

# Dislocations, crystalline anisotropy and plasticity in hexagonal metals

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# Structure

- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink banding
- Twinning in hexagonal metals
- Stacking faults in hexagonal metals
- Texture components in hexagonal metals
- Anisotropy of precipitation strengthening
- Phase transformations; dual- / multiphase systems
- Damage, fracture in hexagonal metals
- Characterization of plasticity carriers in hexagonal metals

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# Crystal structure and Miller-Bravais indices

Reminder: hexagonal crystal structure and Miller-Bravais indices

ABAB stacking sequence

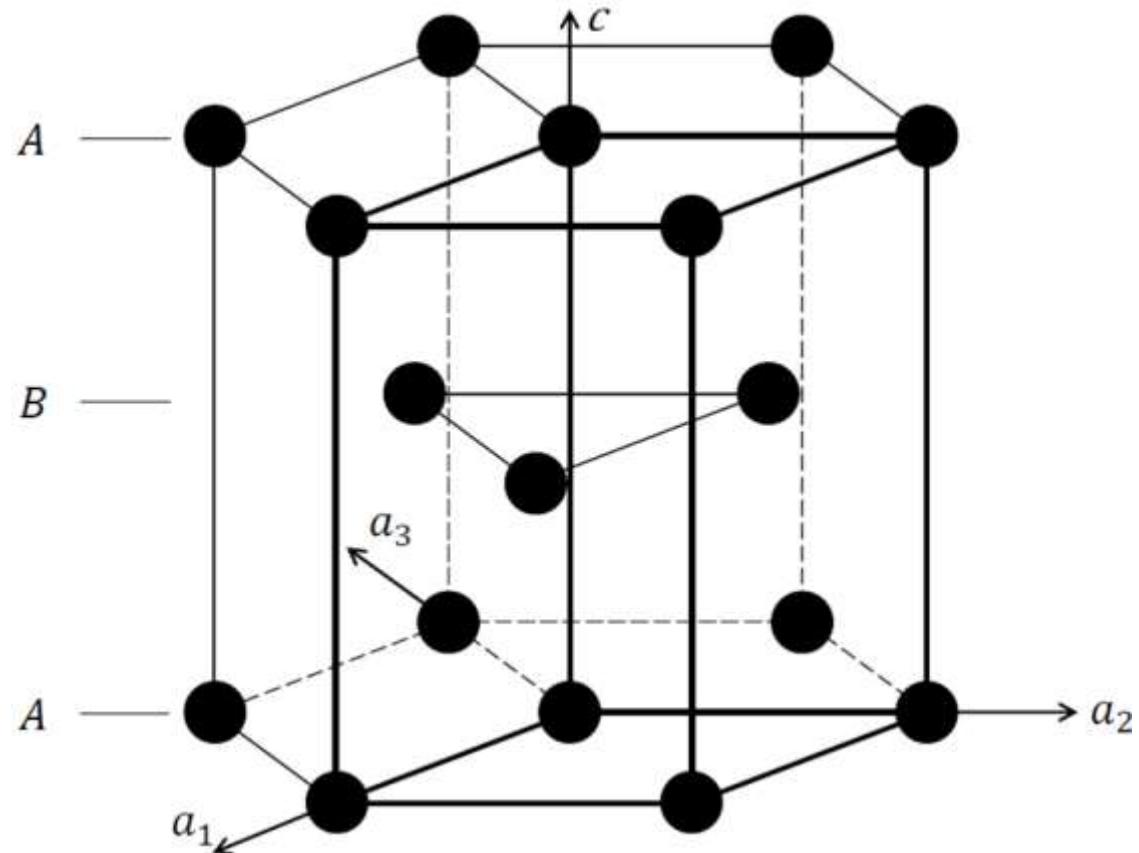
Axes:

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

Angles:

$$a\text{-}c = 90^\circ$$

$$a_1\text{-}a_2 = a_2\text{-}a_3 = a_1\text{-}a_3 = 120^\circ$$



# Crystal structure and Miller-Bravais indices

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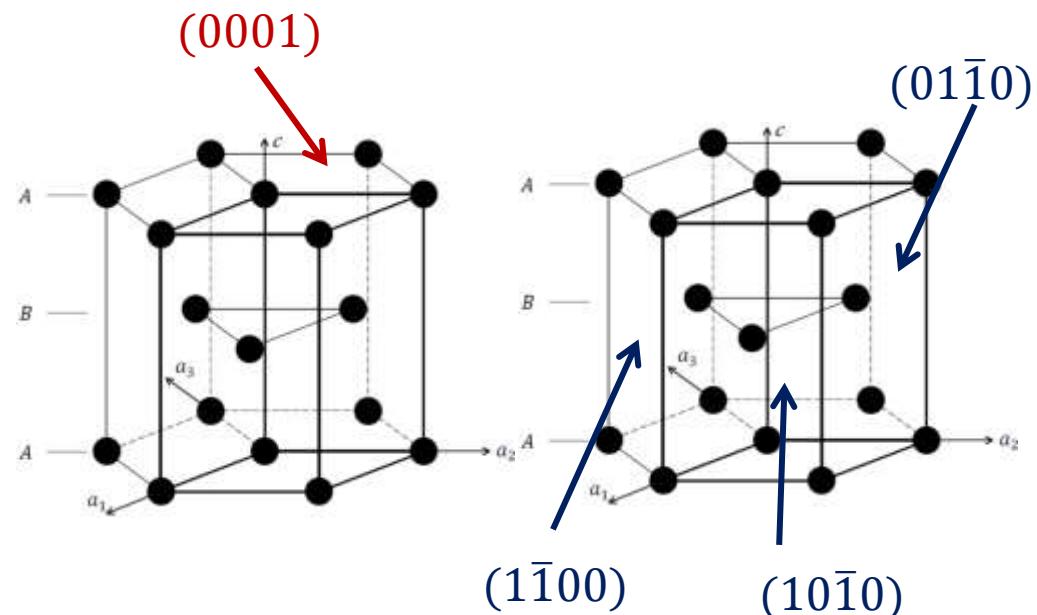
$$a\text{-}c = 90^\circ$$

$$a_1\text{-}a_2 = a_2\text{-}a_3 = a_1\text{-}a_3 = 120^\circ$$

Planes (Miller-Bravais indeces):

$$(hkil) \text{ with } h + k + i = 0$$

$a_3$  is redundant:  $a_3 = -(a_1 + a_2)$



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Reminder: hexagonal crystal structure and Miller-Bravais indices

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Axes:

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

Angles:

$$a-c = 90^\circ$$

$$a_1-a_2 = a_2-a_3 = a_1-a_3 = 120^\circ$$

Planes (Miller-Bravais indeces):

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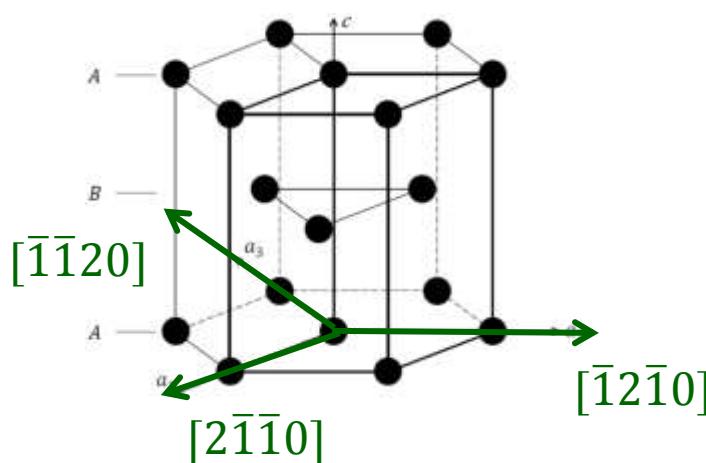
Directions (Miller-Bravais indeces):

$$[uvw\bar{t}] \text{ with } u + v + t = 0$$

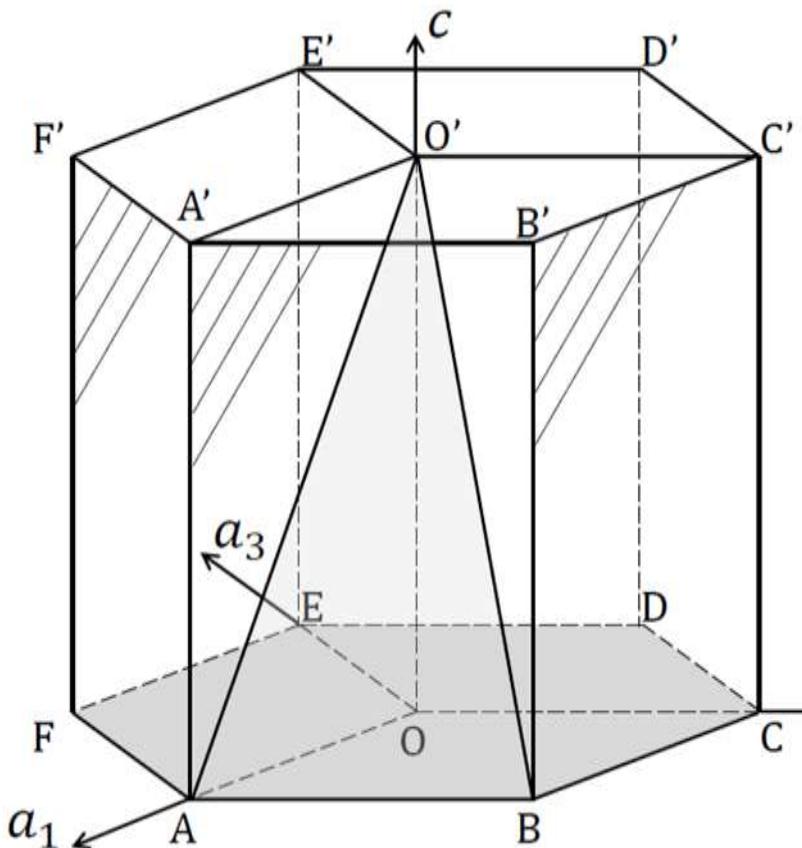
$$u = \frac{1}{3}(2u - v)$$

$$v = \frac{1}{3}(2u - v)$$

$$t = -(u + v)$$



# Crystal structure and Miller-Bravais indices

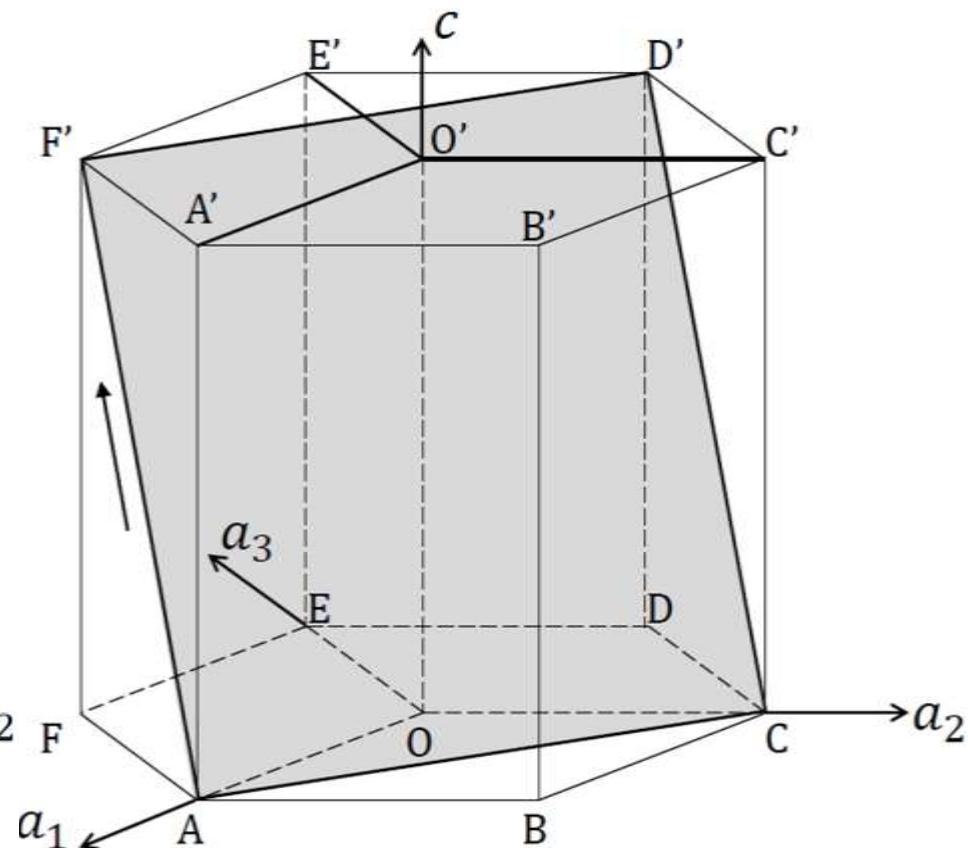


ACE: basal plane

ABB'A': prismatic plane

ABO': first order pyramidal plane

ACD'F': second order pyramidal plane



AB:  $\langle a \rangle$  direction

AF':  $\langle c + a \rangle$  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

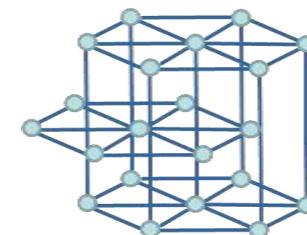
Relevance of hexagonal metals:

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

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HEX  $\neq$  hcp

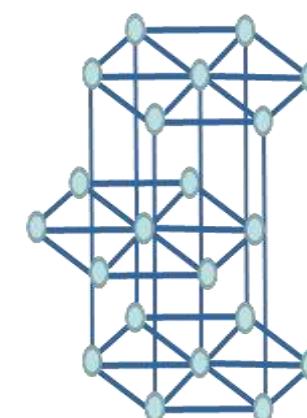
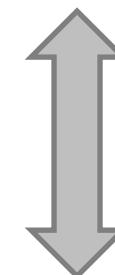


