# Micromechanics of Materials

## Dislocations, crystalline anisotropy and plasticity in hexagonal metals

Institut für Metallkunde und Metallphysik

Max-Planck-Institut für Eisenforschung GmbH

Dr. Stefanie Sandlöbes

sandloebes@imm.rwth-aachen.de

# Topics

- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink bands
- Twinning in hexagonal metals
- Stacking faults in hexagonal metals
- Texture components in hexagonal metals

# Topics

- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink bands
- Twinning in hexagonal metals
- Stacking faults in hexagonal metals
- Texture components in hexagonal metals

# Topics

- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink bands
- Twinning in hexagonal metals
- Stacking faults in hexagonal metals
- Texture components in hexagonal metals

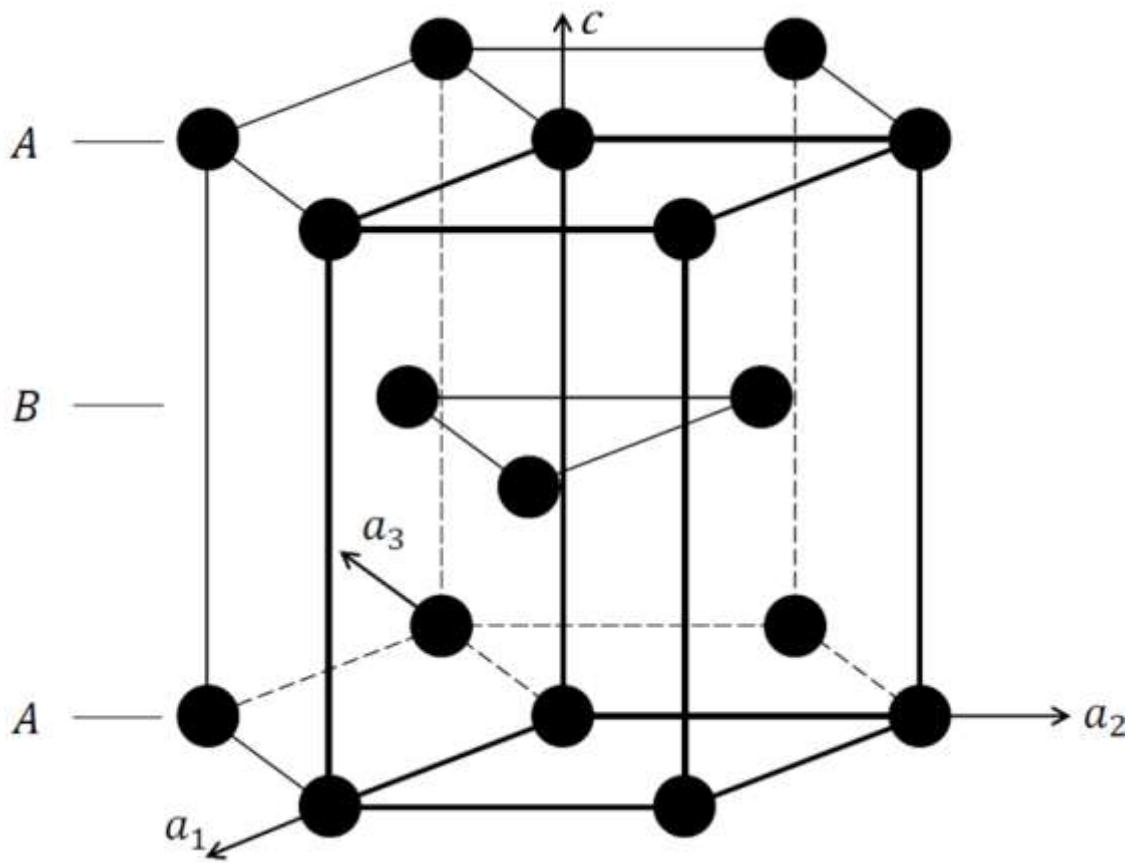
# Crystal structure and Miller-Bravais indices

Reminder: hexagonal crystal structure and Miller-Bravais indices

ABAB stacking sequence

Axes:
$a_1 = a_2 = a_3 \neq c$

Angles:
a-c = 90°
$a_1$-$a_2$ = $a_2$-$a_3$ = $a_1$-$a_3$ = 120°



# Crystal structure and Miller-Bravais indices

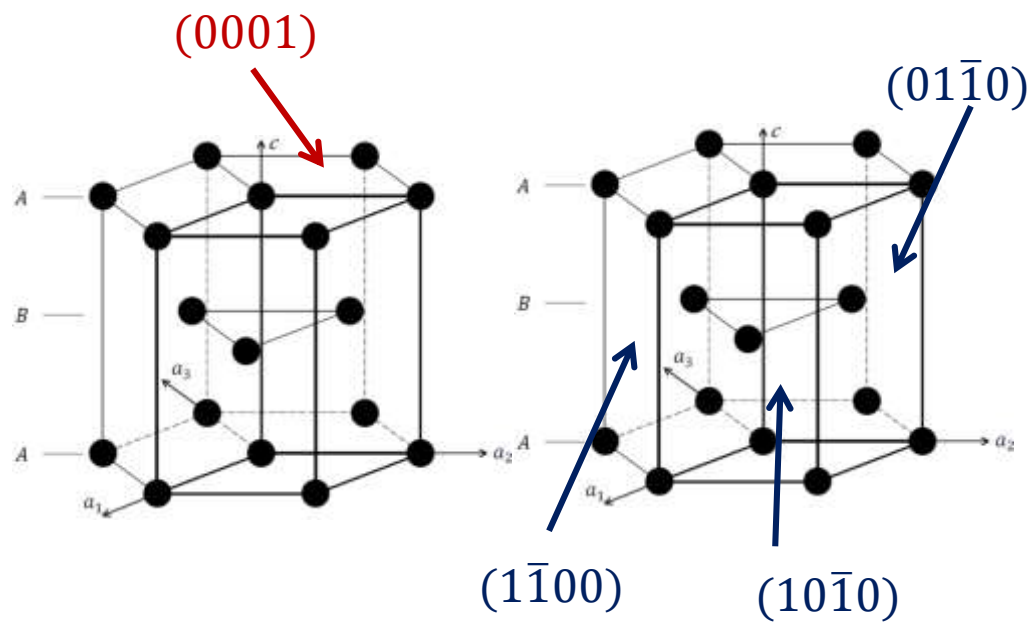
Reminder: hexagonal crystal structure and Miller-Bravais indices

ABAB stacking sequence

Axes:
$a_1 = a_2 = a_3 \neq c$

Angles:
a-c = 90°
$a_1$-$a_2$ = $a_2$-$a_3$ = $a_1$-$a_3$ = 120°

Planes (Miller-Bravais indices):
(*hkil*) with $h + k + i = 0$
$a_3$ is redundant: $a_3 = -(a_1 + a_2)$



# Crystal structure and Miller-Bravais indices

Reminder: hexagonal crystal structure and Miller-Bravais indices

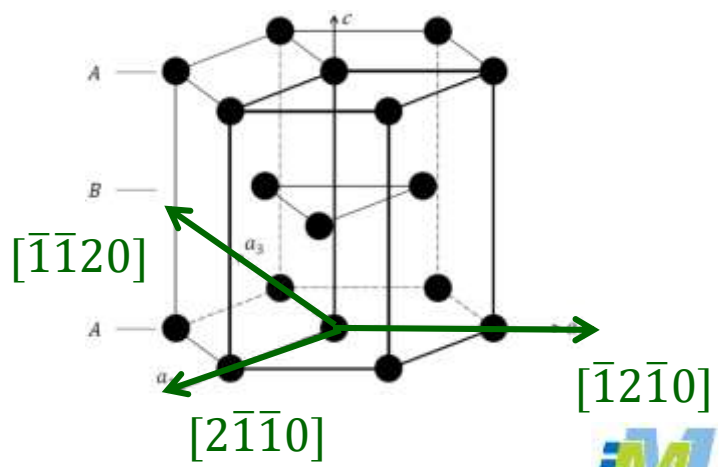
ABAB stacking sequence

Axes:
$a_1 = a_2 = a_3 \neq c$

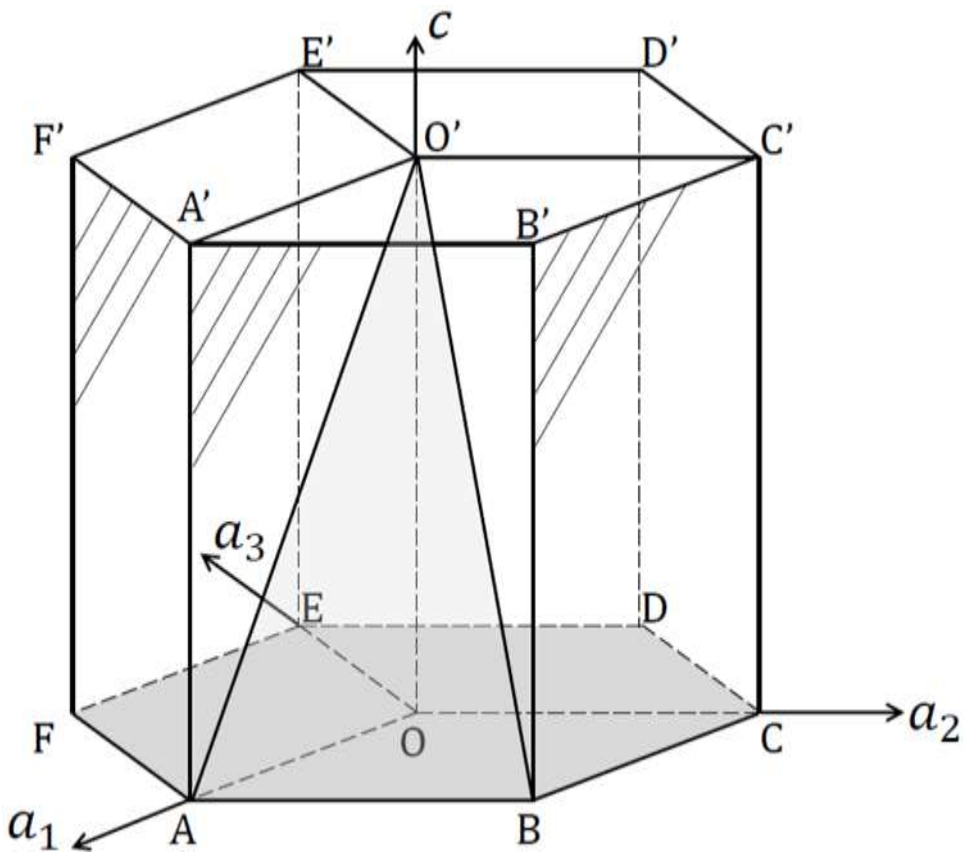
Angles:
a-c = 90°
$a_1$-$a_2$ = $a_2$-$a_3$ = $a_1$-$a_3$ = 120°

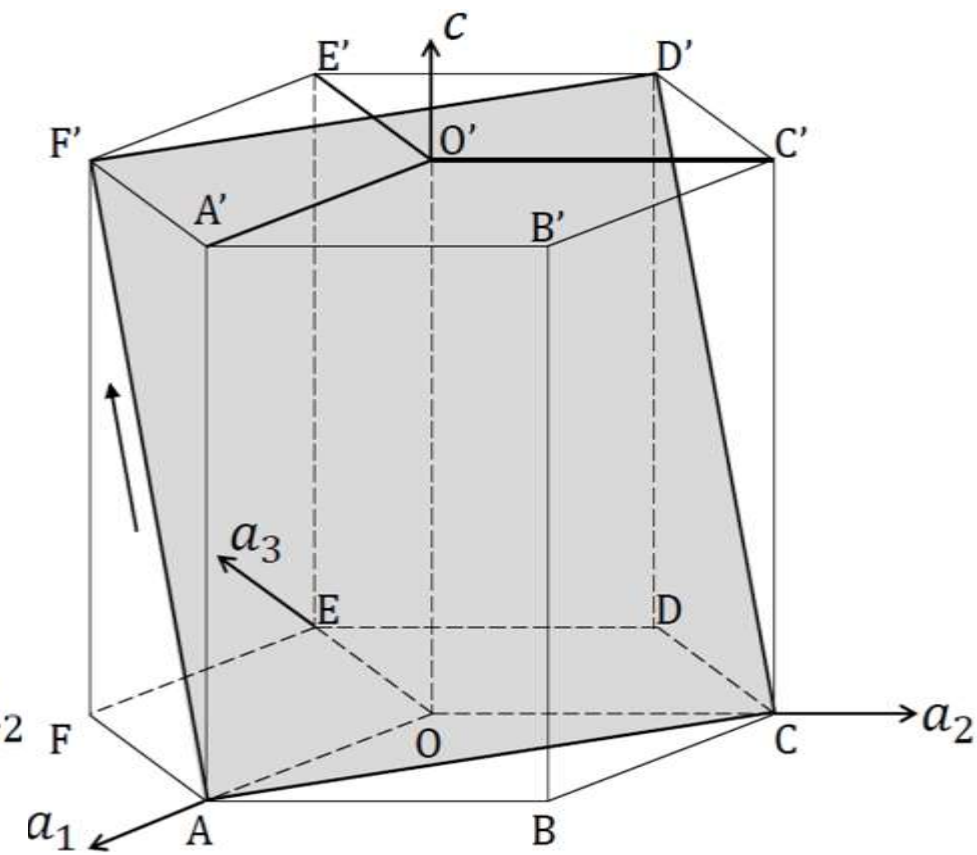
Planes (Miller-Bravais indices):
(*hkil*) with $h + k + i = 0$
$a_3$ is redundant: $a_3 = -(a_1 + a_2)$

Directions (Miller-Bravais indices):
[*uvtw*] with $u + v + t = 0$
$u = \frac{1}{3}(2u - v)$
$v = \frac{1}{3}(2v - u)$
$t = -(u + v)$



# Crystal structure and Miller-Bravais indices




ACE: basal plane

ABB'A': prismatic plane

ABO': first order pyramidal plane $[10\bar{1}1]$

ACD'F': second order pyramidal plane $[11\bar{2}2]$

AB: <a> direction

AF': <c + a> direction

# Crystal structure and Miller-Bravais indices

| Metal | c/a |
|---|---|
| Be | 1.568 |
| Y | 1,572 |
| Os | 1.579 |
| Hf | 1.581 |
| Ru | 1.583 |
| Ti | 1.588 |
| Sc | 1.592 |
| Zr | 1.593 |
| Tl | 1.599 |
| Re | 1.615 |
| Co | 1.623 |
| Mg | 1.623 |
| Zn | 1.856 |
| Cd | 1.886 |

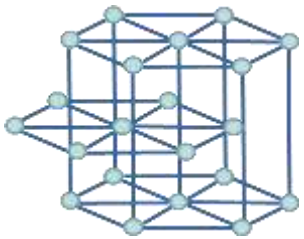
Relevance of hexagonal metals:

- Ti: light-weight; high strength, corrosion resistant
- Mg: light-weight; high specific strength
- Co: high-temperature material; ferromagnetic
- Zn: galvanization; decoration parts, corrosion resistant
- Zr: low neutron absorption
- Be: light-weight; superior specific strength; corrosion resistant
- RE / Y: superior magnetic, optic, electrochemical properties; unique alloying effects

# Crystal structure and Miller-Bravais indices

| Metal | c/a |
|---|---|
| Be | 1.568 |
| Y | 1,572 |
| Os | 1.579 |
| Hf | 1.581 |
| Ru | 1.583 |
| Ti | 1.588 |
| Sc | 1.592 |
| Zr | 1.593 |
| Tl | 1.599 |
| Re | 1.615 |
| Co | 1.623 |
| Mg | 1.623 |
| Zn | 1.856 |
| Cd | 1.886 |

HEX ≠ hcp

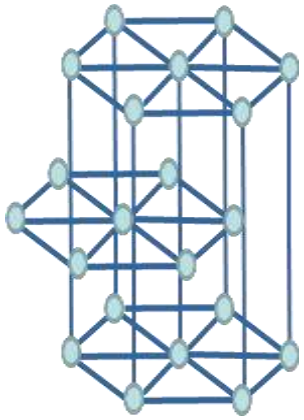


NOT: closed packed crystal structure

Classification as structural materials class „hcp“ not adequat

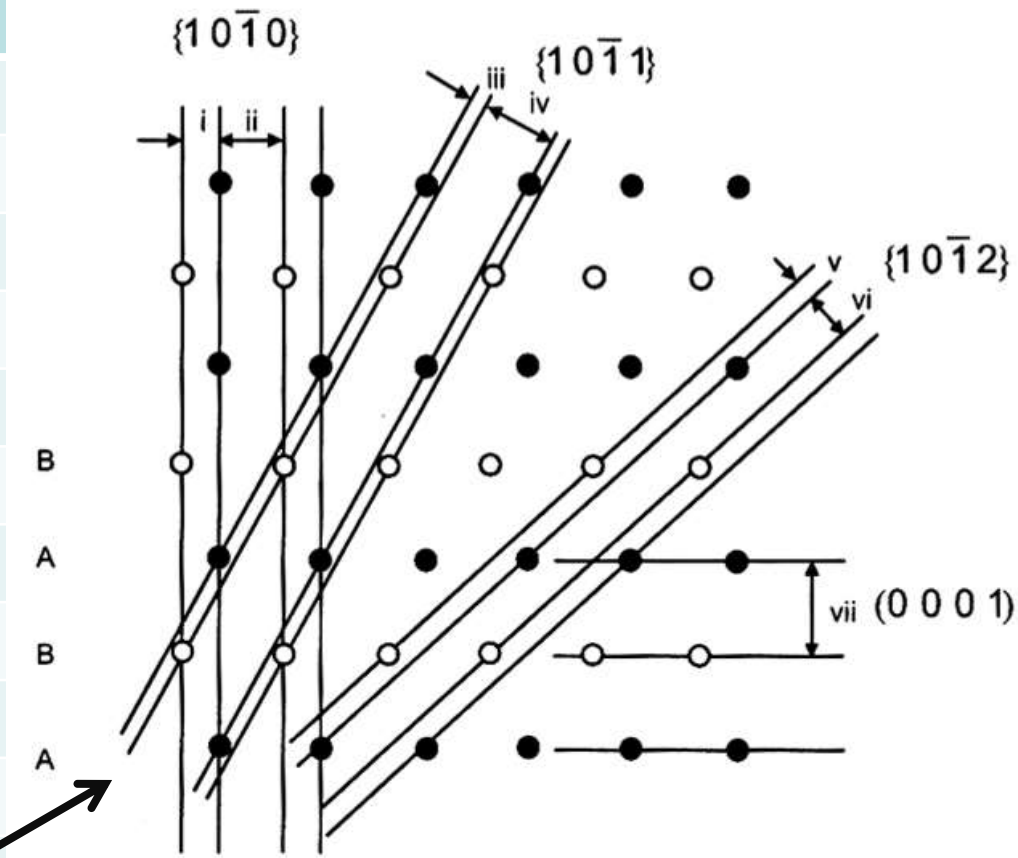
Plastically anisotrop

$$hcp: \sqrt{\frac{8}{3}} = 1.633$$



# Crystal structure and Miller-Bravais indices

| Metal | |
|---|---|
| Be | |
| Y | |
| Os | |
| Hf | |
| Ru | |
| Ti | |
| Sc | |
| Zr | |
| Tl | |
| Re | |
| Co | |
| Mg | 1.623 |
| Zn | 1.856 |
| Cd | 1.886 |



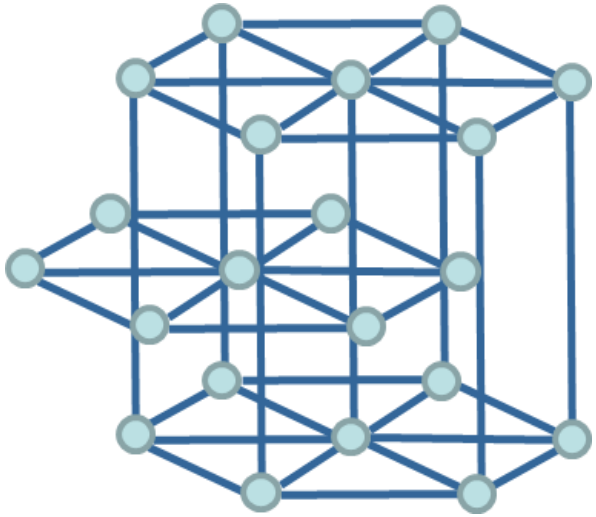

| | Interplanar spacing |
|---|---|
| i | $\frac{a\sqrt{3}}{6}$ |
| ii | $\frac{a\sqrt{3}}{3}$ |
| iii | $\frac{ac\sqrt{3}}{6\sqrt{4c^2+3a^2}}$ |
| iv | $\frac{5ac\sqrt{3}}{6\sqrt{4c^2+3a^2}}$ |
| v | $\frac{ac\sqrt{3}}{6\sqrt{3a^2+c^2}}$ |
| vi | $\frac{ac\sqrt{3}}{3\sqrt{3a^2+c^2}}$ |
| vii | $c/2$ |

$$hcp: \sqrt{\frac{8}{3}} = 1.633$$

Partridge, 1967

# Quiz

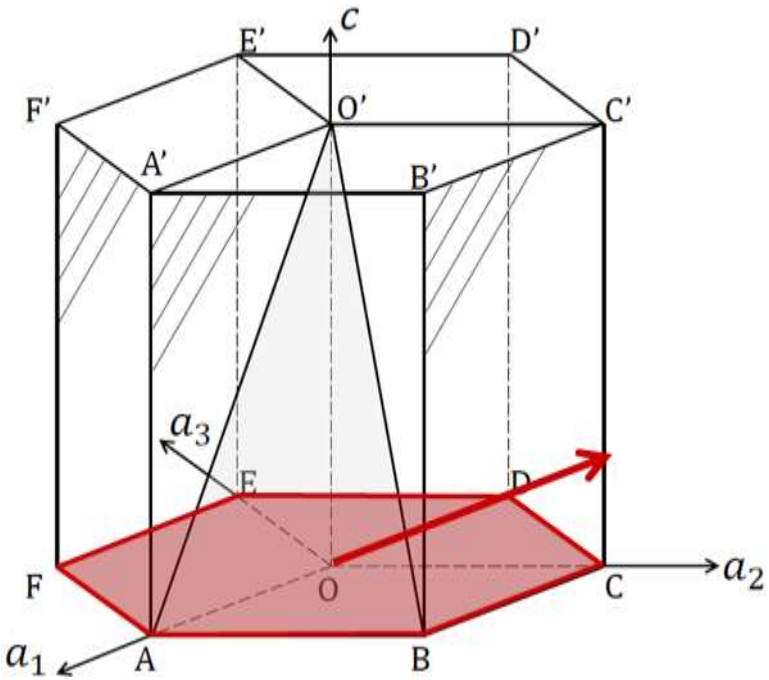
- Why use of Miller-Bravais for hexagonal structure?
- Give the indices and show
  - Basal plane
  - Prismatic plane
  - 1st order pyramidal plane
  - <a> direction
  - <c+a> direction

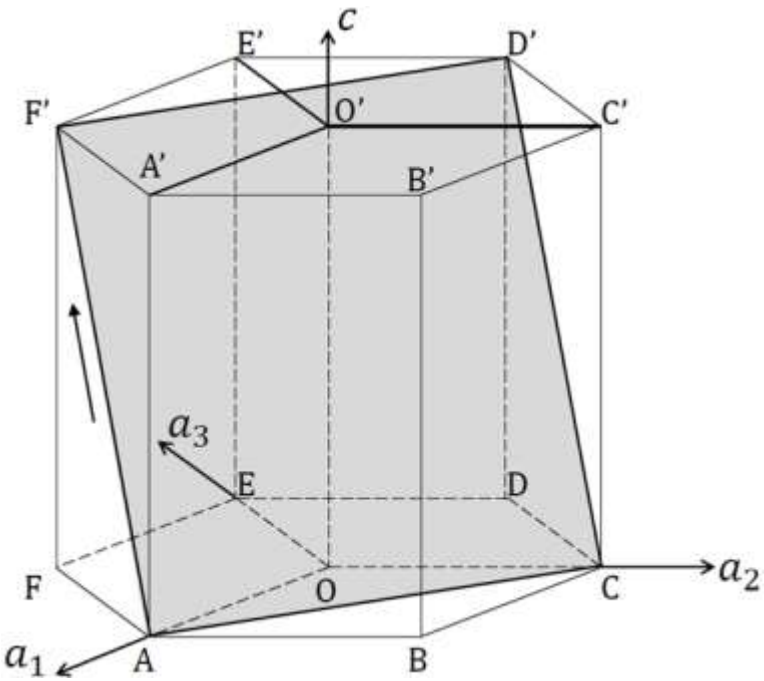


# Topics

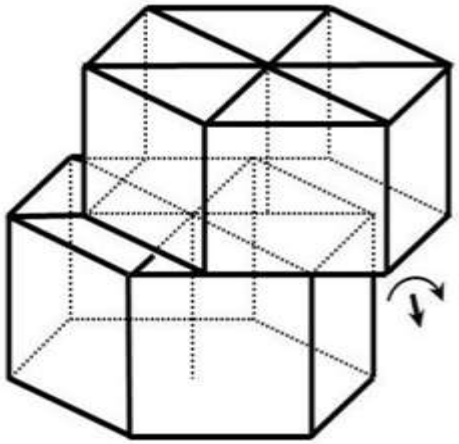
- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink bands
- Twinning in hexagonal metals
- Stacking faults in hexagonal metals
- Texture components in hexagonal metals
- Anisotropy of precipitation strengthening
- Phase transformations; dual- / multiphase systems
- Shear bands in hexagonal metals

# Dislocations in hexagonal metals



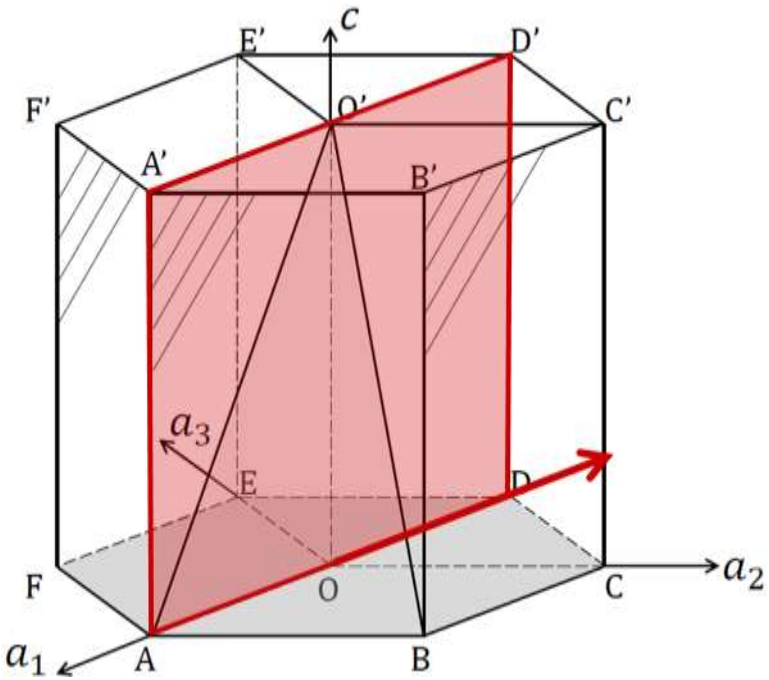



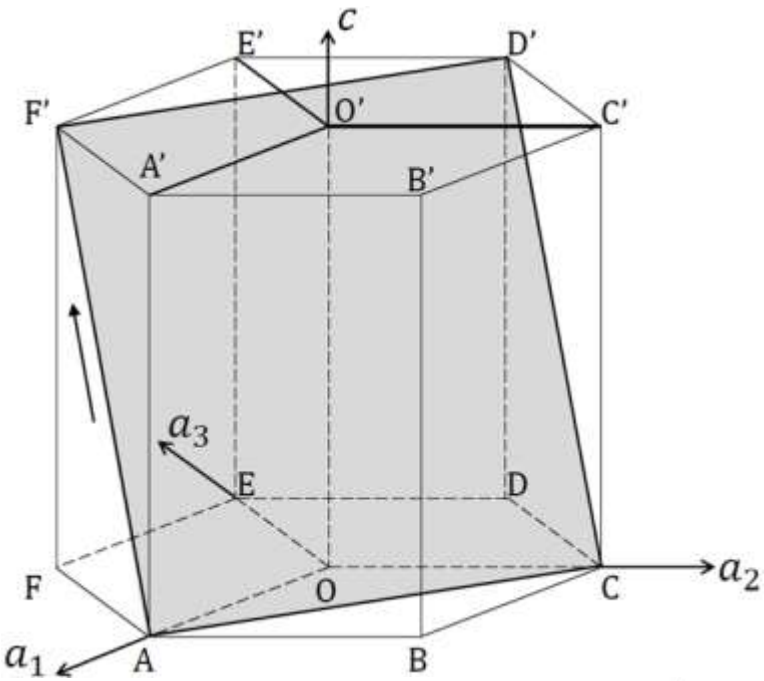

ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane
AB: <a> direction
AF': <c + a> direction



Basal $\{0001\} < 1\bar{2}10 >$

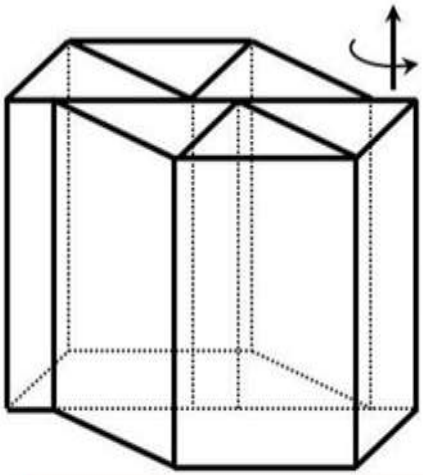
# Dislocations in hexagonal metals



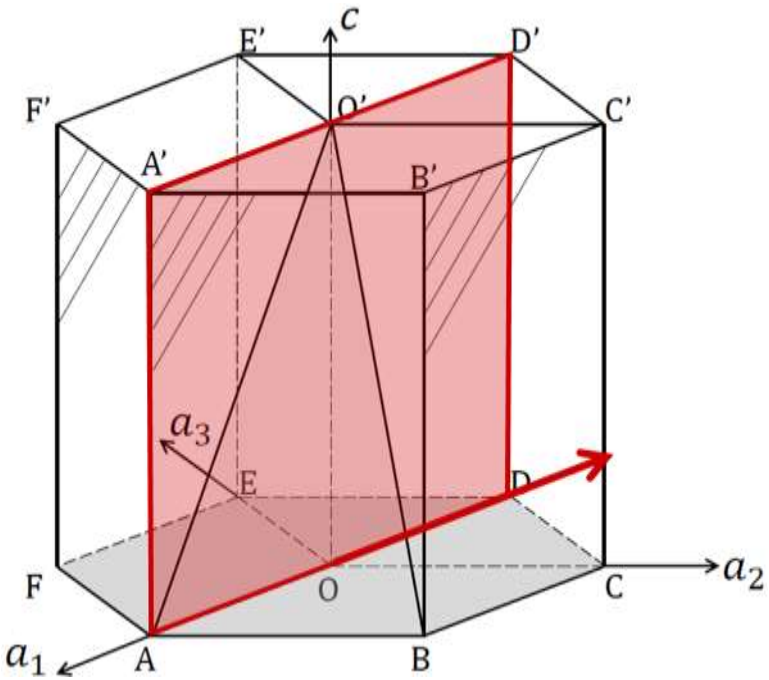

Cross-slip of <a> dislocations on prismatic plane

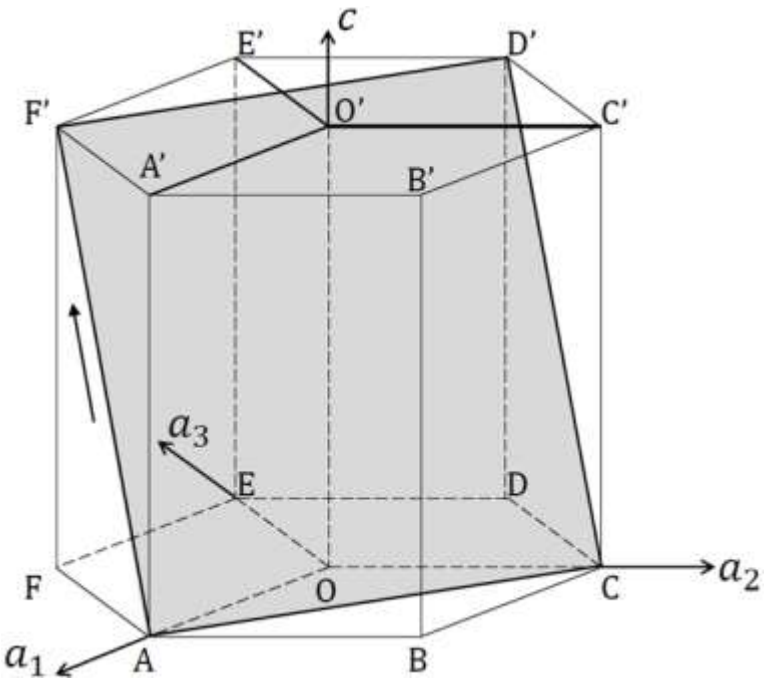
ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane
AB: <a> direction
AF': <c + a> direction



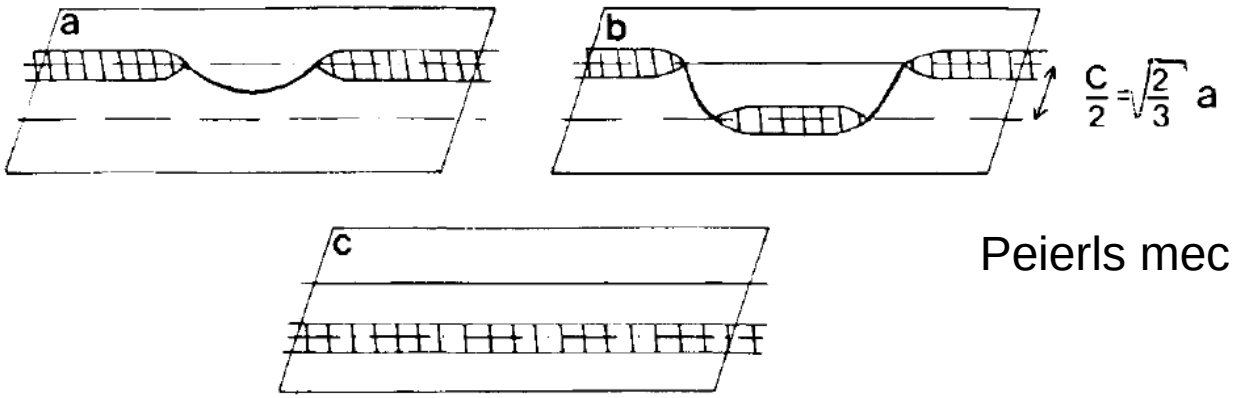
Prism $\{10\bar{1}0\} < 1\bar{2}10 >$

# Dislocations in hexagonal metals



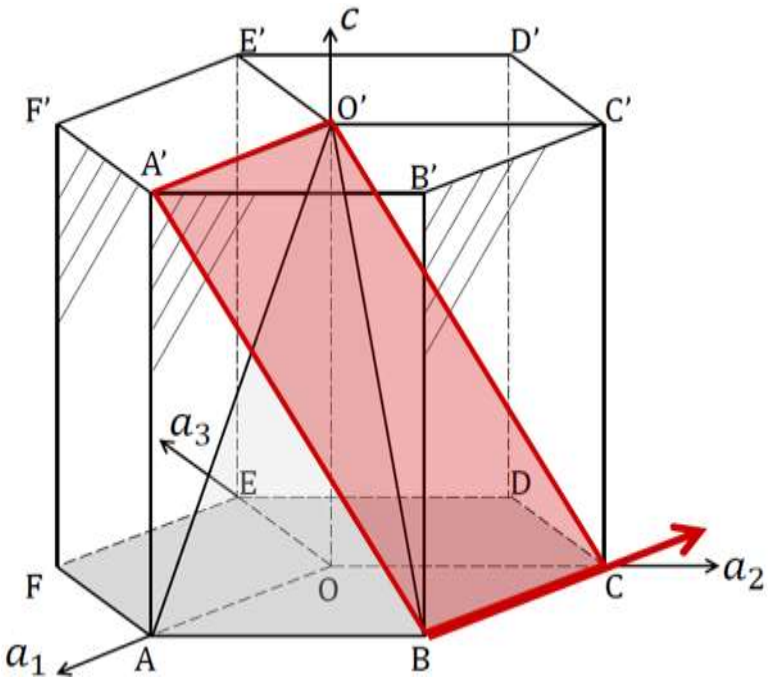



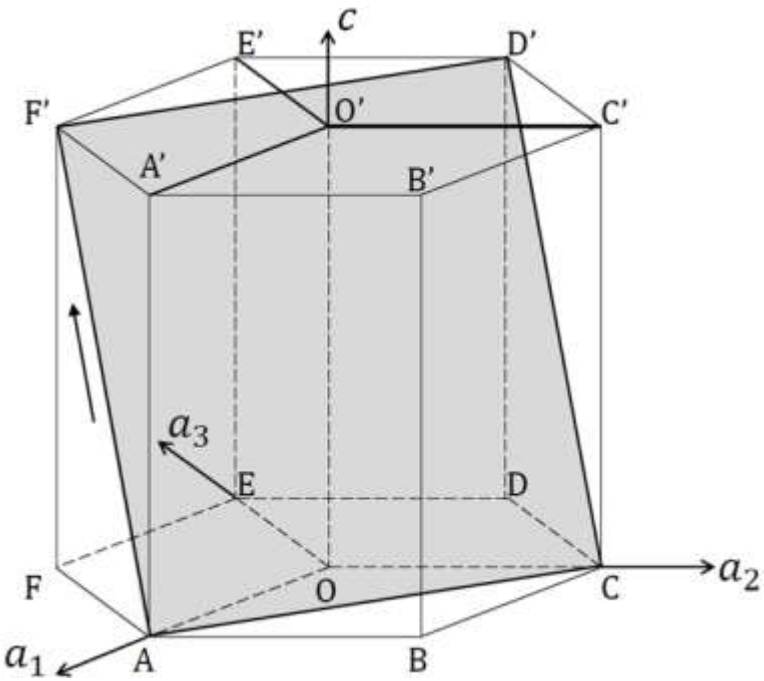

Cross-slip of <a> dislocations on prismatic plane




Peierls mechanisms of cross-slip

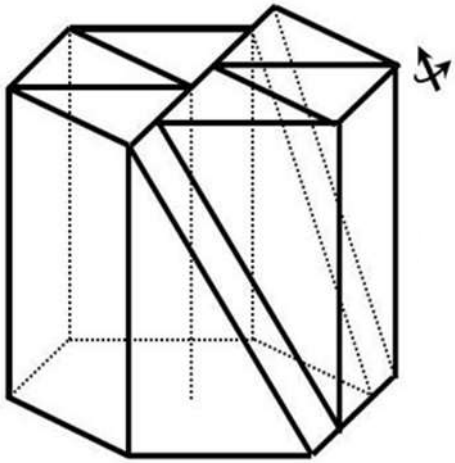
# Dislocations in hexagonal metals



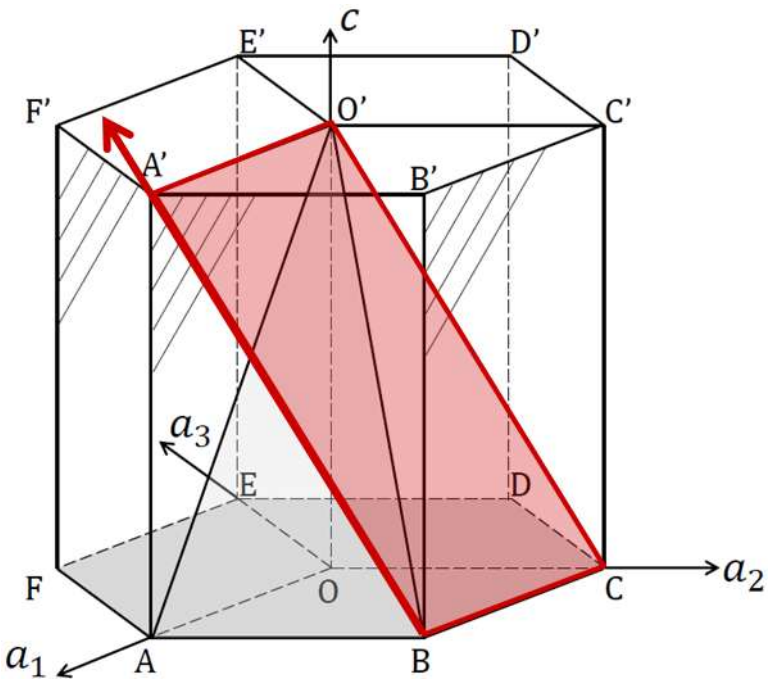

Cross-slip of <a> dislocations on pyramidal plane

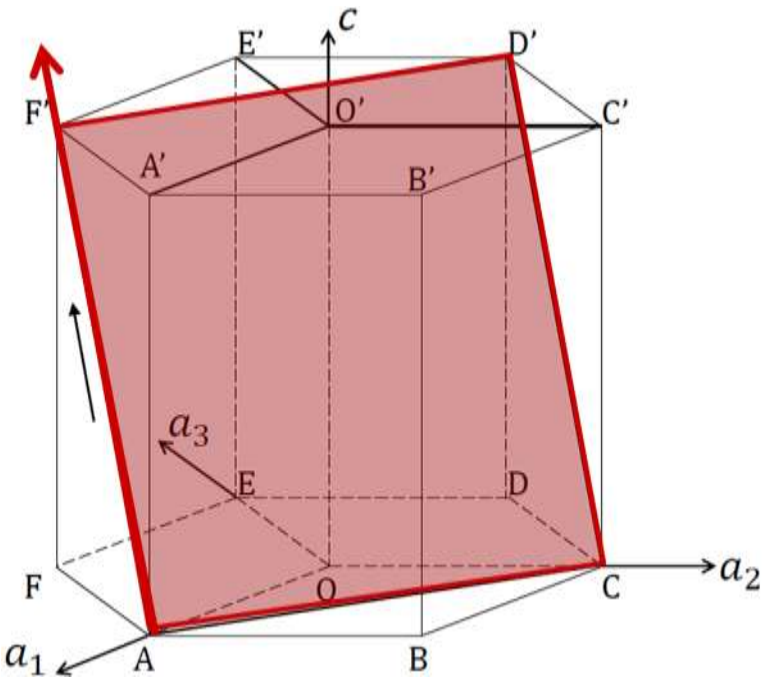
ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane
AB: <a> direction
AF': <c + a> direction

