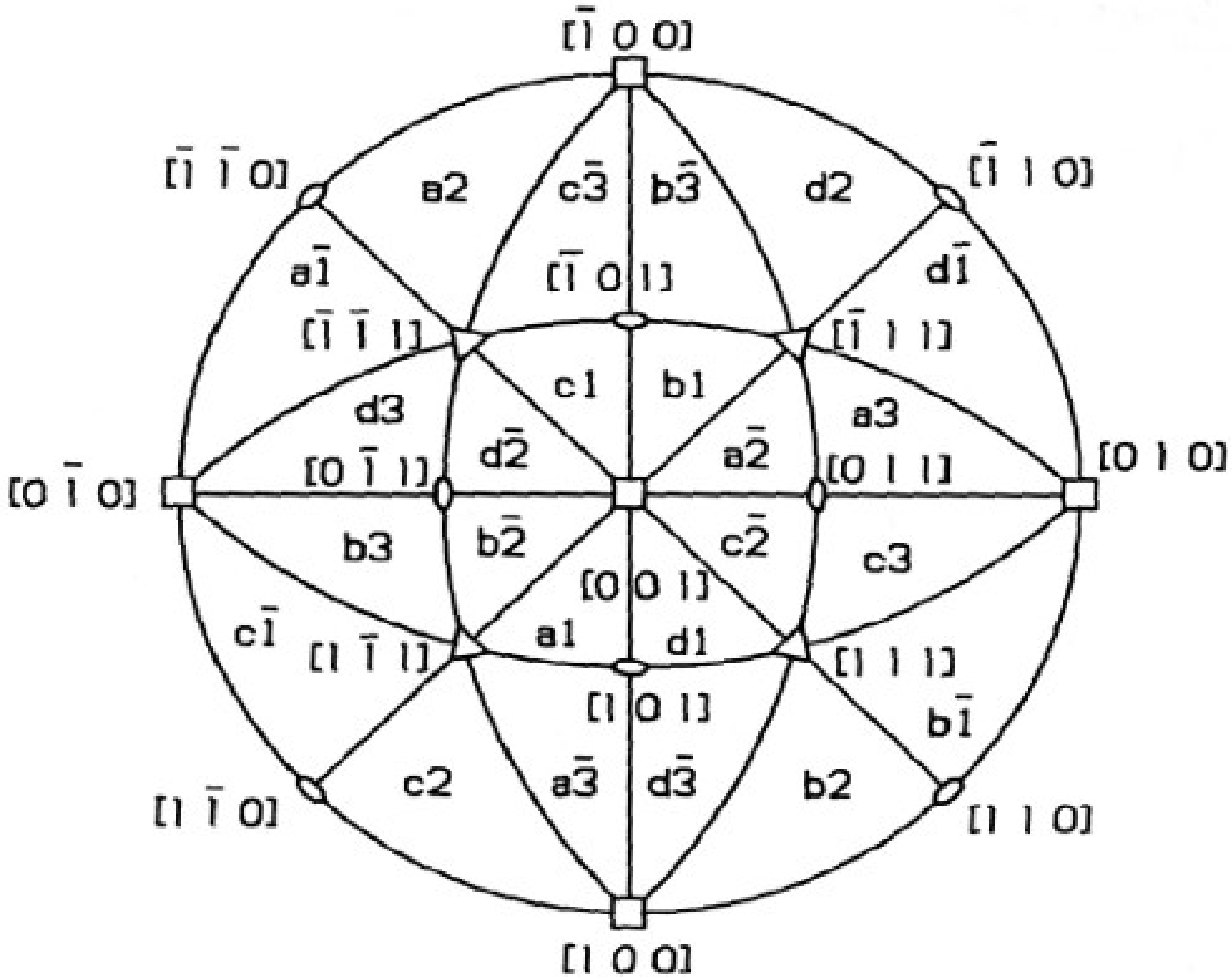



*Image A. Rollett, after Kahn*

# More complex cases

For fcc metals, there is only one type of slip systems → the CRSS is not needed to evaluate with slip plane and directions are activated first.

In other systems, you may have different types of slip systems, with different CRSS. Then, you have to look at the resolved shear stress on all slip systems and see which one is closest to the CRSS.