NOT: closed packed crystal structure

Classification as structural materials class „hcp“ not adequate

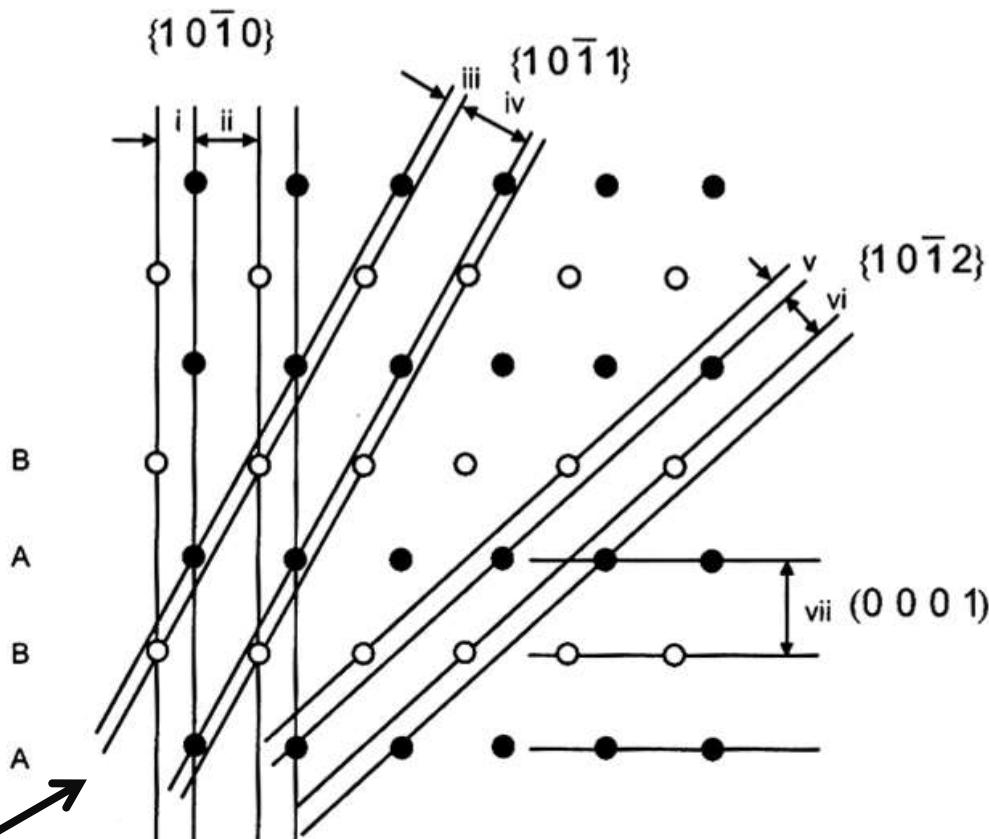
Plastically anisotropic

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	
<b>Mg</b>	<b>1.624</b>
Zn	1.856
Cd	1.886



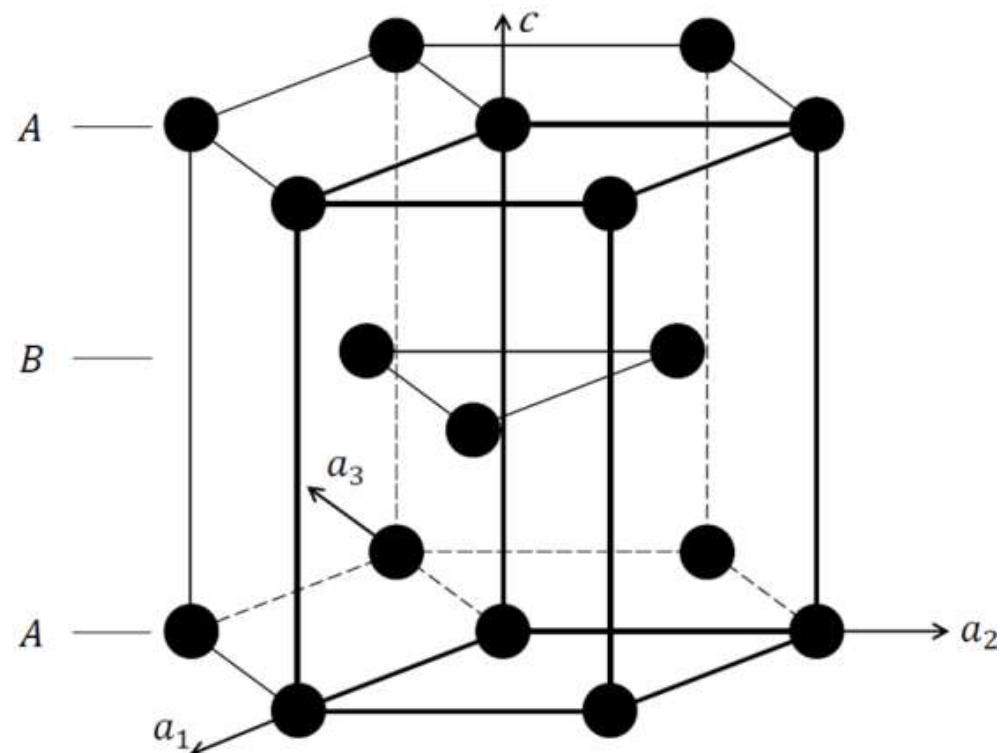
	Interplanar spacing
i	$\frac{a\sqrt{3}}{6}$
ii	$\frac{a\sqrt{3}}{3}$
iii	$\frac{ac\sqrt{3}}{6\sqrt{4c^2 + 3a^2}}$
iv	$\frac{5ac\sqrt{3}}{6\sqrt{4c^2 + 3a^2}}$
v	$\frac{ac\sqrt{3}}{6\sqrt{3a^2 + c^2}}$
vi	$\frac{ac\sqrt{3}}{3\sqrt{3a^2 + c^2}}$
vii	$c/2$

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

Partridge, 1967

# Quiz

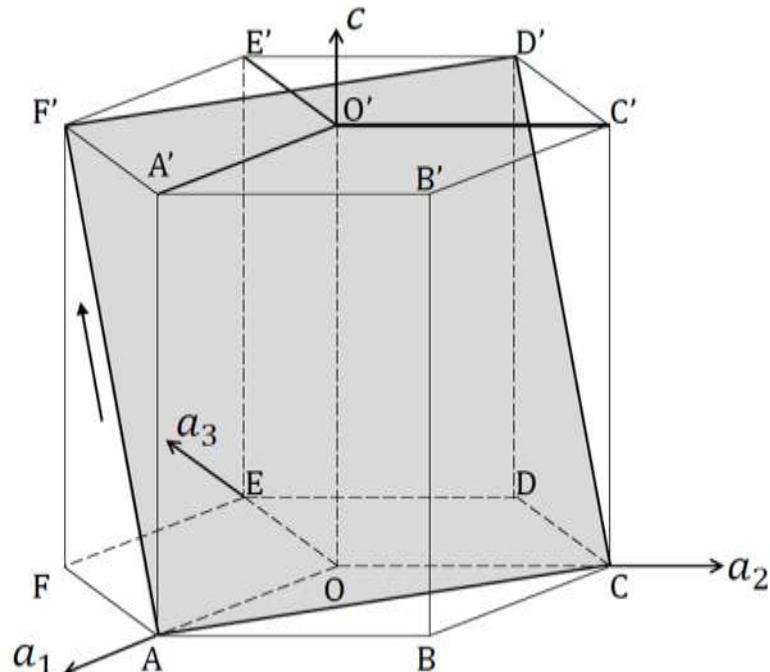
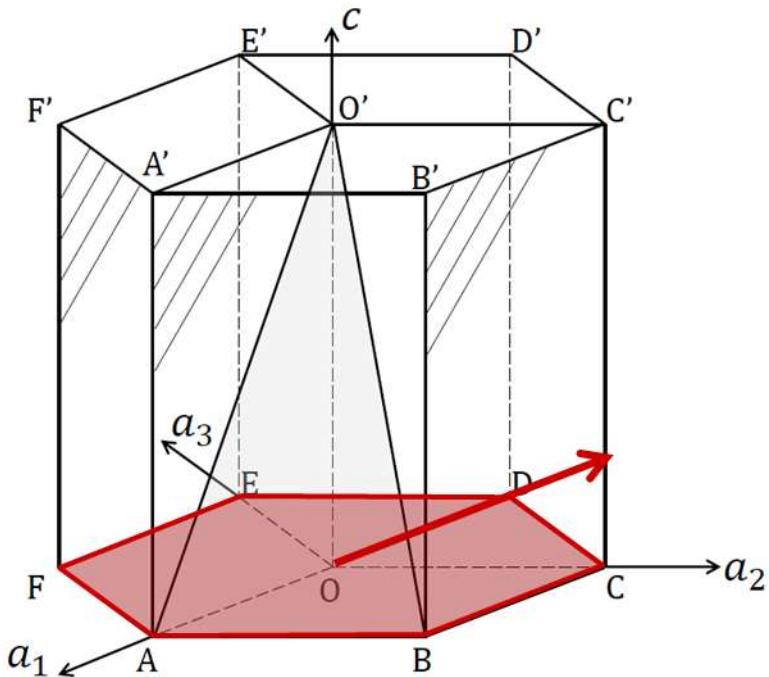
- Why use of Miller-Bravais for hexagonal structure?
- Give the indices and show
  - Basal plane
  - Prismatic plane
  - 1<sup>st</sup> order pyramidal plane
  - $\langle a \rangle$  direction
  - $\langle c+a \rangle$  direction



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# Dislocations in hexagonal metals



ACE: basal plane

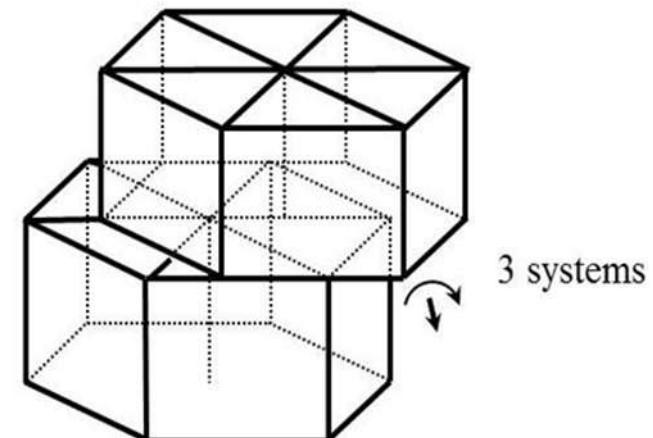
ABB'A': prismatic plane

ABO': first order pyramidal plane

ACD'F': second order pyramidal plane

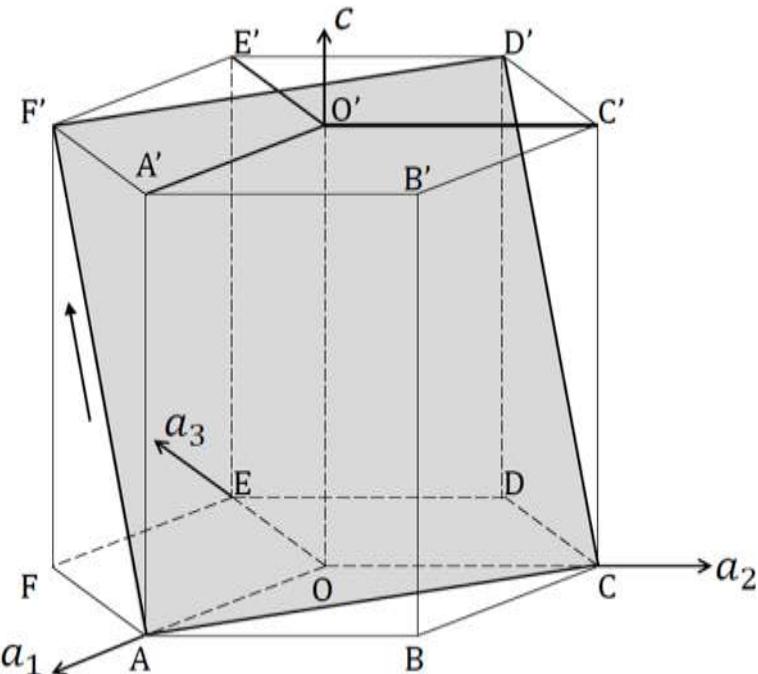
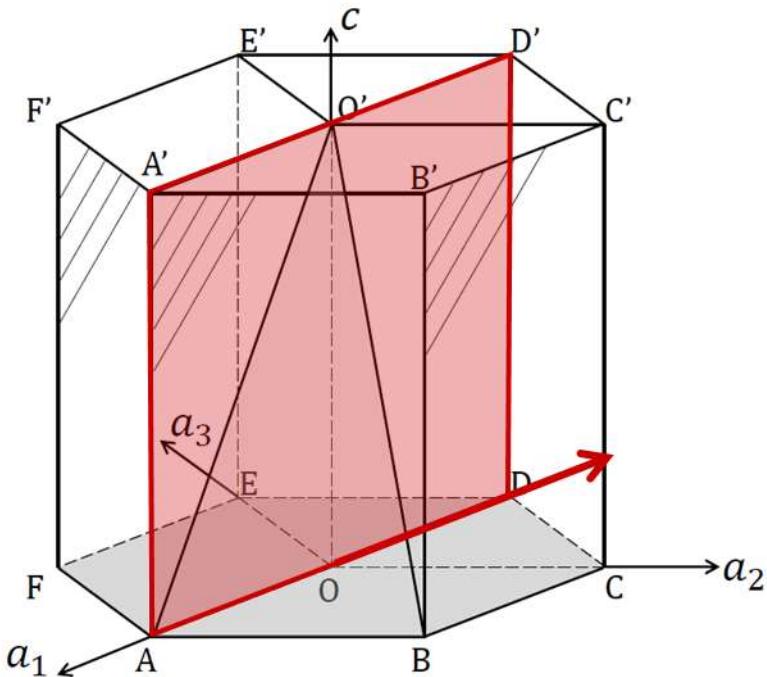
AB:  $\langle a \rangle$  direction