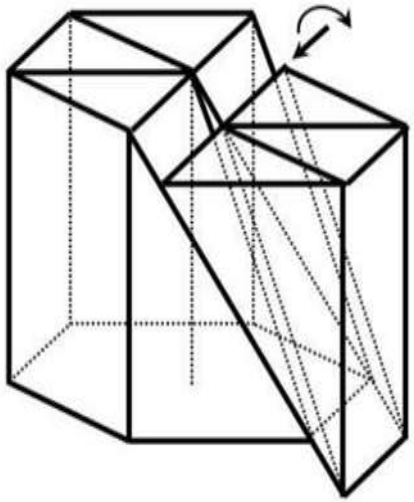


Pyramidal <a> $\{10\bar{1}1\} < 1\bar{2}10 >$

# Dislocations in hexagonal metals



Pyramidal <c+a> $\{10\bar{1}1\} < 2\bar{1}\bar{1}\bar{3} >$

ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane
AB: <a> direction
AF': <c + a> direction

# Dislocations in hexagonal metals

| Slip system type | Burgers vector type | Slip direction | Slip plane | Dislo. Energy | No. of slip systems | |
|---|---|---|---|---|---|---|
| | | | | | Total | Independent |
| basal | $\vec{a}$ | $< 11\bar{2}0 >$ | $(0002)$ | $\lvert a \rvert^2$ | 3 | 2 |
| prismatic | $\vec{a}$ | $< 11\bar{2}0 >$ | $\{10\bar{1}0\}$ | $\lvert a \rvert^2$ | 3 | 2 |
| pyramidal <a> | $\vec{a}$ | $< 11\bar{2}0 >$ | $\{10\bar{1}1\}$ | $\lvert a \rvert^2$ | 6 | 4 |
| pyramidal <c+a> | $\vec{c}+\vec{a}$ | $< 11\bar{2}3 >$ | $\{10\bar{1}1\}$ | $2.63\lvert a \rvert^2$ | 6 | 5 |
| pyramidal <c+a> | $\vec{c}+\vec{a}$ | $< 11\bar{2}3 >$ | $\{11\bar{2}2\}$ | $2.63\lvert a \rvert^2$ | 6 | 5 |
| twinning | | | | | | 0.5 (polar) |

Taylor: at least 5 independent slip systems for plastic poly-crystalline deformation

# Dislocations in hexagonal metals

| Metal | c/a | Primary glide plane(s) | Secondary glide plane(s) |
|---|---|---|---|
| Be | 1.568 | basal <a> | prismatic <a>; pyramidal <a> |
| Y | 1,572 | prismatic <a> | basal <a> |
| Hf | 1.581 | prismatic <a> | basal <a>; pyramidal <a> |
| Ti | 1.588 | prismatic <a> | basal <a>; pyramidal <a> |
| Sc | 1.592 | basal <a> | |
| Zr | 1.593 | prismatic <a> | basal <a>; pyramidal <a> |
| Tl | 1.598 | basal <a>; prismatic <a> | |
| Re | 1.615 | basal <a>; prismatic <a> | |
| Co | 1.623 | basal <a> | |
| Mg | 1.623 | basal <a> | prismatic <a>; pyramidal <c+a> |
| Zn | 1.856 | basal <a> | prismatic <a>; pyramidal <a> pyramidal <c+a>; kinking |
| Cd | 1.886 | basal <a> | prismatic <a>; pyramidal <a> pyramidal <c+a>; kinking |

# Dislocations in hexagonal metals

| Element | c/a | System | d/b | w/b | activated | |
|---|---|---|---|---|---|---|
| | | | | | bei RT | bei HT |
| **Cd** | 1.886 | Basal | 0.94 | 0.83 | XX | X |
| | | Prismatisch | 0.87 | 0.58 | | X |
| | | Pyramidal 1. | 0.79 | 0.64 | X | |
| | | Pyramidal 2. | 0.21 | 0.17 | X | X |
| **Zn** | 1.856 | Basal | 0.93 | 0.67 | XX | X |
| | | Prismatisch | 0.87 | 0.52 | | X |
| | | Pyramidal 1. | 0.79 | 0.49 | X | |
| | | Pyramidal 2. | 0.21 | 0.18 | X | |
| **Mg** | 1.623 | Basal | 0.81 | 0.61 | XX | X |
| | | Prismatisch | 0.87 | 0.62 | X | X |
| | | Pyramidal 1. | 0.76 | 0.56 | X | X |
| | | Pyramidal 2. | 0.22 | 0.17 | | |
| **Co** | 1.623 | Basal | 0.81 | 0.67 | X | X |
| | | Prismatisch | 0.87 | 0.67 | | |
| | | Pyramidal 1. | 0.76 | 0.60 | | |
| | | Pyramidal 2. | 0.22 | 0.14 | | |

| Element | c/a | System | d/b | w/b | activated | |
|---|---|---|---|---|---|---|
| | | | | | bei RT | bei HT |
| **Zr** | 1.593 | Basal | 0.80 | 0.67 | X | |
| | | Prismatisch | 0.87 | 0.65 | XX | X |
| | | Pyramidal 1. | 0.76 | 0.58 | | X |
| | | Pyramidal 2. | 0.23 | 0.16 | | X |
| **Ti** | 1.587 | Basal | 0.80 | 0.57 | X | X |
| | | Prismatisch | 0.87 | 0.68 | XX | X |
| | | Pyramidal 1. | 0.76 | 0.58 | X | X |
| | | Pyramidal 2. | 0.23 | 0.17 | | |
| **Be** | 1.568 | Basal | 0.78 | 0.38 | XX | X |
| | | Prismatisch | 0.87 | 0.47 | X | X |
| | | Pyramidal 1. | 0.76 | 0.40 | X | X |
| | | Pyramidal 2. | 0.23 | 0.12 | | |

Yoo, Wie (1967)

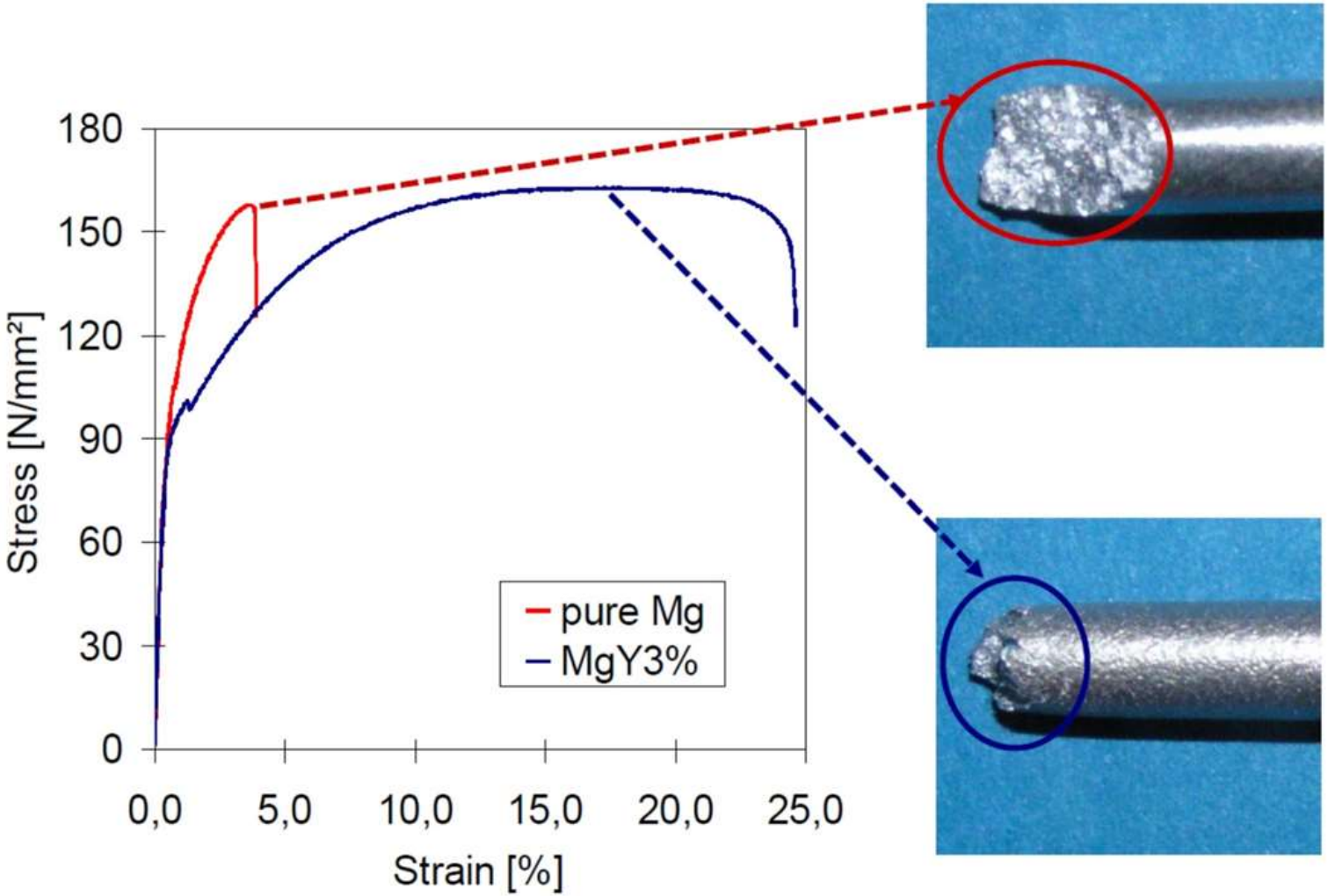
# Dislocations in hexagonal metals

| Metal | c/a | d/b | w/b | Primary glide plane(s) | Secondary glide plane(s) |
|---|---|---|---|---|---|
| Be | 1.568 | 0.78 (B)<br>0.87 (Pr) | 0.38 (B)<br>0.47 (Pr) | basal <a> | prismatic <a>; pyramidal <a> |
| Ti | 1.588 | 0.80 (B)<br>0.87 (Pr) | 0.57 (B)<br>0.68 (Pr) | prismatic <a> | basal <a>; pyramidal <a> |
| Zr | 1.593 | 0.80 (B)<br>0.87 (Pr) | 0.67 (B)<br>0.65 (Pr) | prismatic <a> | basal <a>; pyramidal <a> |
| Co | 1.623 | 0.81 (B) | 0.67 (B) | basal <a> | |
| Mg | 1.623 | 0.81 (B)<br>0.87 (Pr) | 0.61 (B)<br>0.62 (Pr) | basal <a> | prismatic <a>; pyramidal <c+a> |
| Zn | 1.856 | 0.93 (B) | 0.67 (B) | basal <a> | prismatic <a>; pyramidal <a><br>pyramidal <c+a>; kinking |
| Cd | 1.886 | 0.94 (B) | 0.83 (B) | basal <a> | prismatic <a>; pyramidal <a><br>pyramidal <c+a>; kinking |

# Dislocations in hexagonal metals

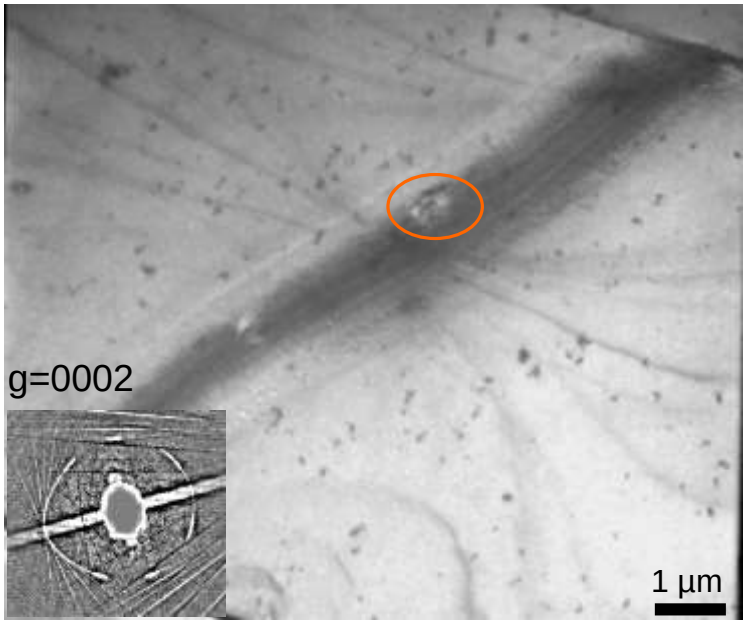
| Metal | c/a | d/b | w/b | Primary glide plane(s) | Secondary glide plane(s) |
|---|---|---|---|---|---|
| Be | 1.568 | 0.78 (B)<br>0.87 (Pr) | 0.38 (B)<br>0.47 (Pr) | basal <a> | prismatic <a>; pyramidal <a> |
| Ti | 1.588 | 0.80 (B)<br>0.87 (Pr) | 0.57 (B)<br>0.68 (Pr) | prismatic <a> | basal <a>; pyramidal <a> |
| Zr | 1.593 | 0.80 (B)<br>0.87 (Pr) | 0.67 (B)<br>0.65 (Pr) | prismatic <a> | basal <a>; pyramidal <a> |
| Co | 1.623 | 0.81 (B) | 0.67 (B) | basal <a> | |
| Mg | 1.623 | 0.81 (B)<br>0.87 (Pr) | 0.61 (B)<br>0.62 (Pr) | basal <a> | prismatic <a>; pyramidal <c+a> |
| Zn | 1.856 | 0.93 (B) | 0.67 (B) | basal <a> | prismatic <a>; pyramidal <a><br>pyramidal <c+a>; kinking |
| Cd | 1.886 | 0.94 (B) | 0.83 (B) | basal <a> | prismatic <a>; pyramidal <a><br>pyramidal <c+a>; kinking |

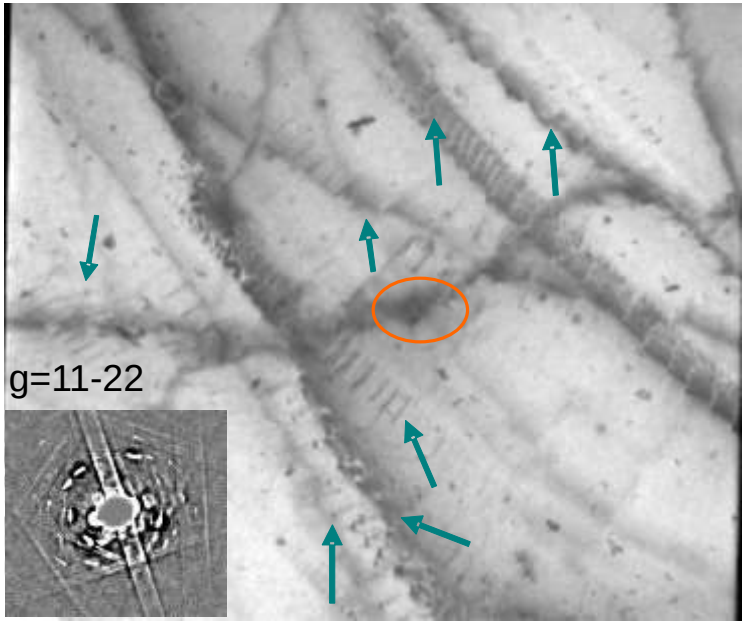
# Dislocations in hexagonal metals




- 5 times higher ductility
- Well-balanced work hardening
- Comparable strength

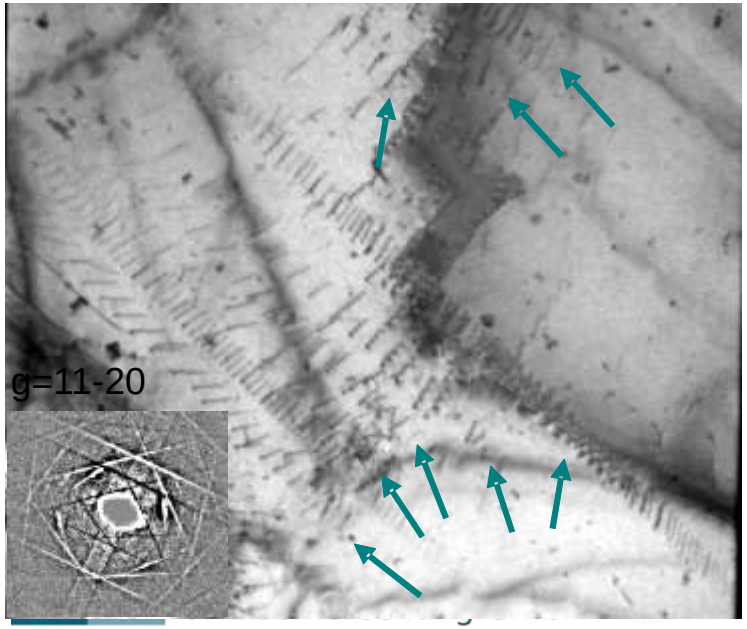
# Dislocations in hexagonal metals




– basal <a>

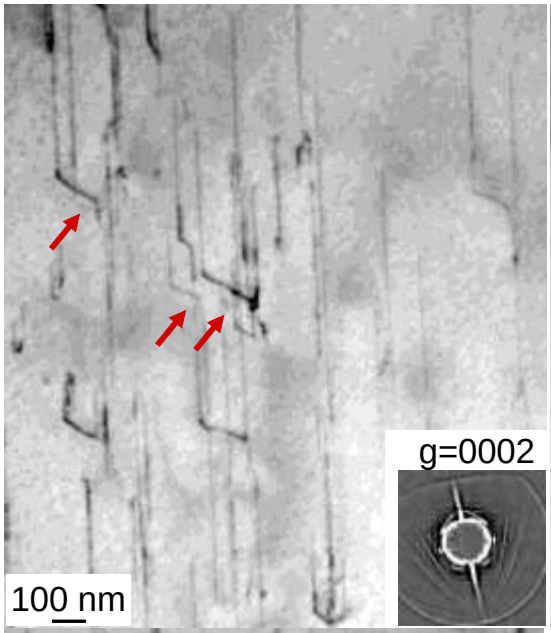
– sessile <c>

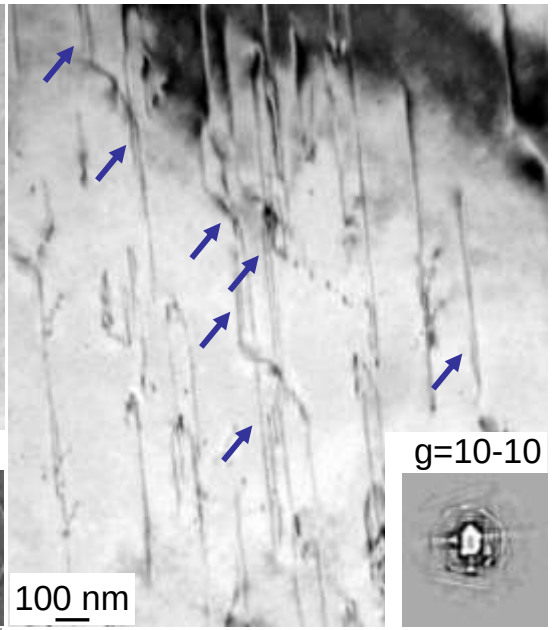


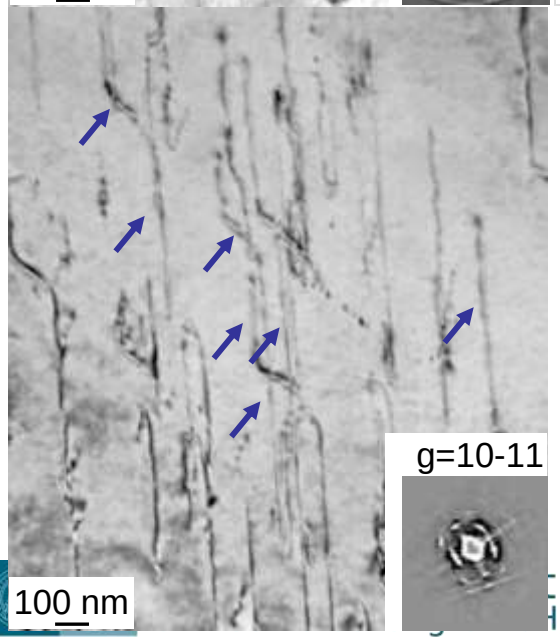

TEM images of dislocations in pure Mg

- High amount of basal <a> dislocations
- Hardly any dislocations with a <c> component
- Basal <a> dislocations lying on defined slip bands

# Dislocations in hexagonal metals



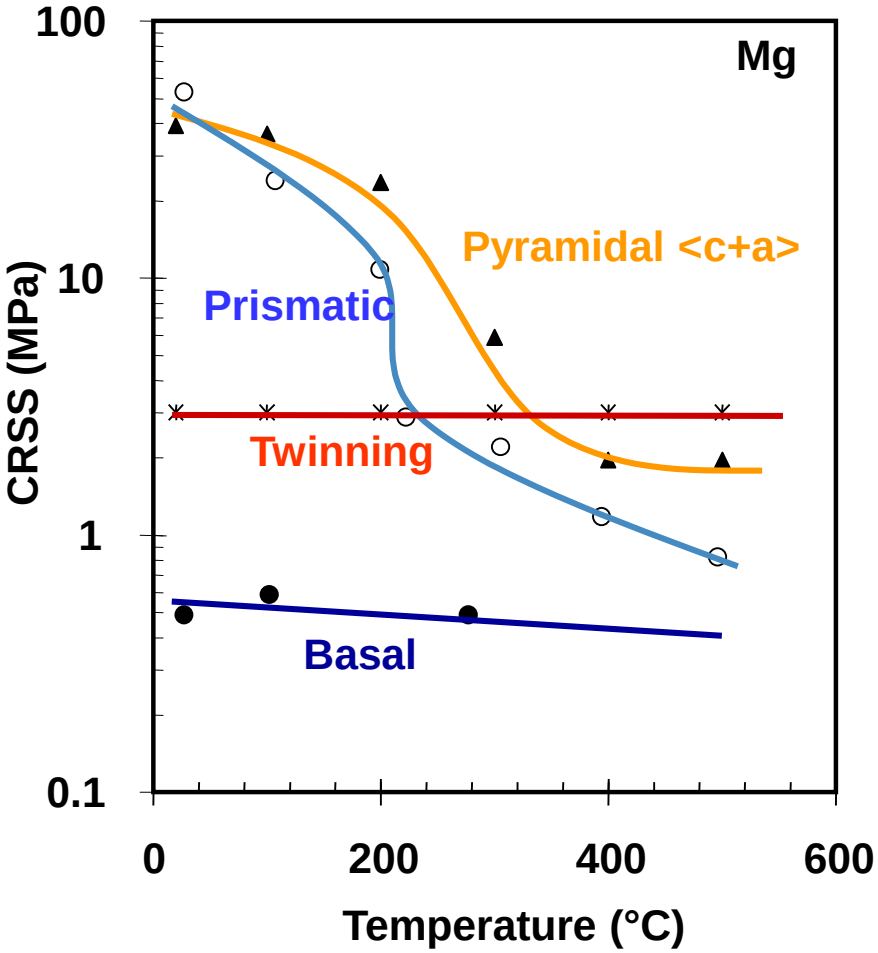



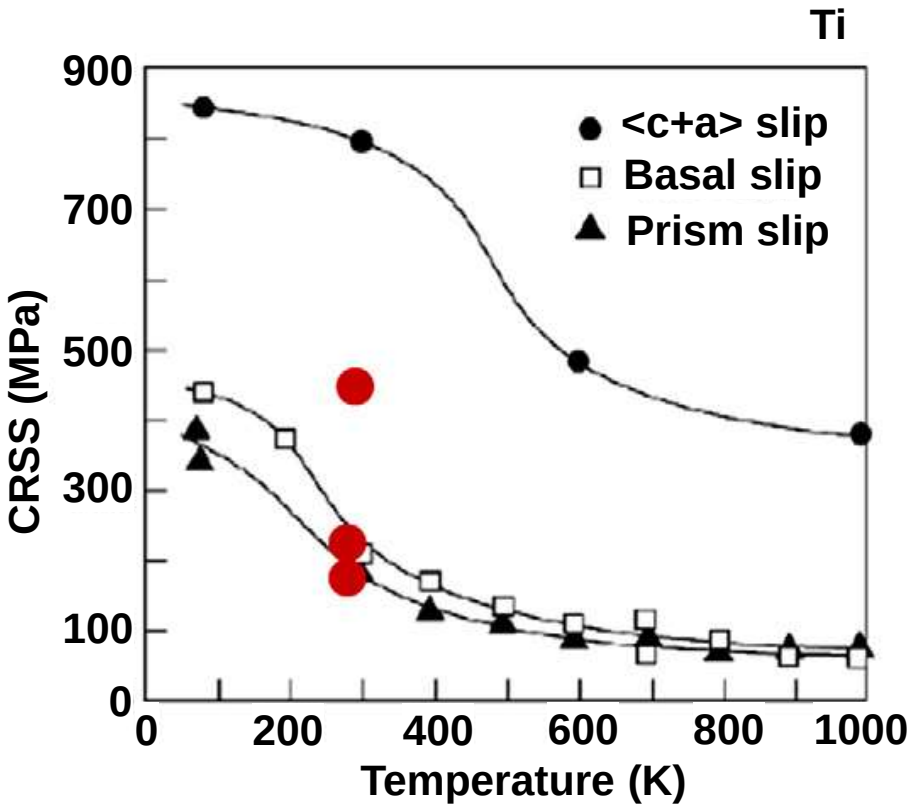

TEM images of <c+a> dislocations in Mg 3 wt-% Y (3.5 % CR)

- Red arrows:
  cross-slip events
- Blue arrows:
  dislocation dissociation on pyramidal planes

# Dislocations in hexagonal metals

Thermal activation – conventional behaviour



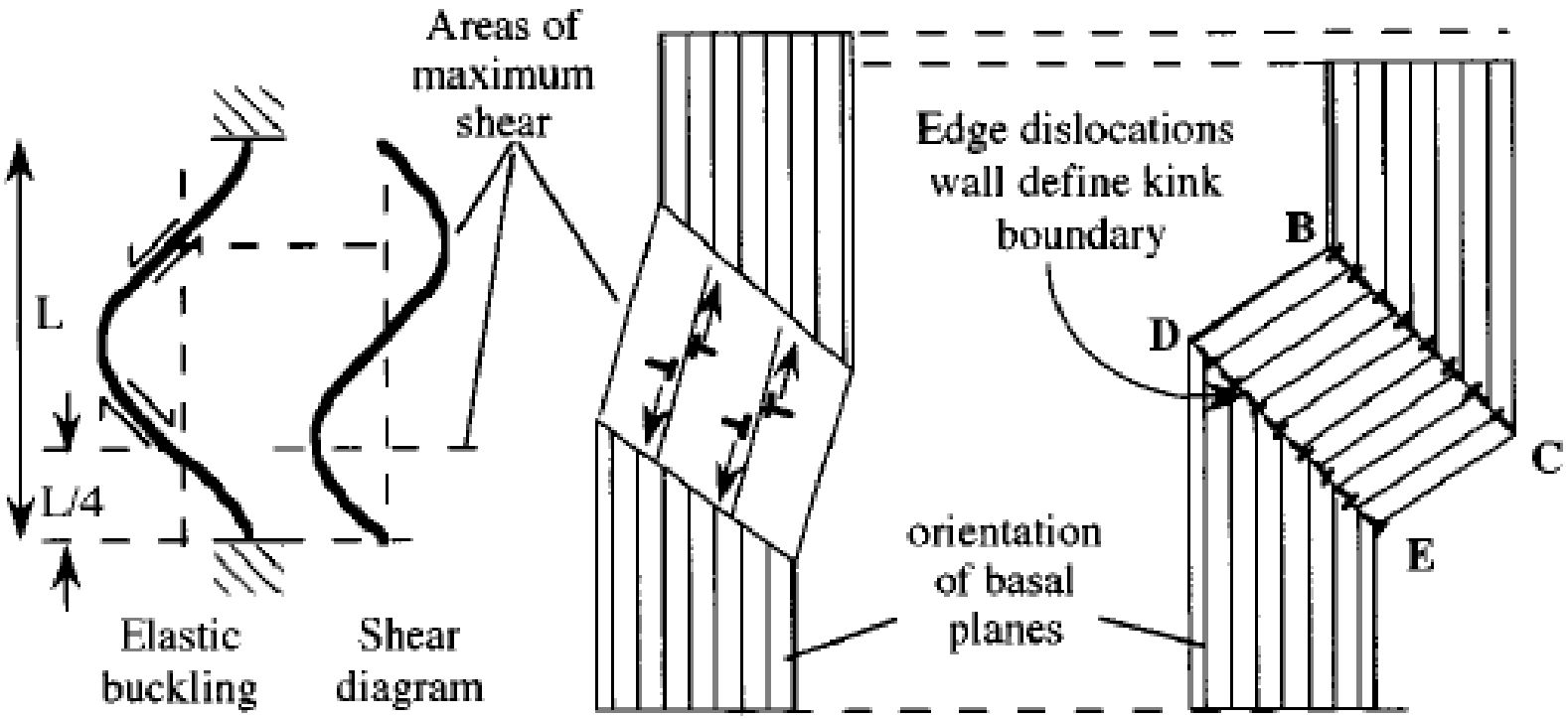

Banerjee, Williams (2013)





Barnett et al. (2002)

# Dislocations in hexagonal metals – Kink bands



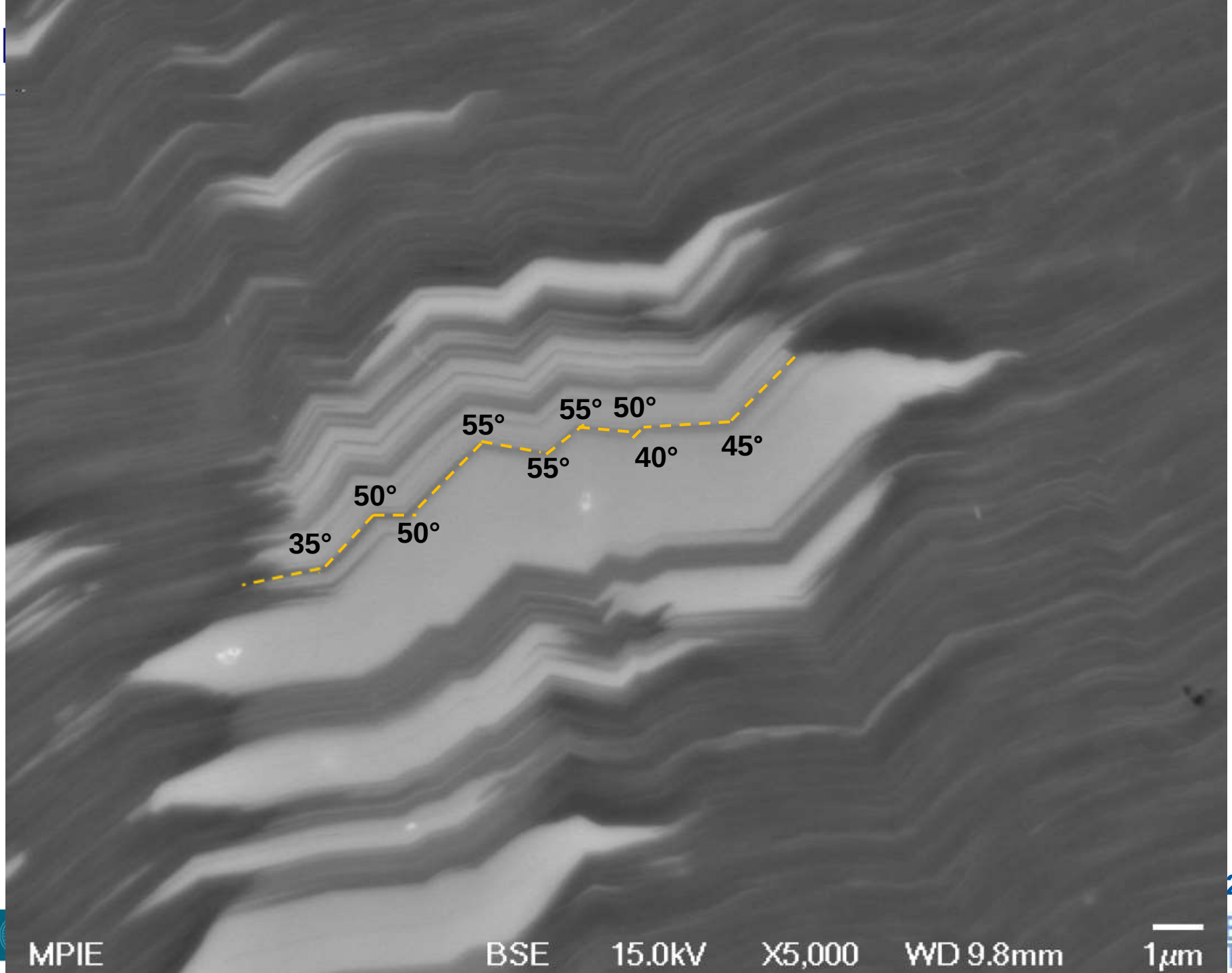

Kink-band formation

- Kink band: a deformation band in which the orientation is changed due to synchronized slipping on several parallel slip planes
- Kinking in hex having c/a ratio > 1.732 (-> twinning is unlikely).