Sometimes, “secondary slip systems” can be activated. Their CRSS is higher, the resolved shear stress is higher, but these systems are required for plastic deformation to work → *von Mises compatibility criterion* (later in the course)

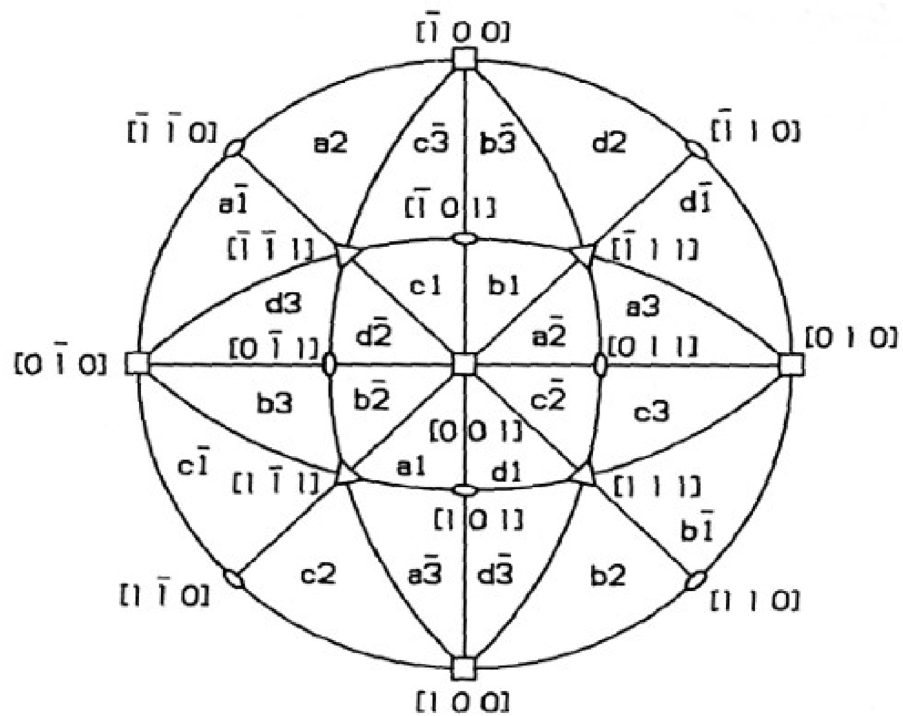
# Practice

Consider a fcc crystal with applied stress parallel to [102]:

- Identify the activated slip systems,
- For each, establish the expression of the rotation tensor,
- Assume that deformation is evenly distributed between all active slip systems and evaluate to complete rotation tensor,
- Describe the effect of the rotation on the crystal

| a1 | a2 | a3 | b1 | b2 | b3 |
|---|---|---|---|---|---|
| (111) | (111) | (111) | $(\bar{1}\bar{1}1)$ | $(\bar{1}\bar{1}1)$ | $(\bar{1}\bar{1}1)$ |
| $[0\bar{1}1]$ | $[10\bar{1}]$ | $[\bar{1}10]$ | [011] | [101] | $[1\bar{1}0]$ |

| c1 | c2 | c3 | d1 | d2 | d3 |
|---|---|---|---|---|---|
| $(\bar{1}11)$ | $(\bar{1}11)$ | $(\bar{1}11)$ | $(1\bar{1}1)$ | $(1\bar{1}1)$ | $(1\bar{1}1)$ |
| $[0\bar{1}1]$ | $[\bar{1}0\bar{1}]$ | [110] | [011] | $[10\bar{1}]$ | $[\bar{1}\bar{1}0]$ |



# Solution

- Activated systems : a1 et d1

$$(111)[0\bar{1}1]$$

$$\mathbf{n} = \frac{1}{\sqrt{3}}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \qquad \mathbf{l} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix}$$

$$\omega_1 = \frac{\gamma}{2\sqrt{6}}\begin{bmatrix} 0 & 1 & -1 \\ -1 & 0 & -2 \\ 1 & 2 & 0 \end{bmatrix}$$

$$(1\bar{1}1)[011]$$

$$\mathbf{n} = \frac{1}{\sqrt{3}}\begin{bmatrix} 1 \\ -1 \\ 1 \end{bmatrix} \qquad \mathbf{l} = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$$

$$\omega_2 = \frac{\gamma}{2\sqrt{6}}\begin{bmatrix} 0 & -1 & -1 \\ 1 & 0 & 2 \\ 1 & -2 & 0 \end{bmatrix}$$

$$\omega_{tot} = \frac{\gamma}{2\sqrt{6}}\begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

# Meaning of $\omega_{ij}$

$\omega_{ij}$ = anti-symmetric component of the deformation gradient
= infinitesimal rotation tensor

Effect on a vector

$$du_i = w_{ij} \;\; u_j$$

$$\begin{bmatrix} du_x \\ du_y \\ du_z \end{bmatrix} = \begin{bmatrix} 0 & -\omega_z & +\omega_y \\ +\omega_z & 0 & -\omega_x \\ -\omega_y & +\omega_x & 0 \end{bmatrix} \begin{bmatrix} u_x \\ u_y \\ u_z \end{bmatrix}$$

***u*** is the vector and ***du*** the displacement. ω is not a “true” rotation matrix, but a tensor.

# 5- Elementary mechanisms
# *c*- Von Mises compatibility criterion

# Von Mises compatibility criterion

Von Mises compatibility criterion

- All strains must be accommodated by plastic deformation,
- All component of the strain tensor must be accommodated,
- Plasticity = constant volume deformation
- $\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} = 0$
- 5 independent component left : $\varepsilon_{11}$, $\varepsilon_{22}$, $\varepsilon_{12}$, $\varepsilon_{13}$, $\varepsilon_{23}$
- The material needs at least 5 independent deformation mechanisms

$$\epsilon_{ij}^{T} = \sum_{k} \frac{1}{2}\gamma^{k}\left(n_j^k l_i^k + n_i^k l_j^k\right)$$

Otherwise:

- There must be another mechanism coming in, otherwise the crystal will break.