AF':  $\langle c + a \rangle$  direction



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

# Dislocations in hexagonal metals



Cross-slip of  $\langle a \rangle$  dislocations on prismatic plane

ACE: basal plane

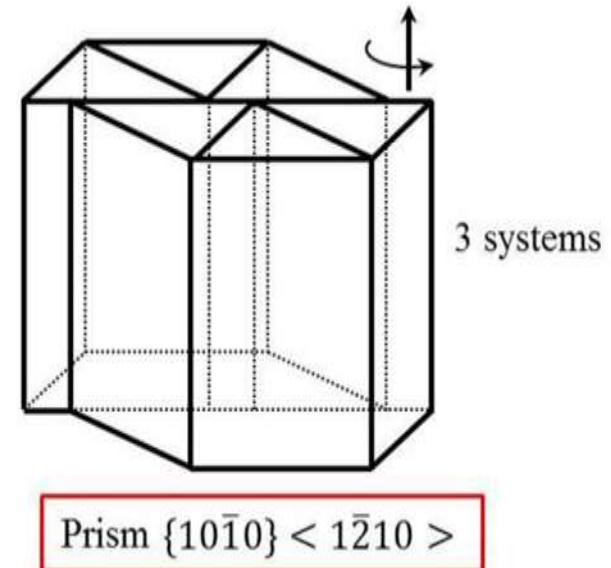
ABB'A': prismatic plane

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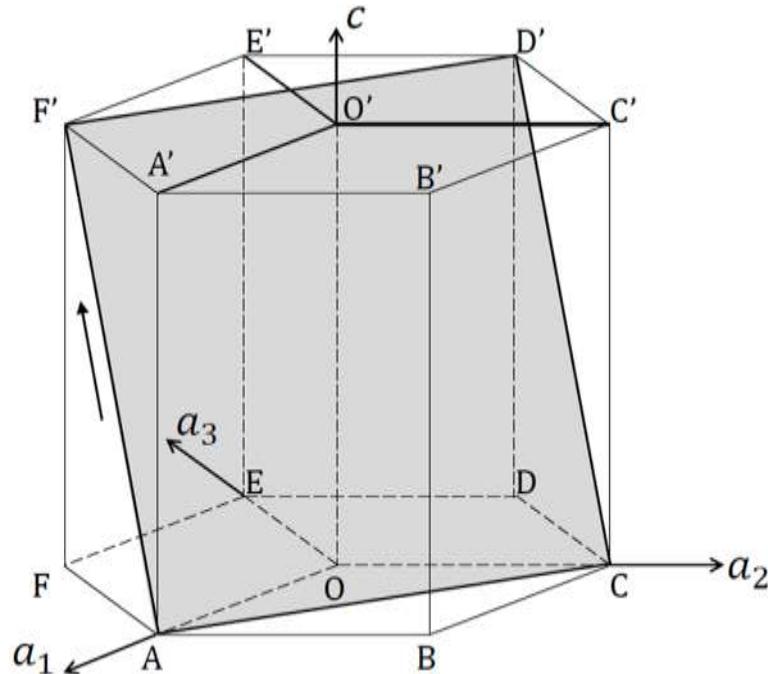
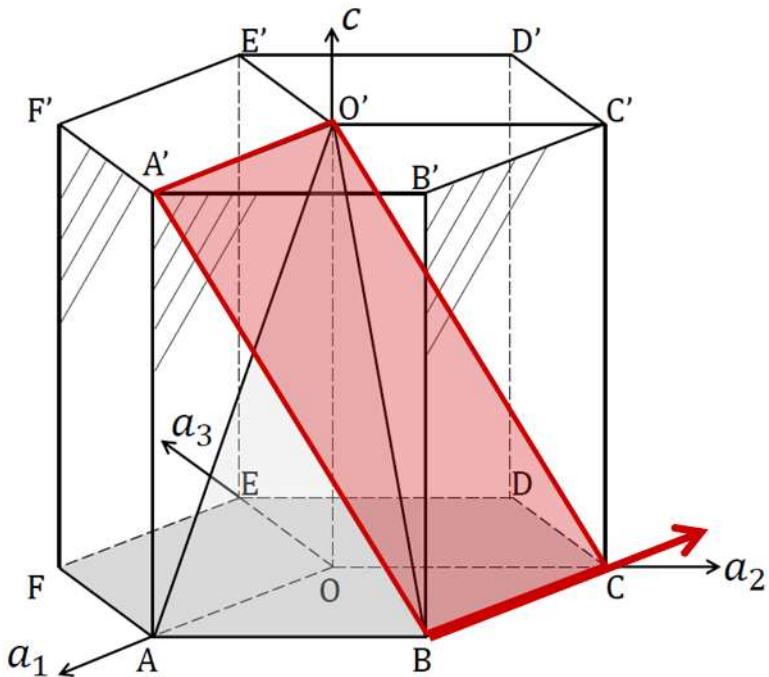
ACD'F': second order pyramidal plane

AB:  $\langle a \rangle$  direction

AF':  $\langle c + a \rangle$  direction



# Dislocations in hexagonal metals



Cross-slip of  $\langle a \rangle$  dislocations on pyramidal plane

ACE: basal plane

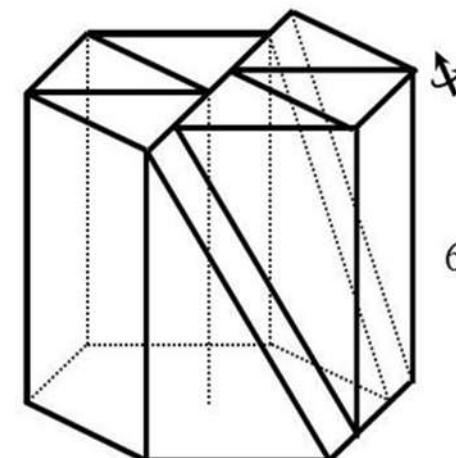
ABB'A': prismatic plane

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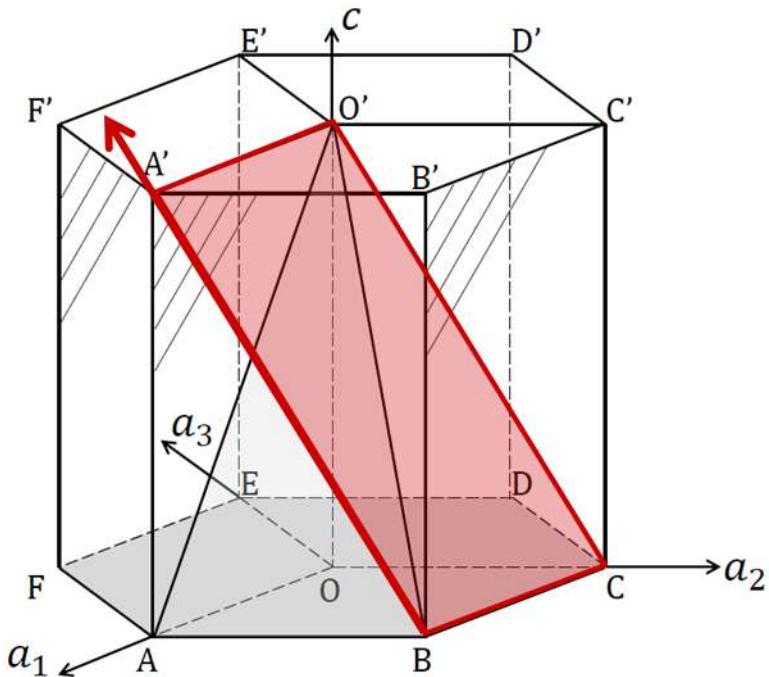
AB:  $\langle a \rangle$  direction

AF':  $\langle c + a \rangle$  direction



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

# Dislocations in hexagonal metals



ACE: basal plane

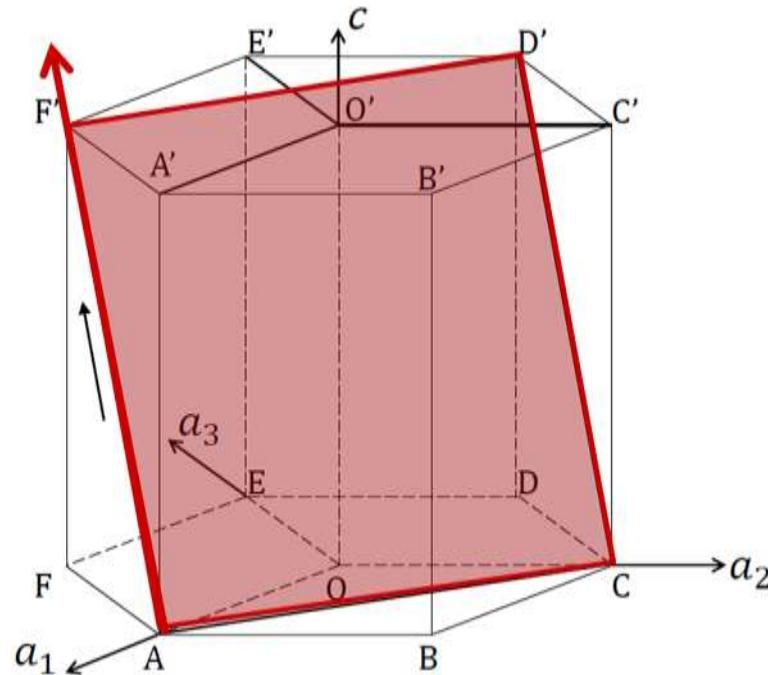
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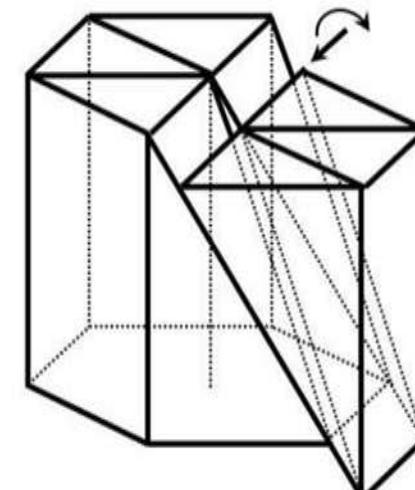
ACD'F': second order pyramidal plane

AB:  $\langle a \rangle$  direction

AF':  $\langle c + a \rangle$  direction



12 systems



Pyramidal  $\langle c+a \rangle$   $\{10\bar{1}1\} < 2\bar{1}13 >$

# 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)	$ a ^2$	3	2
prismatic	$\vec{a}$	$<11\bar{2}0>$	{1010}	$ a ^2$	3	2
pyramidal $\langle a \rangle$	$\vec{a}$	$<11\bar{2}0>$	{1011}	$ a ^2$	6	4
pyramidal $\langle c+a \rangle$	$\vec{c} + \vec{a}$	$<11\bar{2}3>$	{1011}	$2.63 a ^2$	6	5
pyramidal $\langle c+a \rangle$	$\vec{c} + \vec{a}$	$<11\bar{2}3>$	{1122}	$2.63 a ^2$	4	5
twinning						0.5 (polar)

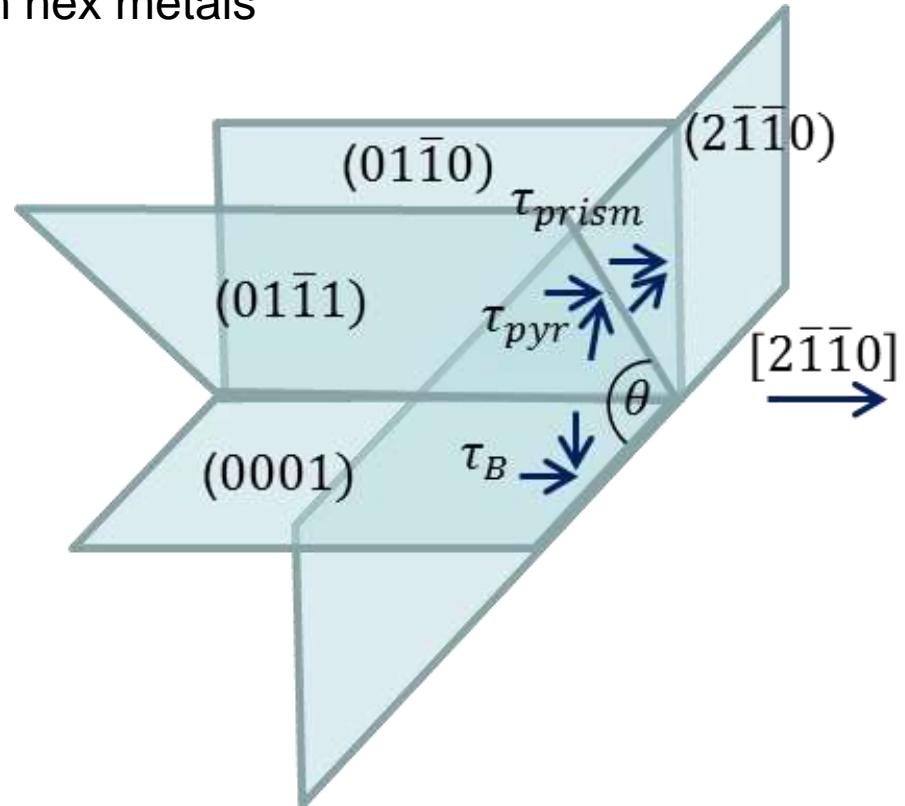
# Dislocations in hexagonal metals

Generalized CRSS for slip systems in hex metals

$$\tau_{crit} = \frac{F}{A} \cdot \cos \kappa \cdot \cos \lambda = \sigma \cdot m$$

$\lambda$ : angle of force to slip direction

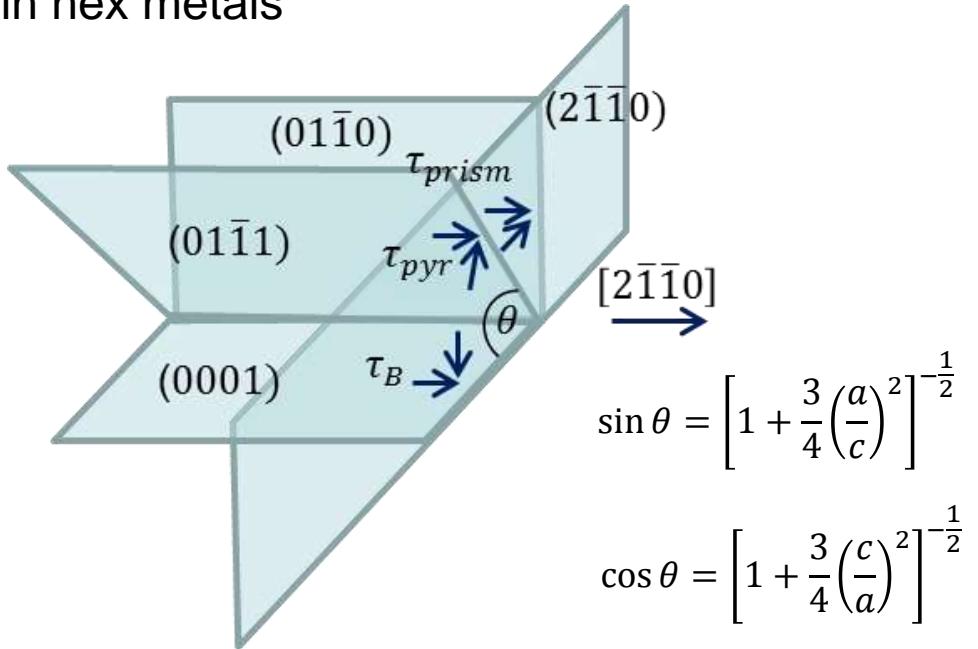
$\kappa$ : angle of force to slip plane normal