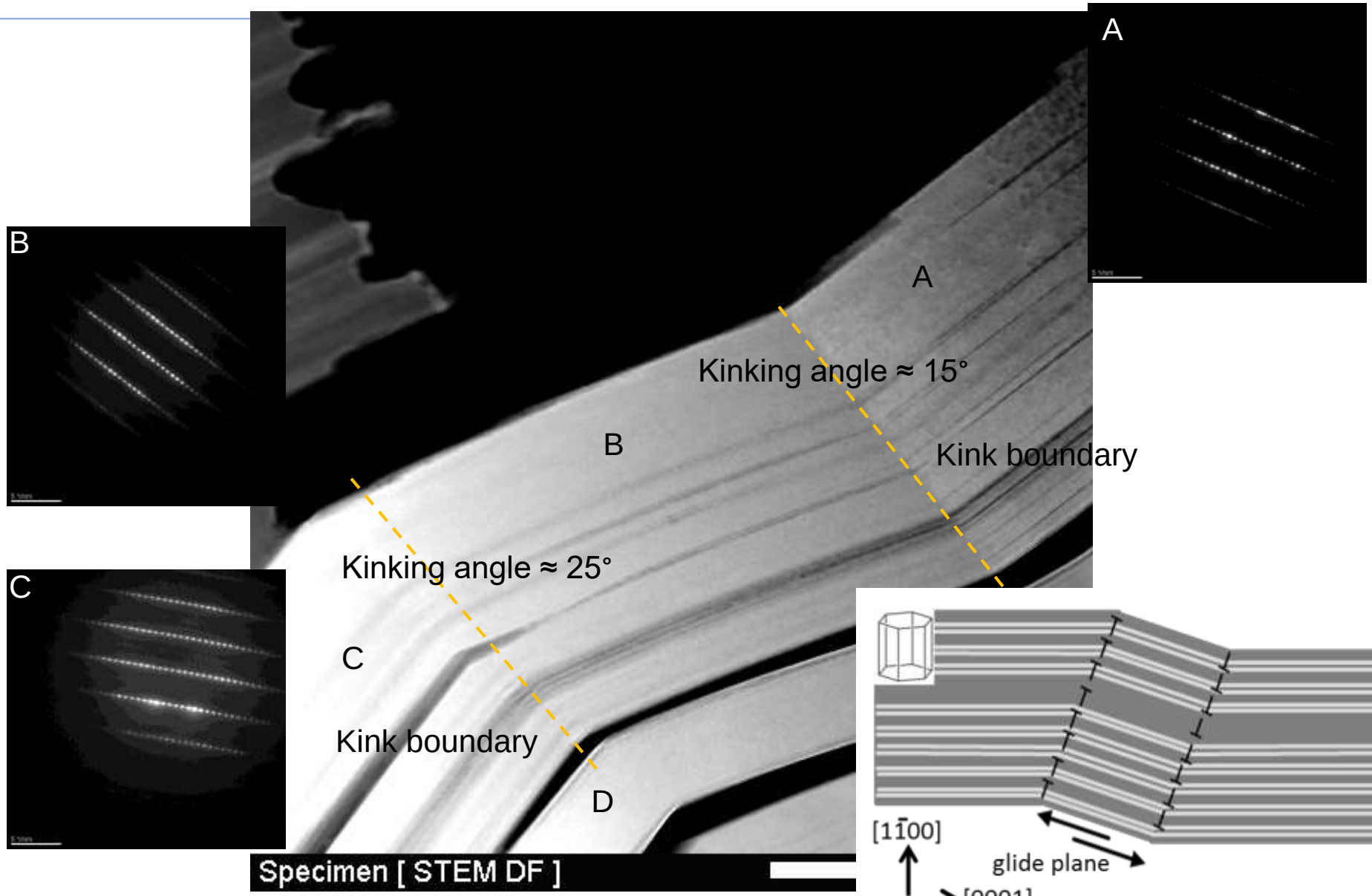




Barsoum et al. (1999)


35°
50°
50°
55°
55°
55°
50°
40°
45°
MPIE
BSE
15.0kV
X5,000
WD 9.8mm
1μm

# Dislocations in hexagonal metals – Kink bands



# Quiz

- How many slip system types in hexagonal metals?
- Which slip system types?
- How many independent systems?
- Which are the most common slip systems?
- Why are metals with basal <a> slip brittle?

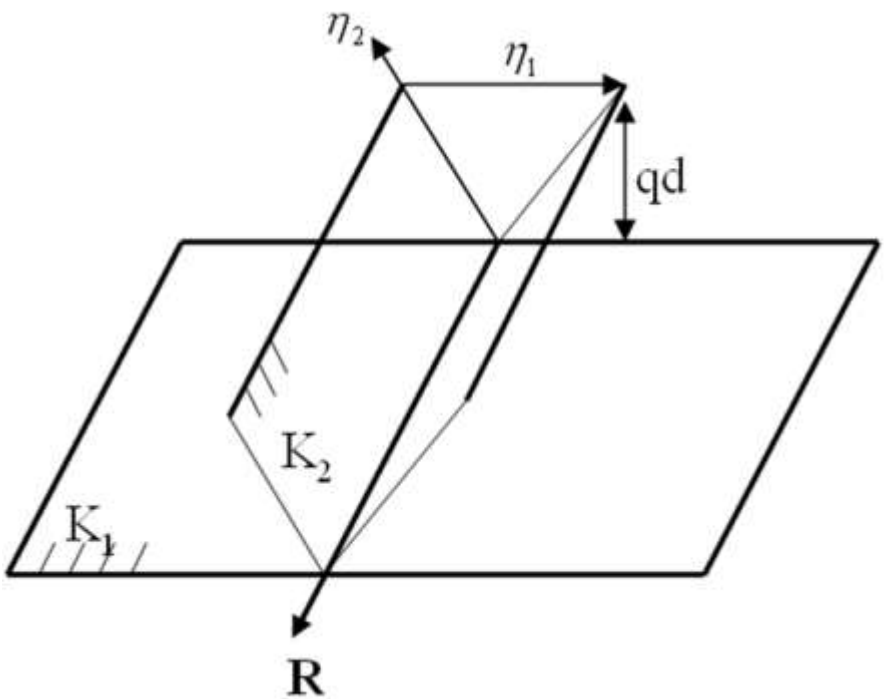
# Topics

- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink bands
- Twinning in hexagonal metals
- Stacking faults in hexagonal metals
- Texture components in hexagonal metals

# Twinning in hexagonal metals

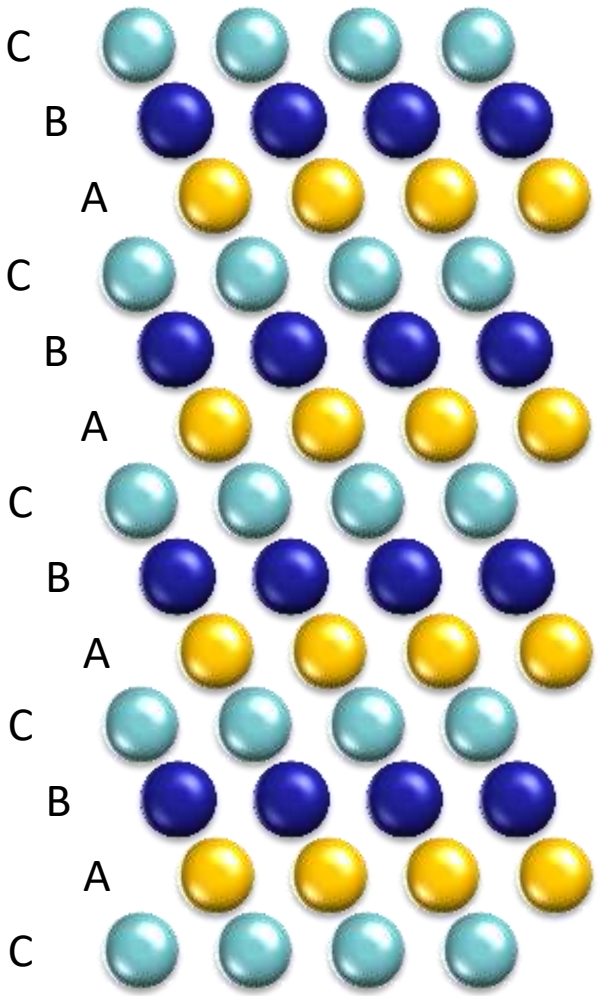
Twinning in hex metals:

- Prevalent deformation mechanism
- ≥ 7 twinning systems, in many metals more than 1 system active
- 6 variants per twinning system
- Twins can consume full grains
  - no dynamic grain refinement
  - deformation inside twins, secondary twinning
- Considered as 0.5 independent deformation systems (polar nature)
- Carry only small shear
- c/a: “atomic shuffling”



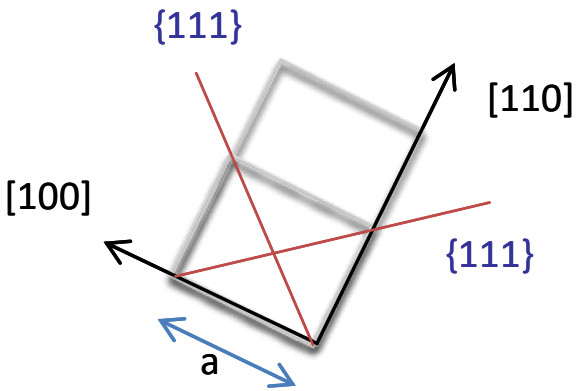

$K_1$ twinning habit plane (invariant plane of twinning shear)
$K_2$ conjugate twinning plane
$\eta_1$ twinning direction
$\eta_2$ conjugate twinning direction
R rotation axis
q number of twin habit planes
d interplanar distance

# Twinning in hexagonal metals



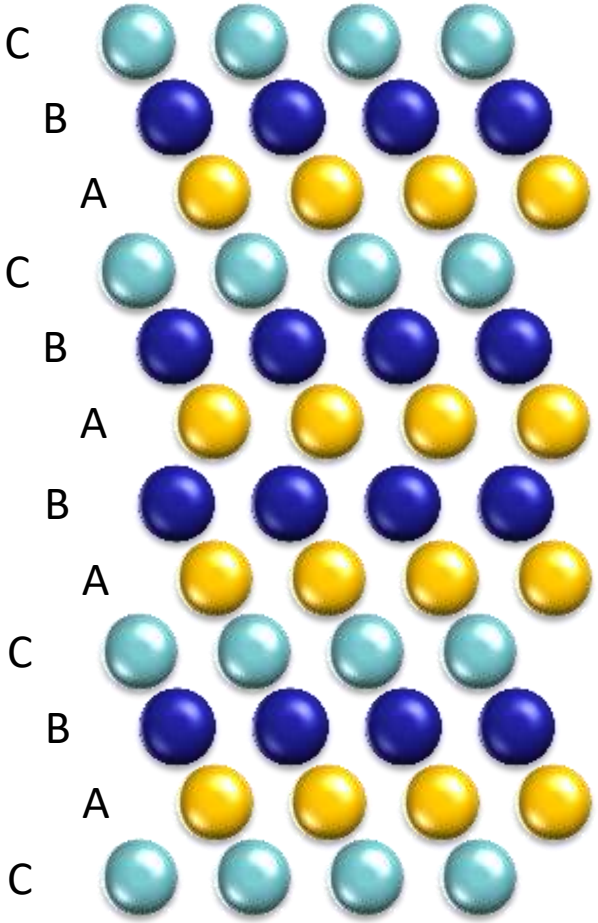

perfect fcc lattice in <110> projection

C-layer is missing: **intrinsic SF** created

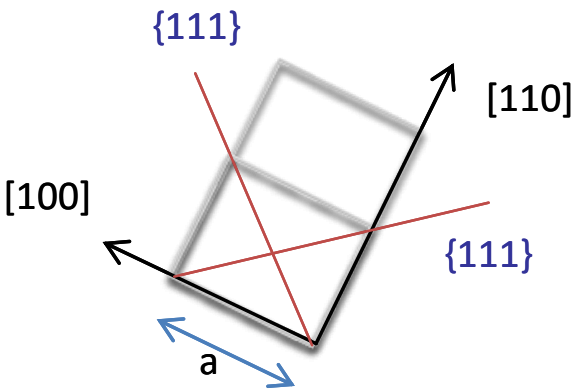



“Easy“ schematics twinning fcc

# Twinning in hexagonal metals

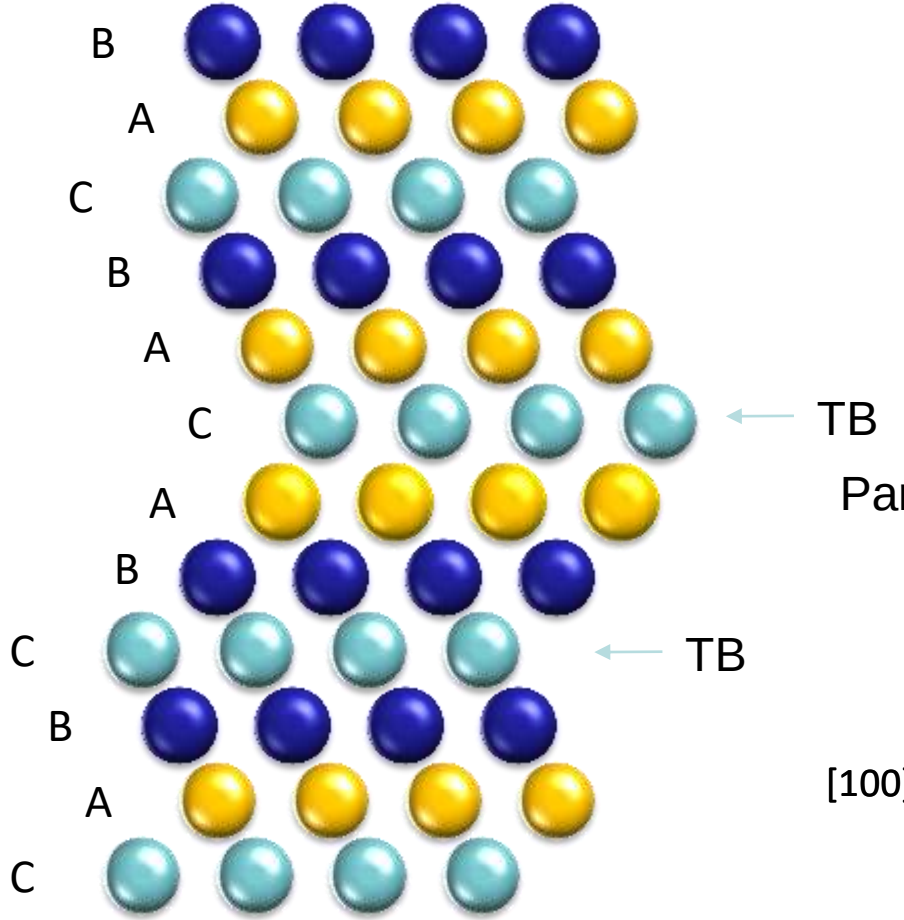



C-layer is missing: **intrinsic SF** created

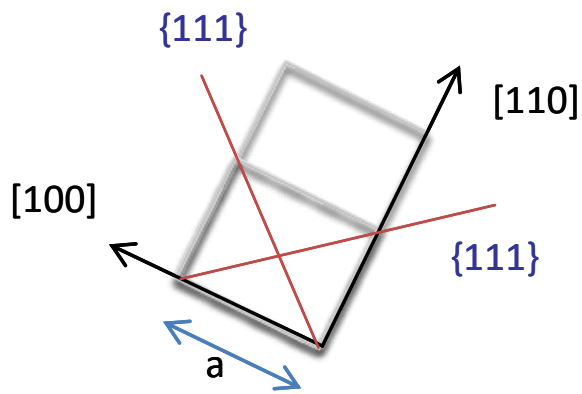



“Easy“ schematics twinning fcc

# Twinning in hexagonal metals

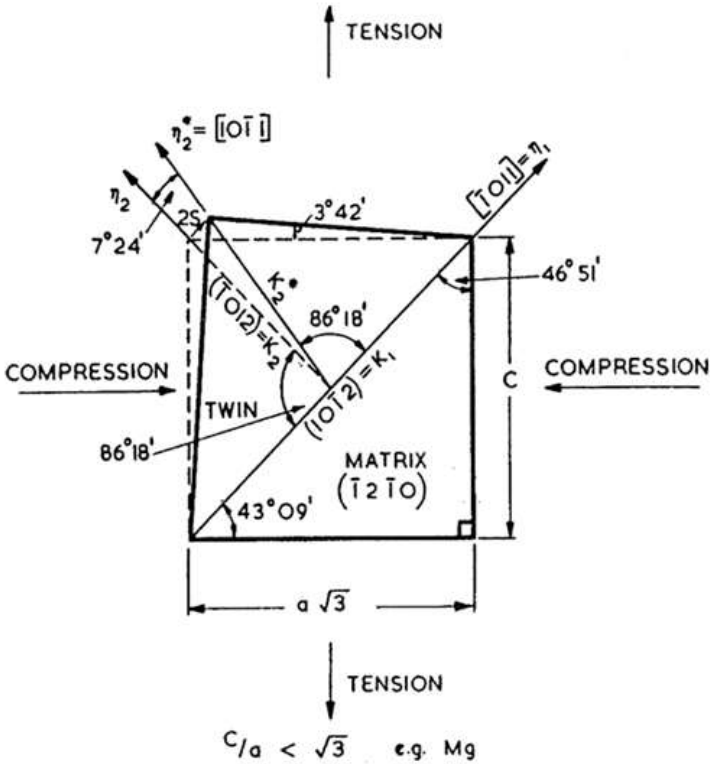



Partial glide on successive {111} planes

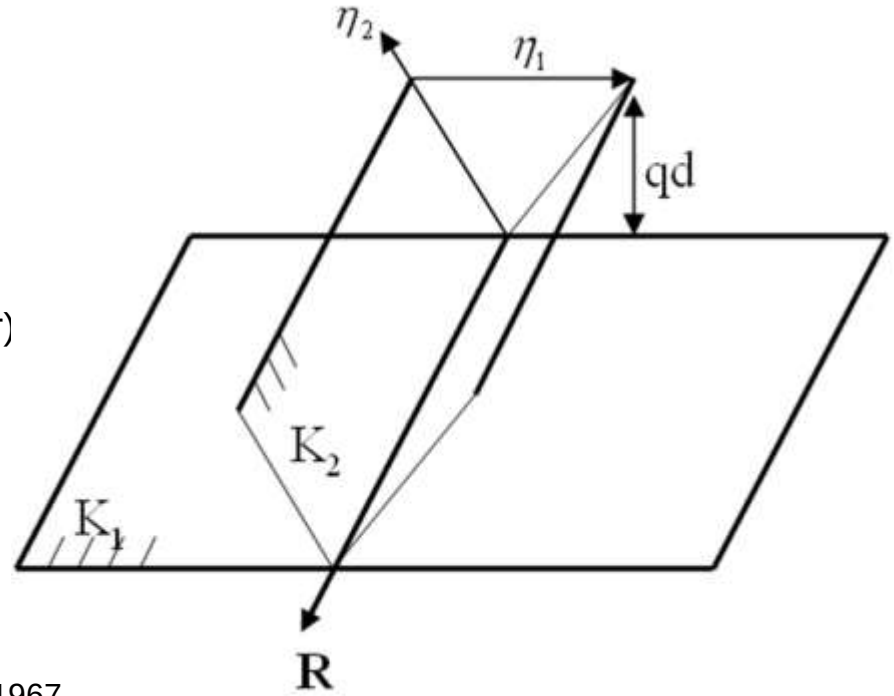



“Easy“ schematics twinning fcc

# Twinning in hexagonal metals



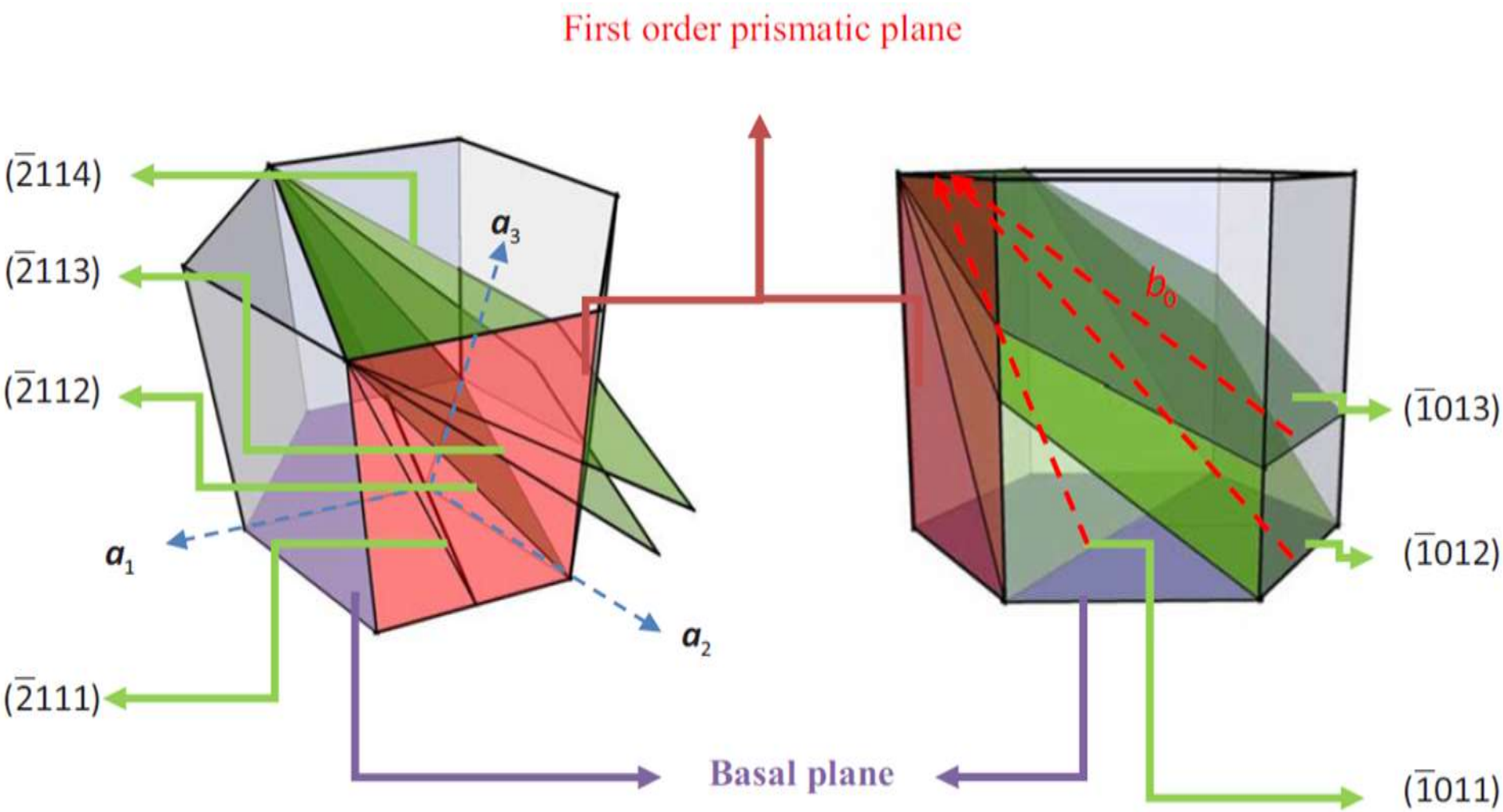

| Twinning planes | Shear directions |
|---|---|
| $(10\bar{1}1)$ | $[\bar{1}011]$ |
| $(10\bar{1}2)$ | $[10\bar{1}\bar{2}]$ |
| $(10\bar{1}3)$ | $\frac{1}{3}[11\bar{2}\bar{3}]$ |
| $(11\bar{2}1)$ | $\frac{1}{3}[11\bar{2}\bar{6}]$ |
| $(11\bar{2}2)$ | $[\bar{2}11\bar{2}]$ |
| $(11\bar{2}3)$ | $[30\bar{3}2]$ |
| $(11\bar{2}4)$ | |




$K_1$ twinning habit plane (invariant plane of twinning shear)
$K_2$ conjugate twinning plane (undistorted rotated plane)
$\eta_1$ twinning direction
$\eta_2$ conjugate twinning direction
R rotation axis
q number of twin habit planes
d interplanar distance

Partridge, 1967

# Twinning in hexagonal metals






Max-Planck-Institut für Eisenforschung GmbH

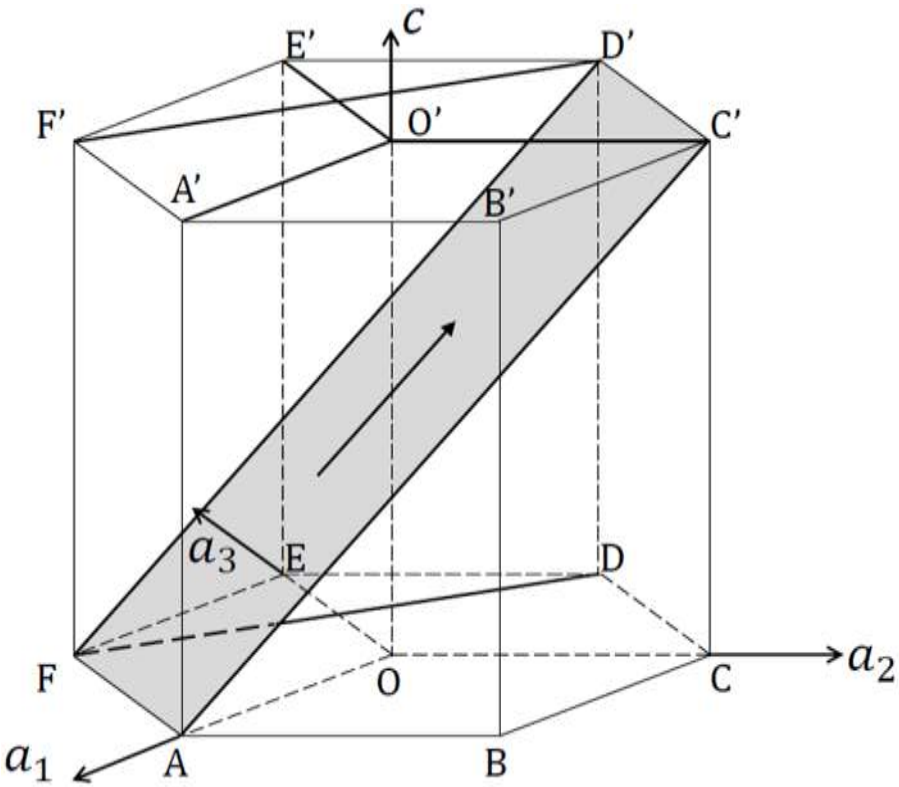
Partridge (1967)
Capolungo et al. (2008)

RWTH AACHEN UNIVERSITY

# Twinning in hexagonal metals

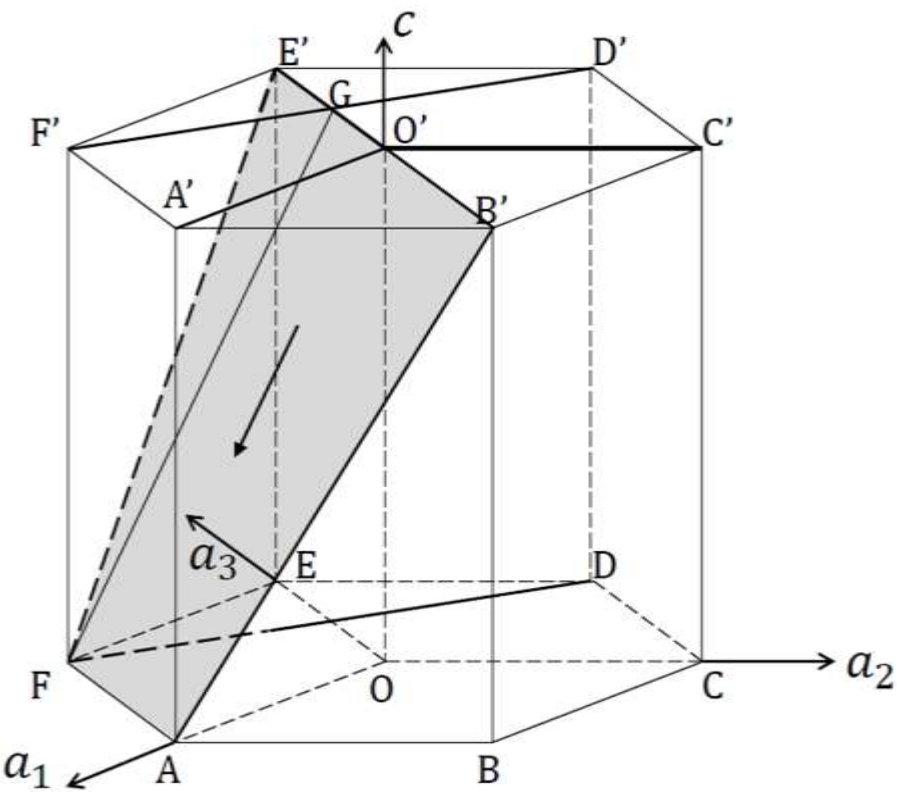
Tensile strain on c-axis

⟶ **tension twin**




Compressive strain on c-axis

⟶ **compression twin**

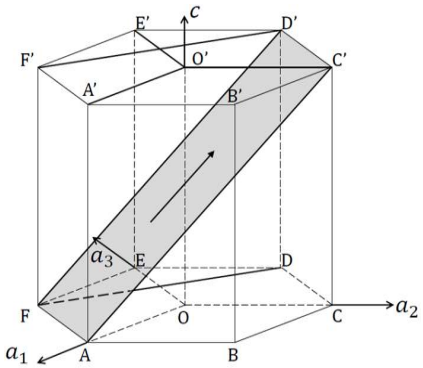



ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane

# Twinning in hexagonal metals

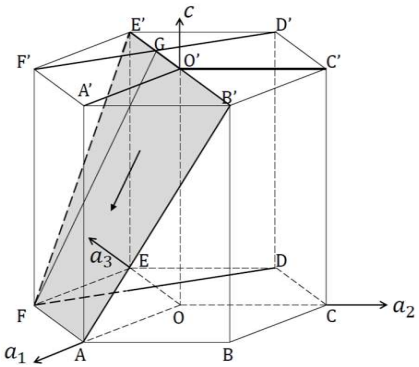
Tensile strain on c-axis

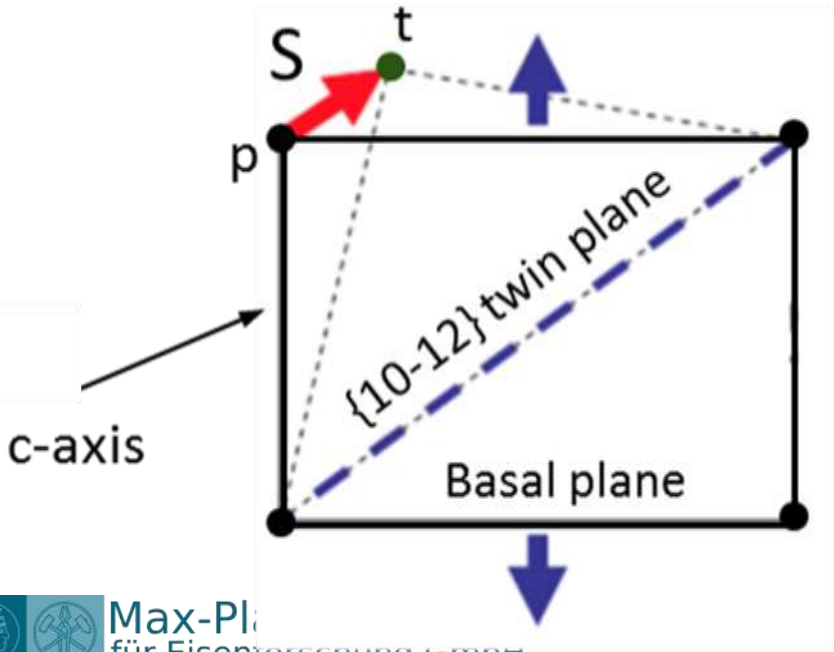
⟶ **tension twin**

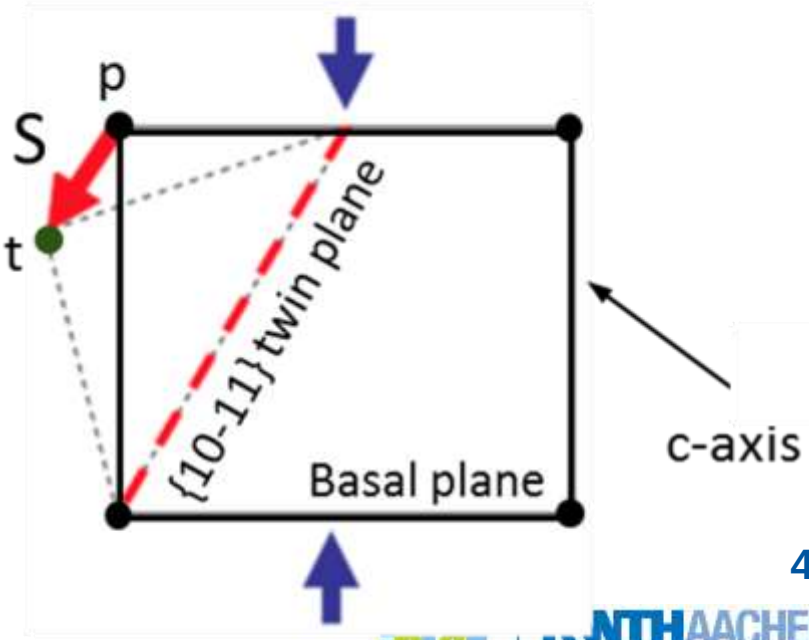



Compressive strain on c-axis

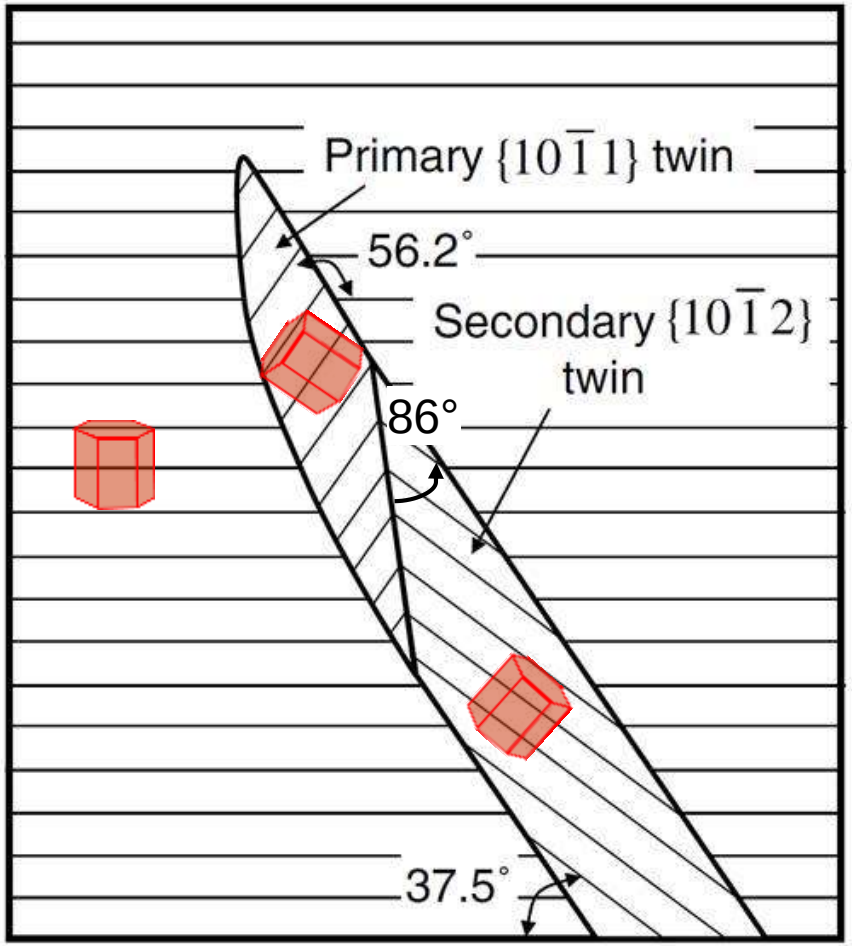
⟶ **compression twin**

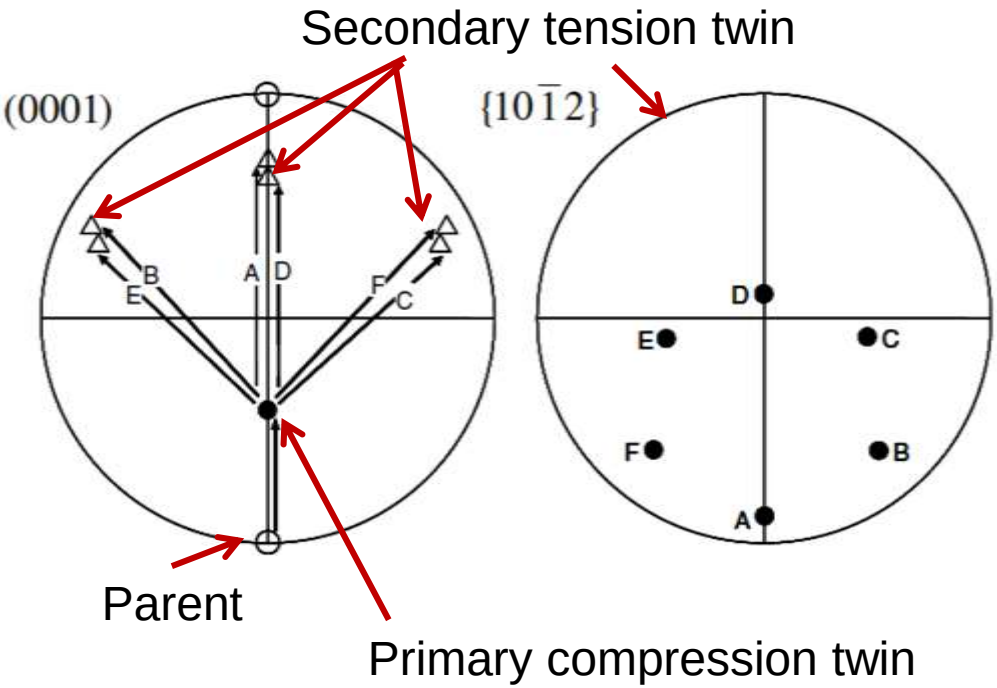


# Twinning in hexagonal metals



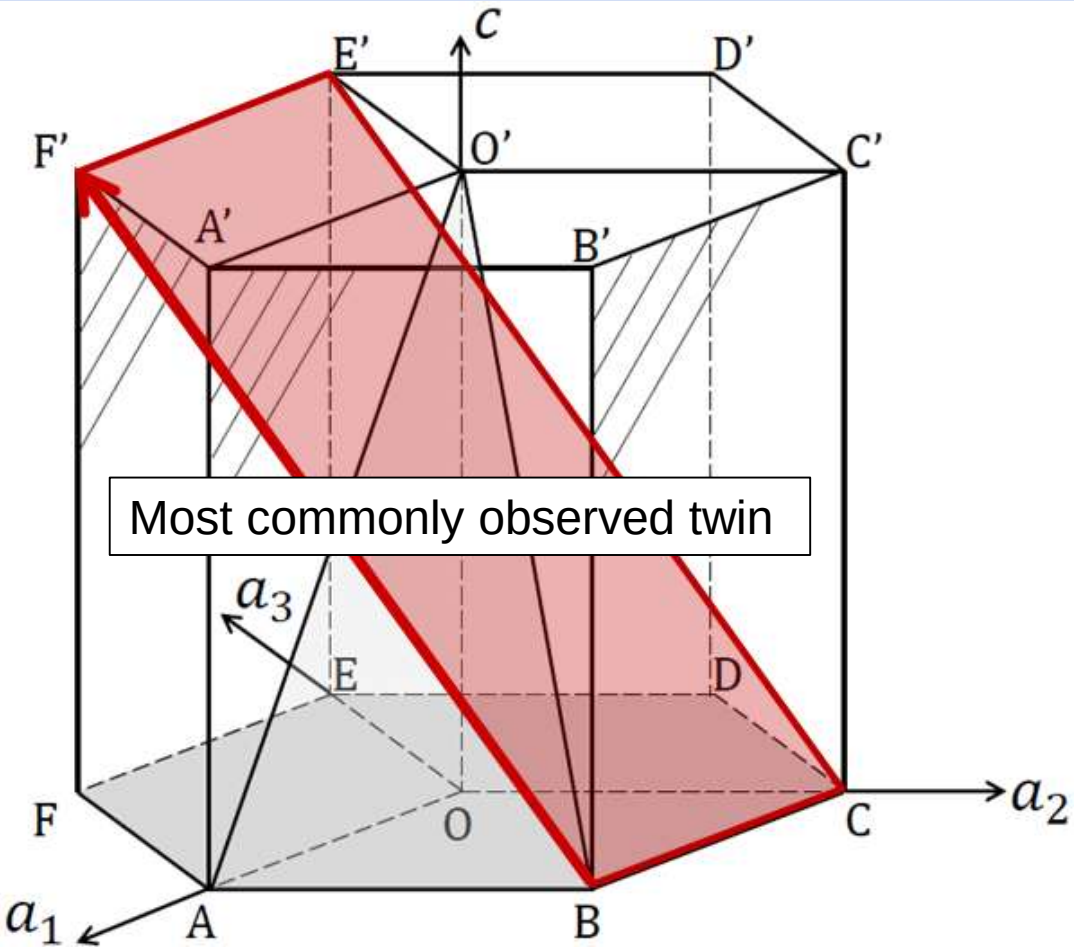




Secondary twin:
"Twin inside twin"
Twin misorientation: primary / secondary twin

Parallel lines are basal plane traces

Barnett (2008)