MgO is a cubic material with a B1 structure, like NaCl

- The {110}<1$\bar{1}$0> slip system is dominant, and has six symmetry equivalents
  - 1 : (110)[$\bar{1}$10]
  - 2 : (1$\bar{1}$0)[110]
  - 3 : (011)[0$\bar{1}$1]
  - 4 : (01$\bar{1}$)[011]
  - 5 : (101)[$\bar{1}$01]
  - 6 : (10$\bar{1}$)[101]
- Are they sufficient to accommodate any form of deformation?

$$\epsilon_{ij} = \frac{1}{2}\gamma\left(n_j l_i + n_i l_j\right) \qquad \omega_{ij} = \frac{1}{2}\gamma\left(n_j l_i - n_i l_j\right)$$

# Practice

MgO is a cubic material with a B1 structure, like NaCl

- The {110}<110> slip system is dominant, and has six symmetry equivalents.
- Are they sufficient to accommodate any form of deformation?

$(110)\,[\bar{1}10]$

$$\epsilon = \frac{\gamma}{2}\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$(011)\,[0\bar{1}1]$

$$\epsilon = \frac{\gamma}{2}\begin{bmatrix} 0 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$(101)\,[\bar{1}01]$

$$\epsilon = \frac{\gamma}{2}\begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

No component of strain off-diagonal

$(\bar{1}10)\,[110]$

$$\epsilon = \frac{\gamma}{2}\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$(01\bar{1})\,[011]$

$$\epsilon = \frac{\gamma}{2}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$(10\bar{1})\,[101]$

$$\epsilon = \frac{\gamma}{2}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Need additional systems such as {100}<1$\bar{1}$0>

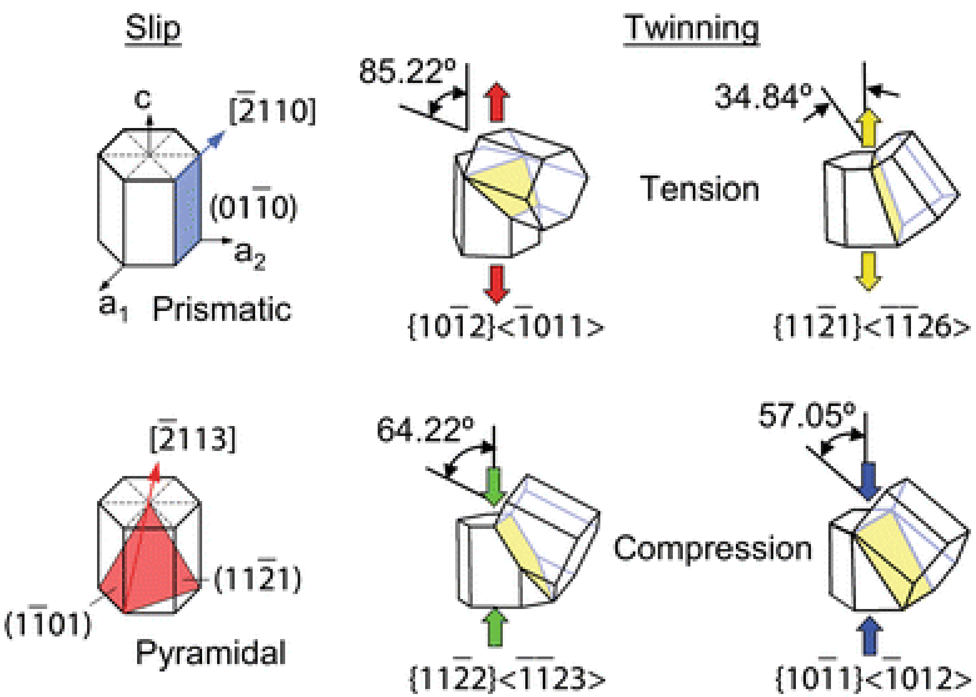
# 5- Elementary mechanisms
# c- Other mechanisms

# Other mechanisms

Dislocations are not the only mechanism that can rotate grains and generate grain orientations.

Other important mechanism: twinning.

Twin: two separate crystals share some of the same crystal lattice points in a symmetrical manner.




Example: deformation mechanisms and orientation in zirconium.

Padilla et al, *Metallurgical and Materials Transactions A*, 2007