# Dislocations in hexagonal metals

Generalized CRSS for slip systems in hex metals

$$\tau_{crit} = \frac{F}{A} \cdot \cos \kappa \cdot \cos \lambda = \sigma \cdot m$$



$$\sin \theta = \left[ 1 + \frac{3}{4} \left( \frac{a}{c} \right)^2 \right]^{-\frac{1}{2}}$$

$$\cos \theta = \left[ 1 + \frac{3}{4} \left( \frac{c}{a} \right)^2 \right]^{-\frac{1}{2}}$$

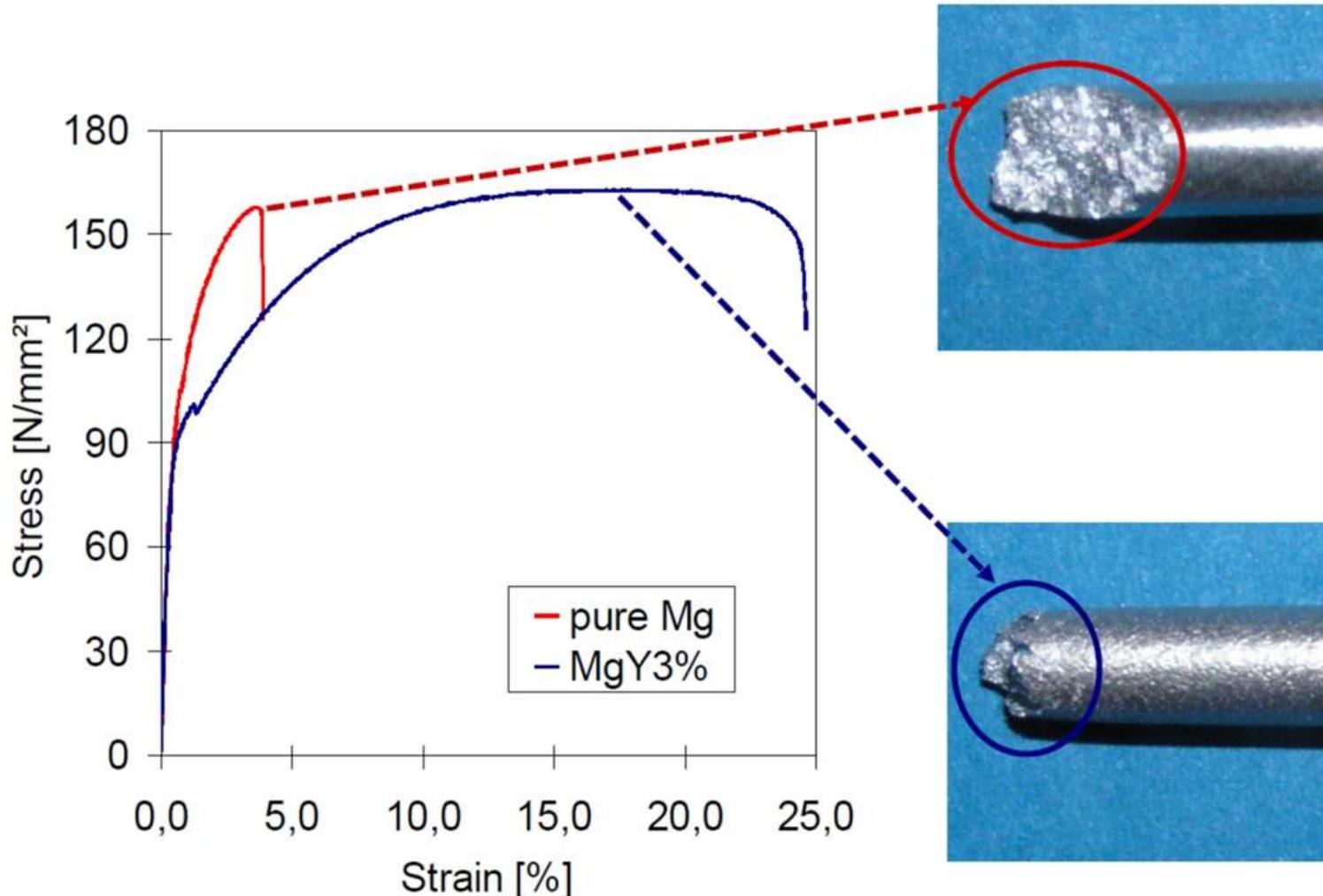
Examples:

$$(0002)[\bar{1}2\bar{1}0]: \tau_{crit} (0002)[\bar{1}2\bar{1}0] = \frac{\sigma_{zx}}{2} + \frac{\sqrt{3}}{2} \cdot \sigma_{zy}$$

$$(10\bar{1}0)[\bar{1}2\bar{1}0]: \tau_{crit} (10\bar{1}0)[\bar{1}2\bar{1}0] = \frac{\sqrt{3}}{4} \cdot (\sigma_{xx} - \sigma_{yy}) + \frac{\sigma_{xy}}{2}$$

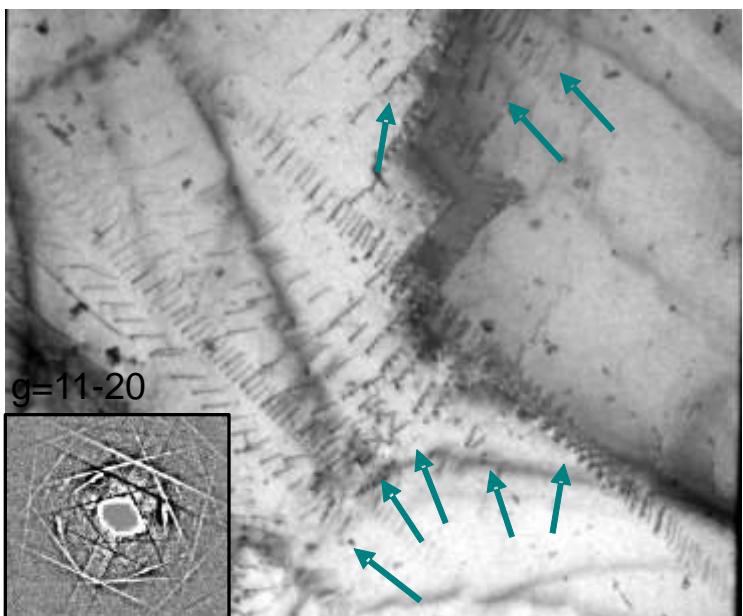
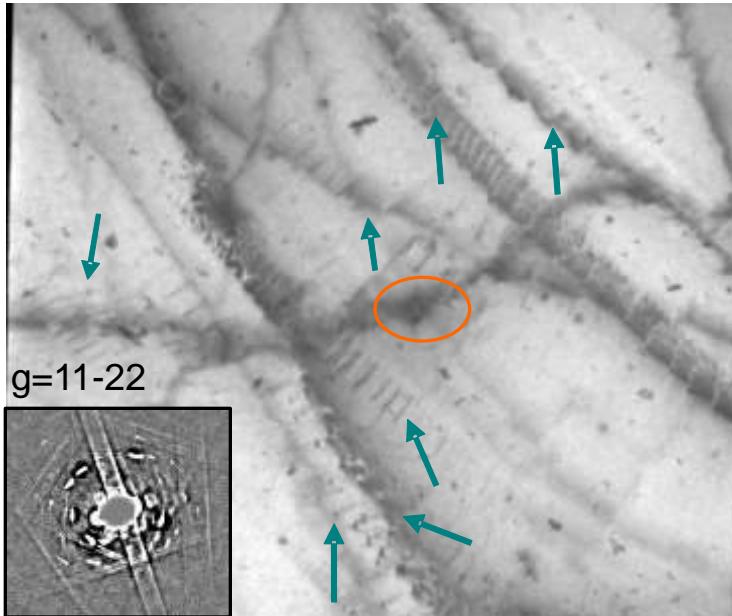
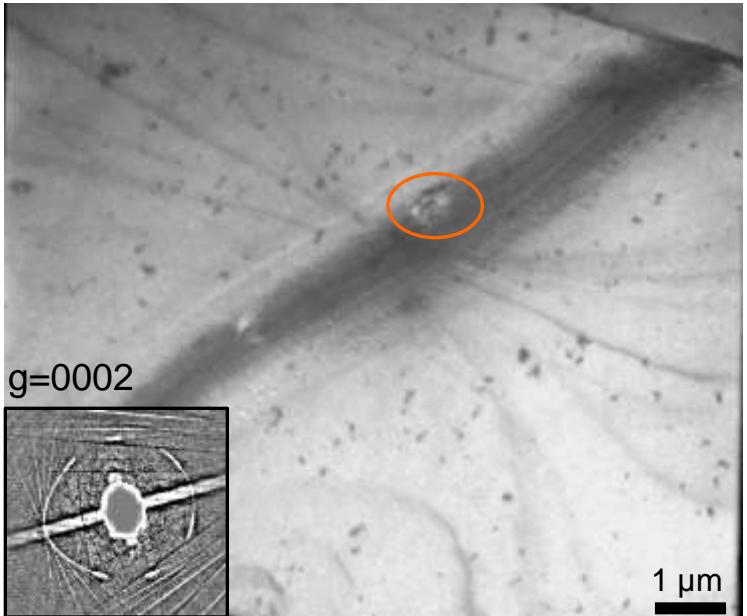
$$(10\bar{1}1)[\bar{1}2\bar{1}0]: \tau_{crit} (10\bar{1}1)[\bar{1}2\bar{1}0] = \frac{\sqrt{3}}{4} \cdot \sin \theta (\sigma_{xx} - \sigma_{yy}) - \sin \theta \frac{\sigma_{xy}}{2} - \cos \theta \frac{\sigma_{zx}}{2} + \frac{\sqrt{3}}{2} \cos \theta \sigma_{zy}$$

# Dislocations in hexagonal metals



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

# Dislocations in hexagonal metals

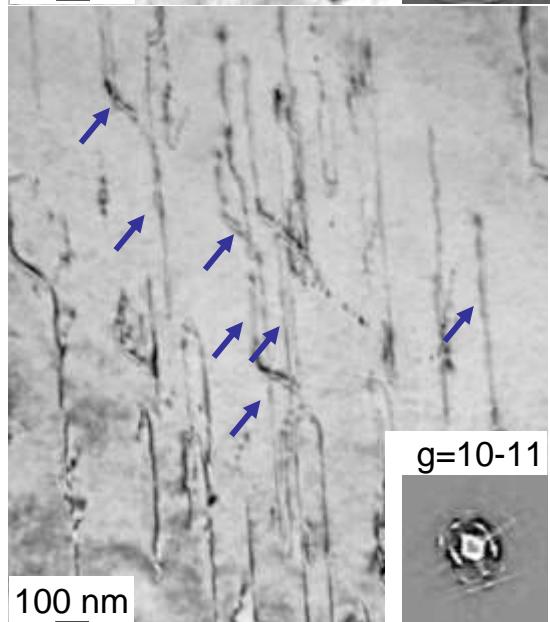
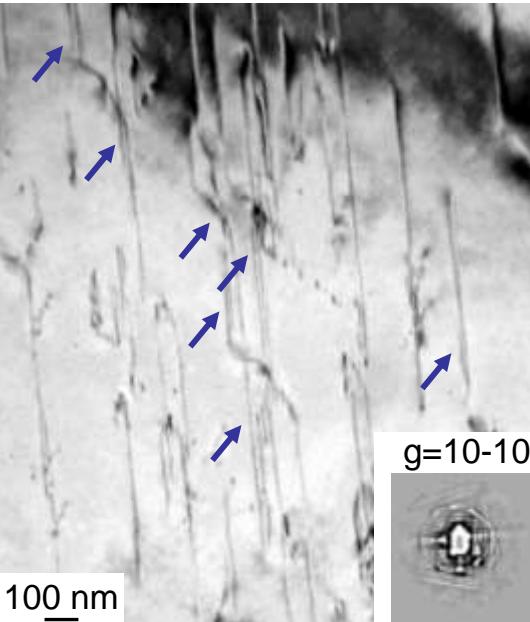
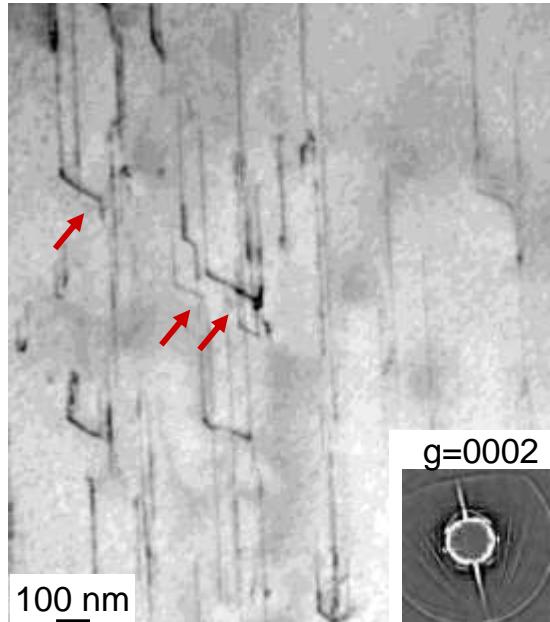


- basal  $\langle a \rangle$
- sessile  $\langle c \rangle$

TEM images of dislocations in pure Mg

- High amount of basal  $\langle a \rangle$  dislocations
- Hardly any dislocations with a  $\langle c \rangle$  component
- Basal  $\langle a \rangle$  dislocations lying on defined slip bands

# Dislocations in hexagonal metals



TEM images of  $\langle c+a \rangle$  dislocations in  
Mg 3 wt-% Y (3.5 % CR)