# Twinning in hexagonal metals




ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane

$\{10\bar{1}2\}\langle\bar{1}011\rangle$ tension twin
(compression: Zn, Cd)

Basal plane rotation: $86°\ \langle 1\bar{2}10\rangle$

$K_1$: $\{10\bar{1}2\}$
$K_2$: $\{10\bar{1}\bar{2}\}$
$\eta_1$: $\langle 10\bar{1}\bar{1}\rangle$
$\eta_2$: $\langle 10\bar{1}1\rangle$

$$b_{twn\eta_1} : \frac{\left(\frac{c}{a}\right)^2 - 3}{\left(\frac{c}{a}\right)^2 + 3} \qquad (*)$$

$$b_{twn\eta_2} : \frac{\left(\frac{c}{a}\right)^2 - 3}{\left(\frac{c}{a}\right)^2 + 3} \qquad (*)$$

Twinning shear: $\dfrac{\left(\frac{c}{a}\right)^2 - 3}{\left(\frac{c}{a}\right)\sqrt{3}}$

(*) $b_{twn\eta i}$ : Bugers vector of zonal twin dislocation $\eta_i$ - „simple“ geometrical description of complex atomic shuffling to form twin

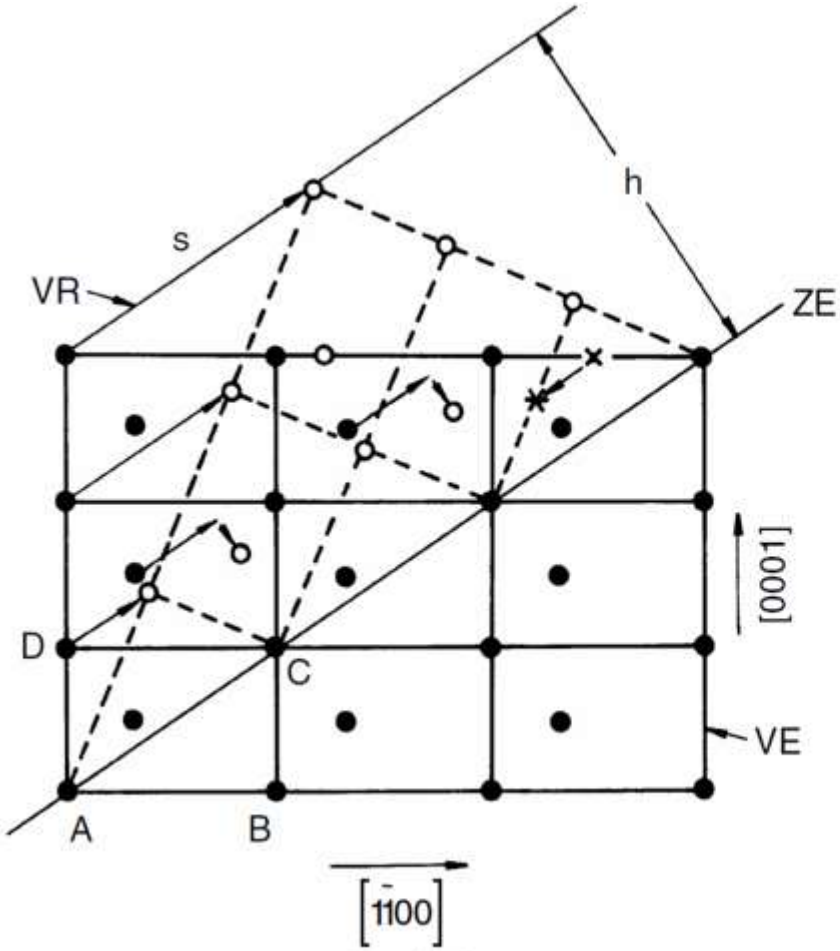
# Twinning in hexagonal metals

Tensile strain on c-axis

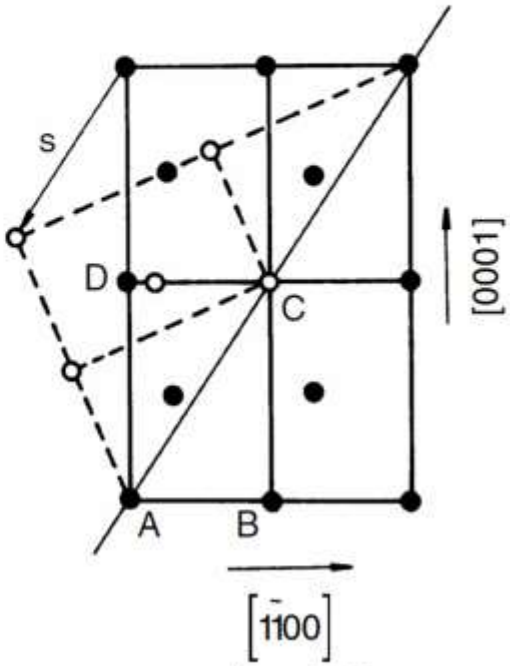
⟶ **tension twin**

Compressive strain on c-axis

⟶ **compression twin**



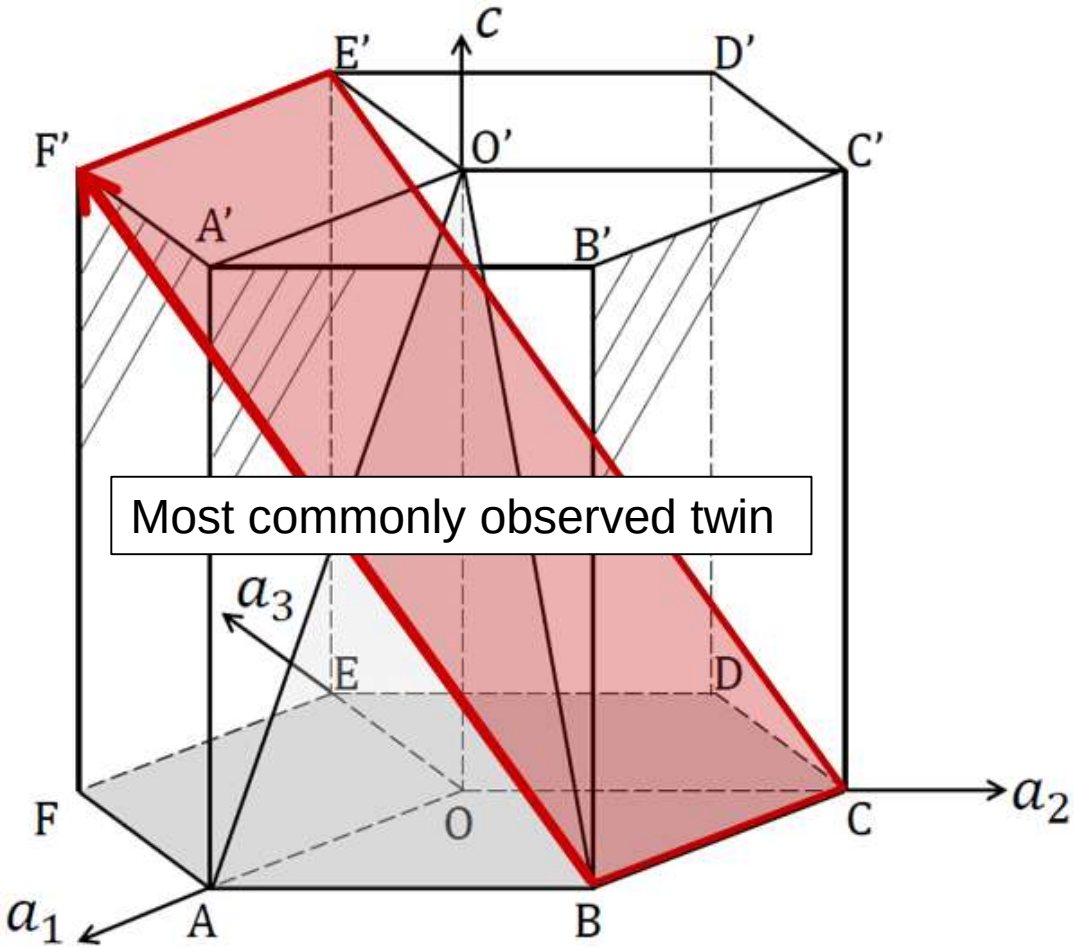

c/a < 1.73




c/a > 1.73

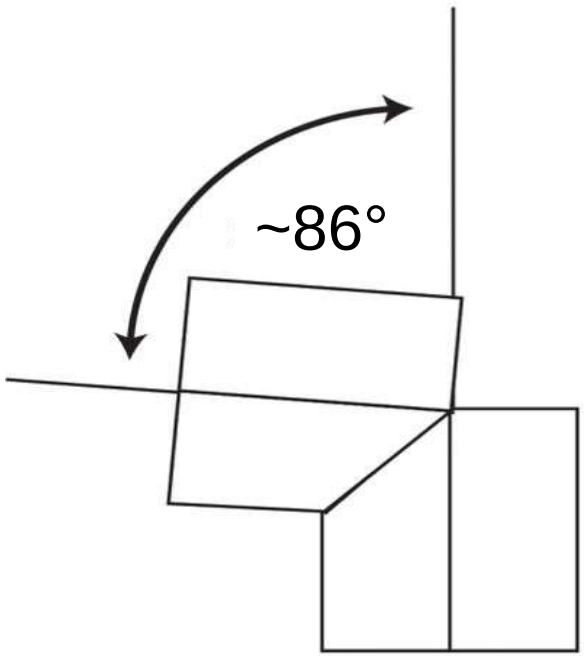
$\{10\bar{1}2\}\langle\bar{1}011\rangle$ twin

# Twinning in hexagonal metals




$\{10\bar{1}2\}\langle\bar{1}011\rangle$ tension twin
(compression: Zn, Cd)

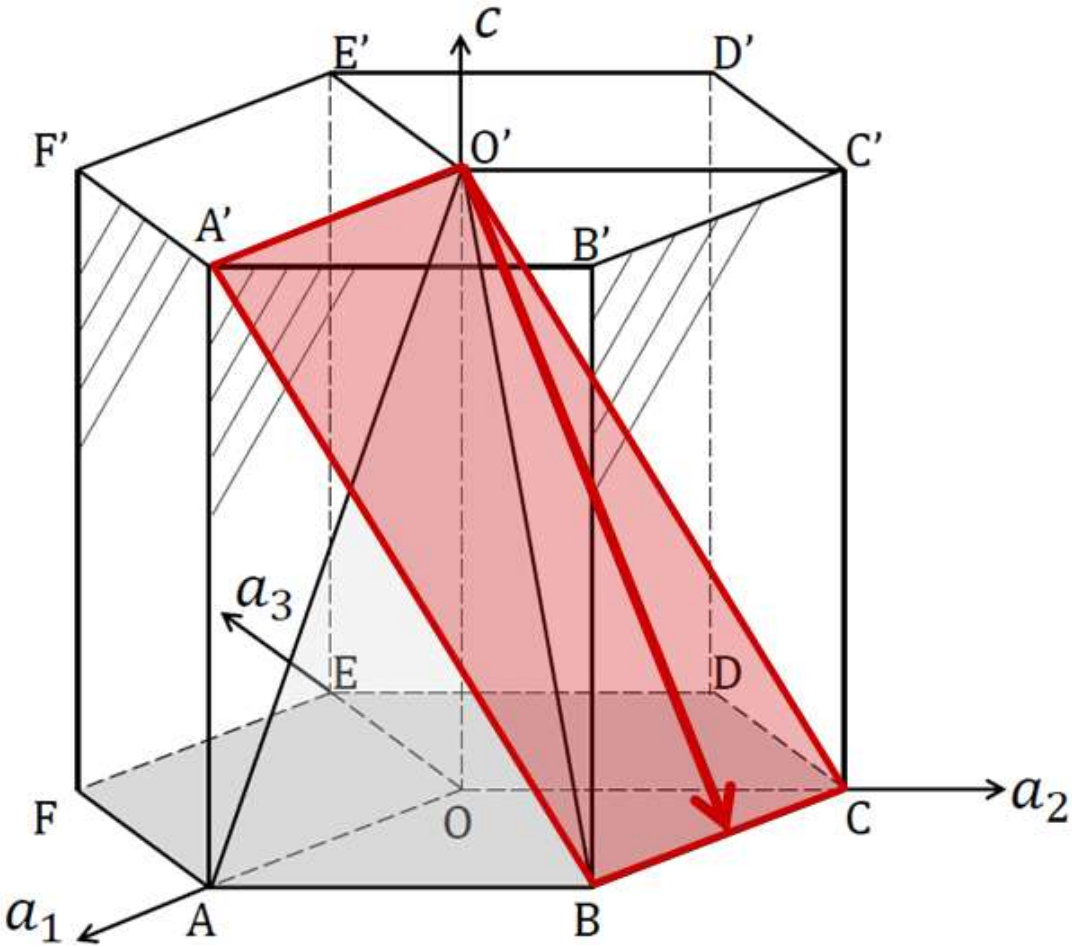
Basal plane rotation:~86° $\langle 1\bar{2}10\rangle$




ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane

(*) $b_{twnl}$ : Bugers vector of zonal twin dislocation $\eta_i$ - „simple“ geometrical description of complex atomic shuffling to form twin

# Twinning in hexagonal metals




ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane

$\{10\bar{1}1\}\langle 10\bar{1}\bar{2}\rangle$ compression twin

Basal plane rotation: $56°\ \langle \bar{1}2\bar{1}0\rangle$

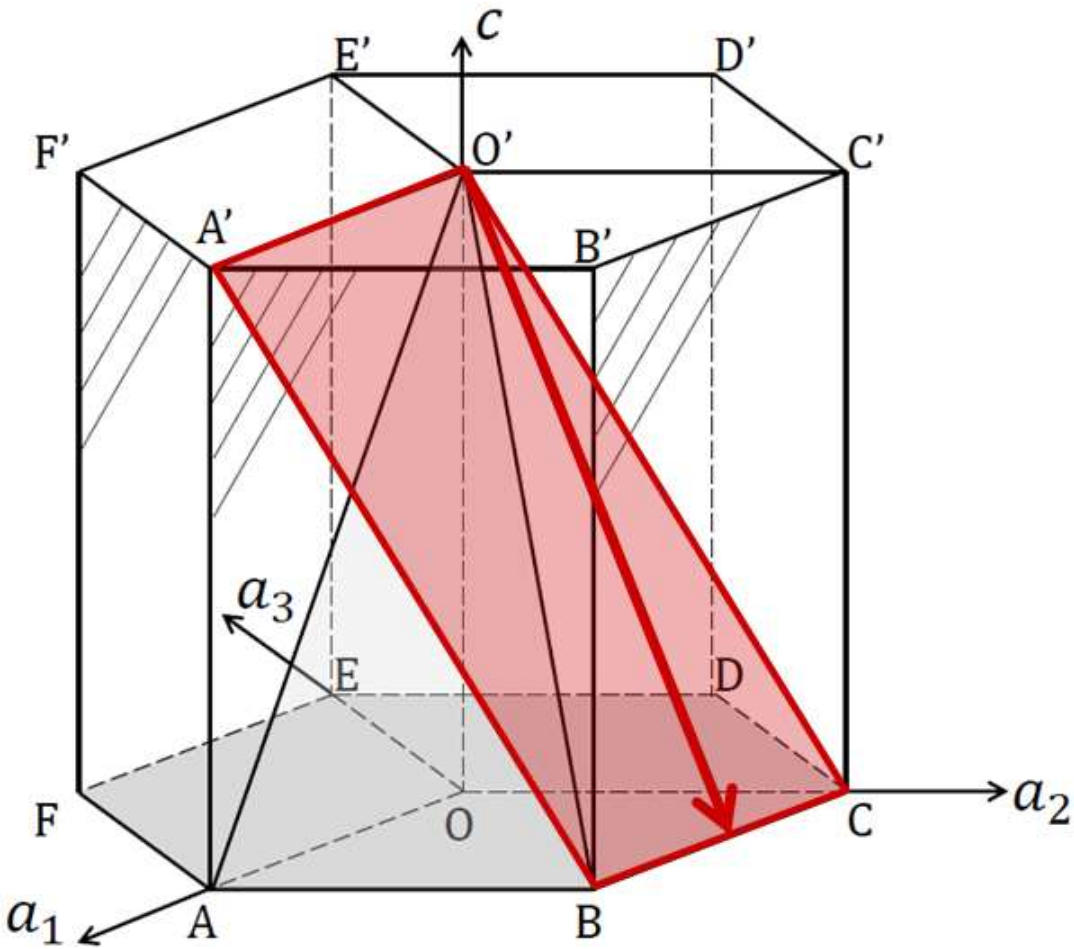
$K_1$: $\{10\bar{1}1\}$
$K_2$: $\{10\bar{1}\bar{3}\}$
$\eta_1$: $\langle 10\bar{1}\bar{2}\rangle$
$\eta_2$: $\langle 30\bar{3}2\rangle$

$$b_{twn\eta_1} : \frac{4\left(\frac{c}{a}\right)^2 - 9}{4\left(\frac{c}{a}\right)^2 + 3} \quad (*)$$

$$b_{twn\eta_2} : \frac{4\left(\frac{c}{a}\right)^2 - 9}{4\left(\frac{c}{a}\right)^2 + 27} \quad (*)$$

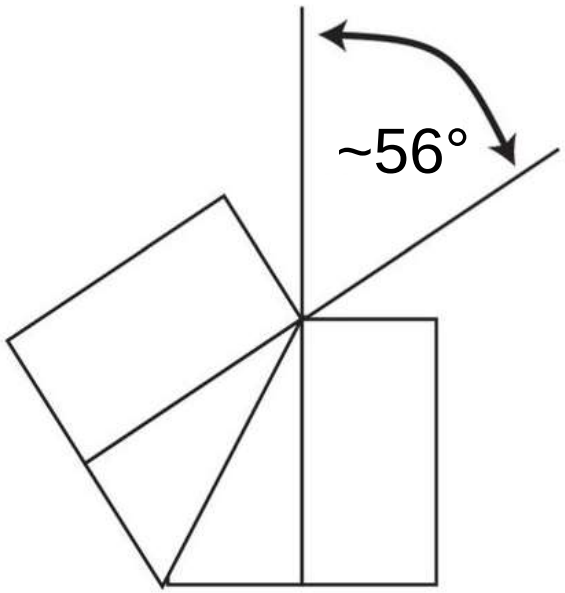
Twinning shear: $\dfrac{4\left(\frac{c}{a}\right)^2 - 9}{4\left(\frac{c}{a}\right)\sqrt{3}}$

# Twinning in hexagonal metals



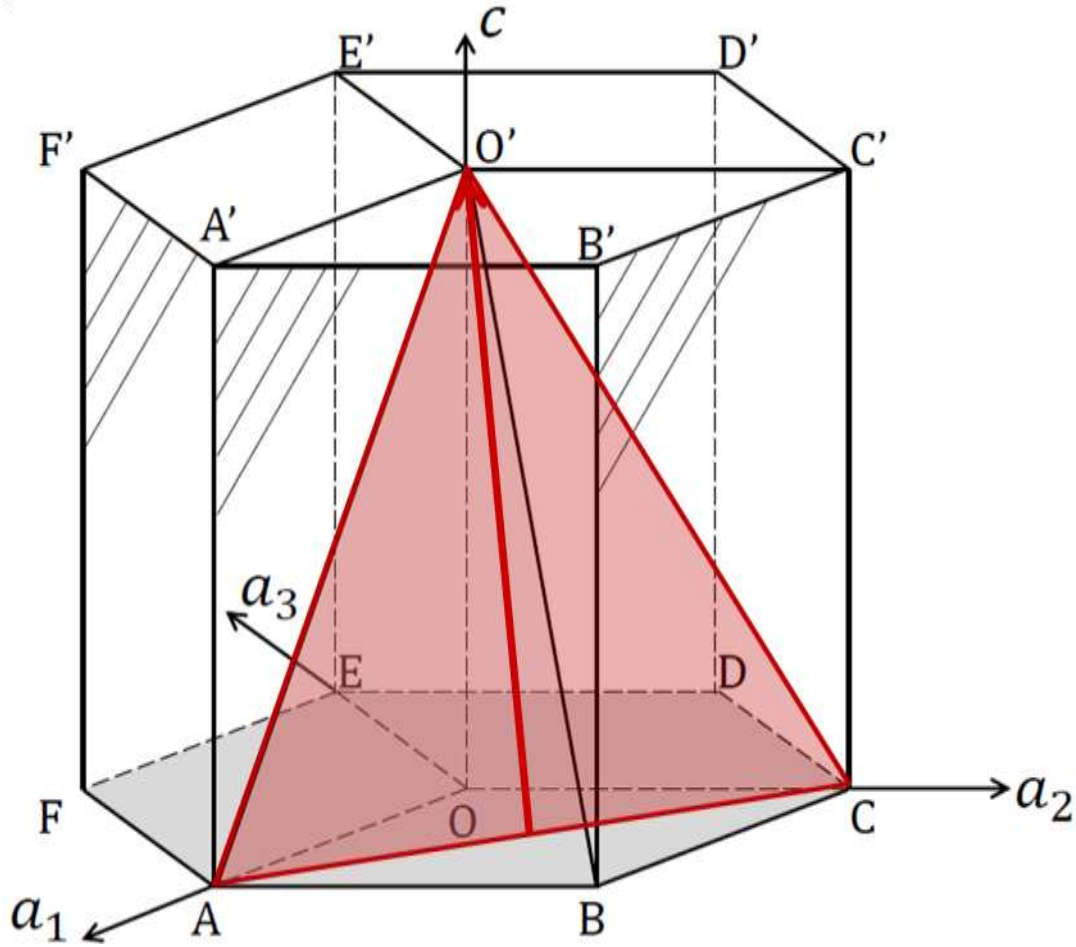

$\{10\bar{1}1\}\langle 10\bar{1}\bar{2}\rangle$ compression twin

Basal plane rotation: ~56° $\langle \bar{1}2\bar{1}0\rangle$




ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane

# Twinning in hexagonal metals




$\{10\bar{2}1\}\langle\bar{1}\bar{1}26\rangle$ tension twin

Basal plane rotation: $35°\ \langle 1\bar{1}00\rangle$

$K_1$: $\{11\bar{2}1\}$
$K_2$: $(0002)$
$\eta_1$: $\frac{1}{3}\langle\bar{1}\bar{1}26\rangle$
$\eta_2$: $\frac{1}{3}\langle 11\bar{2}0\rangle$

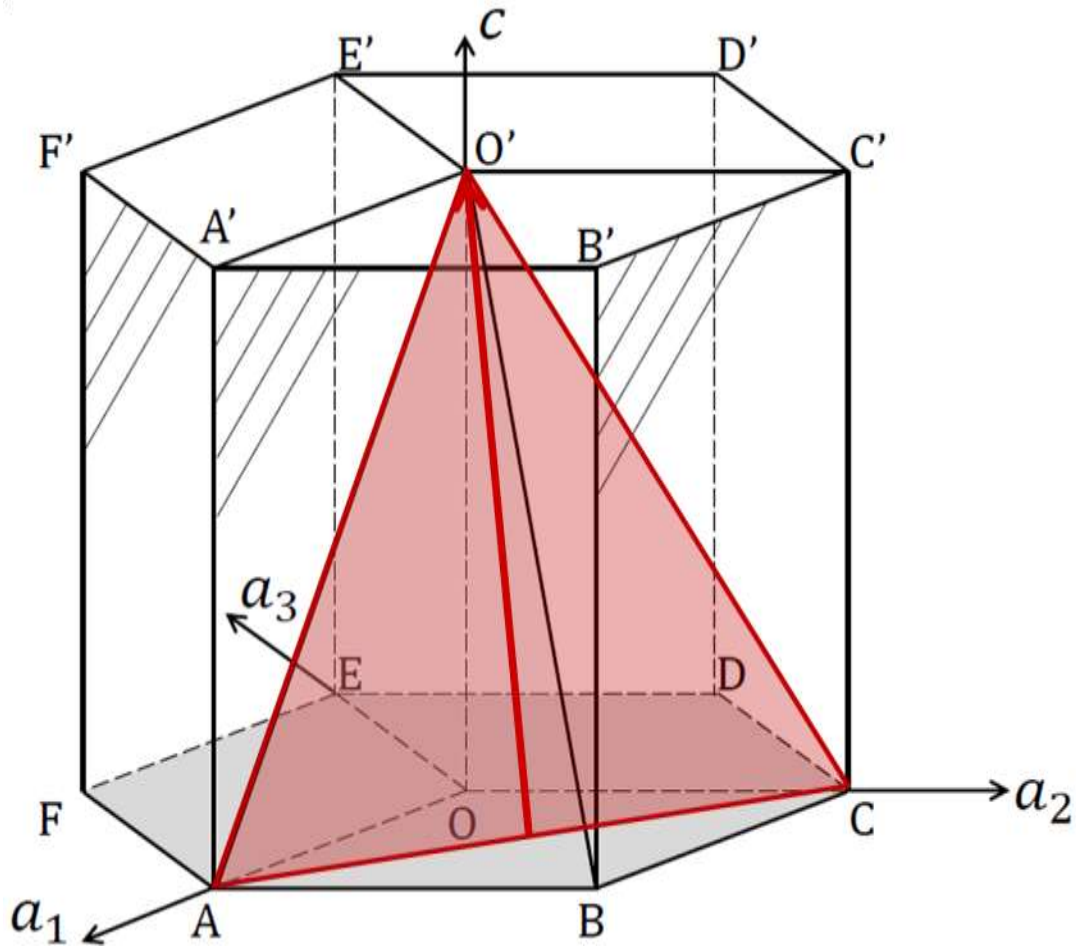
$b_{twn\eta_1}$ : $\dfrac{1}{4\left(\frac{c}{a}\right)^2+1}$ (*)

$b_{twn\eta_2}$ : $1$ (*)

Twinning shear: $\dfrac{1}{\left(\frac{c}{a}\right)}$

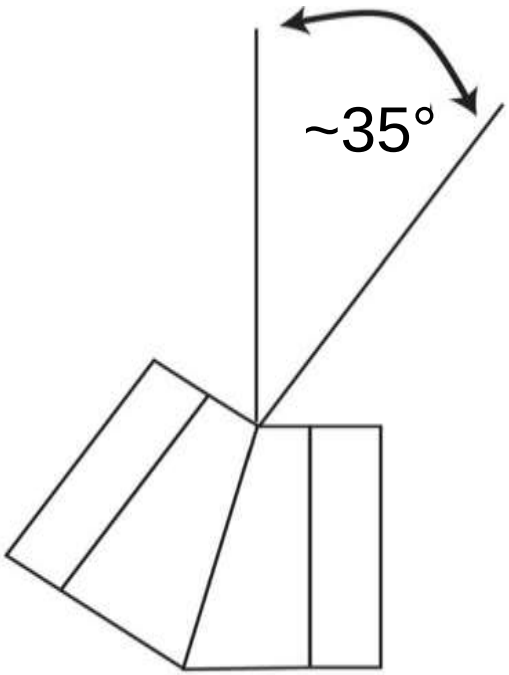
ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane

# Twinning in hexagonal metals



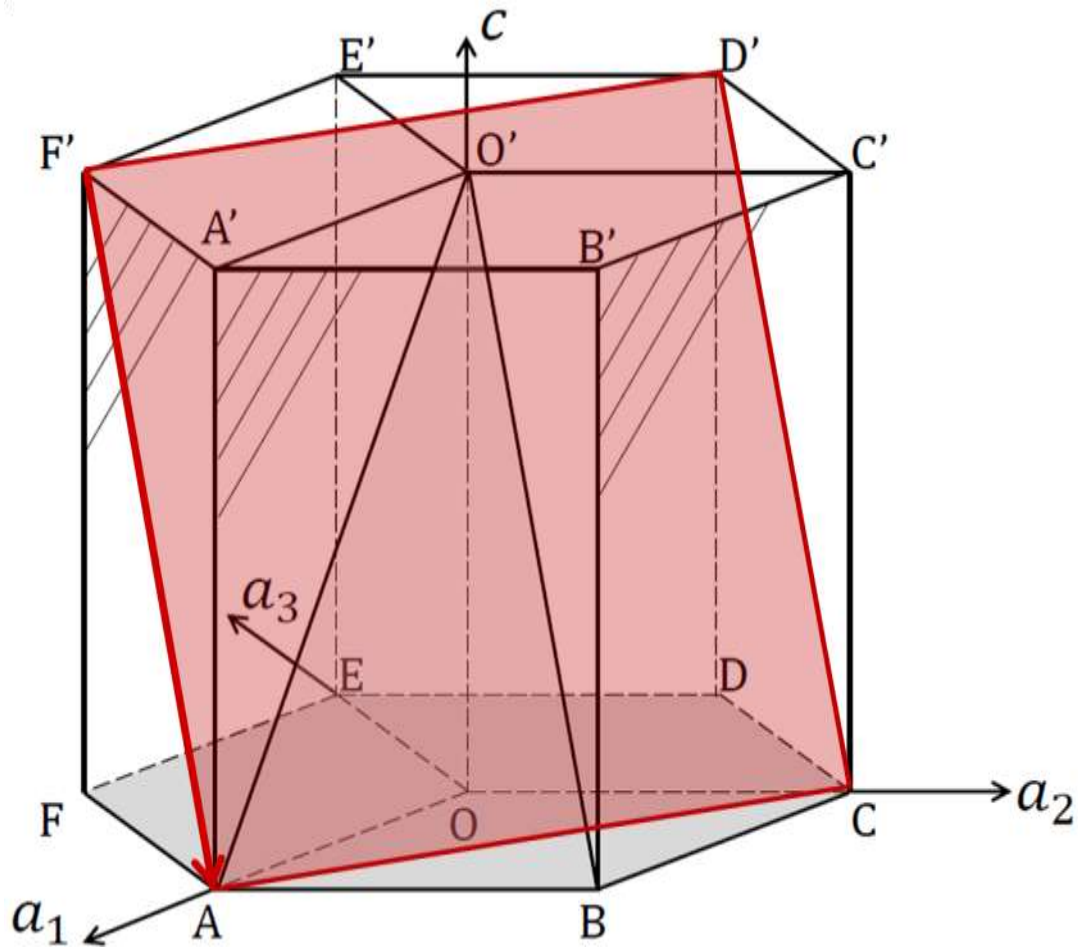

$\{10\bar{2}1\}\langle\bar{1}\bar{1}26\rangle$ tension twin

Basal plane rotation: ~35° $\langle 1\bar{1}00\rangle$




ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane

# Twinning in hexagonal metals




ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane

$\{11\bar{2}2\}\langle 11\bar{2}\bar{3}\rangle$ compression twin

Basal plane rotation: 55° $\langle \bar{1}100\rangle$

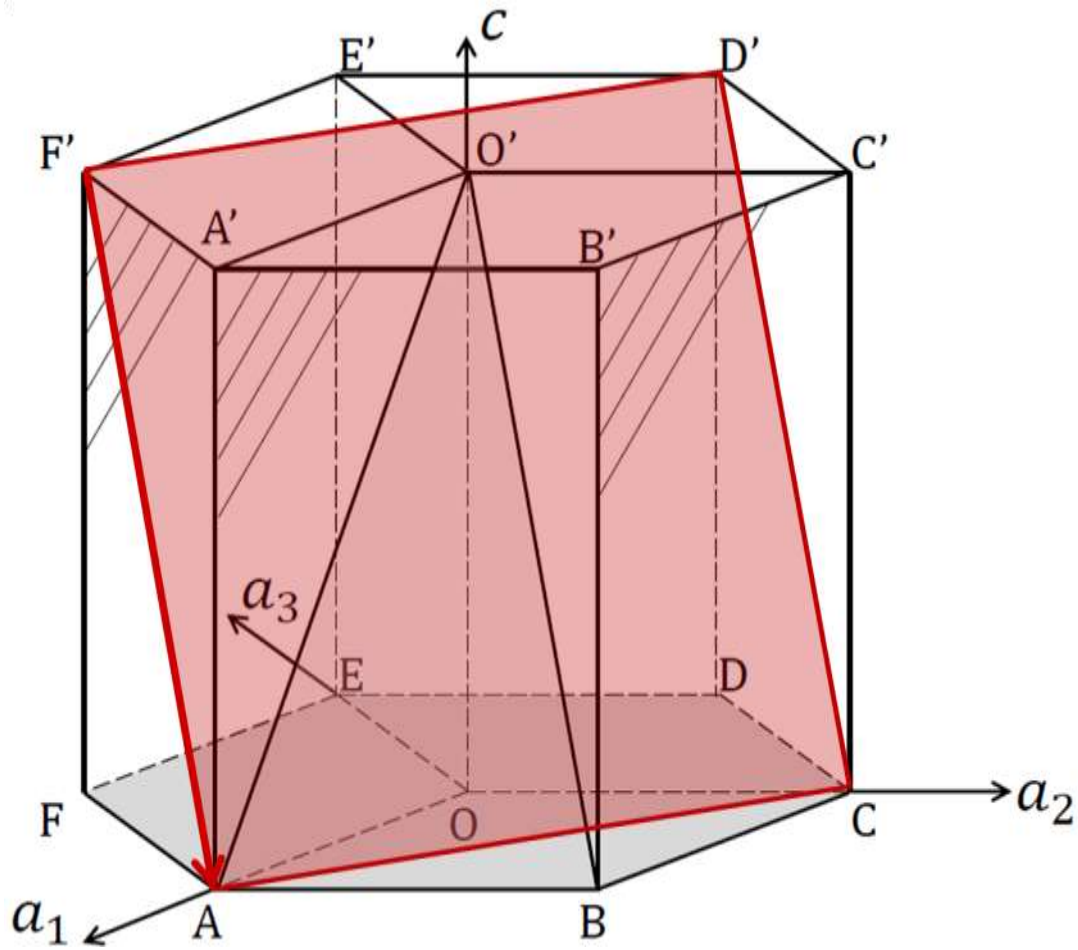
$K_1$: $\{11\bar{2}2\}$
$K_2$: $\{11\bar{2}\bar{4}\}$
$\eta_1$: $\frac{1}{3}\langle 11\bar{2}\bar{3}\rangle$
$\eta_2$: $\frac{1}{3}\langle 22\bar{4}3\rangle$

$$b_{tw\eta_1} : \frac{\left(\frac{c}{a}\right)^2 - 2}{\left(\frac{c}{a}\right)^2 + 2} \qquad (*)$$

$$b_{tw\eta_2} : \frac{\left(\frac{c}{a}\right)^2 - 2}{\left(\frac{c}{a}\right)^2 + 4} \qquad (*)$$

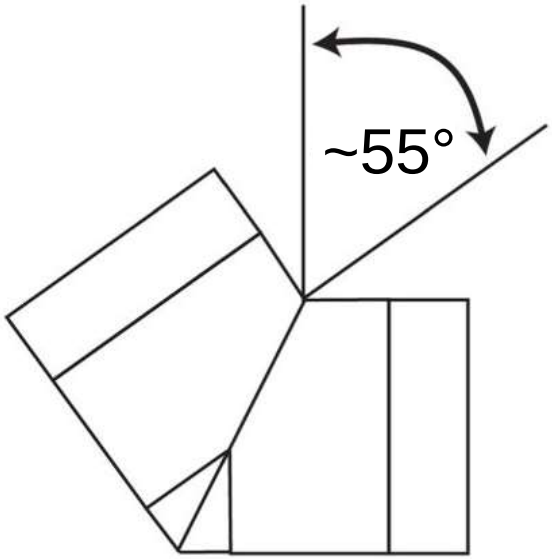
Twinning shear: $\dfrac{2\left(\left(\frac{c}{a}\right)^2 - 2\right)}{3\left(\frac{c}{a}\right)}$

# Twinning in hexagonal metals




$\{11\bar{2}2\}\langle 11\bar{2}\bar{3}\rangle$ compression twin

Basal plane rotation: $\sim 55°\ \langle \bar{1}100\rangle$




ACE: basal plane
ABB'A': prismatic plane
ABO': first order pyramidal plane
ACD'F': second order pyramidal plane

# Twinning in hexagonal metals

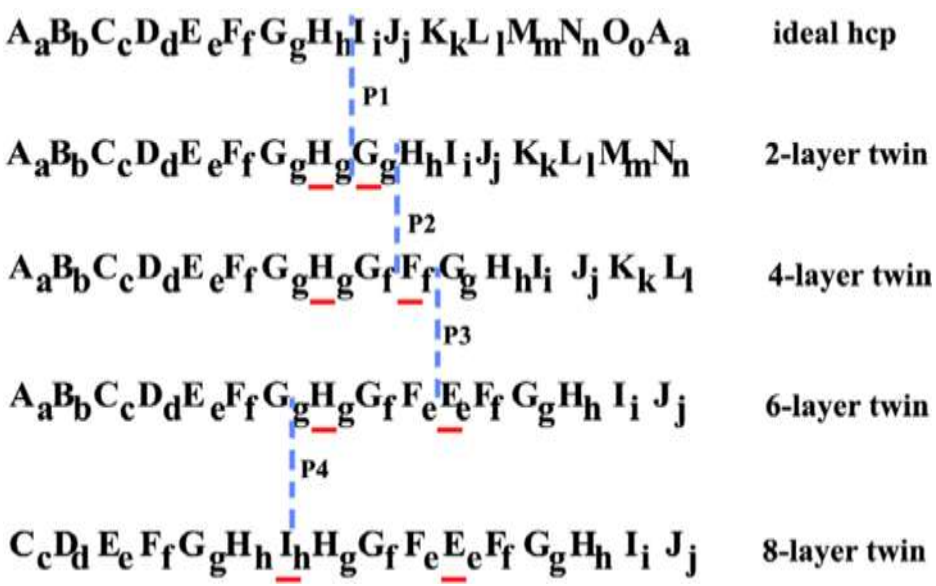
Twin nucleation

- “Normal“ twinning mechanism
  Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism
  Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations