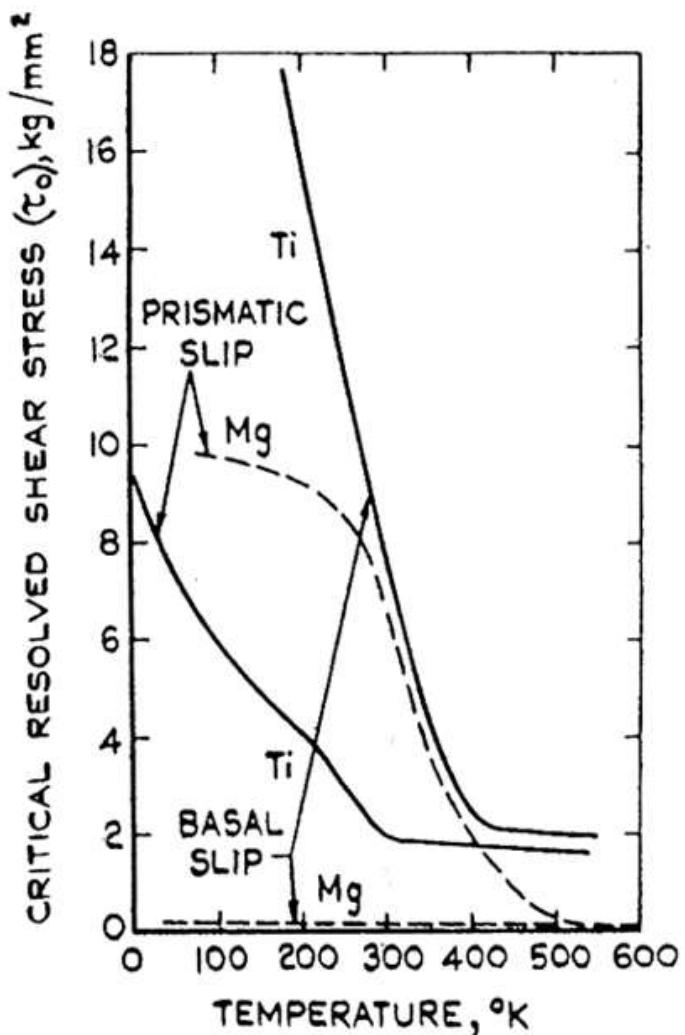
- Red arrows:  
cross-slip events
- Blue arrows:  
dislocation dissociation on  
pyramidal planes

# Dislocations in hexagonal metals

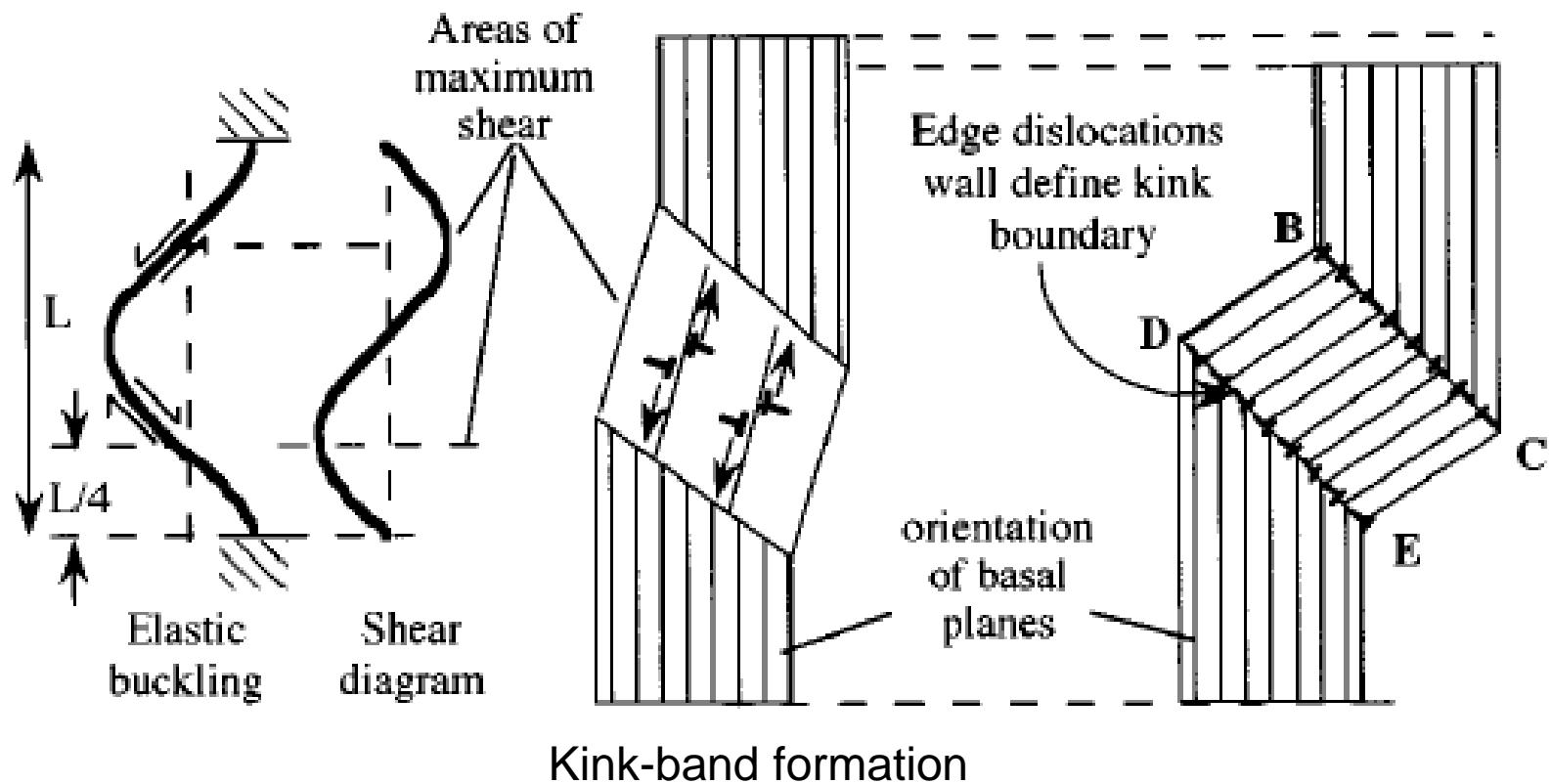
Metal	c/a	Primary glide plane	Secondary glide plane(s)
Be	1.568	basal <a>	prismatic <a>; pyramidal <a>
Y	1.572	prismatic <a>	basal <a>
Hf	1.581	prismatic <a>	basal <a>; pyramidal <a>
Ti	1.588	prismatic <a>	basal <a>; pyramidal <a>
Sc	1.592	basal <a>	
Zr	1.593	prismatic <a>	basal <a>; pyramidal <a>
Tl	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

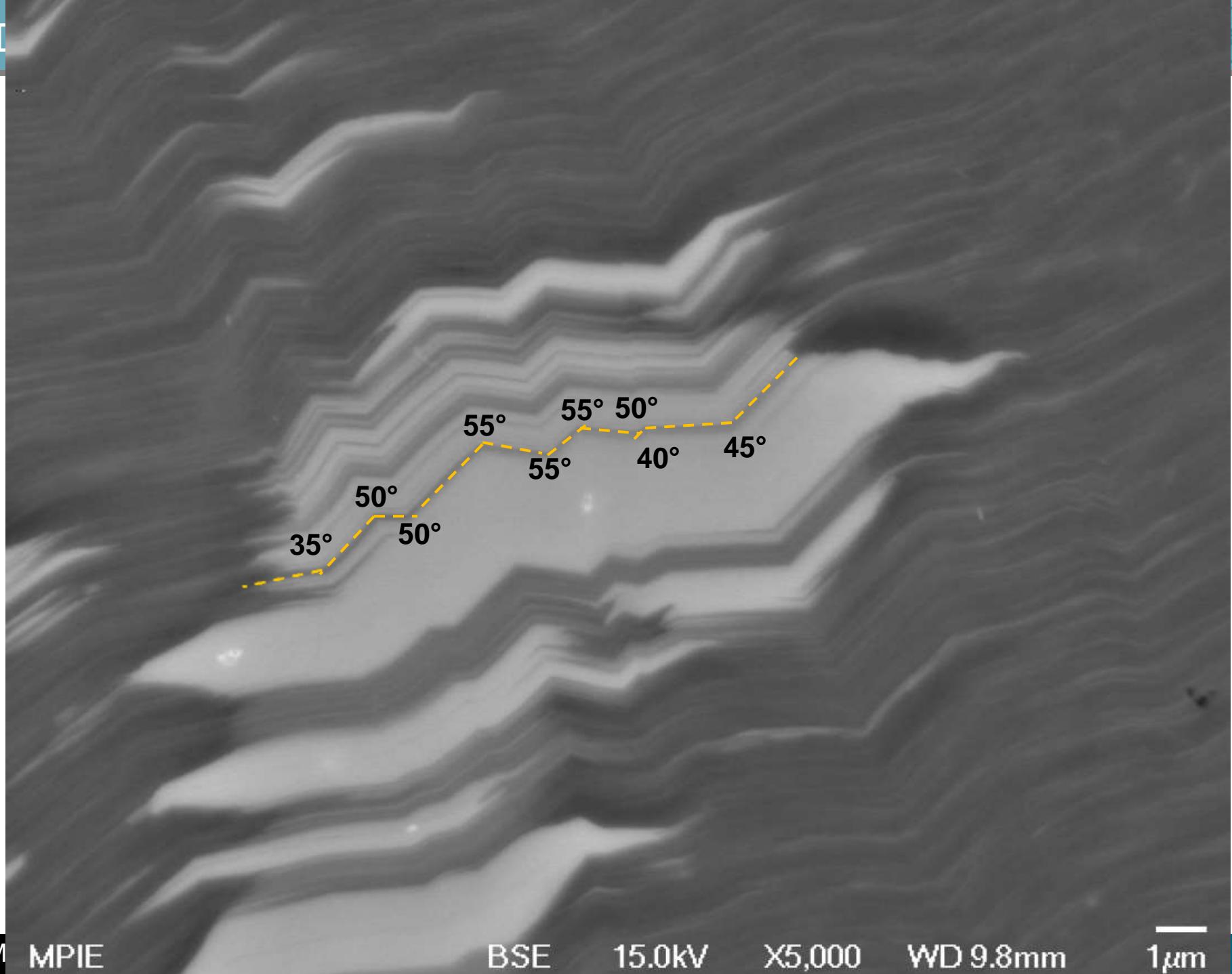
Metal	c/a	Primary glide plane	Secondary glide plane(s)
Be	1.568	basal <a>	p
Y	1.572	prismatic <a>	b
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Cd	1.886	basal <a>	p p



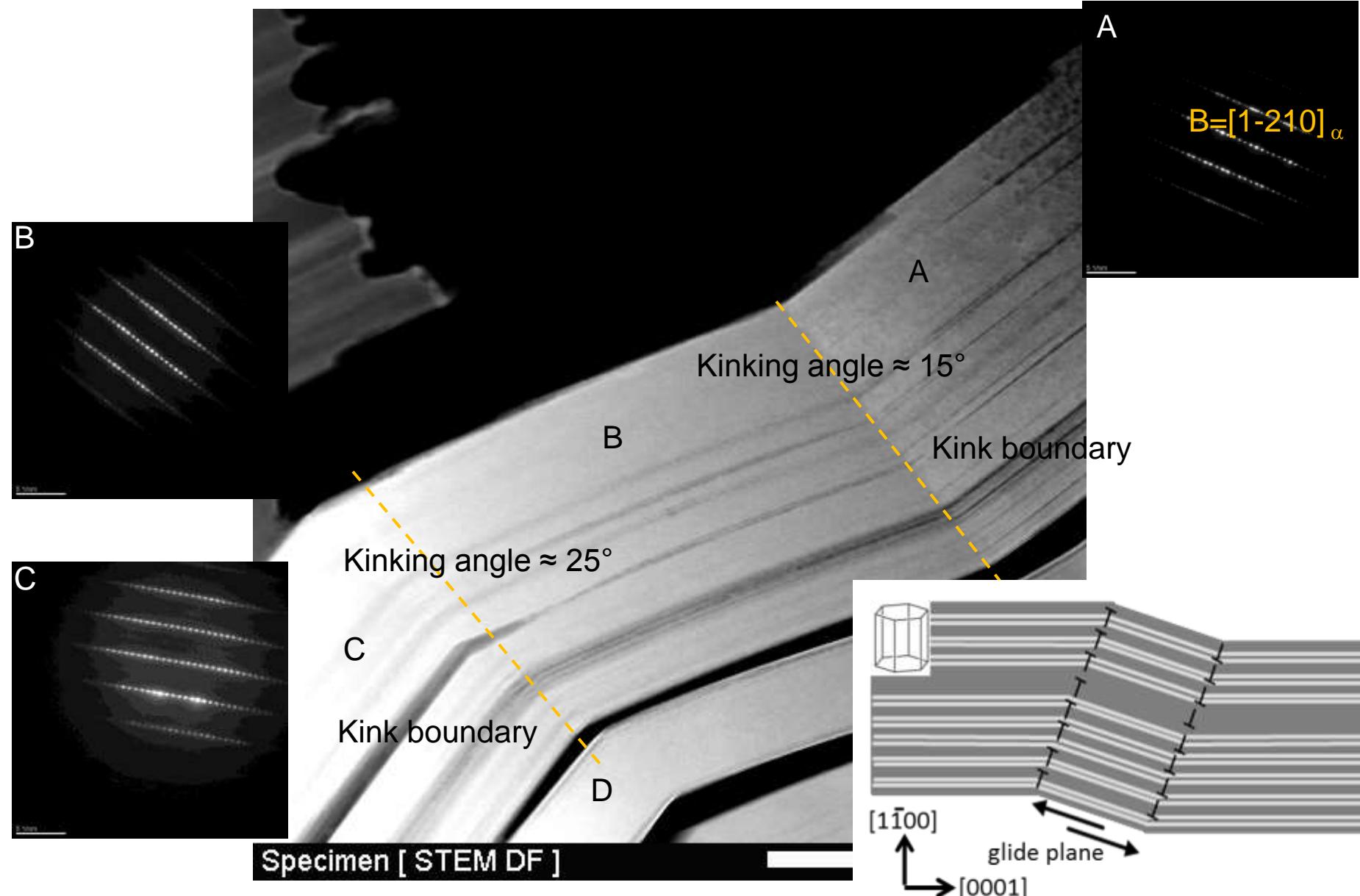
Partridge, 1967



- 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).



# Dislocations in hexagonal metals – special case kink banding



# Quiz

- How many slip system types in hexagonal metals?
- Which slip system types?
- How many independent system?
- Which are the most common slip systems?
- Why are metals with basal  $\langle a \rangle$  slip brittle?

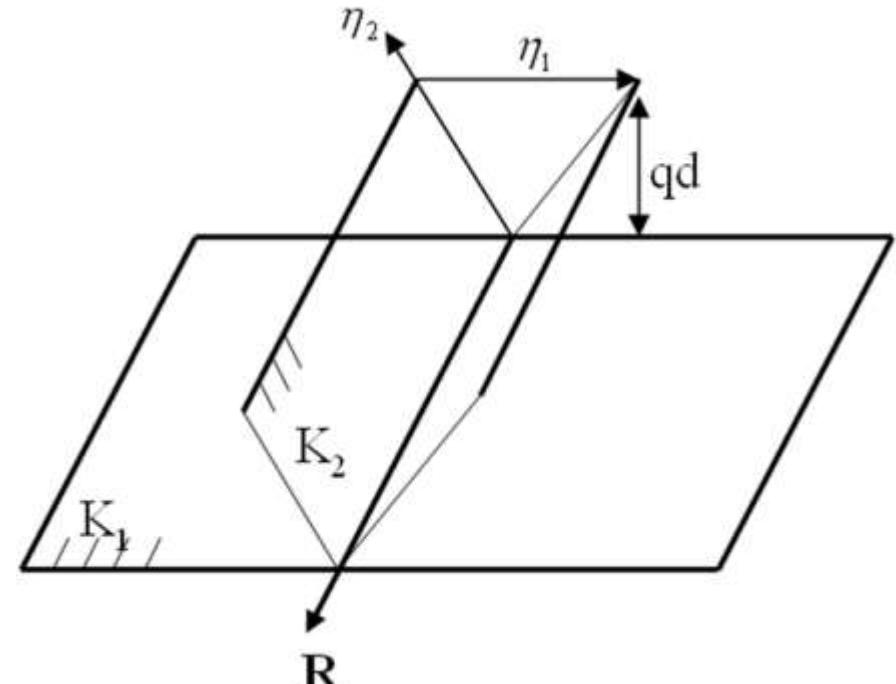
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# Twinning in hexagonal metals

Twinning in hex metals:

- Prevalent deformation mechanism
- $\geq 7$  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

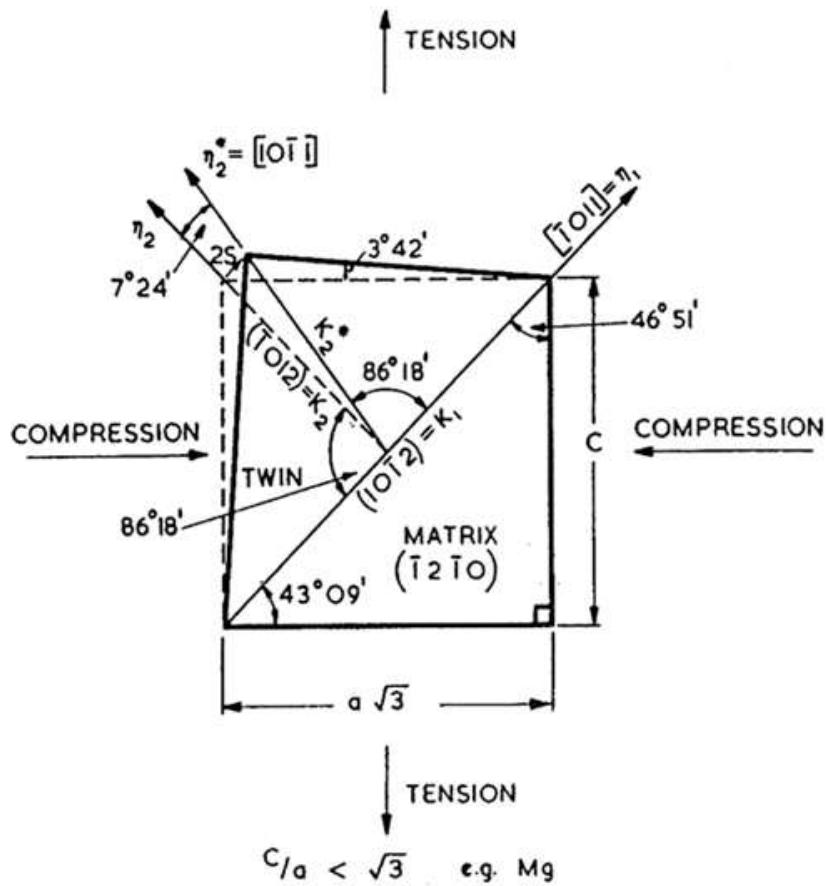
$\eta_2$  conjugate twinning direction

$R$  rotation axis

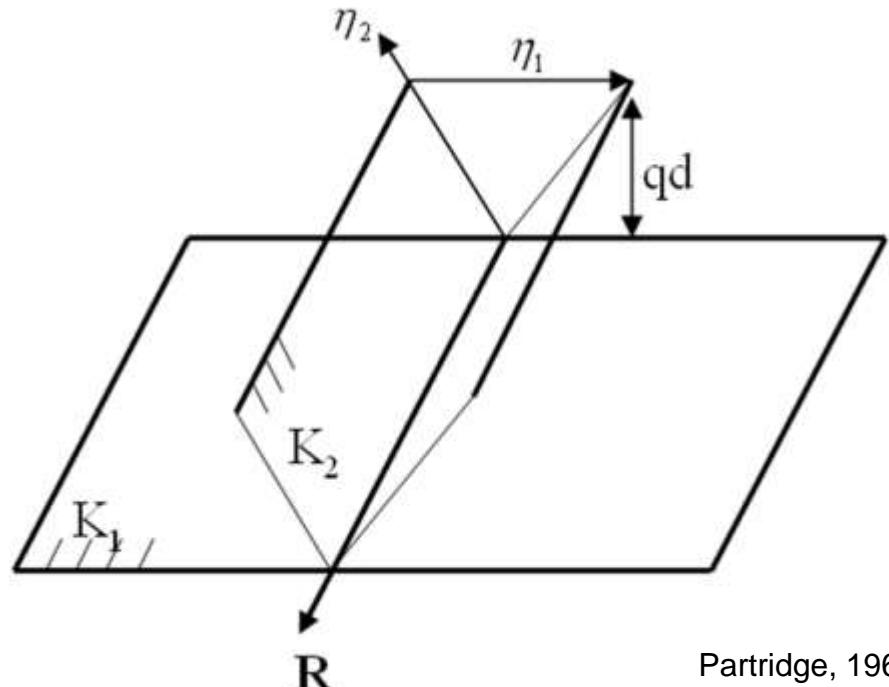
$q$  number of twin habit planes

$d$  interplanar distance

# Twinning in hexagonal metals



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



Partridge, 1967

$K_1$  twinning habit plane (invariant plane of twinning shear)

$K_2$  conjugate twinning plane (undistorted rotated plane)