# Twinning in hexagonal metals

Twin nucleation

- “Normal“ twinning mechanism
  Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism
  Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations




“Normal“ twinning



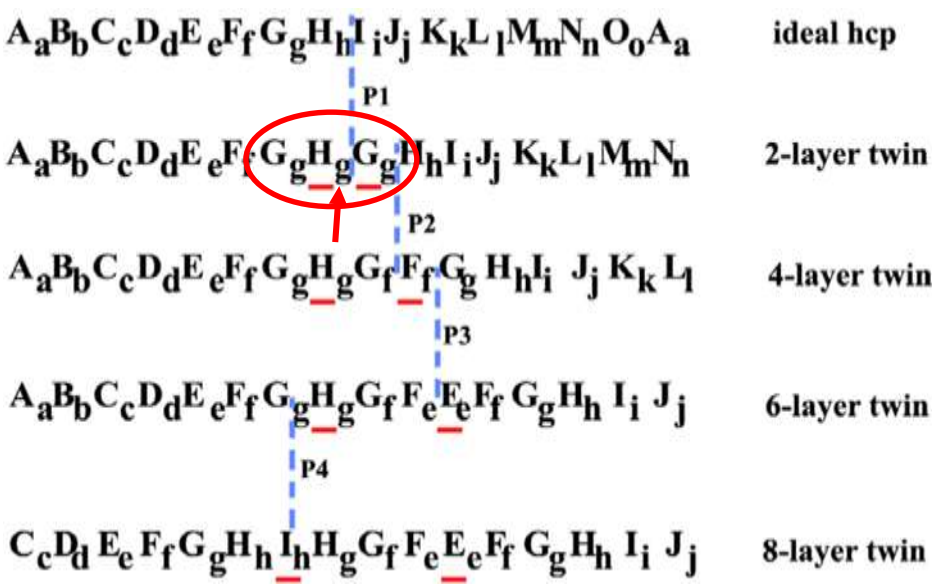


Tomé et al. (2009)

# Twinning in hexagonal metals

Twin nucleation

- “Normal“ twinning mechanism
  Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism
  Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations




“Normal“ twinning



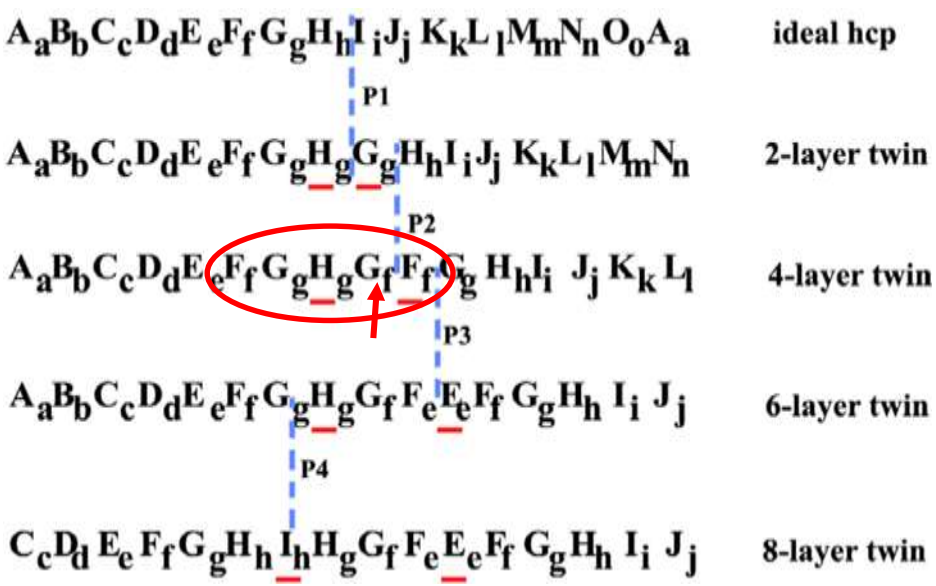


Tomé et al. (2009)

# Twinning in hexagonal metals

Twin nucleation

- “Normal“ twinning mechanism
  Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism
  Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations




“Normal“ twinning



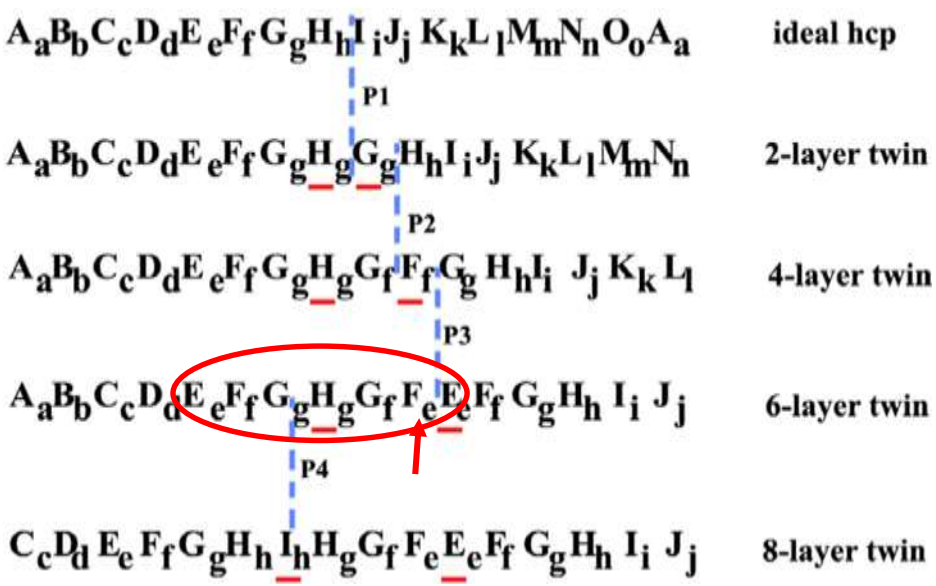


Tomé et al. (2009)

# Twinning in hexagonal metals

Twin nucleation

- “Normal“ twinning mechanism
  Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism
  Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations




“Normal“ twinning



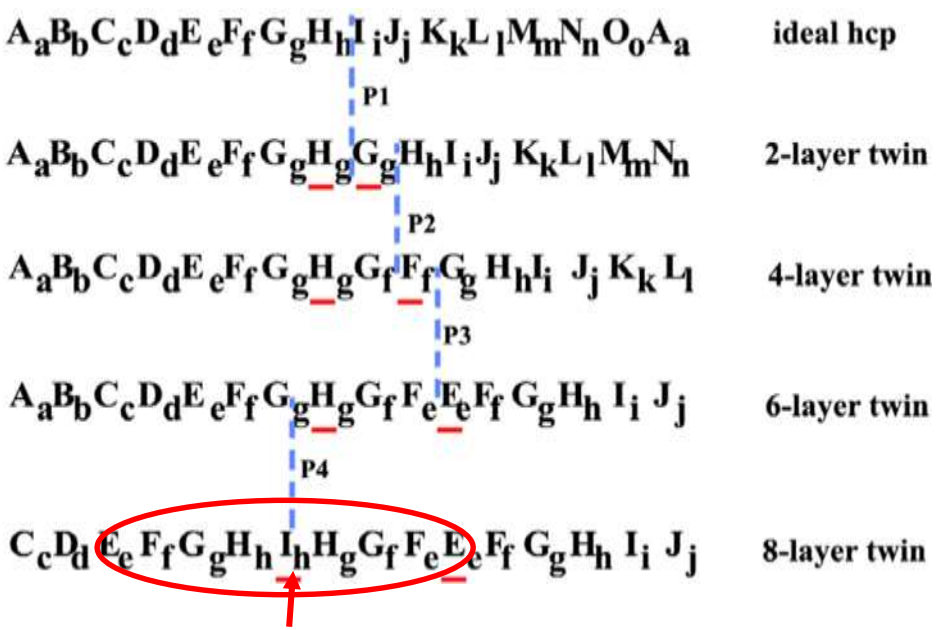


Tomé et al. (2009)

# Twinning in hexagonal metals

Twin nucleation

- “Normal“ twinning mechanism
  Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism
  Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations




“Normal“ twinning



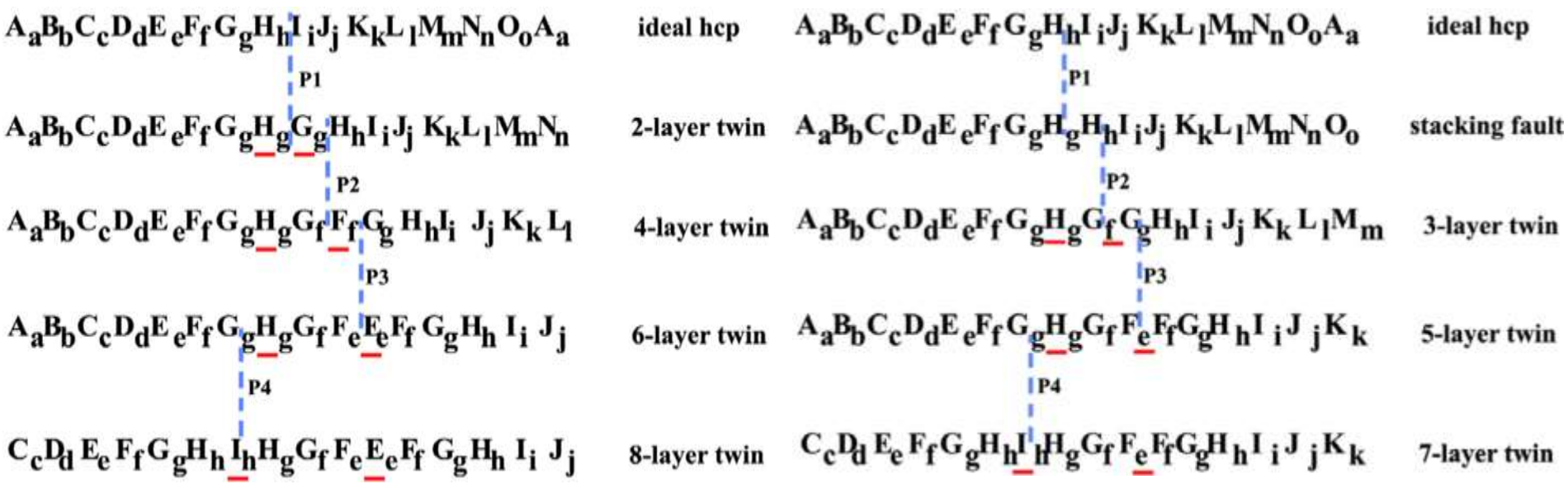


Tomé et al. (2009)

# Twinning in hexagonal metals

Twin nucleation

- “Normal“ twinning mechanism
  Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism
  Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations




“Normal“ twinning

“Zonal“ twinning



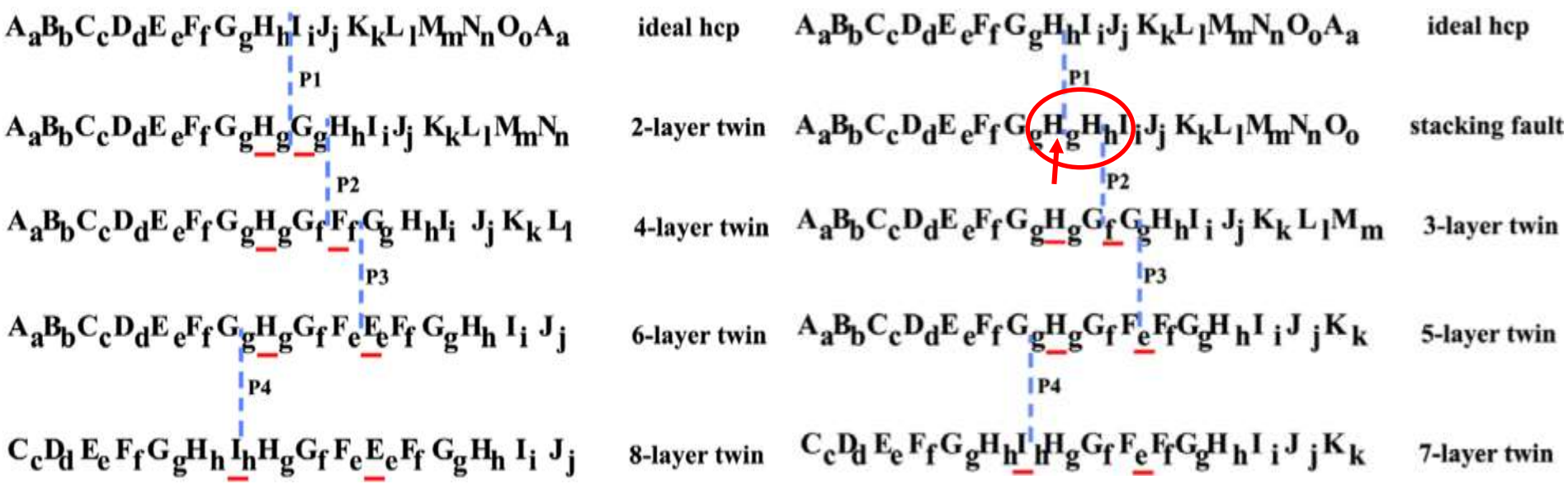


Tomé et al. (2009)

# Twinning in hexagonal metals

Twin nucleation

- “Normal“ twinning mechanism
  Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism
  Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations




“Normal“ twinning

“Zonal“ twinning



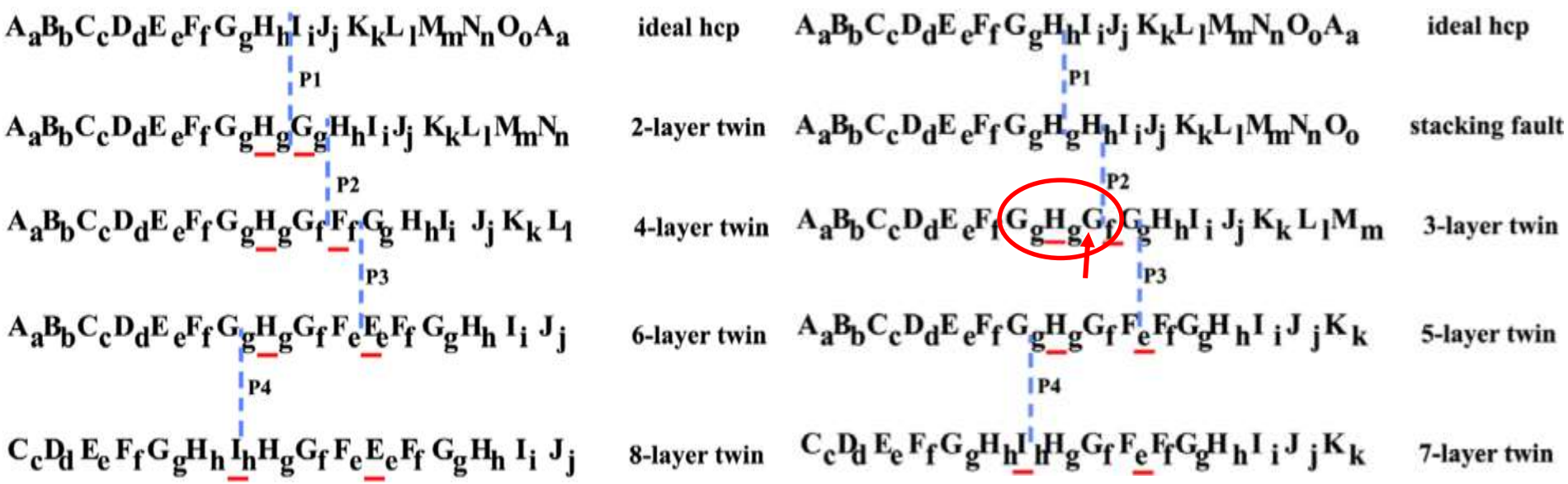


Tomé et al. (2009)

# Twinning in hexagonal metals

Twin nucleation

- “Normal“ twinning mechanism
  Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism
  Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations




“Normal“ twinning

“Zonal“ twinning



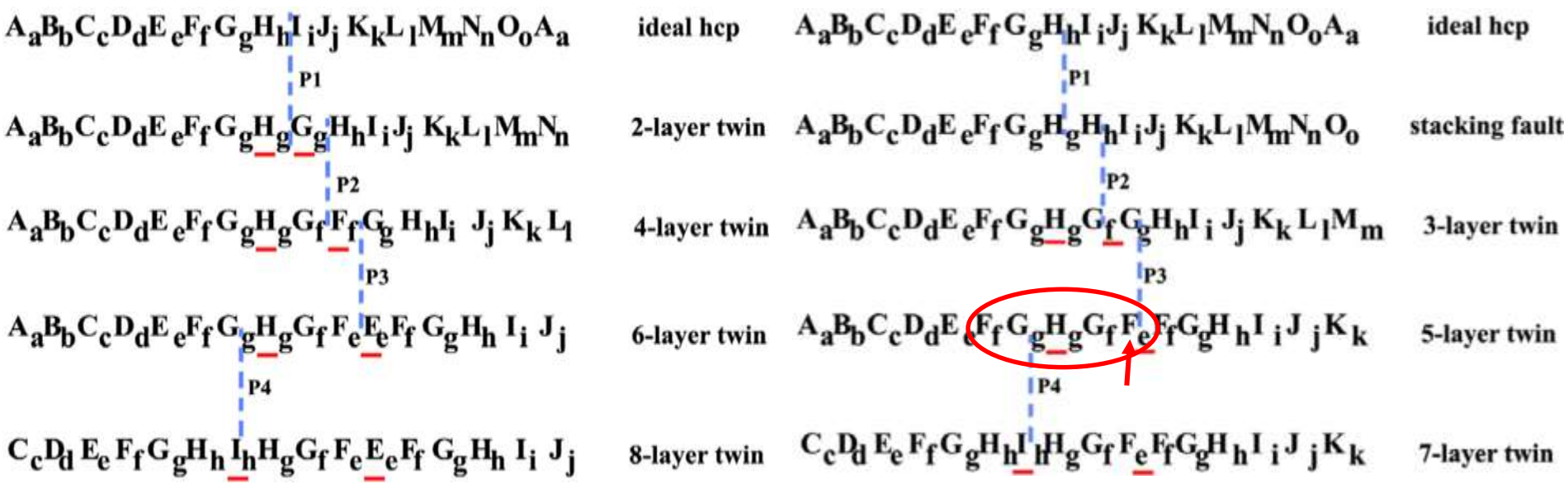


Tomé et al. (2009)

# Twinning in hexagonal metals

Twin nucleation

- “Normal“ twinning mechanism
  Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism
  Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations




“Normal“ twinning

“Zonal“ twinning



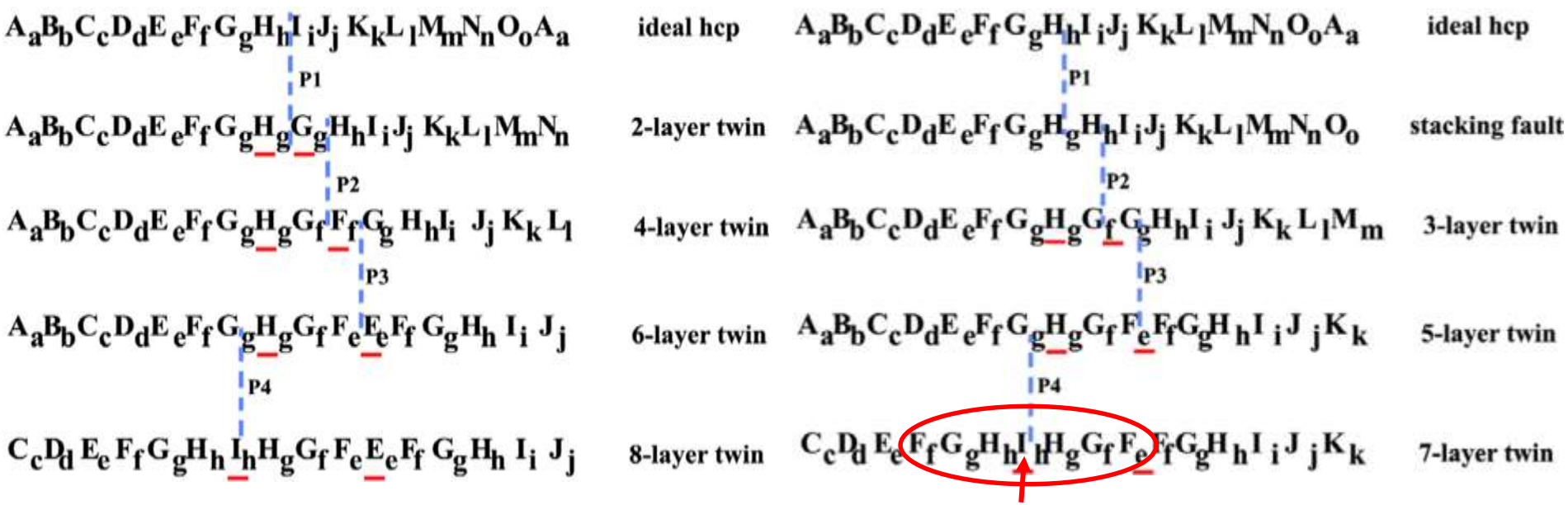


Tomé et al. (2009)

# Twinning in hexagonal metals

Twin nucleation

- “Normal“ twinning mechanism
  Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism
  Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations




“Normal“ twinning

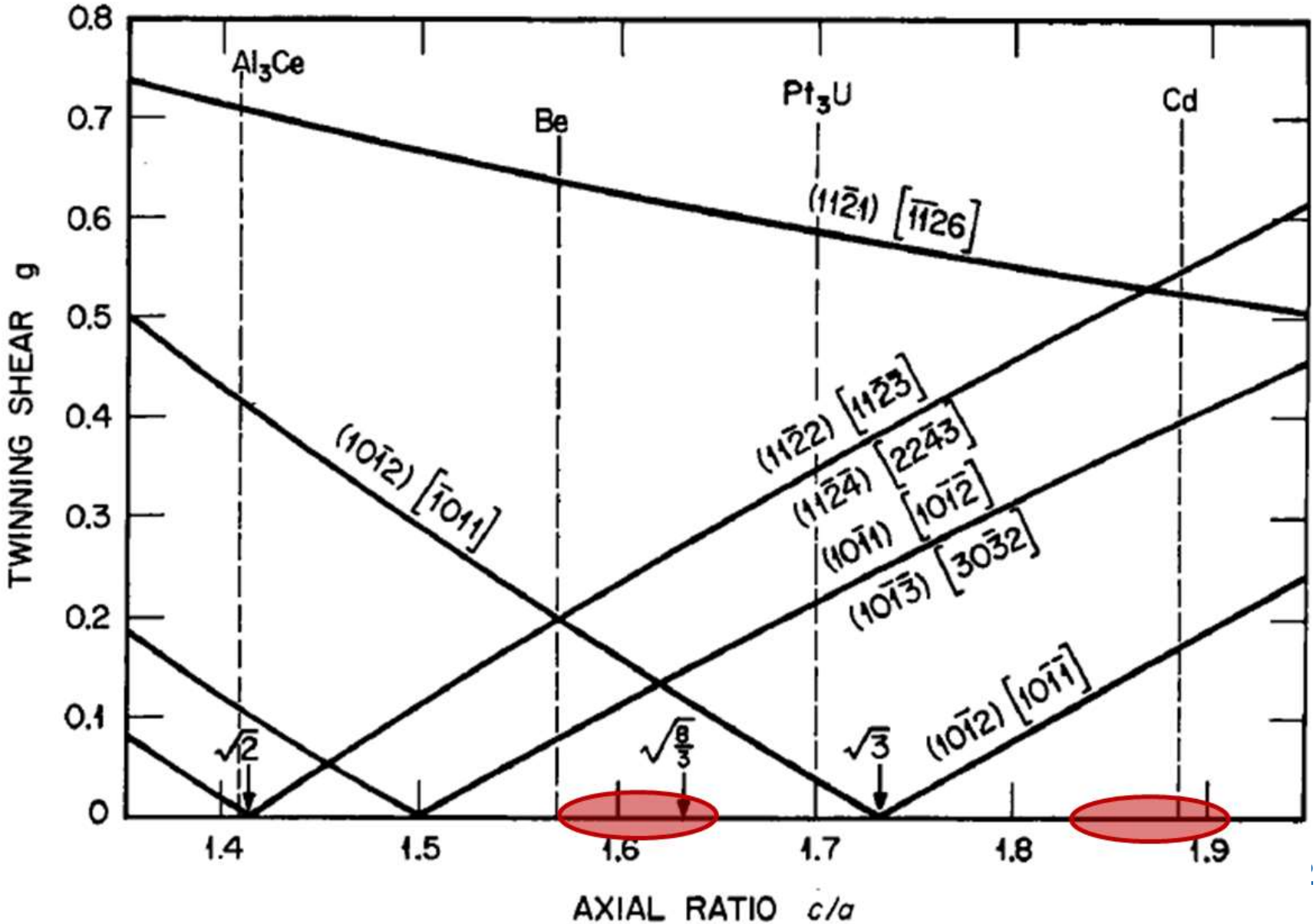
“Zonal“ twinning





Tomé et al. (2009)

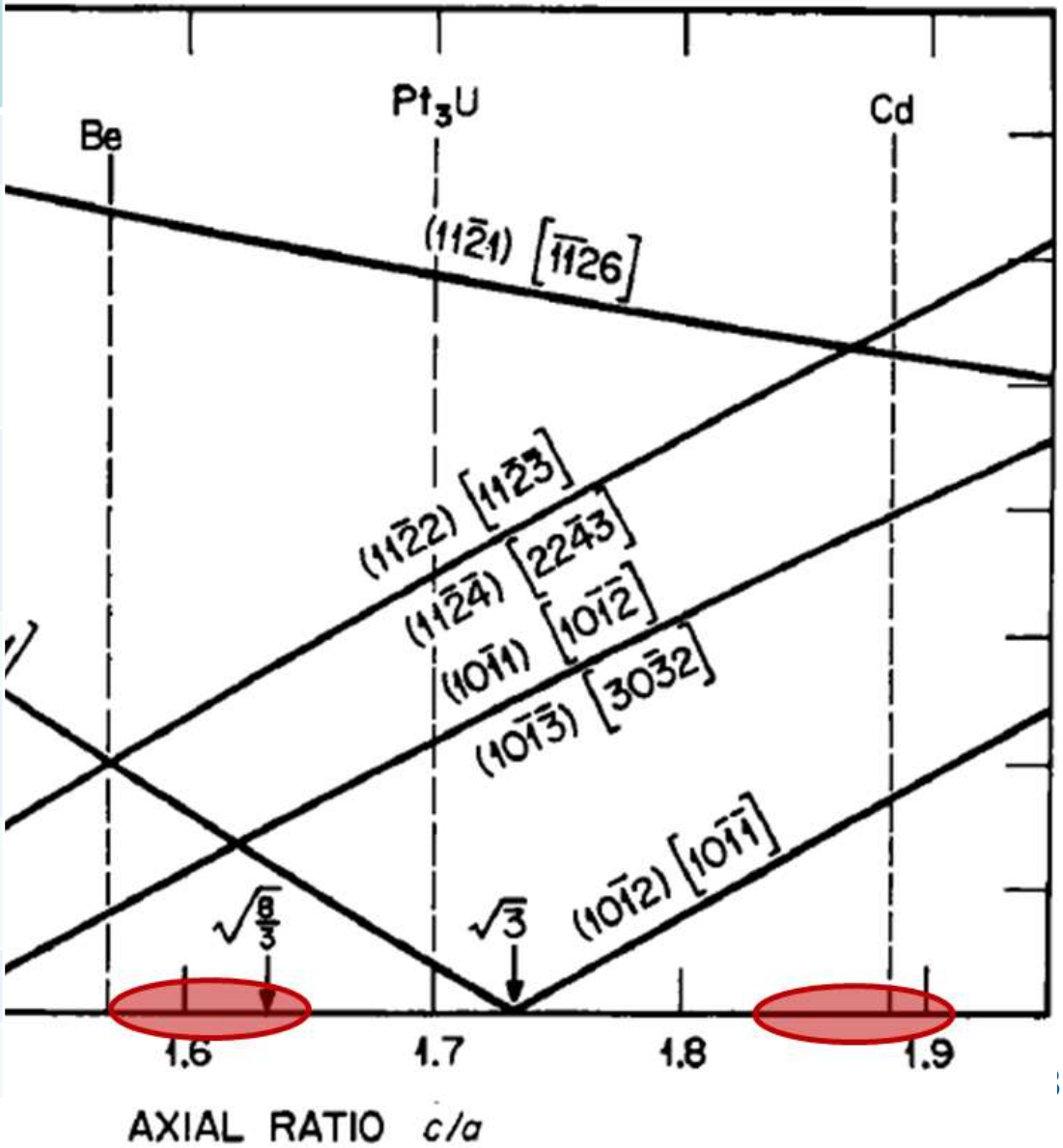
# Twinning in hexagonal metals




Yoo (1981)

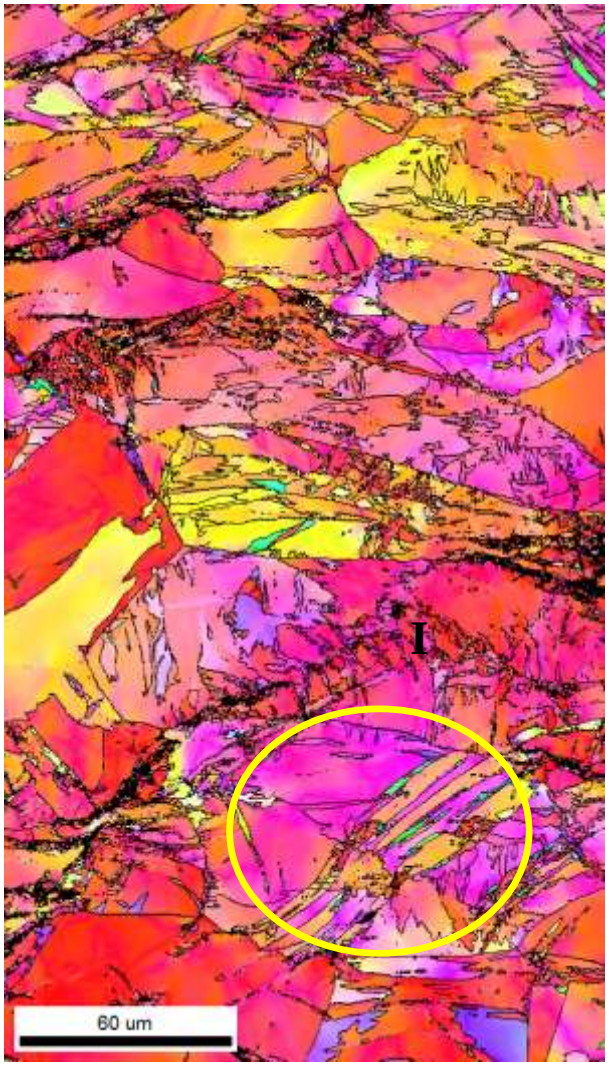
# Twinning in hexagonal metals

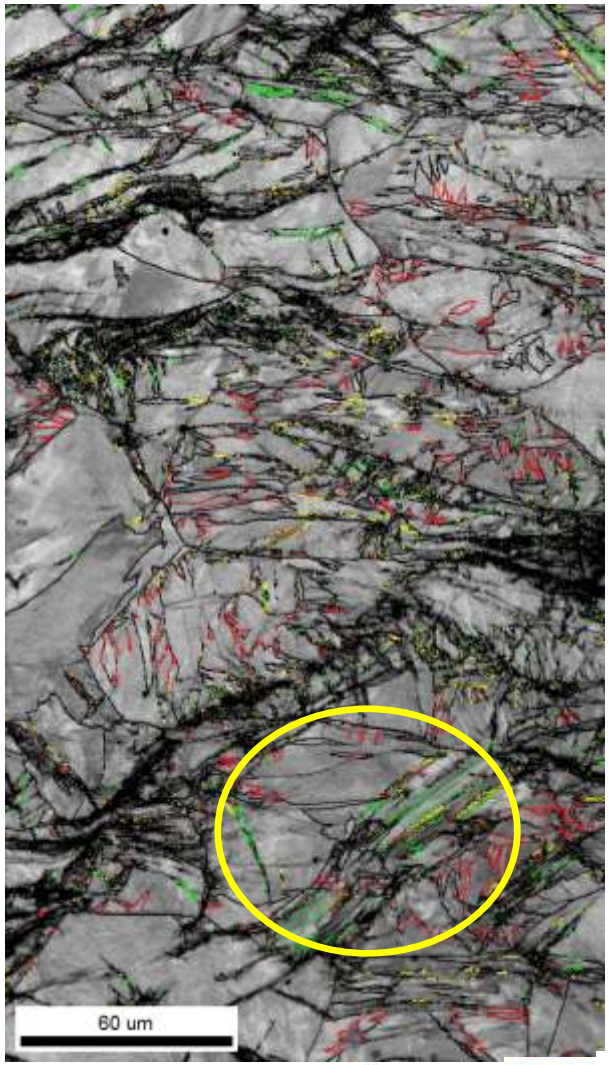
| Metal | c/a | Active twinning system(s) |
|---|---|---|
| Be | 1.568 | $\{10\bar{1}2\}\langle\bar{1}011\rangle$ |
| Ti | 1.588 | $\{10\bar{1}2\}\langle\bar{1}011\rangle$<br>$\{10\bar{1}1\}\langle10\bar{1}\bar{2}\rangle$<br>$\{10\bar{2}1\}\langle\bar{1}\bar{1}26\rangle$<br>$\{11\bar{2}2\}\langle11\bar{2}\bar{3}\rangle$ |
| Zr | 1.593 | $\{10\bar{1}2\}\langle\bar{1}011\rangle$<br>$\{10\bar{2}1\}\langle\bar{1}\bar{1}26\rangle$<br>$\{11\bar{2}2\}\langle11\bar{2}\bar{3}\rangle$ |
| Re | 1.615 | $\{10\bar{2}1\}\langle\bar{1}\bar{1}26\rangle$ |
| Co | 1.623 | $\{10\bar{1}2\}\langle\bar{1}011\rangle$<br>$\{10\bar{2}1\}\langle\bar{1}\bar{1}26\rangle$ |
| Mg | 1.623 | $\{10\bar{1}2\}\langle\bar{1}011\rangle$<br>$\{10\bar{1}1\}\langle10\bar{1}\bar{2}\rangle$ |
| Zn | 1.856 | $\{10\bar{1}2\}\langle\bar{1}011\rangle$ |
| Cd | 1.886 | $\{10\bar{1}2\}\langle\bar{1}011\rangle$ |

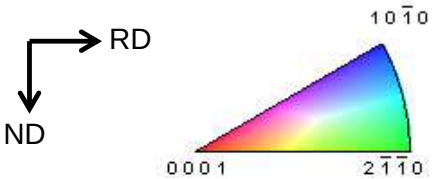



Yoo (1981)

# Twinning in hexagonal metals

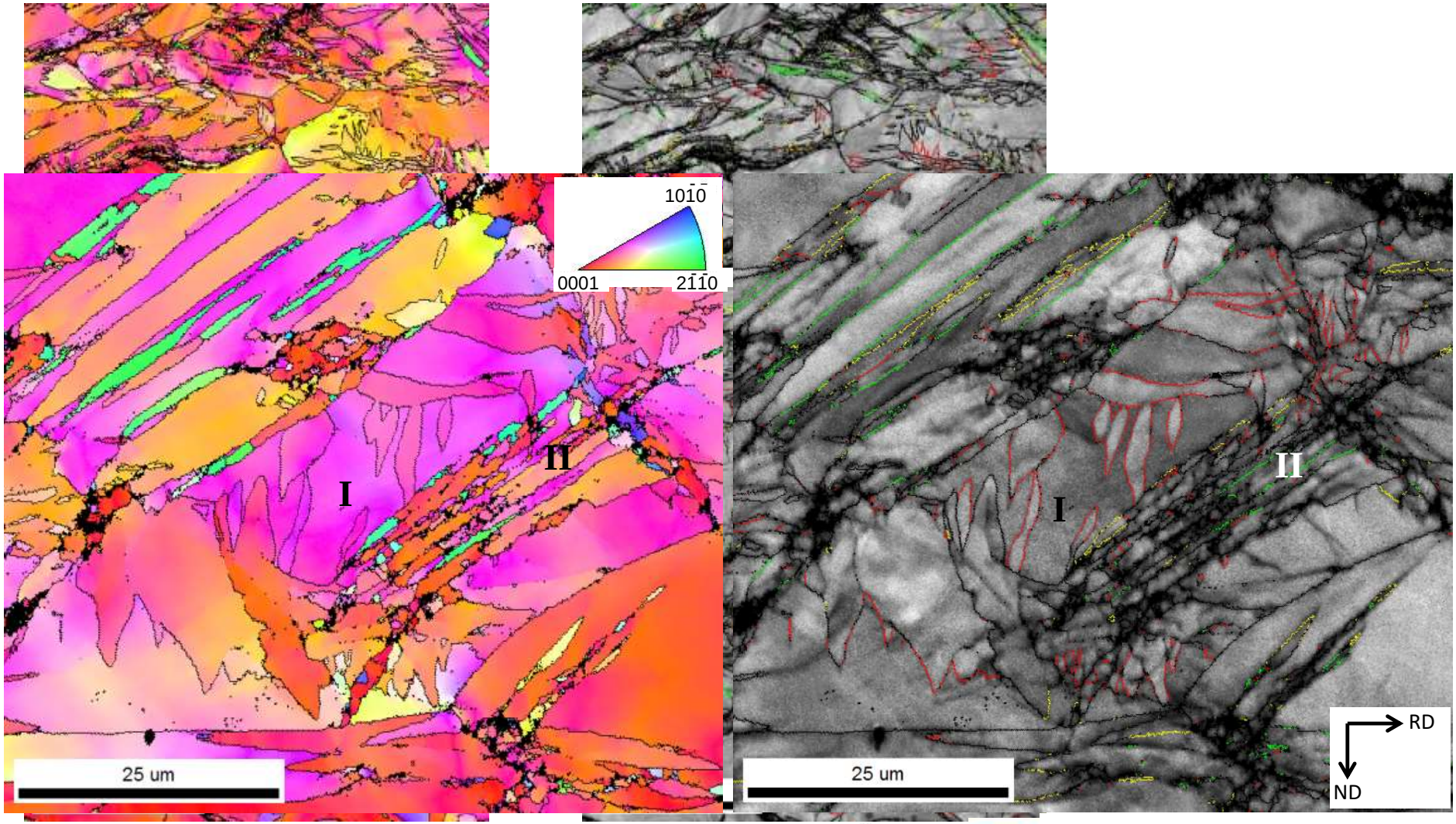


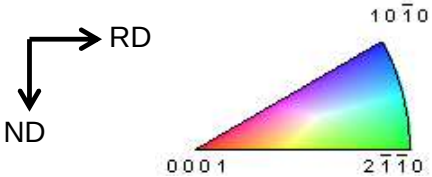




Tensile twin (86°@11-20)
Compression twin (56°@11-20)
Secondary twin (38°@11-20)
HAGB (>15°)

# Twinning in hexagonal metals




Tensile twin (86°@11-20)
Compression twin (56°@11-20)
Secondary twin (38°@11-20)
HAGB (>15°)

# Quiz

- How many twinning systems in hexagonal metals?
- Which twinning systems do you remember?
- What is a tension twin?
- What is a compression twin?
- What is a secondary twin?
- What is a twinning dislocation?
- Why using the concept of twinning dislocations in hexagonal metals?