$\eta_1$  twinning direction

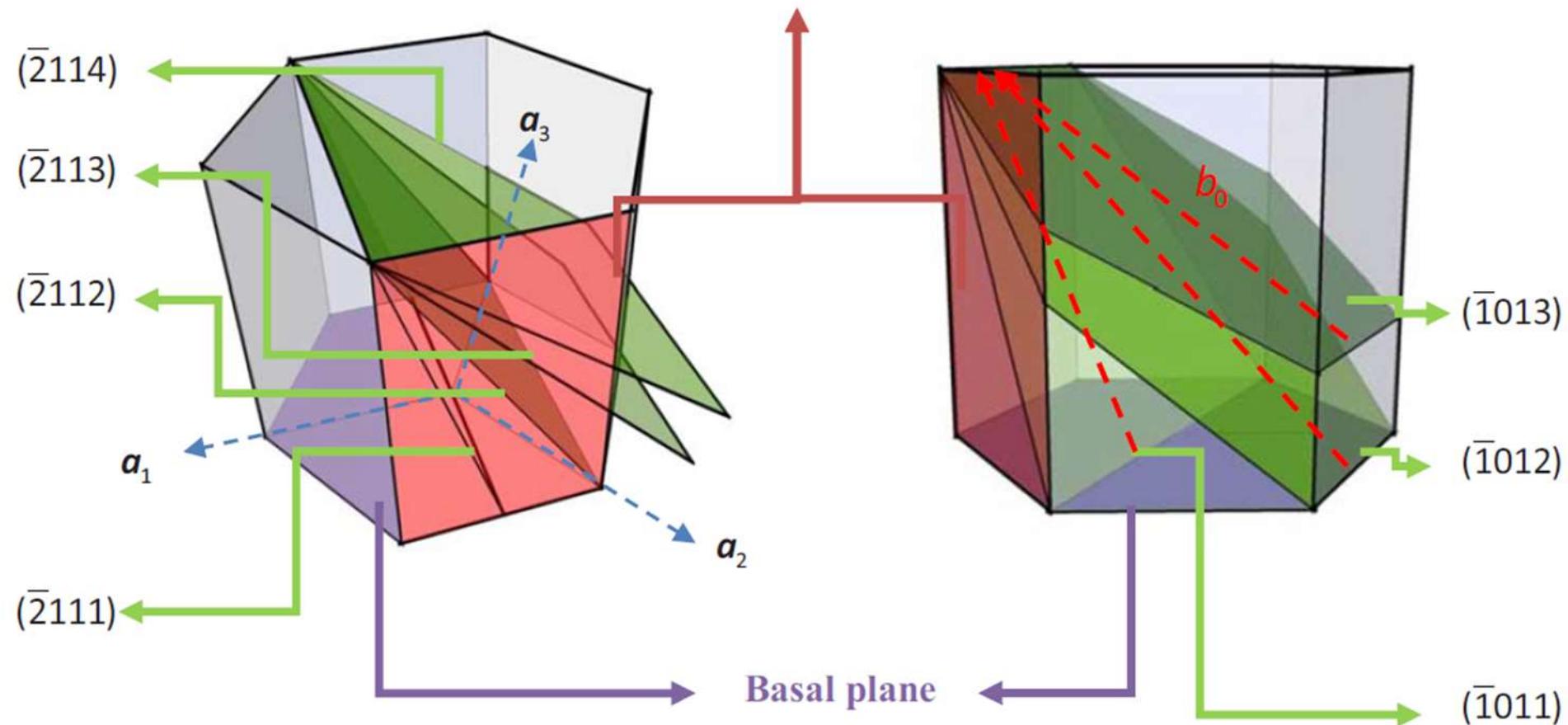
$\eta_2$  conjugate twinning direction

R rotation axis

q number of twin habit planes

d interplanar distance

First order prismatic plane



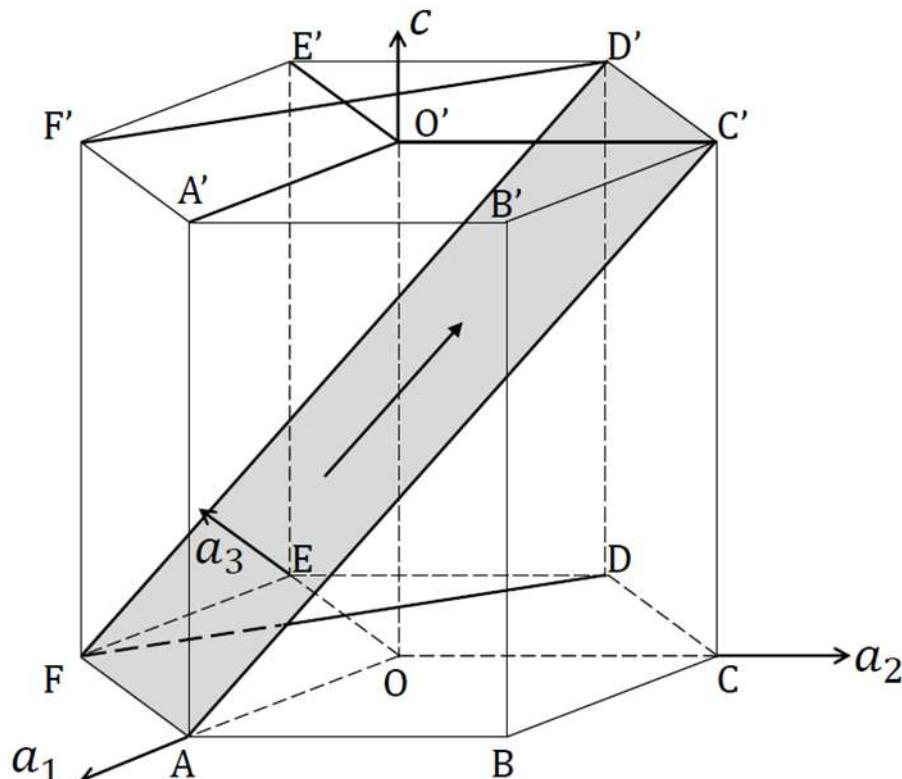
Partridge, 1967

Capolungo et al., 2008

# Deformation HEX

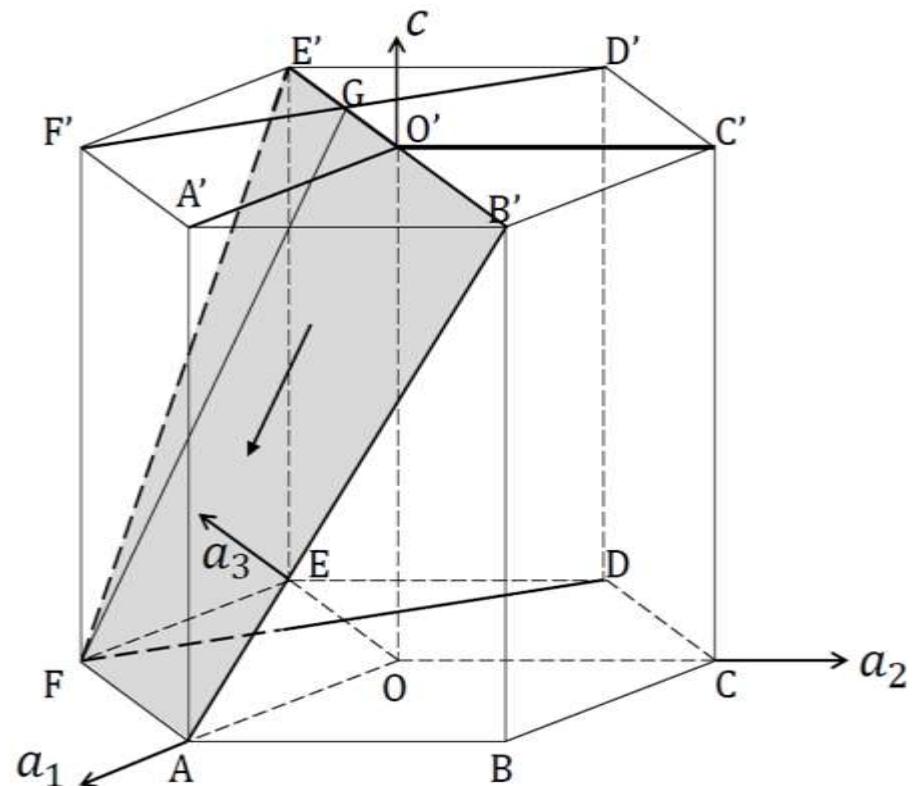
Tensile strain on c-axis

→ tension twin



Compressive strain on c-axis

→ compression twin



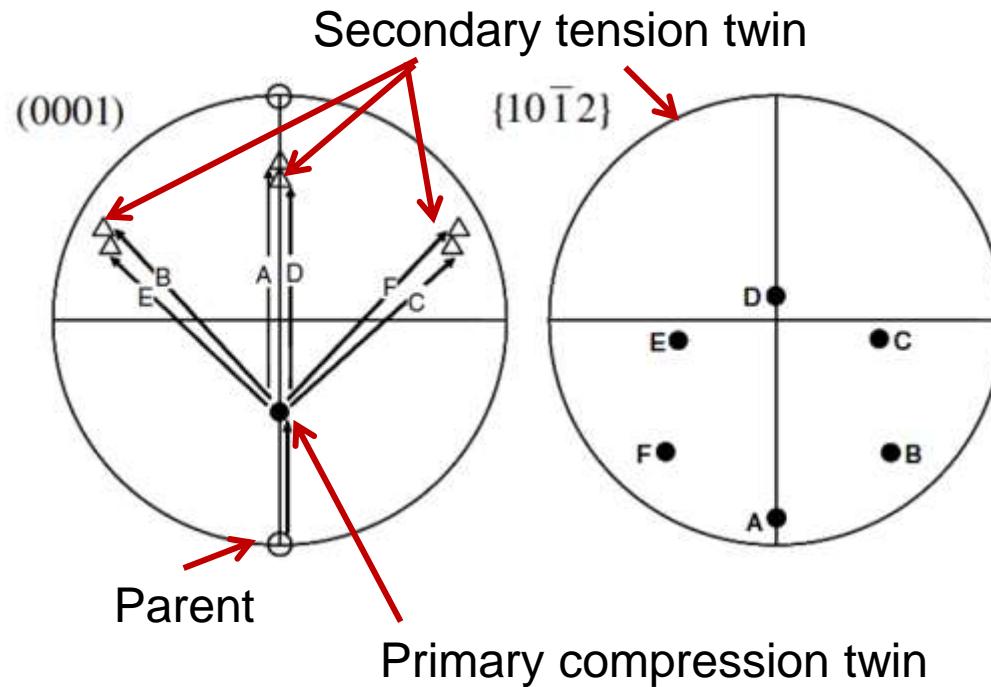
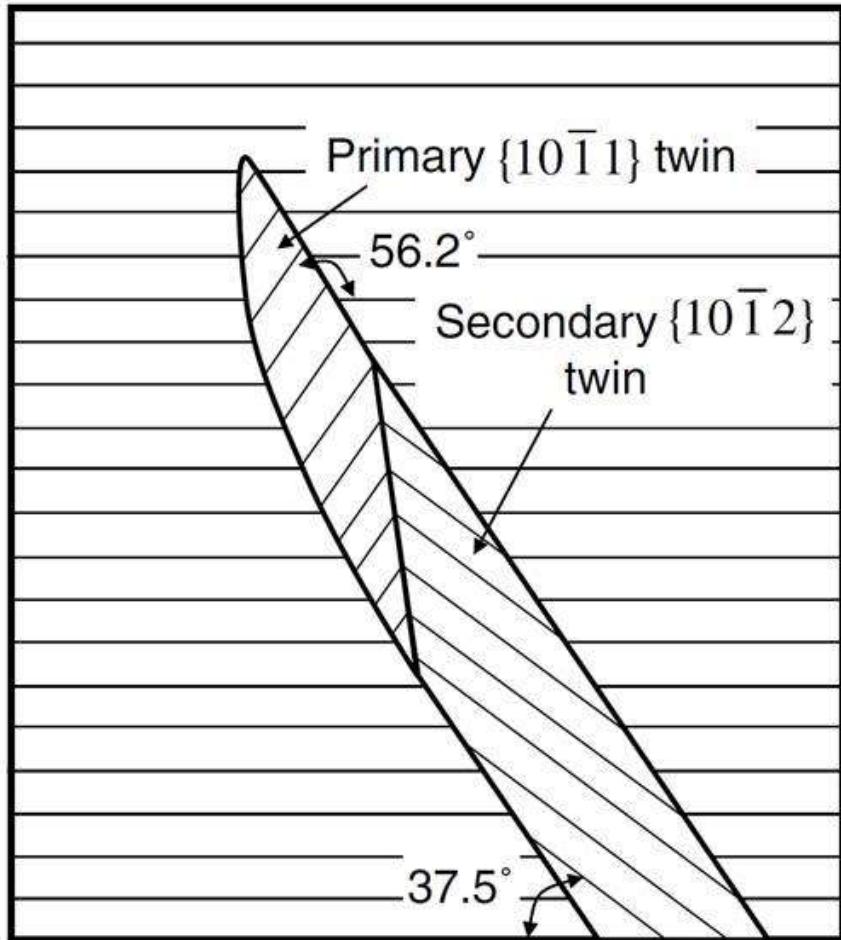
ACE: basal plane

ABB'A': prismatic plane

ABO': first order pyramidal plane

ACD'F': second order pyramidal plane

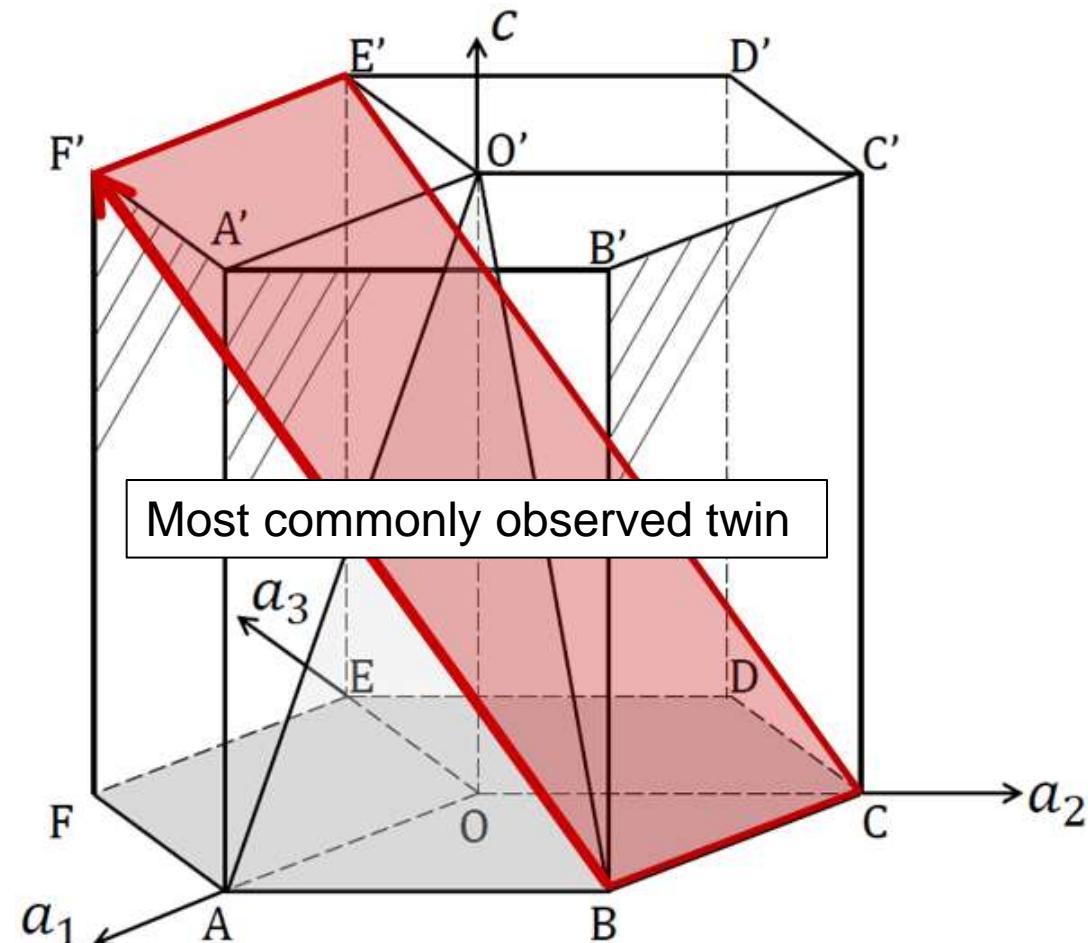
# Deformation HEX



Secondary twin:  
“Twin inside twin”  
Twin misorientation: primary / secondary twin

Parallel lines are basal plane traces

# 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:  $86^\circ$   $\langle 1\bar{2}10 \rangle$

$K_1: \{10\bar{1}2\}$

$K_2: \{10\bar{1}\bar{2}\}$

$\eta_1: \langle 10\bar{1}\bar{1} \rangle$

$\eta_2: \langle 10\bar{1}1 \rangle$

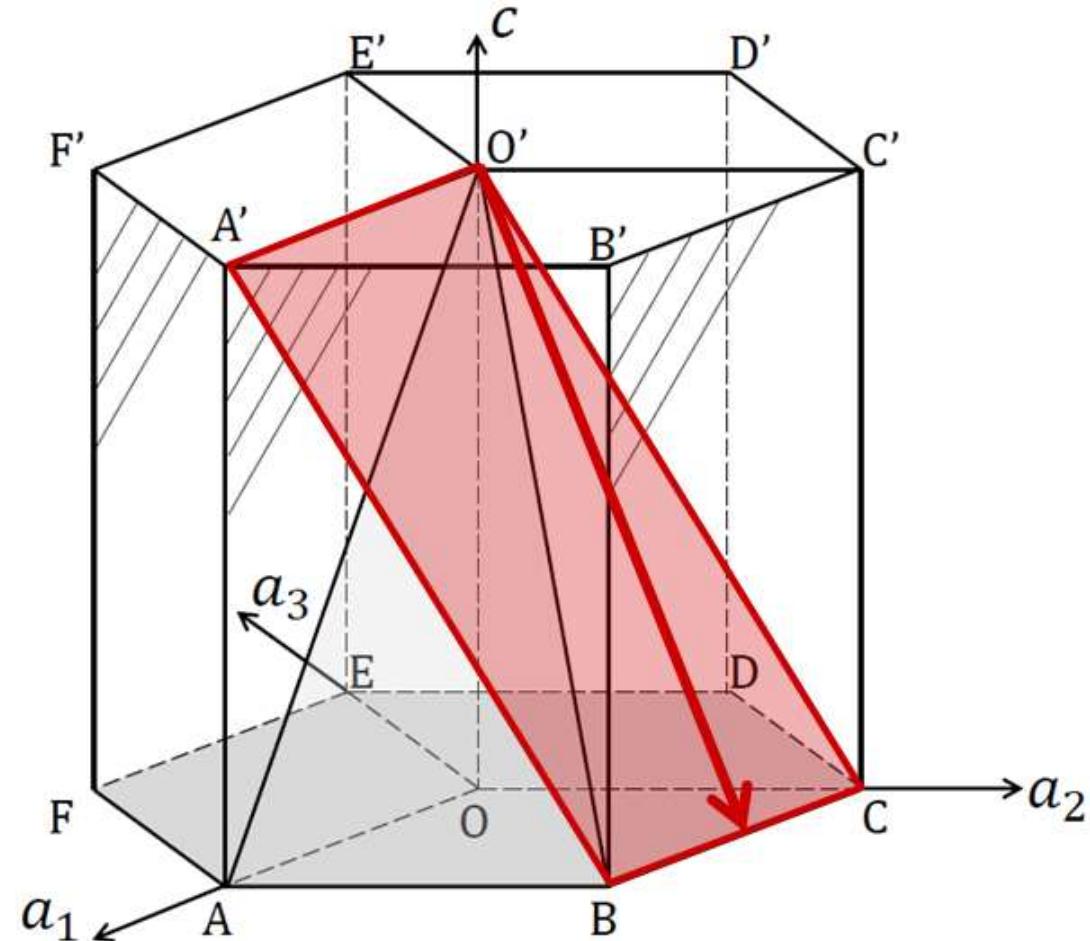
$$b_{\text{twn}_1} : \frac{\left(\frac{c}{a}\right)^2 - 3}{\left(\frac{c}{a}\right)^2 + 3} \quad (*)$$

$$b_{\text{twn}_2} : \frac{\left(\frac{c}{a}\right)^2 - 3}{\left(\frac{c}{a}\right)^2 + 3} \quad (*)$$

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

(\*)  $b_{\text{twn}_i}$ : Burgers 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

$\{10\bar{1}1\}\langle10\bar{1}\bar{2}\rangle$  compression twin

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

$K_1: \{10\bar{1}1\}$

$K_2: \{10\bar{1}\bar{3}\}$

$\eta_1: \langle10\bar{1}\bar{2}\rangle$

$\eta_2: \langle30\bar{3}2\rangle$

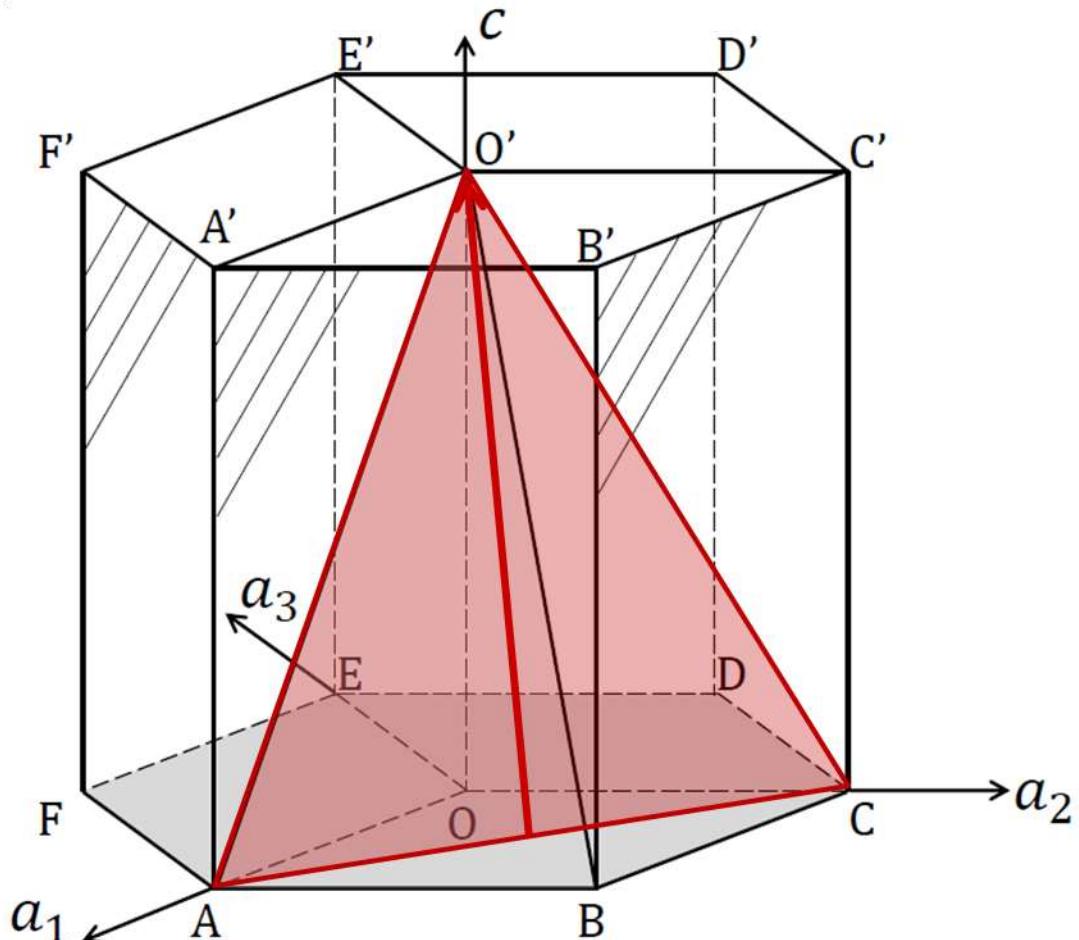
$$b_{\text{twn}_1} : \frac{4\left(\frac{c}{a}\right)^2 - 9}{4\left(\frac{c}{a}\right)^2 + 3} \quad (*)$$

$$b_{\text{twn}_2} : \frac{4\left(\frac{c}{a}\right)^2 - 9}{4\left(\frac{c}{a}\right)^2 + 27} \quad (*)$$