# Topics

- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink bands
- Twinning in hexagonal metals
- Stacking faults in hexagonal metals
- Texture components in hexagonal metals

# Stacking faults in hexagonal metals

Basal stacking faults in hex metals:

$I_1$- stacking sequence …ABABCBCBC…

$I_2$ - stacking sequence …ABCACAC…

E - stacking sequence …ABABCABAB…

Non-basal stacking faults in hex metals:

~ 80 possible dislocation dissociation reactions

Relevant for twin nucleation

Confirmation only by MD yet

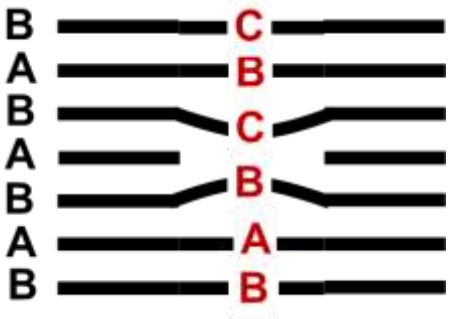
Stacking fault energies determine:

- Energy needed for the dissociation of a perfect dislocation
  - Dislocation core structure
  - Dislocation mobility
  - Cross-slip probability

# Stacking faults in hexagonal metals

Basal stacking faults in hex metals:

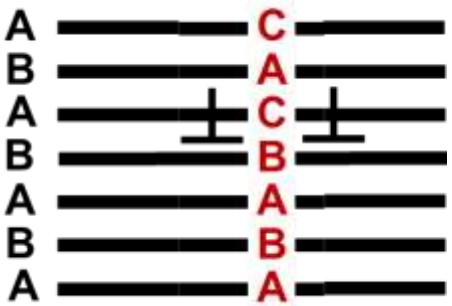
$I_1$- stacking sequence …ABABCBCBC…
Shockley-type basal <a> partial and
Frank-type $\frac{1}{2}$<c+a> partial
→ sessile, proposed as Frank-Read source <c+a>



# Stacking faults in hexagonal metals

Basal stacking faults in hex metals:

$I_1$- stacking sequence …ABABCBCBC…
Shockley-type basal <a> partial and
Frank-type $\frac{1}{2}$<c+a> partial
→ sessile, proposed as Frank-Read source <c+a>




$I_2$ - stacking sequence …ABCACAC…
2 Shockley-type basal partials :
$\frac{1}{3}[\bar{1}2\bar{1}0] \rightarrow \frac{1}{3}[01\bar{1}0] + \frac{1}{3}[\bar{1}100]$
"equivalent" to ISF in fcc
proposed as measure for cross-slip probability

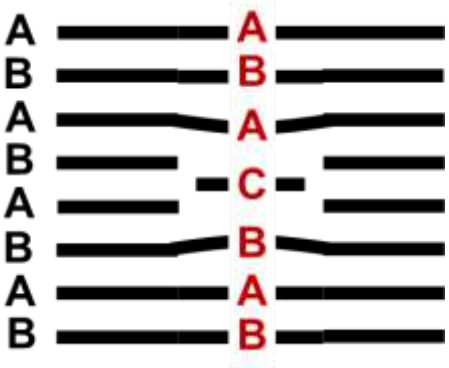
# Stacking faults in hexagonal metals

Basal stacking faults in hex metals:

$I_1$- stacking sequence …ABABCBCBC…
Shockley-type basal <a> partial and
Frank-type $\frac{1}{2}$<c+a> partial
→ sessile, proposed as Frank-Read source <c+a>

$I_2$ - stacking sequence …ABABCACAC…
2 Shockley-type basal partials :
$\frac{1}{3}[\bar{1}2\bar{1}0] \rightarrow \frac{1}{3}[01\bar{1}0] + \frac{1}{3}[\bar{1}100]$
"equivalent" to ISF in fcc
proposed as measure for cross-slip probability

E - stacking sequence …ABABCABAB…
energetically unfavorable



# Stacking faults in hexagonal metals

($I_2$-type) GSFEs for hexagonal metals

SFE:

Dissociation and formation of SFI2 on basal plane

Cross-slip on prismatic planes

USFE:

Nucleation of <a> dislocations

# Stacking faults in hexagonal metals

| Metal | c/a | d/b | w/b | Primary glide plane(s) | Secondary glide plane(s) |
|---|---|---|---|---|---|
| Be | 1.568 | 0.78 (B)<br>0.87 (Pr) | 0.38 (B)<br>0.47 (Pr) | basal <a> | prismatic <a>; pyramidal <a> |
| Ti | 1.588 | 0.80 (B)<br>0.87 (Pr) | 0.57 (B)<br>0.68 (Pr) | prismatic <a> | basal <a>; pyramidal <a> |
| Zr | 1.593 | 0.80 (B)<br>0.87 (Pr) | 0.67 (B)<br>0.65 (Pr) | prismatic <a> | basal <a>; pyramidal <a> |
| Co | 1.623 | 0.81 (B) | 0.67 (B) | basal <a> | |
| Mg | 1.623 | 0.81 (B)<br>0.87 (Pr) | 0.61 (B)<br>0.62 (Pr) | basal <a> | prismatic <a>; pyramidal <c+a> |
| Zn | 1.856 | 0.93 (B) | 0.67 (B) | basal <a> | prismatic <a>; pyramidal <a><br>pyramidal <c+a>; kinking |
| Cd | 1.886 | 0.94 (B) | 0.83 (B) | basal <a> | prismatic <a>; pyramidal <a><br>pyramidal <c+a>; kinking |

# Stacking faults in hexagonal metals

| Metal | c/a | d/b | w/b | Primary glide plane(s) | Secondary glide plane(s) |
|---|---|---|---|---|---|
| Mg | 1.623 | 0.81 (B)<br>0.87 (Pr) | 0.61 (B)<br>0.62 (Pr) | basal <a> | prismatic <a>; pyramidal <c+a> |

Why basal <a> and not prismatic <a>?

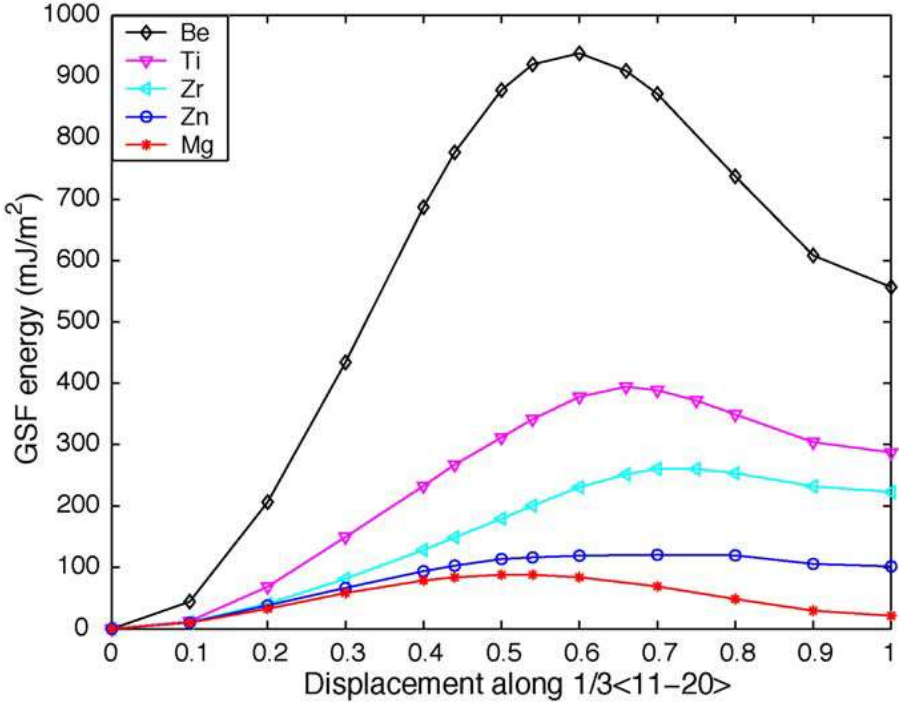
# Stacking faults in hexagonal metals

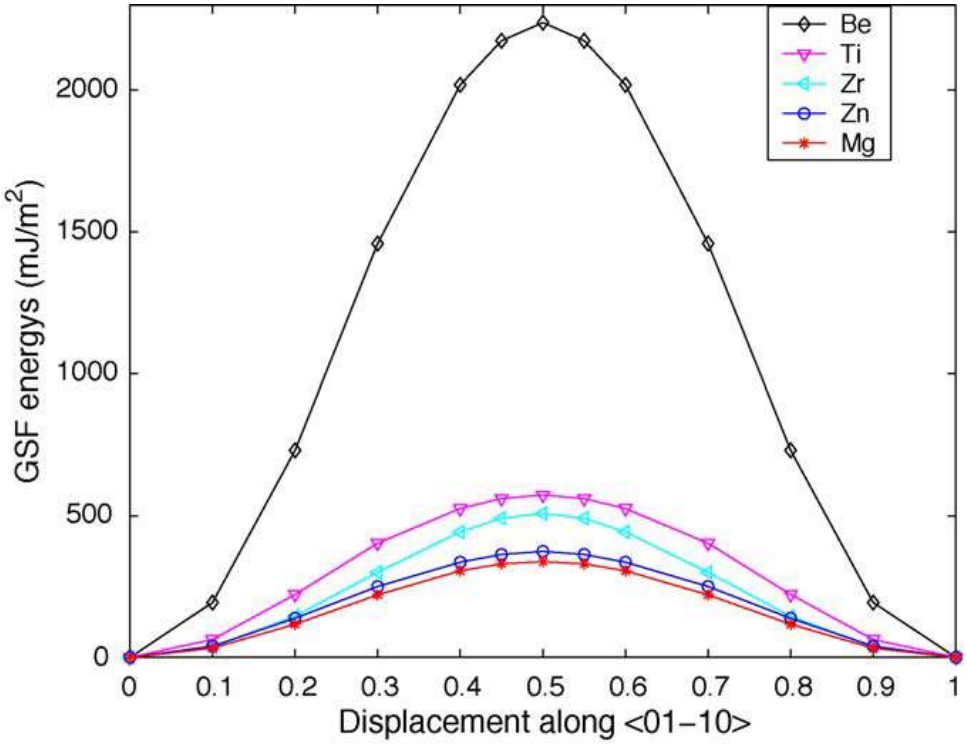
($I_2$-type) GSFEs for hexagonal metals

SFE:

Dissociation and formation of $SFI_2$ on basal plane

Cross-slip on prismatic planes








Wu et al. (2010)

# Stacking faults in hexagonal metals

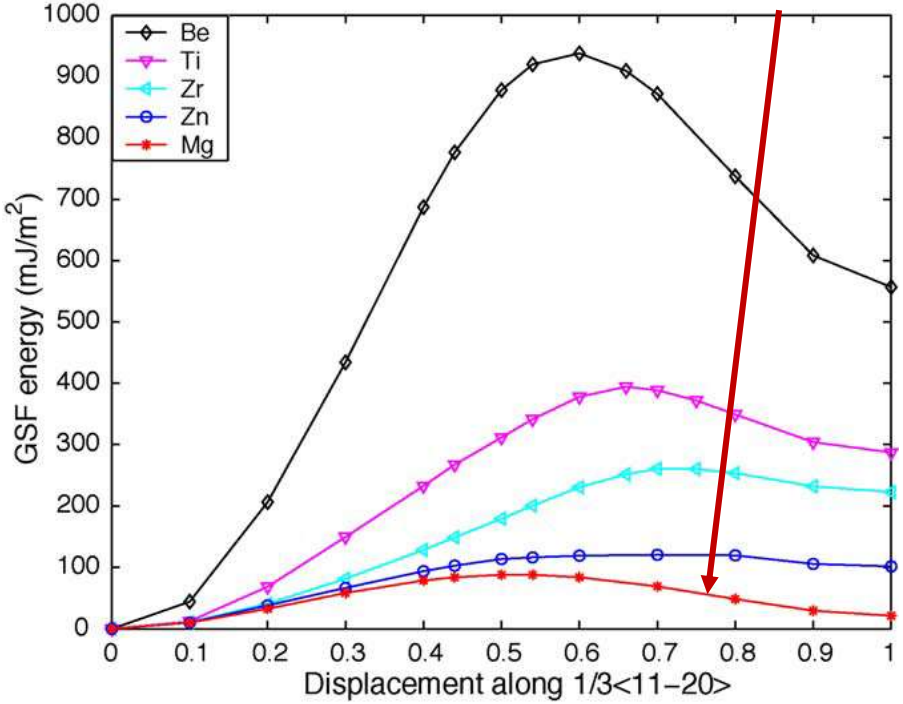
($I_2$-type) GSFEs for hexagonal metals

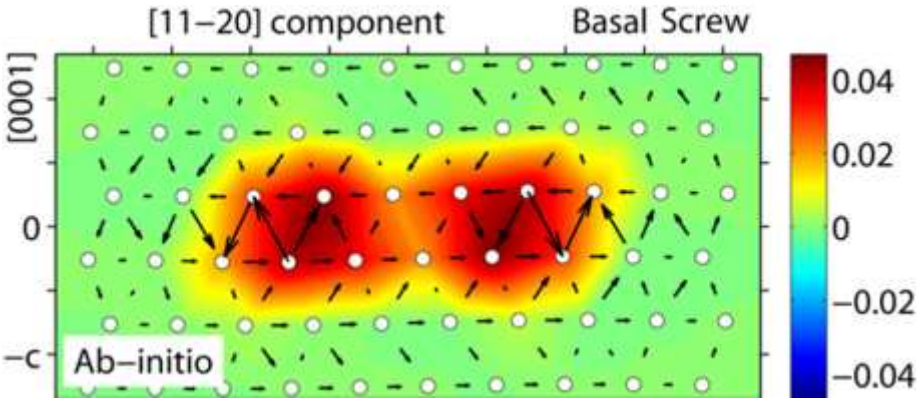
SFE:

Dissociation and formation of $SFI_2$ on basal plane

Cross-slip on prismatic planes

Low SFE $I_2$: dissociated dislocation core → cross-slip difficult



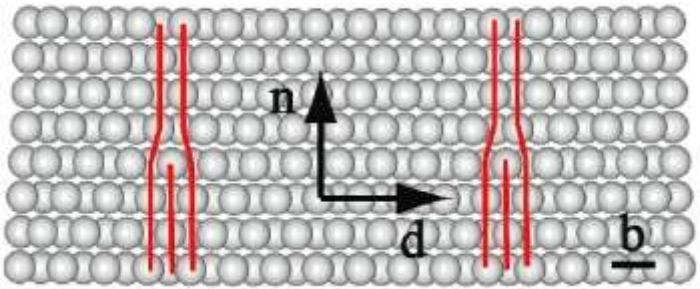

Dissociated ($I_2$-type) basal screw dislocation core

Yasi et al. (2009)

Wu et al. (2010)

# Stacking faults and dislocation cores

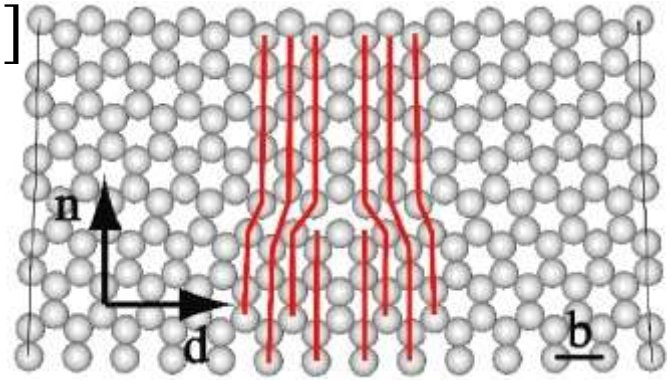
$[1\bar{1}00]$




$[11\bar{2}0]$

Mg: basal <a> -edge dislocation

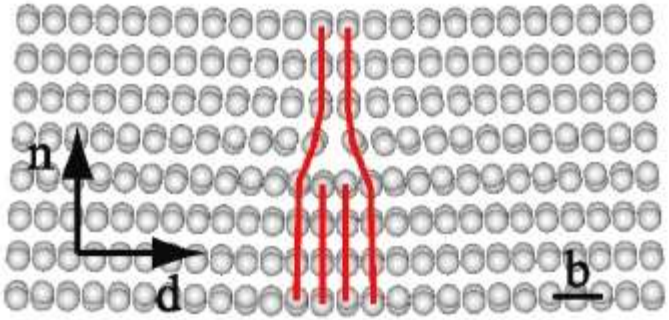
$[0001]$




$[11\bar{2}0]$

Mg: prismatic <a> -edge dislocation

$\perp [1\bar{1}01]$




$[11\bar{2}0]$

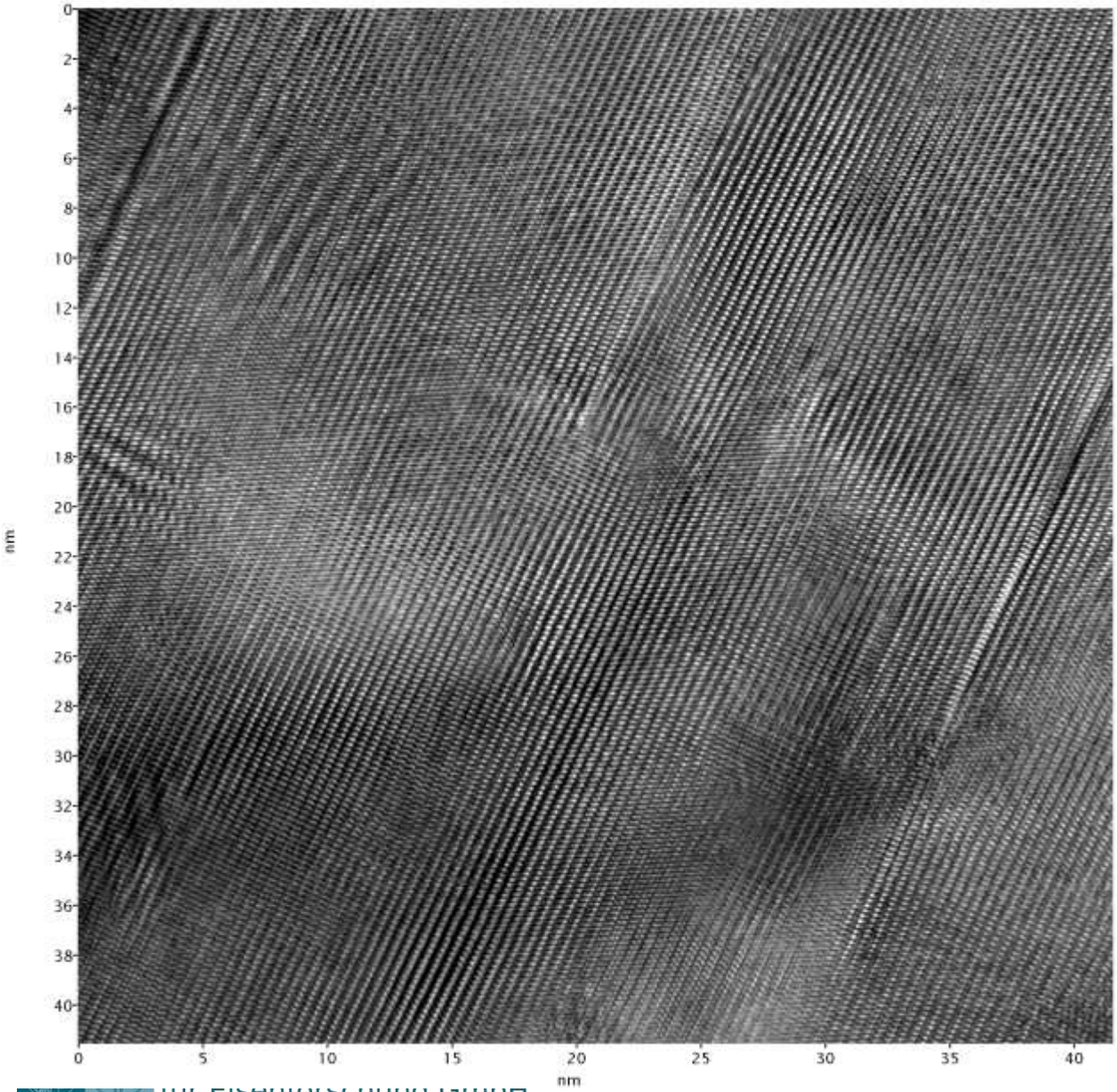
Mg: pyramidal <a> -edge dislocation





Groh et al. (2009)

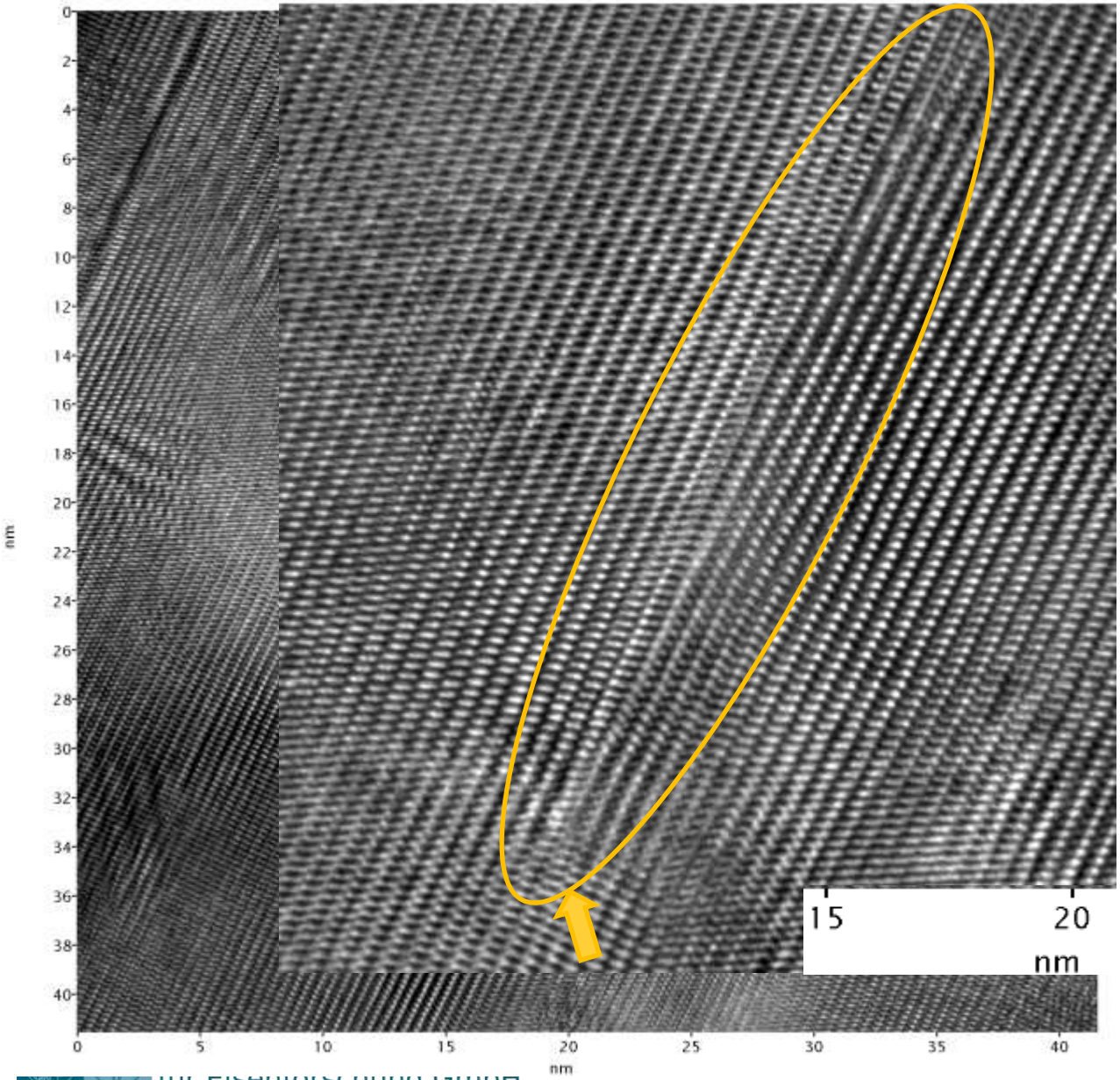
# Stacking faults and dislocation cores




Mg:
basal <a> -edge dislocation

B=$[1\bar{1}00]$

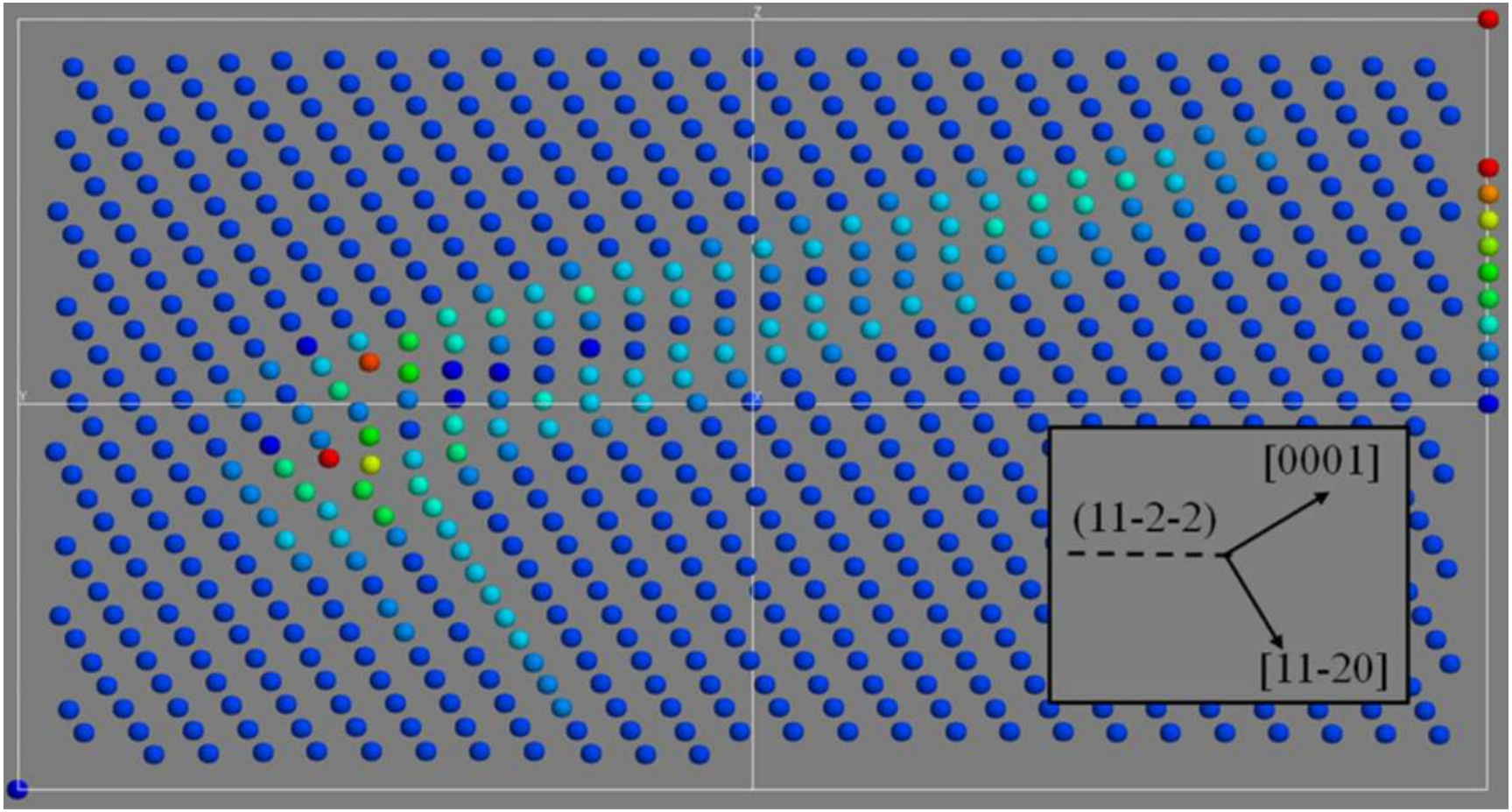
# Stacking faults and dislocation cores




Mg:
basal <a> -edge dislocation

$B=[1\bar{1}00]$

# Stacking faults and dislocation cores




Mg: pyramidal <c+a> edge dislocation

Yasi et al. (2009)

# Stacking faults in hexagonal metals

| Metal | c/a | d/b | w/b | Primary glide plane(s) | Secondary glide plane(s) |
|---|---|---|---|---|---|
| Be | 1.568 | 0.78 (B)<br>0.87 (Pr) | 0.38 (B)<br>0.47 (Pr) | basal <a> | prismatic <a>; pyramidal <a> |
| Ti | 1.588 | 0.80 (B)<br>0.87 (Pr) | 0.57 (B)<br>0.68 (Pr) | prismatic <a> | basal <a>; pyramidal <a> |
| Zr | 1.593 | 0.80 (B)<br>0.87 (Pr) | 0.67 (B)<br>0.65 (Pr) | prismatic <a> | basal <a>; pyramidal <a> |
| Co | 1.623 | 0.81 (B) | 0.67 (B) | basal <a> | |
| Mg | 1.623 | 0.81 (B)<br>0.87 (Pr) | 0.61 (B)<br>0.62 (Pr) | basal <a> | prismatic <a>; pyramidal <c+a> |
| Zn | 1.856 | 0.93 (B) | 0.67 (B) | basal <a> | prismatic <a>; pyramidal <a><br>pyramidal <c+a>; kinking |
| Cd | 1.886 | 0.94 (B) | 0.83 (B) | basal <a> | prismatic <a>; pyramidal <a><br>pyramidal <c+a>; kinking |

# Stacking faults in hexagonal metals

| Metal | c/a | d/b | w/b | Primary glide plane(s) | Secondary glide plane(s) |
|---|---|---|---|---|---|
| Be | 1.568 | 0.78 (B)<br>0.87 (Pr) | 0.38 (B)<br>0.47 (Pr) | basal <a> | prismatic <a>; pyramidal <a> |

Why basal <a> and not prismatic <a>?

# Stacking faults in hexagonal metals

($I_2$-type) GSFEs for hexagonal metals

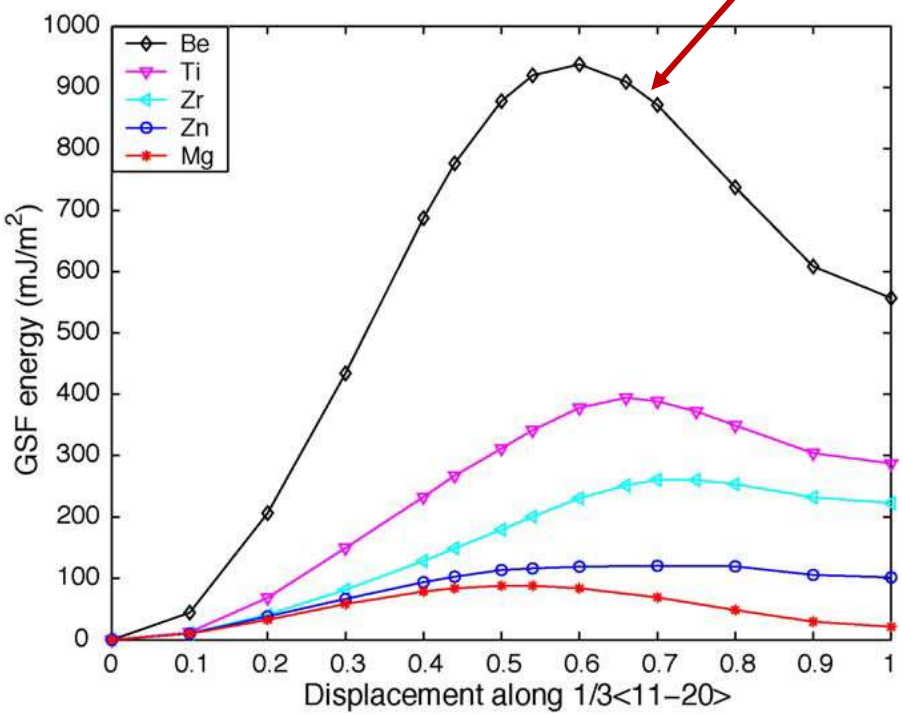
SFE:

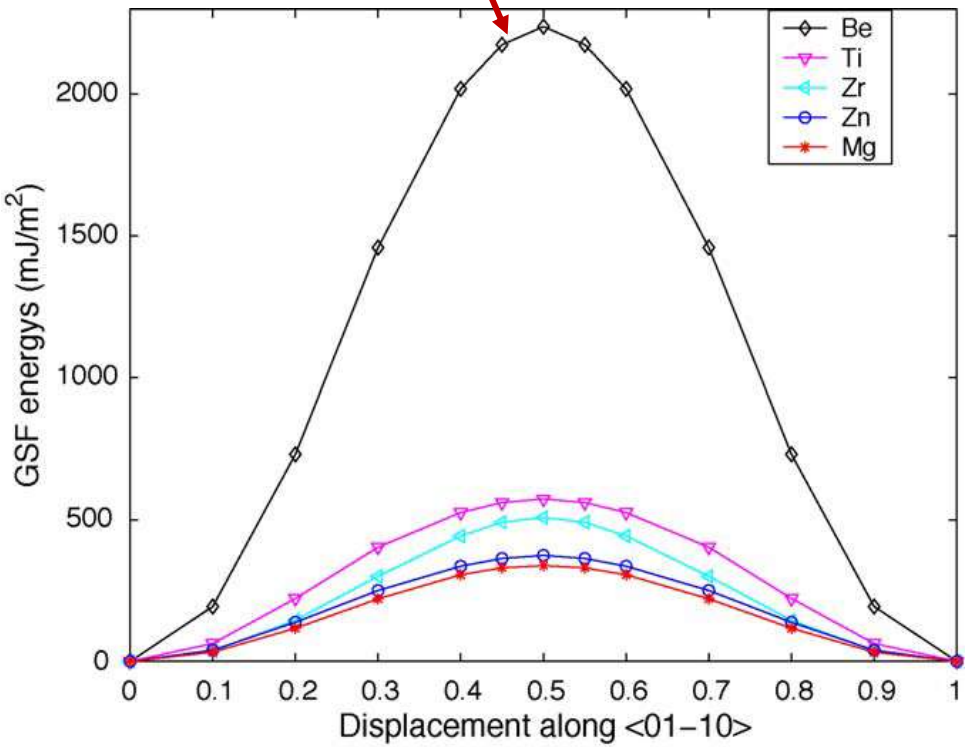
Dissociation and formation of $SFI_2$ on basal plane

Cross-slip on prismatic planes

Dislocation stability on competing planes

→ higher stability on basal plane




Wu et al. (2010)

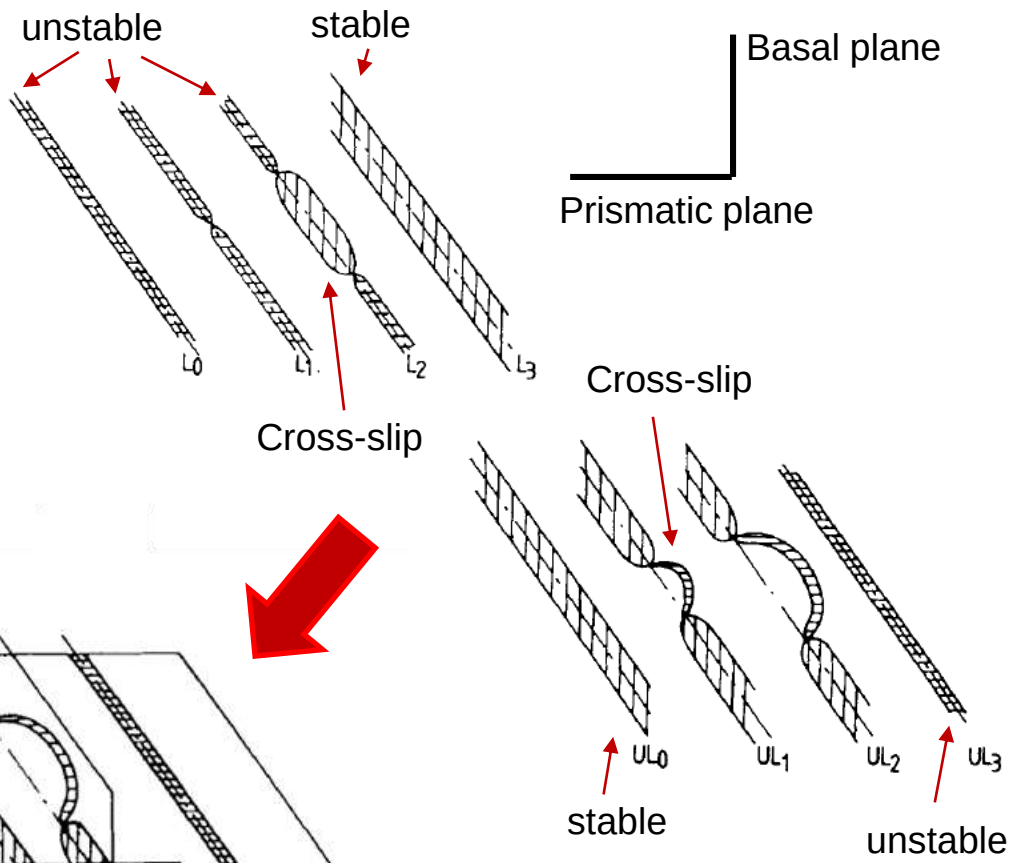
# Stacking faults in hexagonal metals

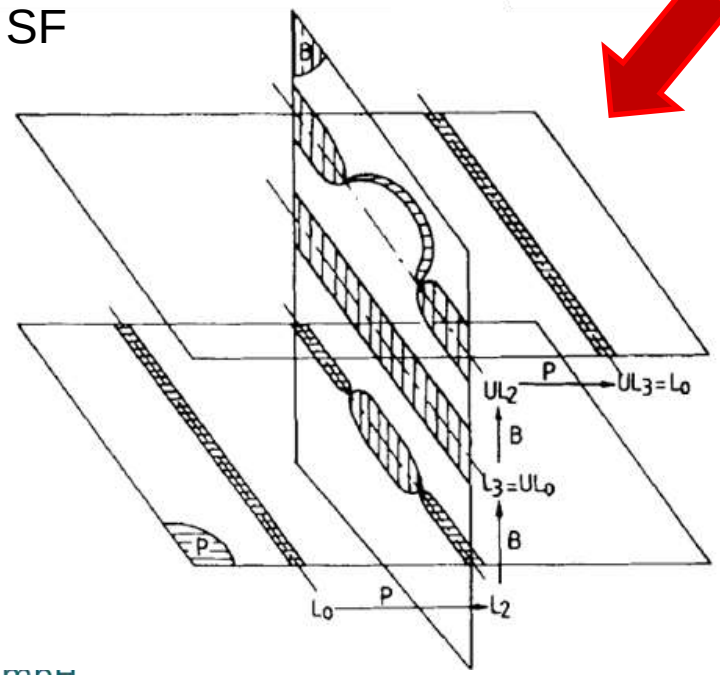
Prismatic plane:

- Much higher SFE
- Unstable dislocation core
- Immobilization (“locking“)
- Stress: cross-slip of segments on basal plane

Basal plane:

- Lower SFE
- Spreading of core
- Stable, glissile SF



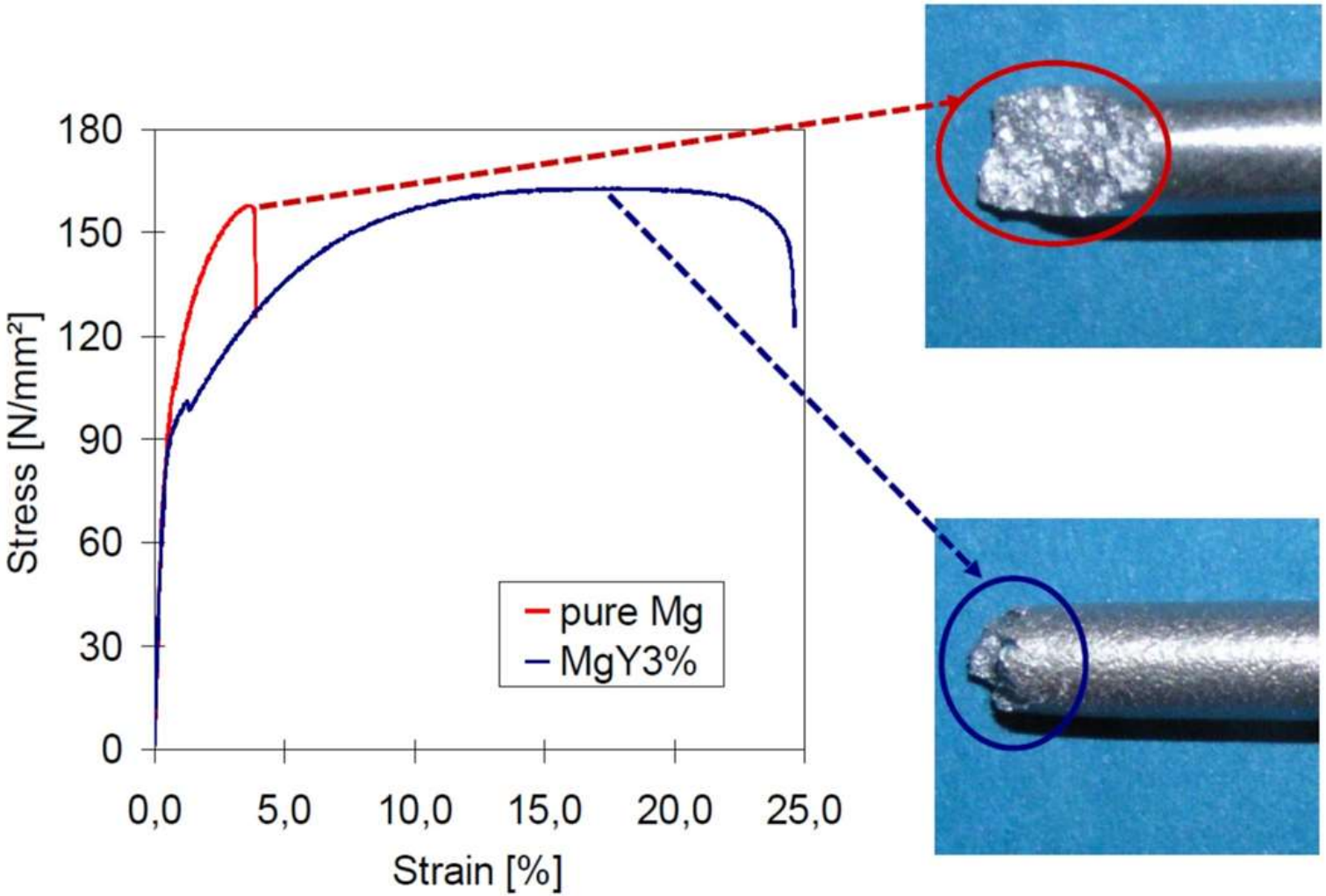

Regnier, Dupouy (1970)

# Stacking faults in hexagonal metals

($I_1$-type) GSFEs for hexagonal metals

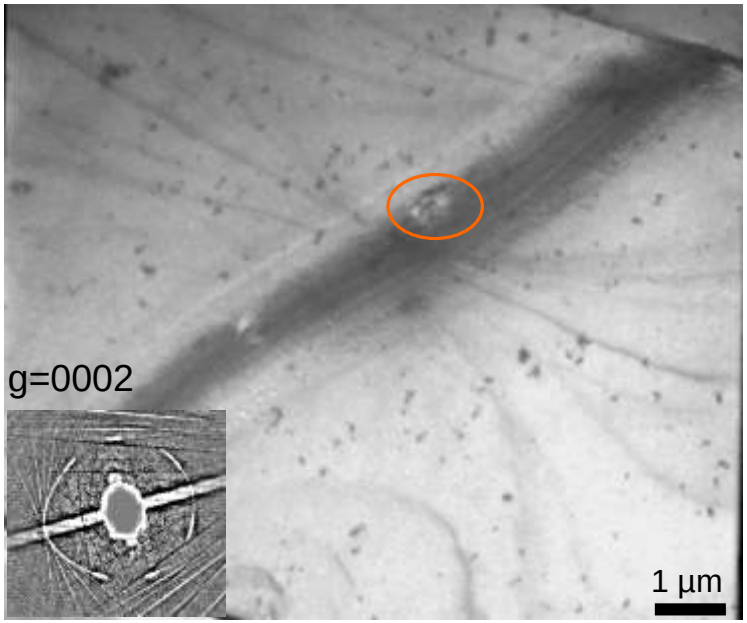
SF:
Nucleation of <c+a> dislocations?

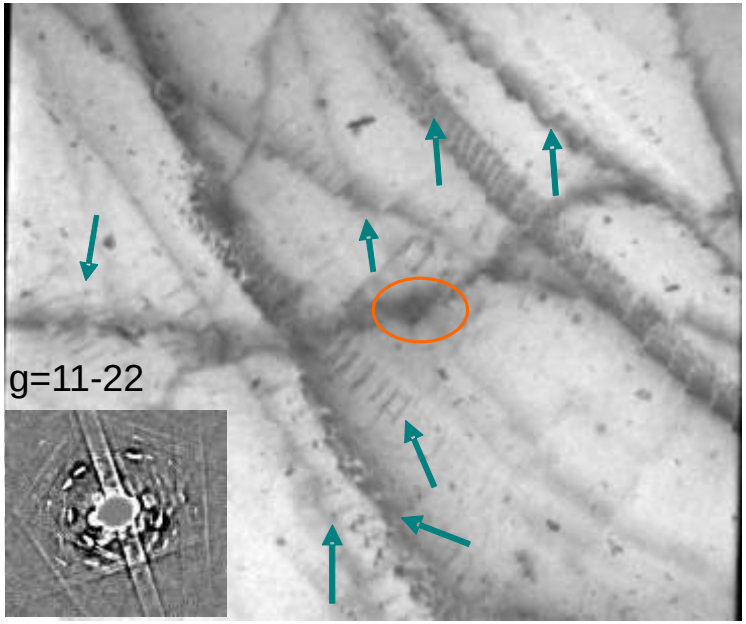
# Stacking faults in hexagonal metals




- 5 times higher ductility
- Well-balanced work hardening
- Comparable strength

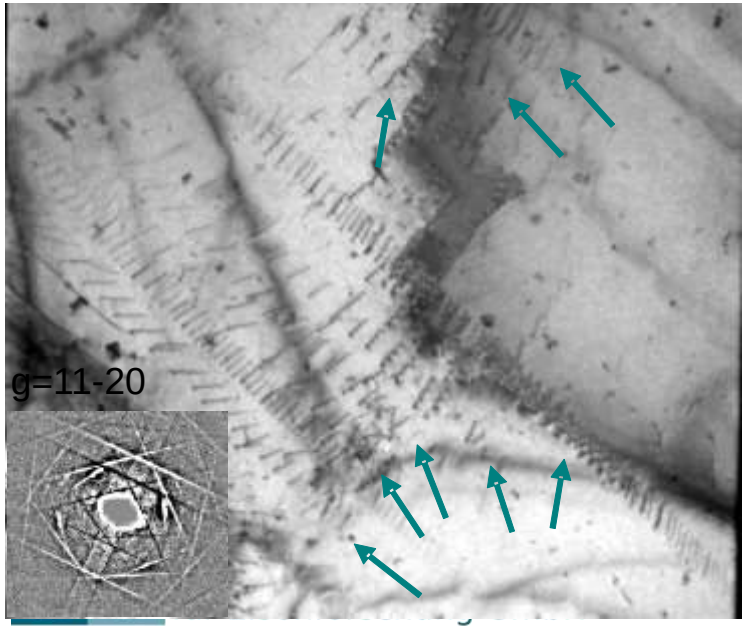
# Stacking faults in hexagonal metals




– basal <a>

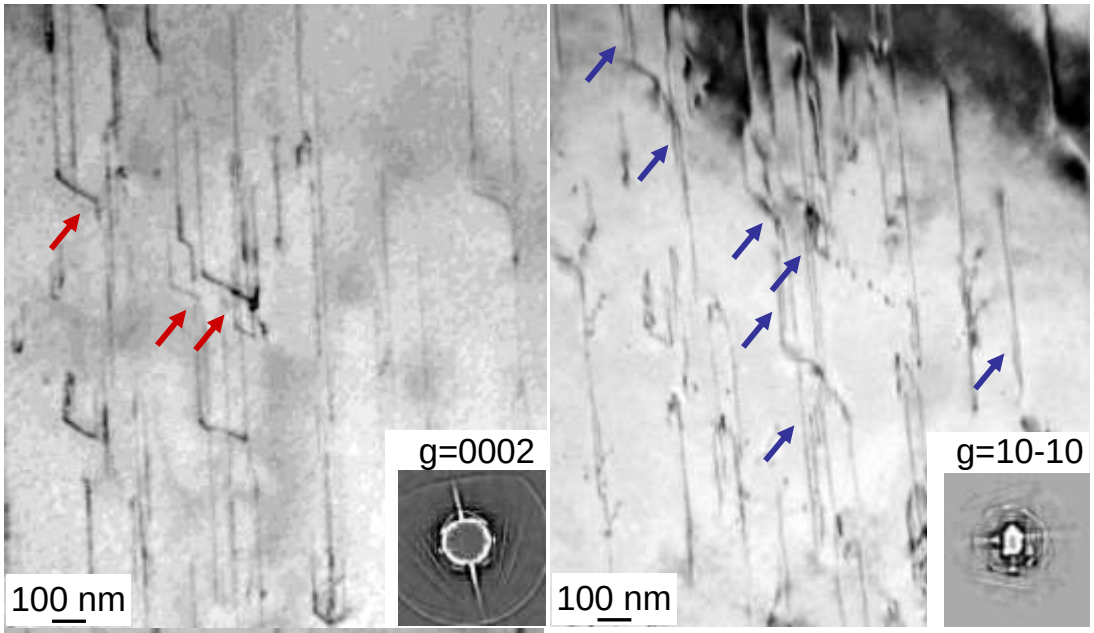
– sessile <c>

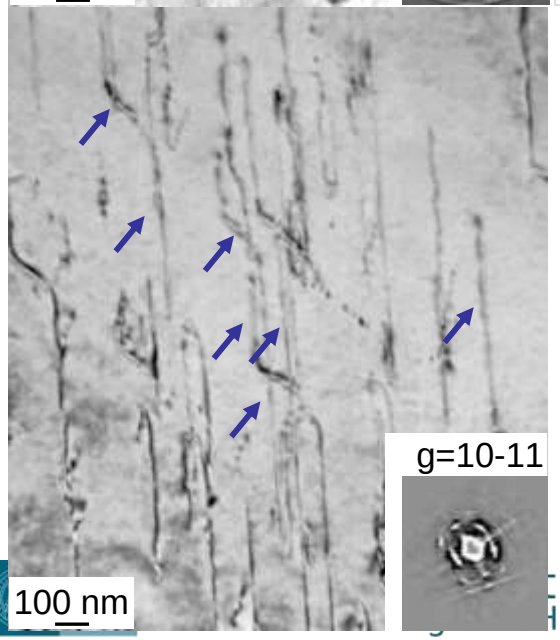



TEM images of dislocations in pure Mg

- High amount of basal <a> dislocations
- Hardly any dislocations with a <c> component
- Basal <a> dislocations lying on defined slip bands

# Stacking faults in hexagonal metals




TEM images of <c+a> dislocations in Mg 3 wt-% Y (3.5 % CR)

- Red arrows:
  cross-slip events
- Blue arrows:
  dislocation dissociation on pyramidal planes

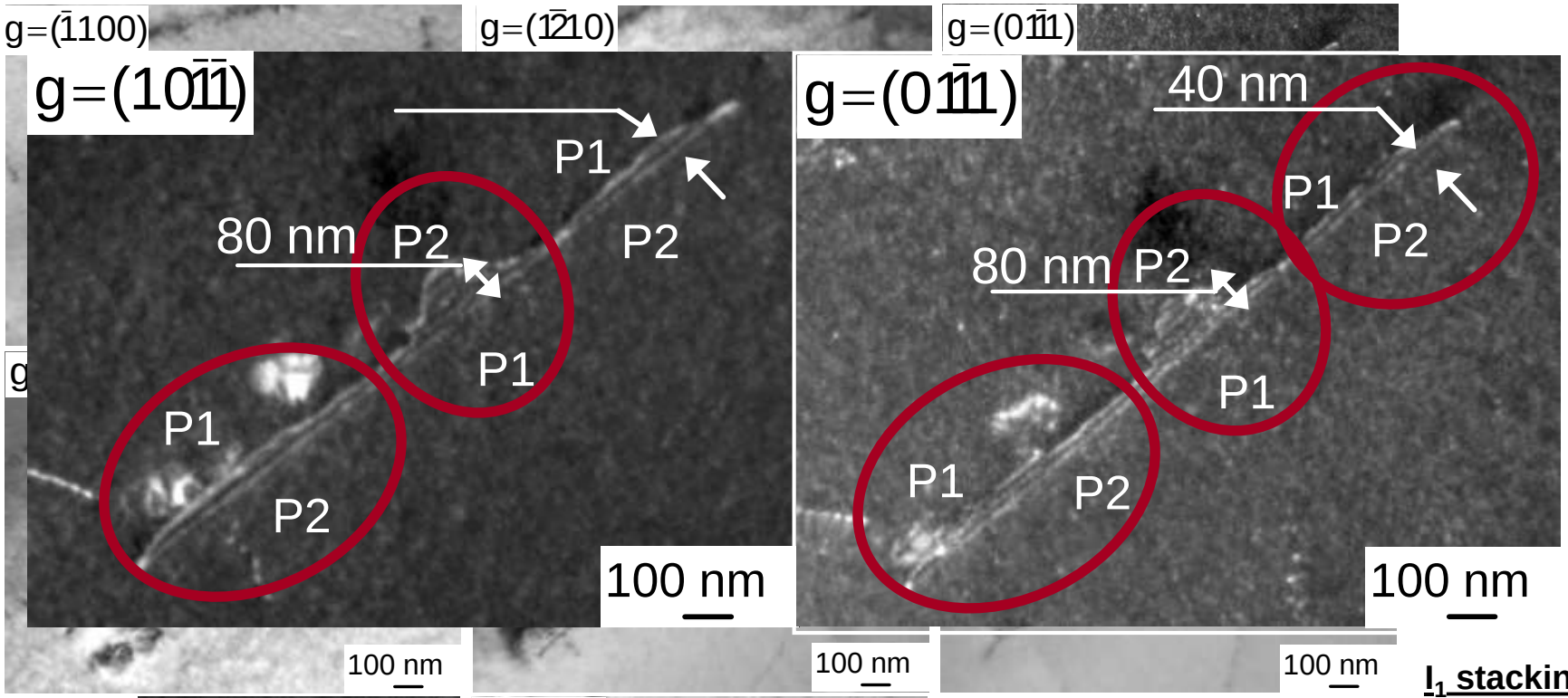
# … but mechanisms?

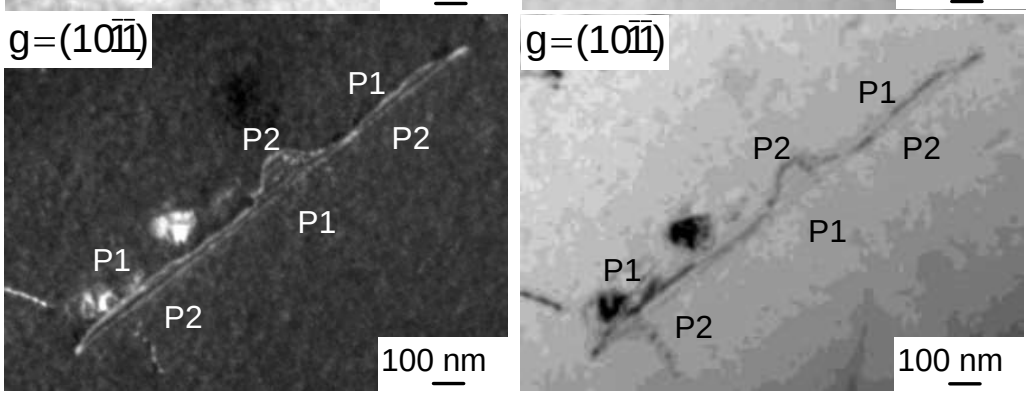
Mg3Y

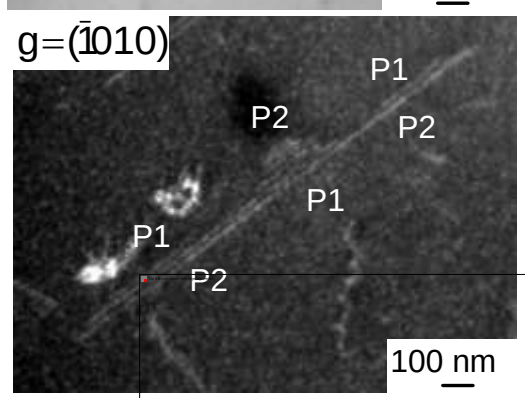
- **Why** high activity of compression twins and <c+a> slip?
  - Shear bands not mechanism for ductility, but for failure
  - Not related to particles (e.g. precipitation hardening)
  - No purification effect
  - Not caused by grain refinement
  - c/a ratio not decisive
  - Changed Peierls potentials can not explain high twin activity

➔ Changes in the SFE(s) !

# Stacking faults in hexagonal metals




**$I_1$ stacking fault: ~ 0.5-1.5 mJ/m²**

# Stacking faults in hexagonal metals

Stacking fault energy:

$$\gamma = \frac{E_{SF} - E_0}{A_{2D}}$$

- $E_{SF}$: energy of a crystal with a stacking fault
- $E_0$: energy of a perfect crystal
- $A_{2D}$: stacking fault area

**Axial Next Nearest Neighbor Ising ANNNI model [5]**

Expansion of the energy, assuming layers $S_i$ interact via $J_n$:

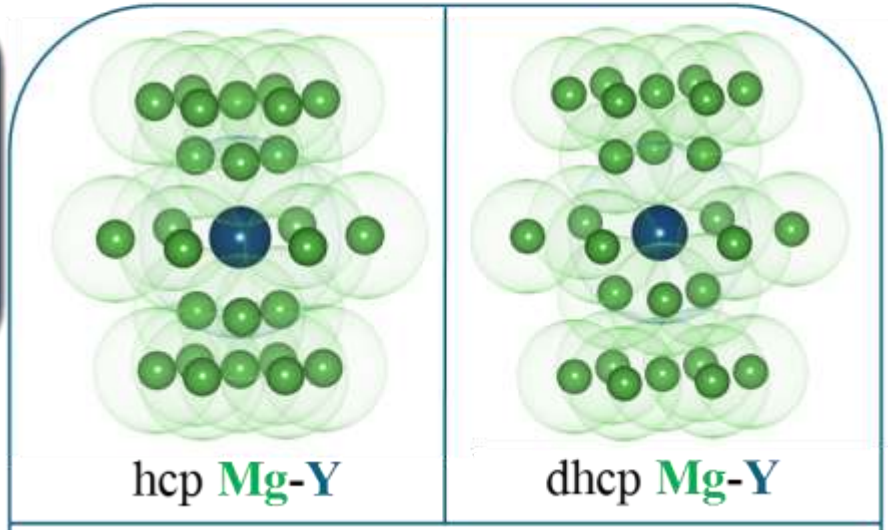
$$E = -\sum_n \sum_i J_n S_i S_{i+n}$$

2nd order approximation:

$J_1 = ½ (E_{hcp} - E_{fcc})$,

$J_2 = ½ (E_{dhcp} - E_{fcc} - J_1)$

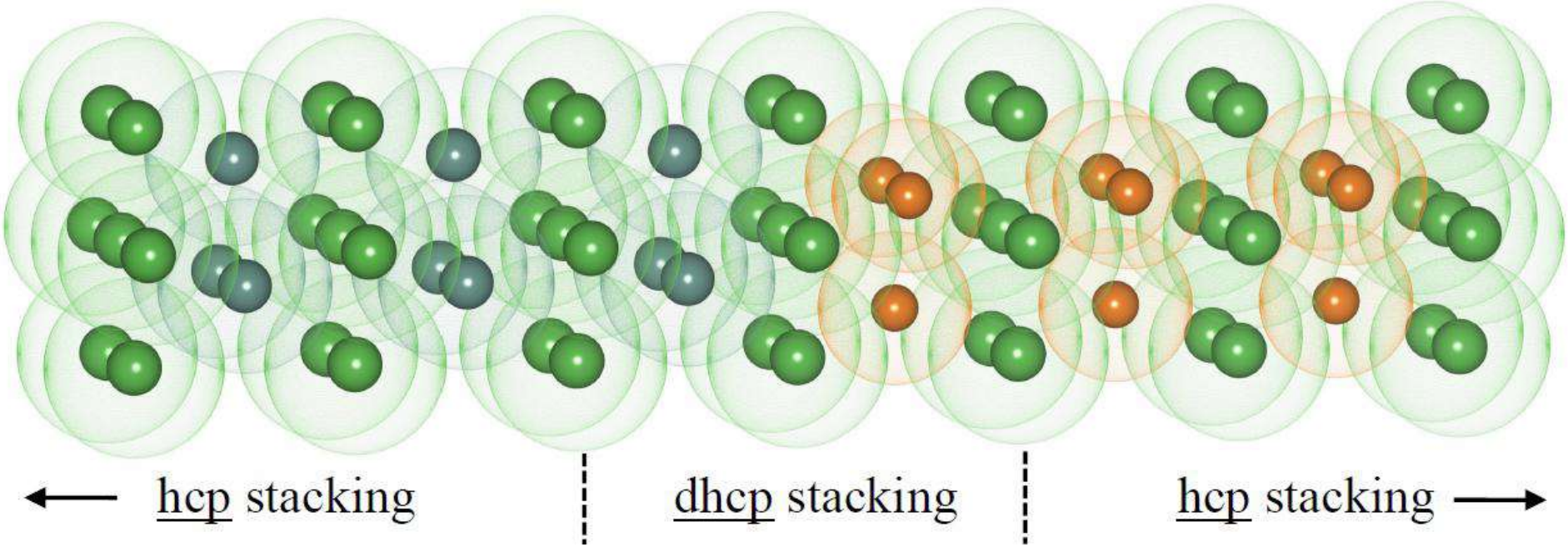
$$E_{SF1} - E_0 \approx 4J_2 - 2J_1 = 2(E_{dhcp} - E_{hcp})$$




Density functional theory (DFT) calculations of Mg-Y hcp and dhcp supercells employing the VASP code, PAW potentials, GGA-PBE, 400 eV cut-off energy, and 60 000 ***k***-points atoms.

# Stacking faults in hexagonal metals

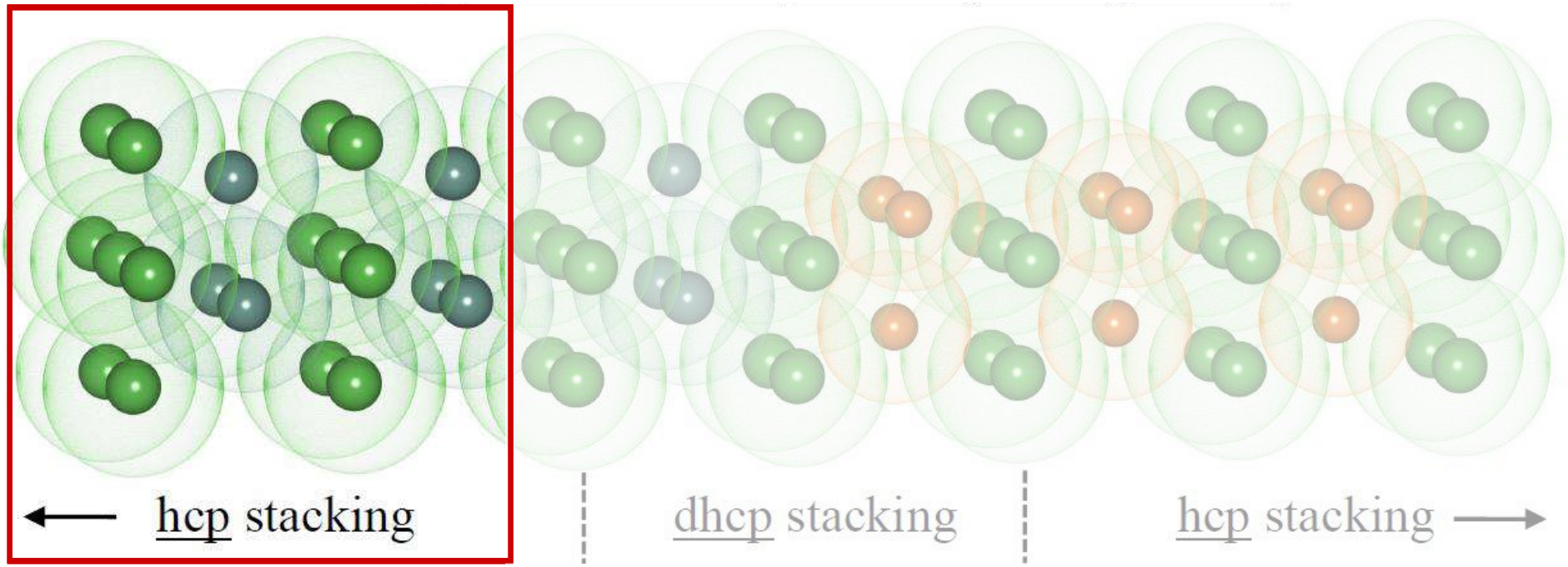
$I_1$- stacking sequence …ABABCBCBC… ⟶ 20-40 $mJm^{-2}$ from DFT in pure Mg




SFE: $\gamma = \frac{F_{SF} - F_0}{A_{2D}}$ $\quad F = -\sum_n \sum_i J_n S_i S_{i+n}$

# Stacking faults in hexagonal metals

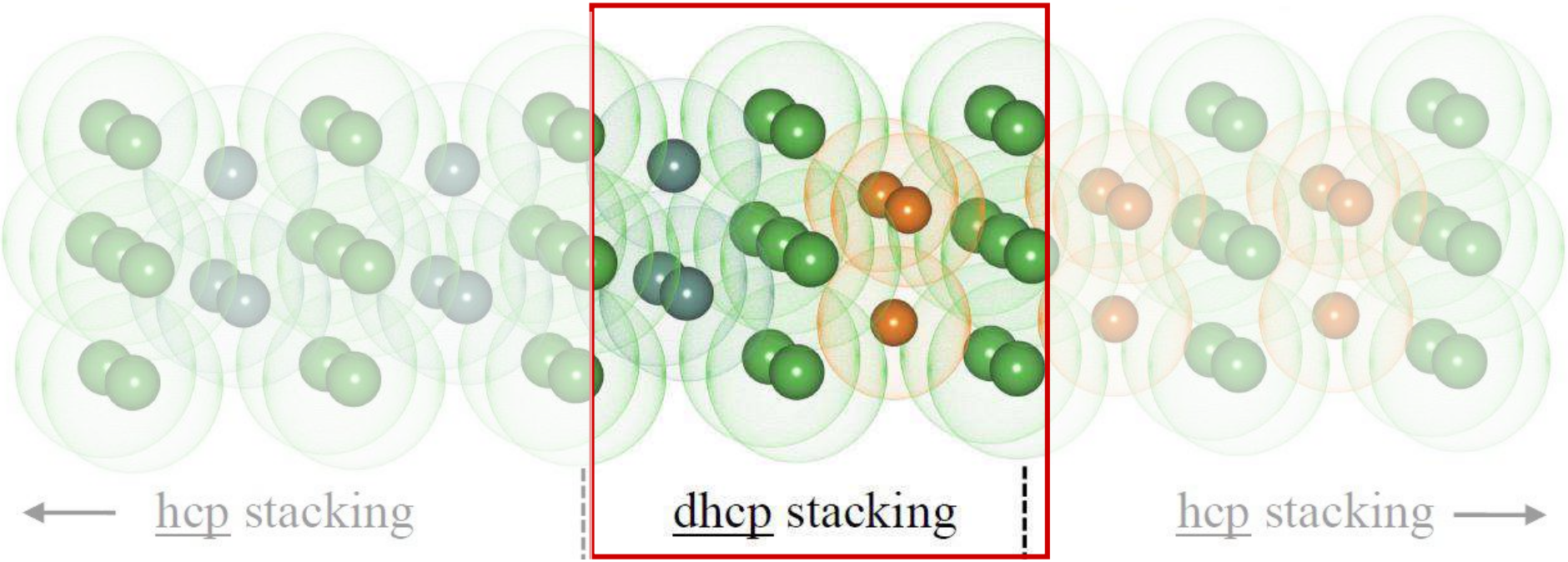
$I_1$- stacking sequence …ABABCBCBC… ⟶ 20-40 $mJm^{-2}$ from DFT in pure Mg




SFE: $\gamma = \dfrac{F_{SF} - F_0}{A_{2D}}$ $\quad F = -\sum_n \sum_i J_n S_i S_{i+n}$

# Stacking faults in hexagonal metals

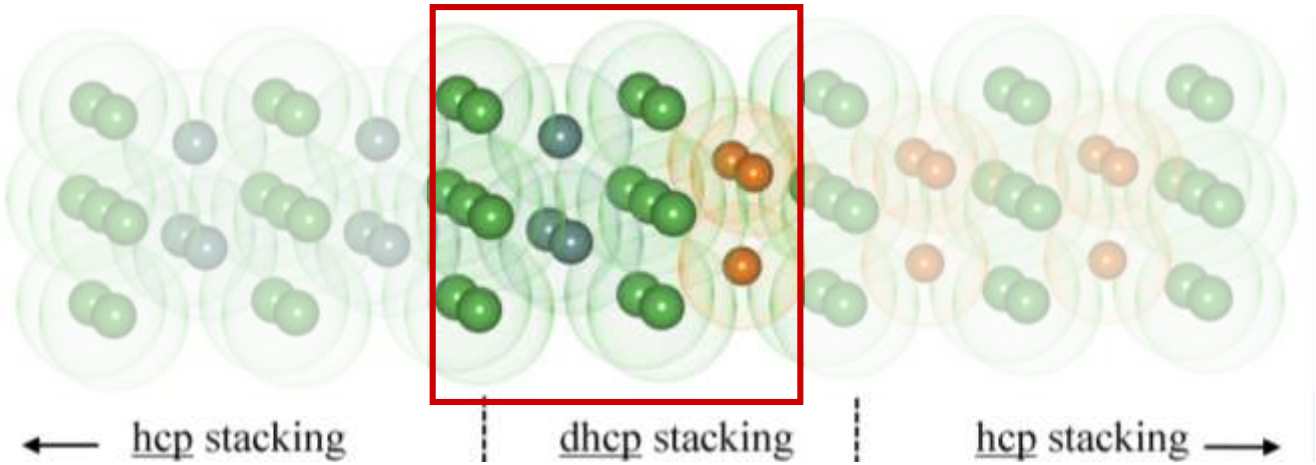
$I_1$- stacking sequence …ABABCBCB… → 20-40 $mJm^{-2}$ from DFT in pure Mg

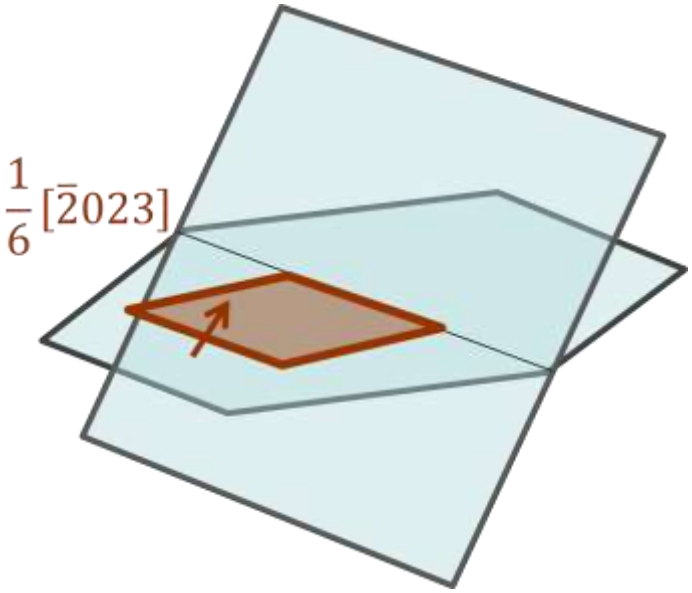



SFE: $\gamma = \dfrac{F_{SF} - F_0}{A_{2D}}$ $\quad F = -\sum_n \sum_i J_n S_i S_{i+n}$

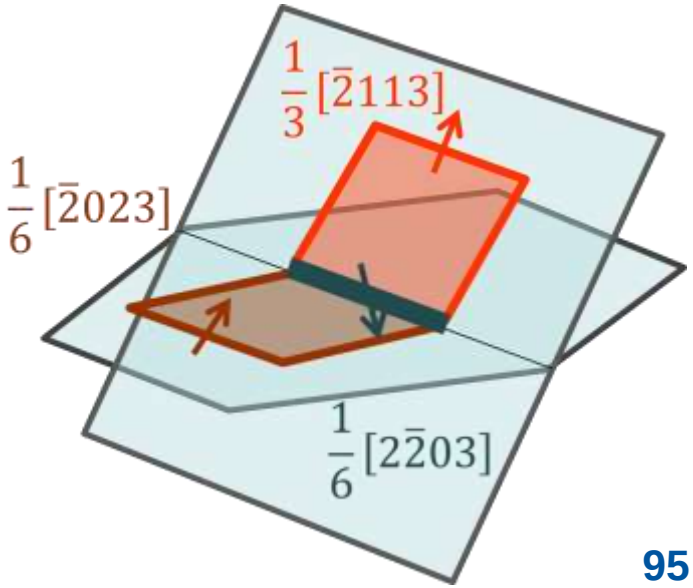
# Stacking faults in hexagonal metals

$I_1$- stacking sequence …ABABCBCBC… ⟶ 20-40 $mJm^{-2}$ from DFT in pure Mg

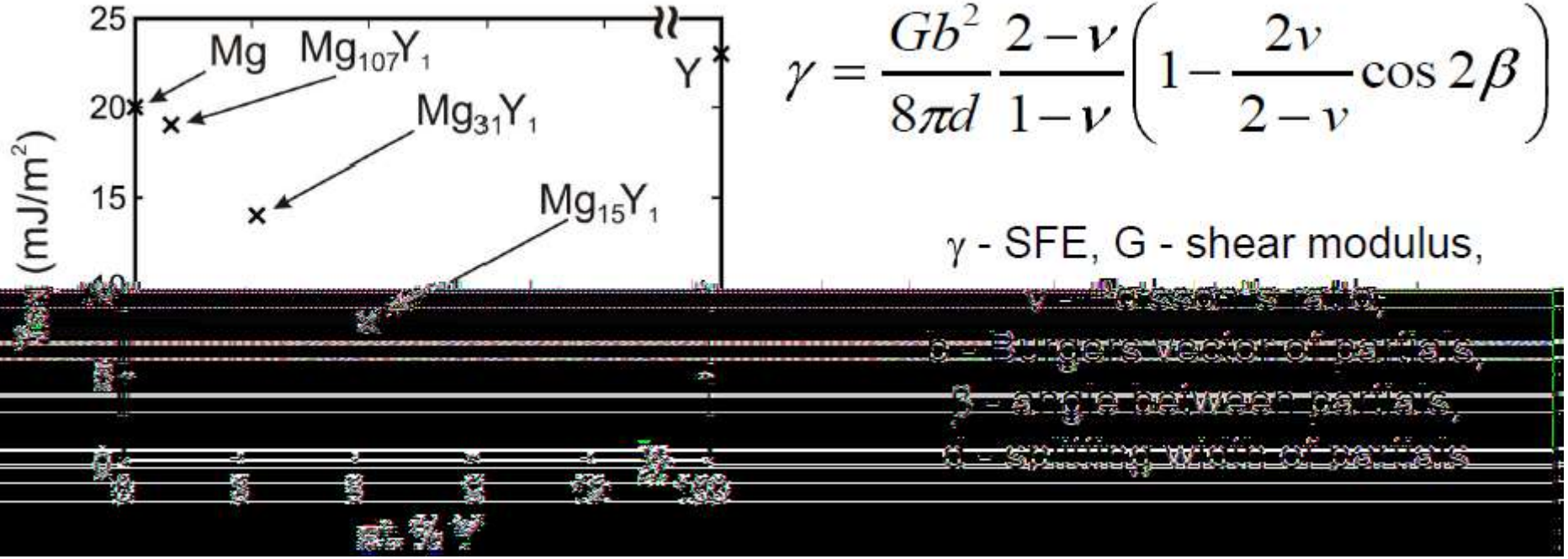



Source mechanism:
glissile <c+a>



# Stacking faults in hexagonal metals



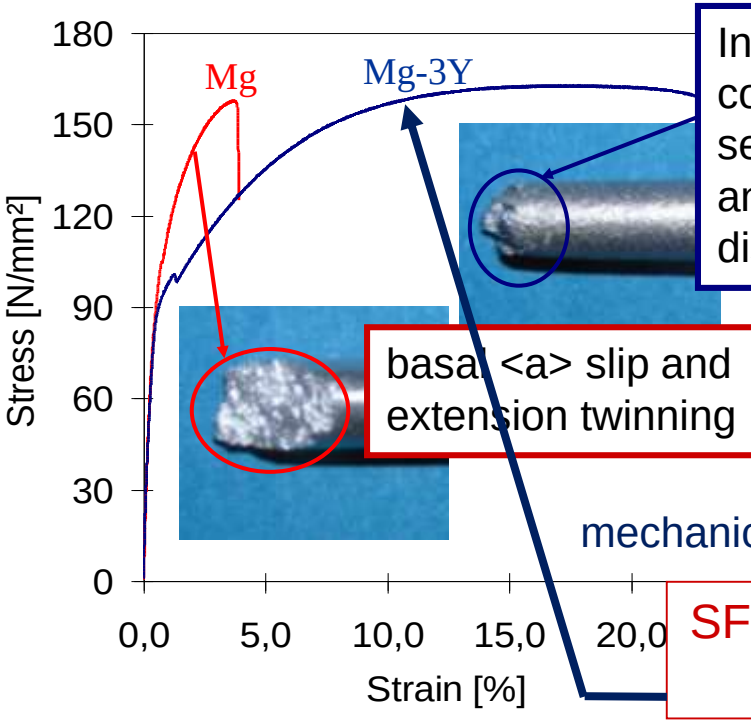

$$\gamma = \frac{Gb^2}{8\pi d}\frac{2-\nu}{1-\nu}\left(1-\frac{2\nu}{2-\nu}\cos 2\beta\right)$$

γ - SFE, G - shear modulus,
ν - Poisson's ratio,
b - Burgers vector of partials,
β - angle between partials,
d - splitting width of partials

$I_1$ SFE in Mg-3wt.-%-Y: 0.5-1.5 mJ/m$^{-2}$
(after 1.5% cold deformation)

$I_1$ SFE in Mg-1wt.-%-Y: 2.5-3.5 mJ/m$^{-2}$
(after 1.5% cold deformation)

# Stacking faults in hexagonal metals



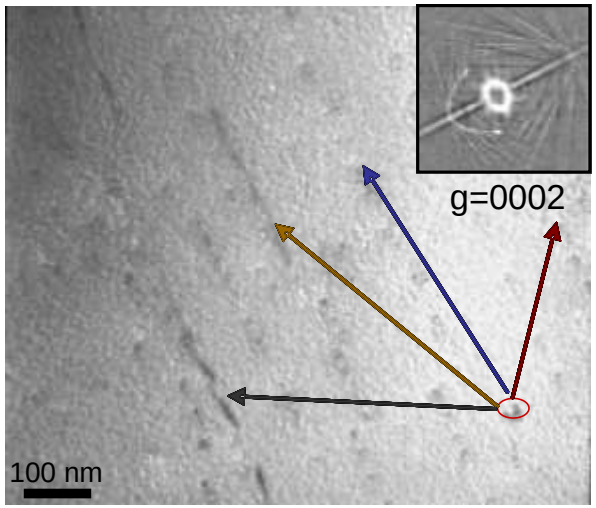

Increased activation contraction twinning, secondary twinning and pyramidal <c+a> dislocation slip

basal <a> slip and extension twinning

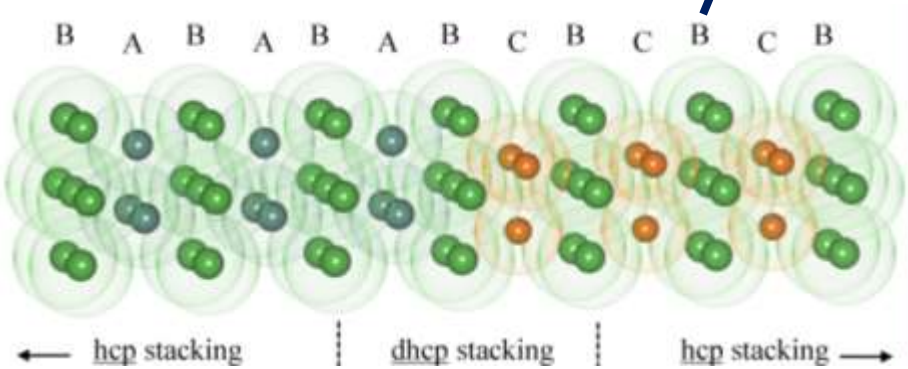
Improved mechanical properties

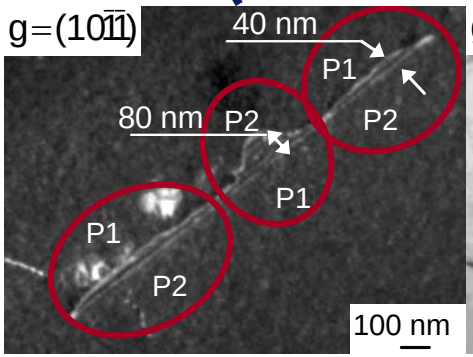
SFE significant decreased through Y addition

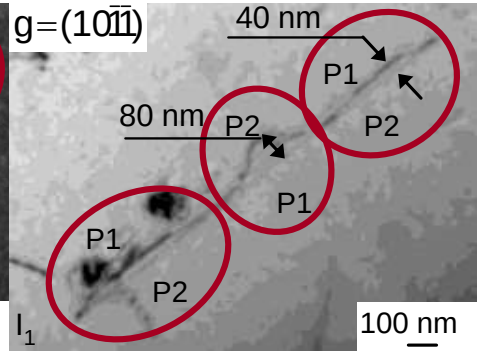
Enhanced <c+a> dislocations



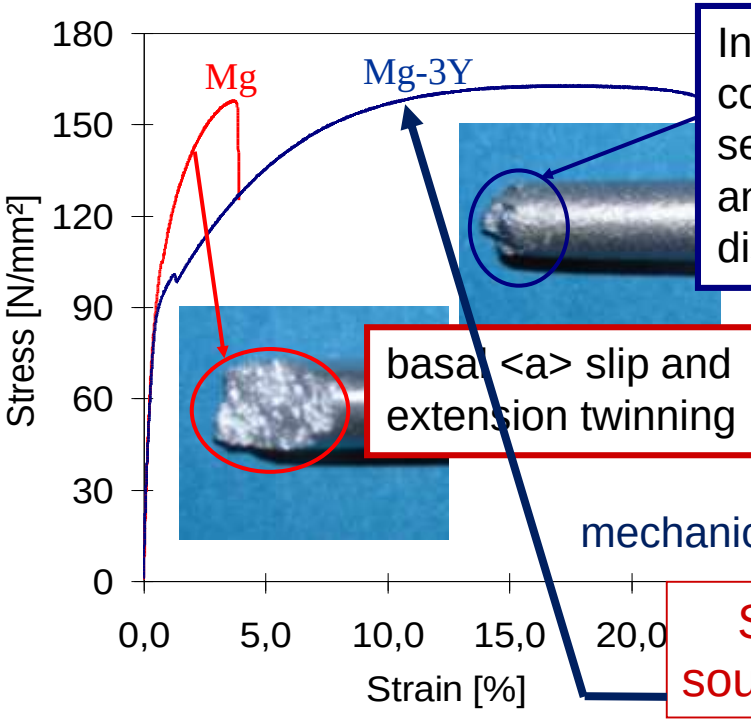

Assumption: SFE Modification



# Stacking faults in hexagonal metals

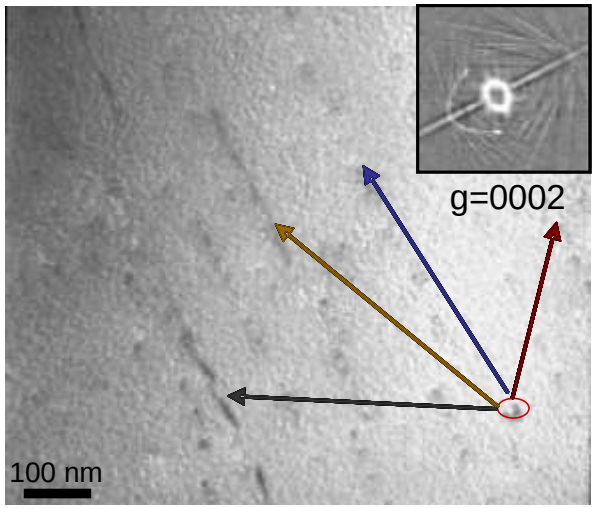



Increased activation contraction twinning, secondary twinning and pyramidal <c+a> dislocation slip

basal <a> slip and extension twinning

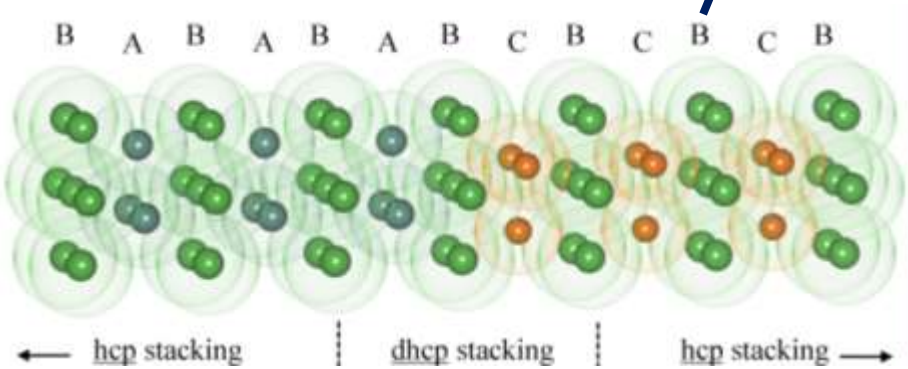
Improved mechanical properties

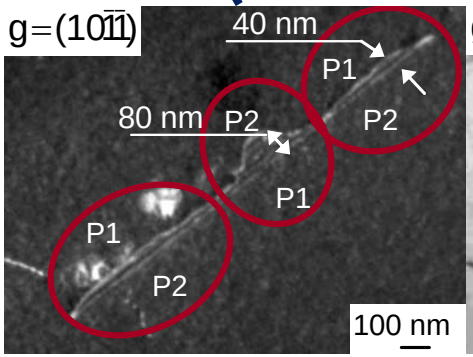
Enhanced <c+a> dislocations

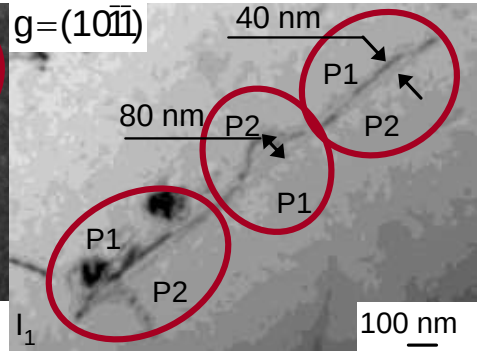



Assumption: SFE Modification

$SFI_1$ acts as nucleations source for <c+a> dislocations



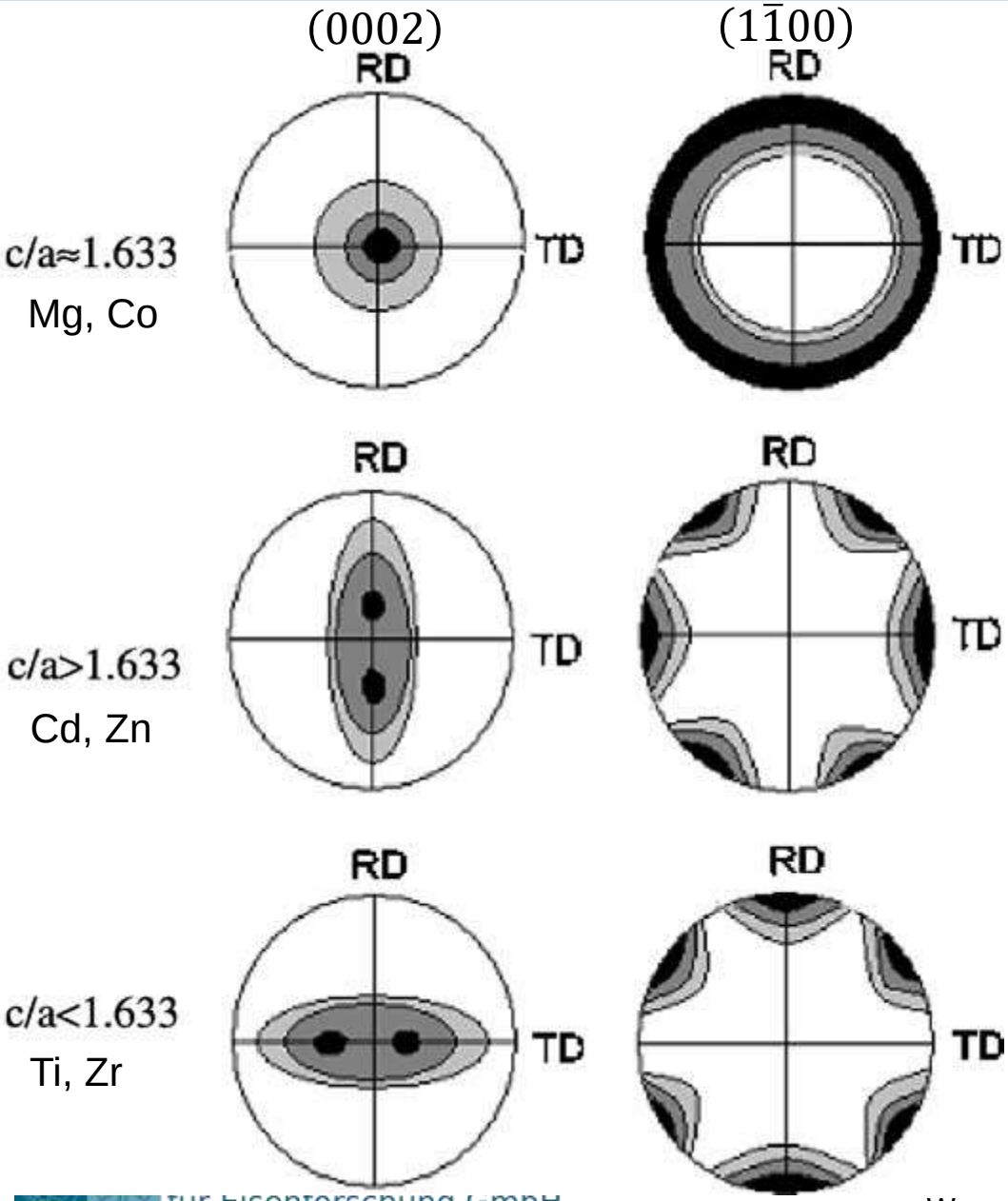
# Quiz

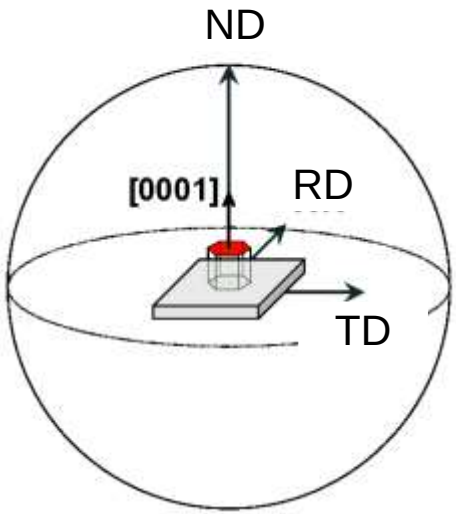
- Which stacking faults in hexagonal metals do you remember?
- How do the stacking fault energy(s) influence the deformation behavior of hexagonal metals?

# Topics

- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink bands
- Twinning in hexagonal metals
- Stacking faults in hexagonal metals
- Texture components in hexagonal metals

# Texture components in hexagonal metals



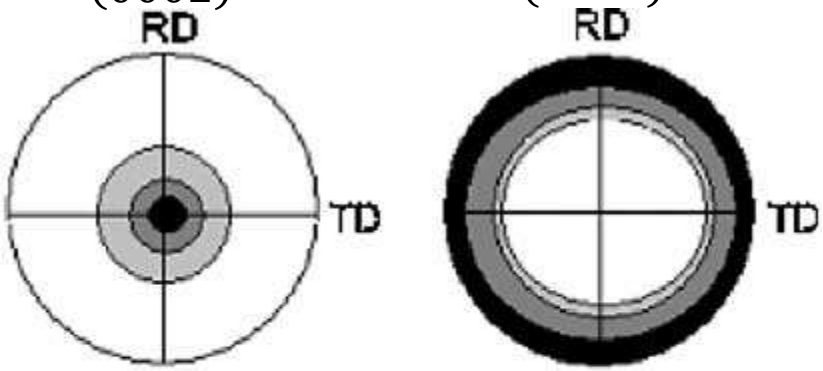

K. Hantzsche

Wang et al. (2003)

# Texture components in hexagonal metals

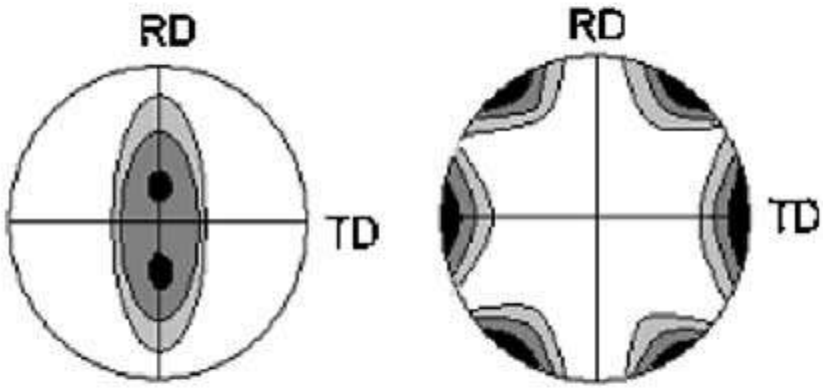
$(0002)$ $(1\bar{1}00)$

c/a≈1.633
Mg, Co




Basal <a> slip + tension twinning

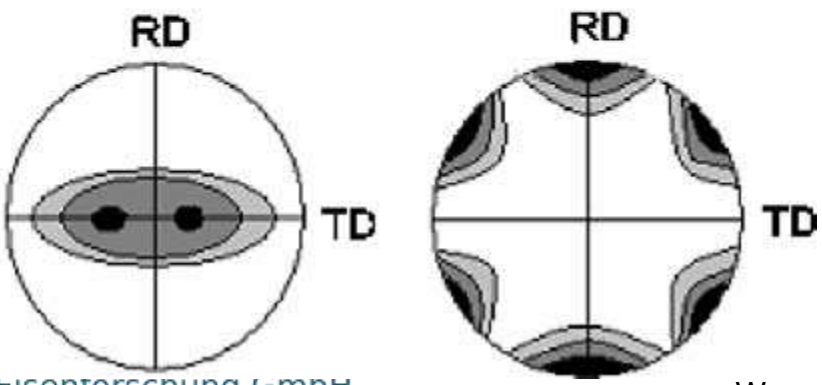
c/a>1.633
Cd, Zn




Basal <a> slip + pyramidal slip

plastic anisotropy

c/a<1.633
Ti, Zr

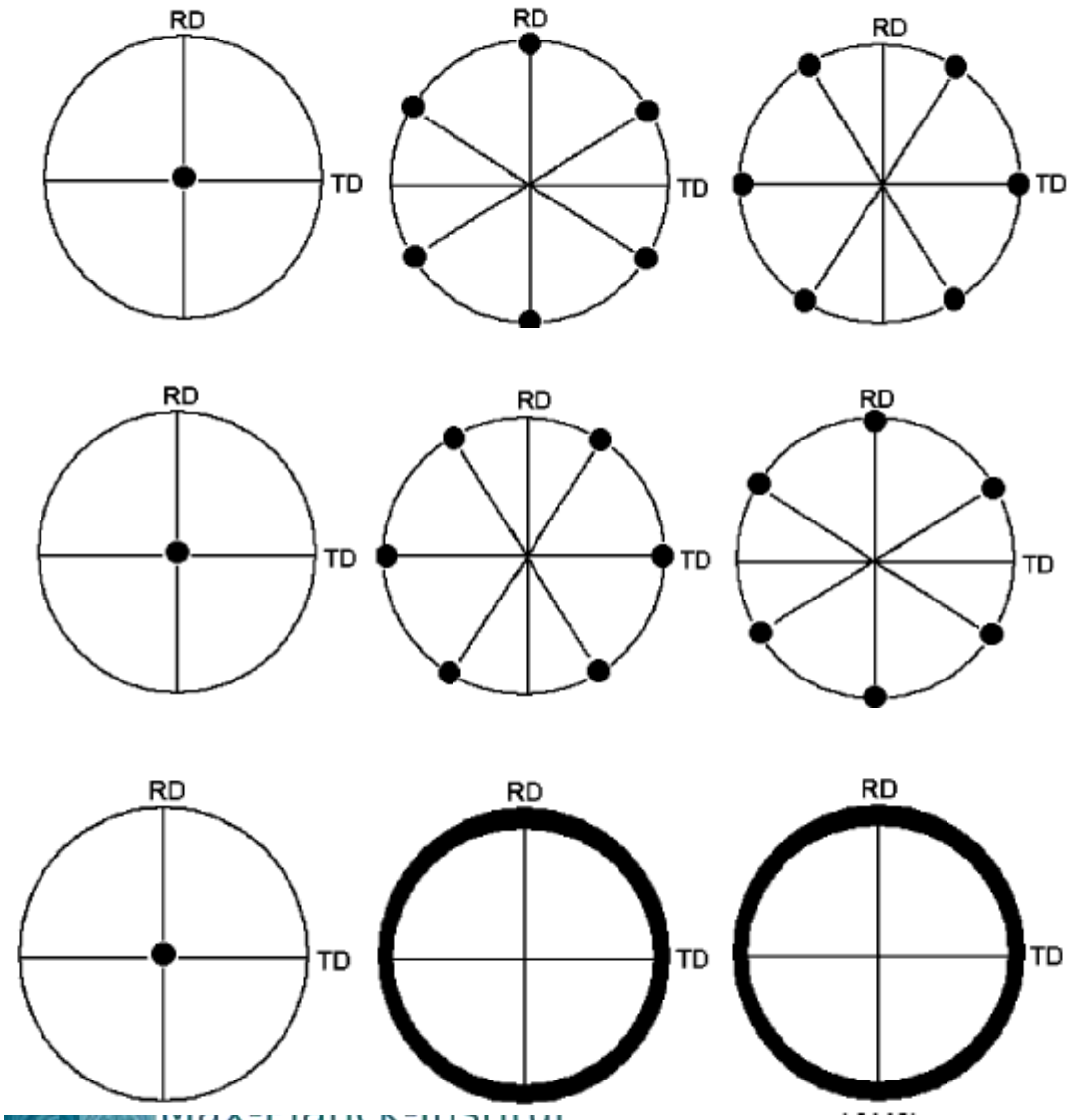


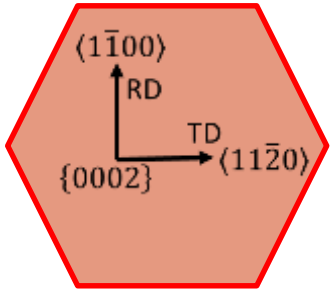

Prismatic <a> slip + basal <a>slip

Wang et al. (2003)

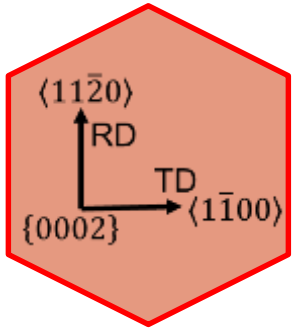
# Texture components in hexagonal metals

$(0002)$ $(1\bar{1}00)$ $(11\bar{2}0)$

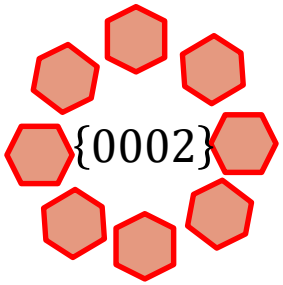



$\{0001\}\langle 1\bar{1}00\rangle$
Basal texture




$\{0001\}\langle 11\bar{2}0\rangle$
Basal texture

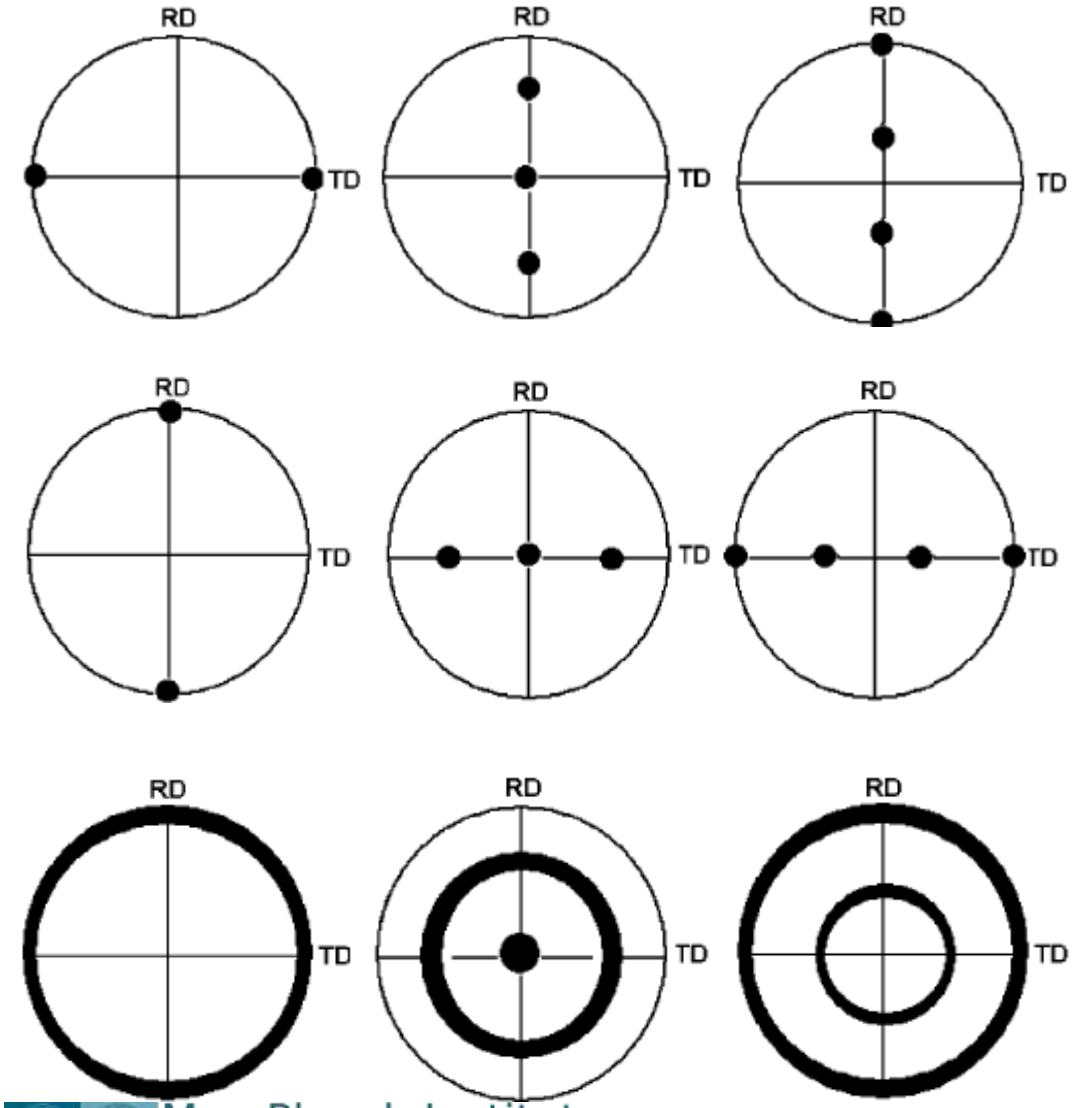


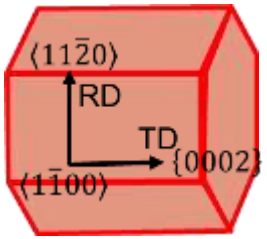

Basal fiber texture

Wang et al. (2003)

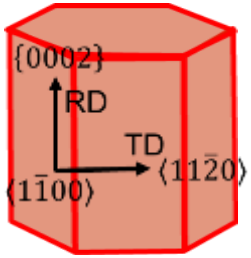
# Texture components in hexagonal metals

$(0002)$ $(1\bar{1}00)$ $(11\bar{2}0)$

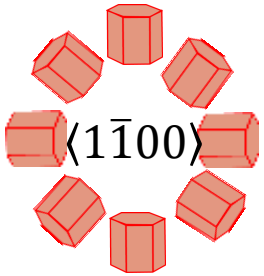



$\{1\bar{1}00\}\langle 11\bar{2}0\rangle$
Prismatic texture




$\{1\bar{1}00\}\langle 0001\rangle$
Prismatic texture



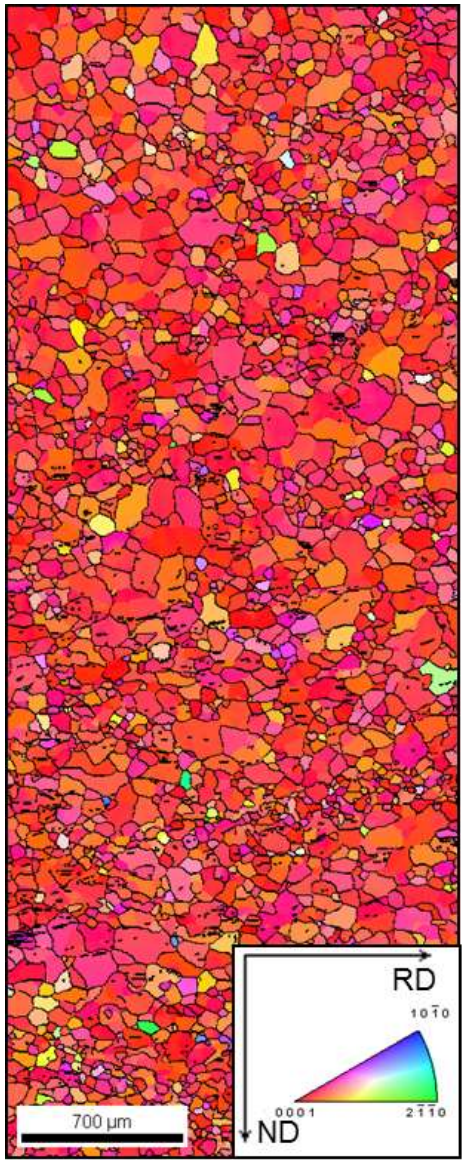

Prismatic
fiber texture

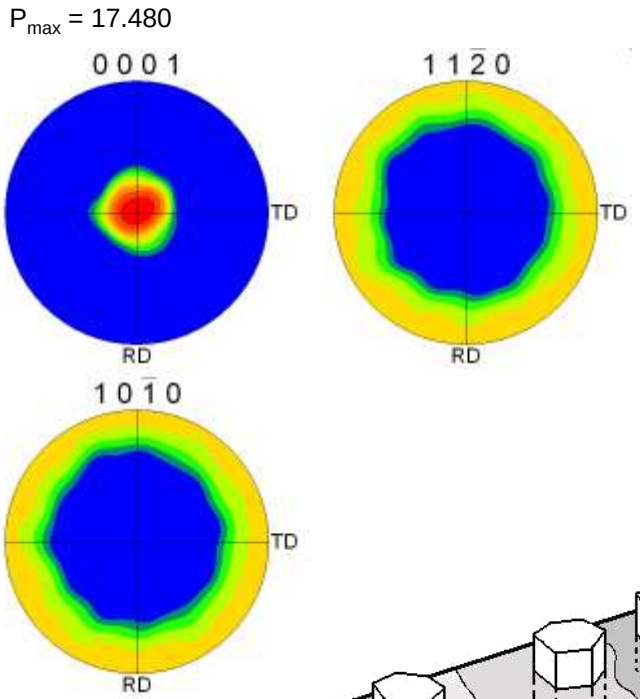


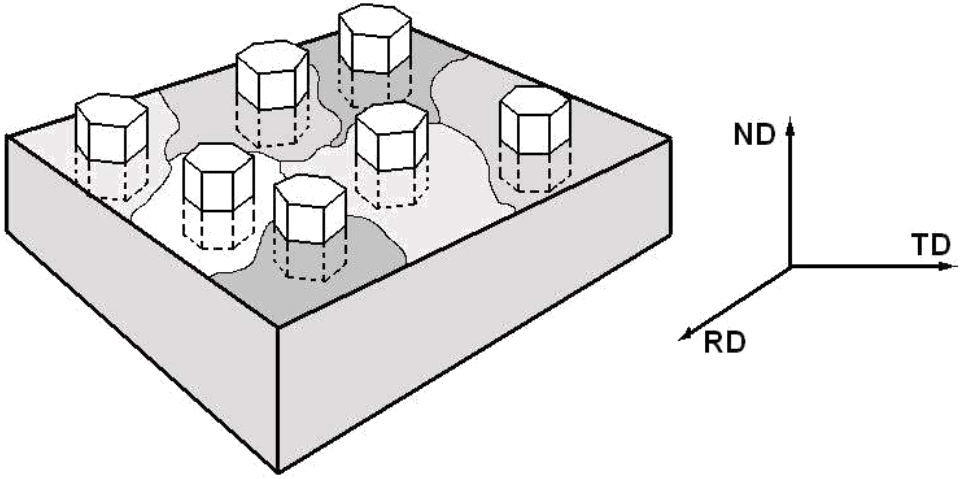


Wang et al. (2003)

# Texture components in hexagonal metals



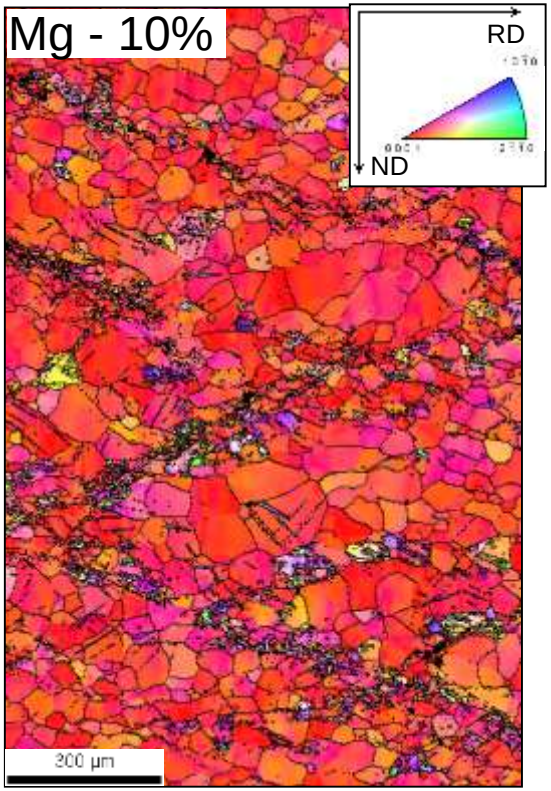



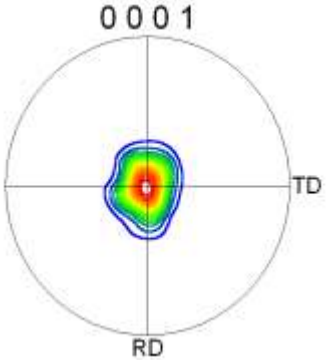




Example for strong basal texturing: Mg

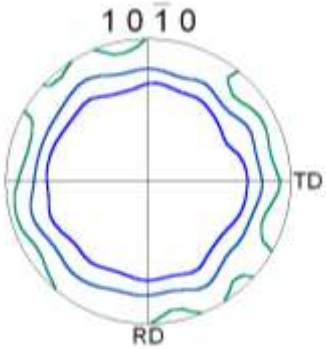
# Texture components in hexagonal metals

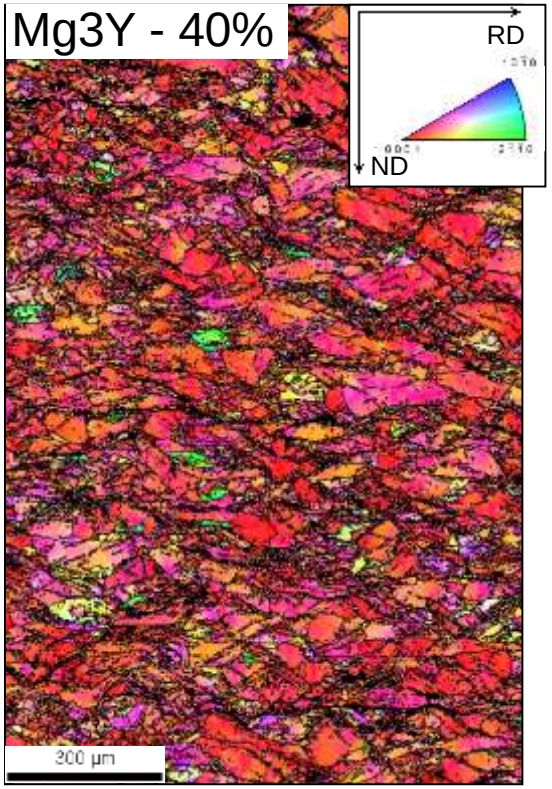
Deformation texture at fracture begin

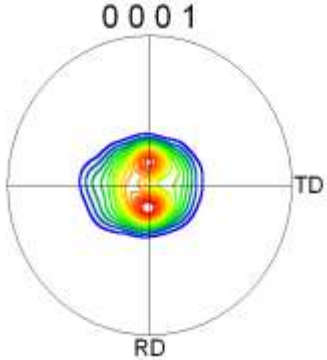


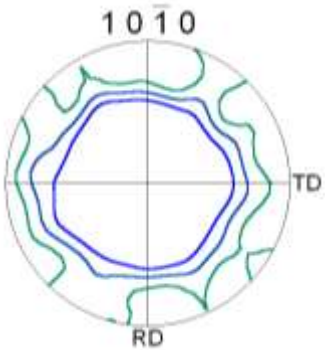

$P_{max}$ = 17.165




$P_{max}$ = 8.230




- Strong basal type texture
- Matrix grains (0001)||ND
- Basal slip and tensile twinning

- Weaker (0.5) basal texture intensity
- r-type texture ((0001) 15° tow. RD)
- non-basal deformation mechanisms

Questions?

Ask now

or:

sandloebes@imm.rwth-aachen.de
raabe@mpie.de