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

(\*)  $b_{\text{twn}_i}$ : Burgers vector of zonal twinning 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

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

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

$K_1: \{11\bar{2}1\}$

$K_2: (0002)$

$\eta_1: \frac{1}{3}\langle\bar{1}\bar{1}26\rangle$

$\eta_2: \frac{1}{3}\langle11\bar{2}0\rangle$

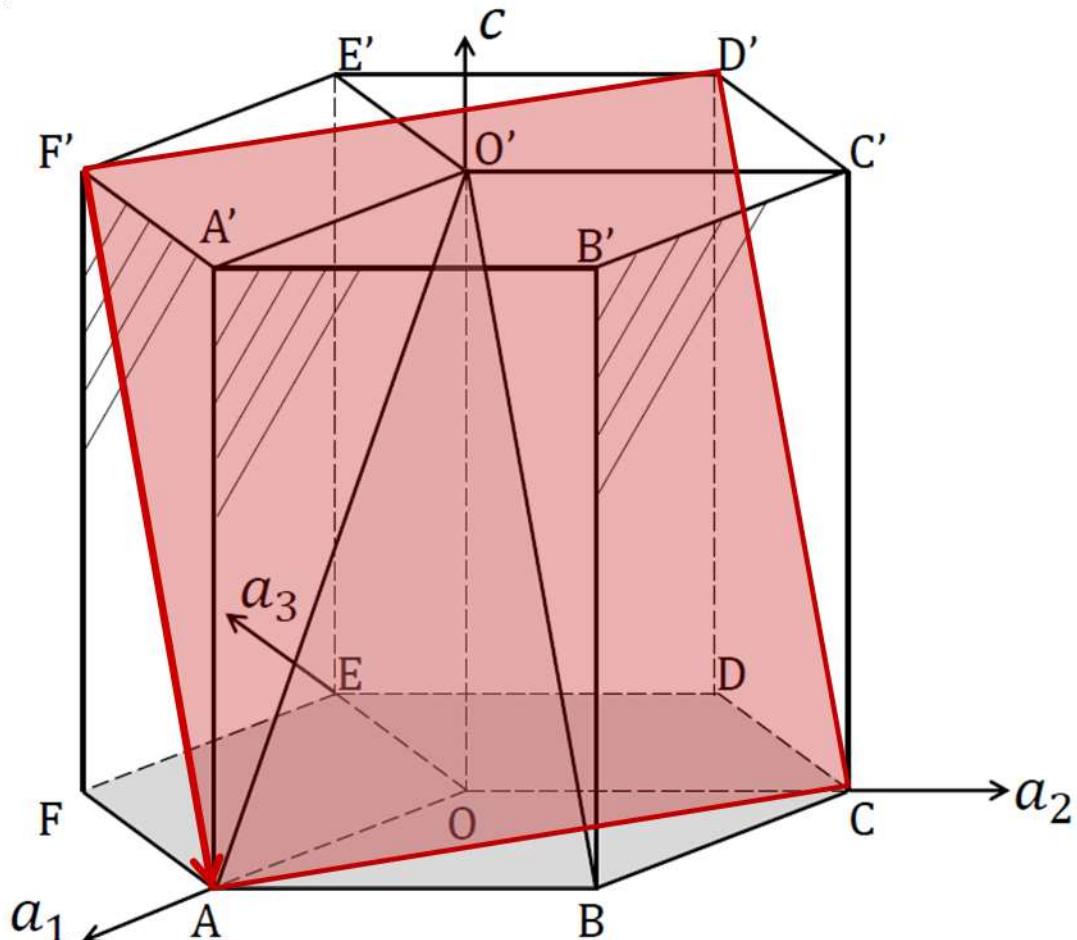
$$b_{tw\eta_1} : \frac{1}{4\left(\frac{c}{a}\right)^2 + 1} \quad (*)$$

$$b_{tw\eta_2} : 1 \quad (*)$$

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

(\*)  $b_{tw\eta_i}$ : Burgers vector of zonal twinning 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

$\{11\bar{2}2\}\langle11\bar{2}\bar{3}\rangle$  compression twin

Basal plane rotation:  $65^\circ \langle\bar{1}100\rangle$

$K_1: \{11\bar{2}2\}$

$K_2: \{11\bar{2}\bar{4}\}$

$\eta_1: \frac{1}{3}\langle11\bar{2}\bar{3}\rangle$

$\eta_2: \frac{1}{3}\langle22\bar{4}3\rangle$

$$b_{\text{twn}_1} : \frac{\left(\frac{c}{a}\right)^2 - 2}{\left(\frac{c}{a}\right)^2 + 2} \quad (*)$$

$$b_{\text{twn}_2} : \frac{\left(\frac{c}{a}\right)^2 - 2}{\left(\frac{c}{a}\right)^2 + 4} \quad (*)$$

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

(\*)  $b_{\text{twn}_i}$ : Burgers vector of zonal twinning dislocation  $\eta_i$  - „simple“ geometrical description of complex atomic shuffling to form twin

# Twinning in hexagonal metals

## Twin nucleation

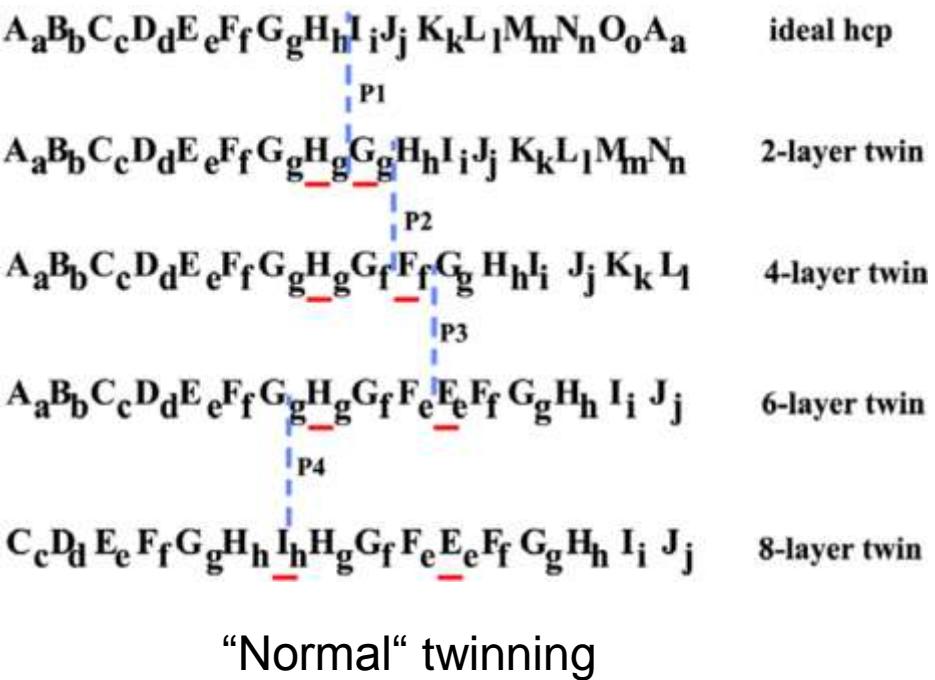
- “Normal“ twinning mechanism  
Simultaneous glide of multiple twinning dislocations
- “Zonal“ twinning mechanism  
Simultaneous glide of a zonal dislocation („super-dislocation“ of partial dislocations) and multiple twinning dislocations

Twining dislocation: line defect with dislocation and step character (“zonal”)

# 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 dislocation: line defect with dislocation and step character (“zonal”)

Tomé, 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

$A_aB_bC_cD_dE_eF_fG_gH_hI_iJ_jK_kL_lM_mN_nO_oA_a$

ideal hcp

$A_aB_bC_cD_dE_eF_fG_gH_gH_gH_hI_iJ_jK_kL_lM_mN_n$

2-layer twin

$A_aB_bC_cD_dE_eF_fG_gH_gG_fF_fG_gH_hI_iJ_jK_kL_l$

4-layer twin

$A_aB_bC_cD_dE_eF_fG_gH_gG_fF_eF_fG_gH_hI_iJ_j$

6-layer twin

$C_cD_dE_eF_fG_gH_hI_hH_gG_fF_eF_fG_gH_hI_iJ_j$

8-layer twin

“Normal“ twinning

$A_aB_bC_cD_dE_eF_fG_gH_hI_iJ_jK_kL_lM_mN_nO_oA_a$

ideal hcp

$A_aB_bC_cD_dE_eF_fG_gH_gH_gH_hI_iJ_jK_kL_lM_mN_nO_o$

stacking fault

$A_aB_bC_cD_dE_eF_fG_gH_gG_fG_gH_hI_iJ_jK_kL_lM_m$

3-layer twin

$A_aB_bC_cD_dE_eF_fG_gH_gG_fF_eF_fG_gH_hI_iJ_jK_k$

5-layer twin

$C_cD_dE_eF_fG_gH_hI_hH_gG_fF_eF_fG_gH_hI_iJ_jK_k$

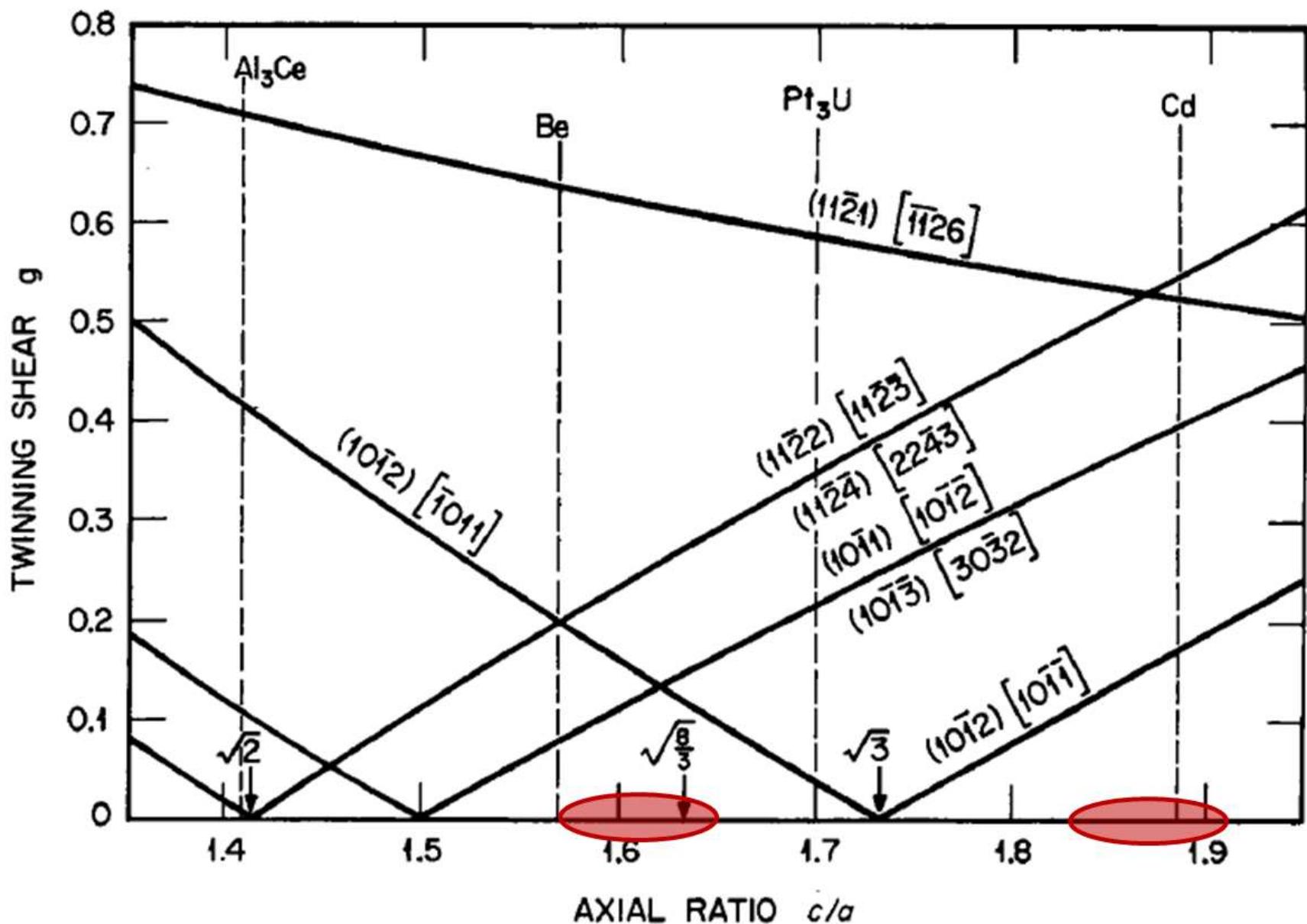
7-layer twin

“Zonal“ twinning

Twinning dislocation: line defect with dislocation and step character (“zonal“)

Tomé, 2009

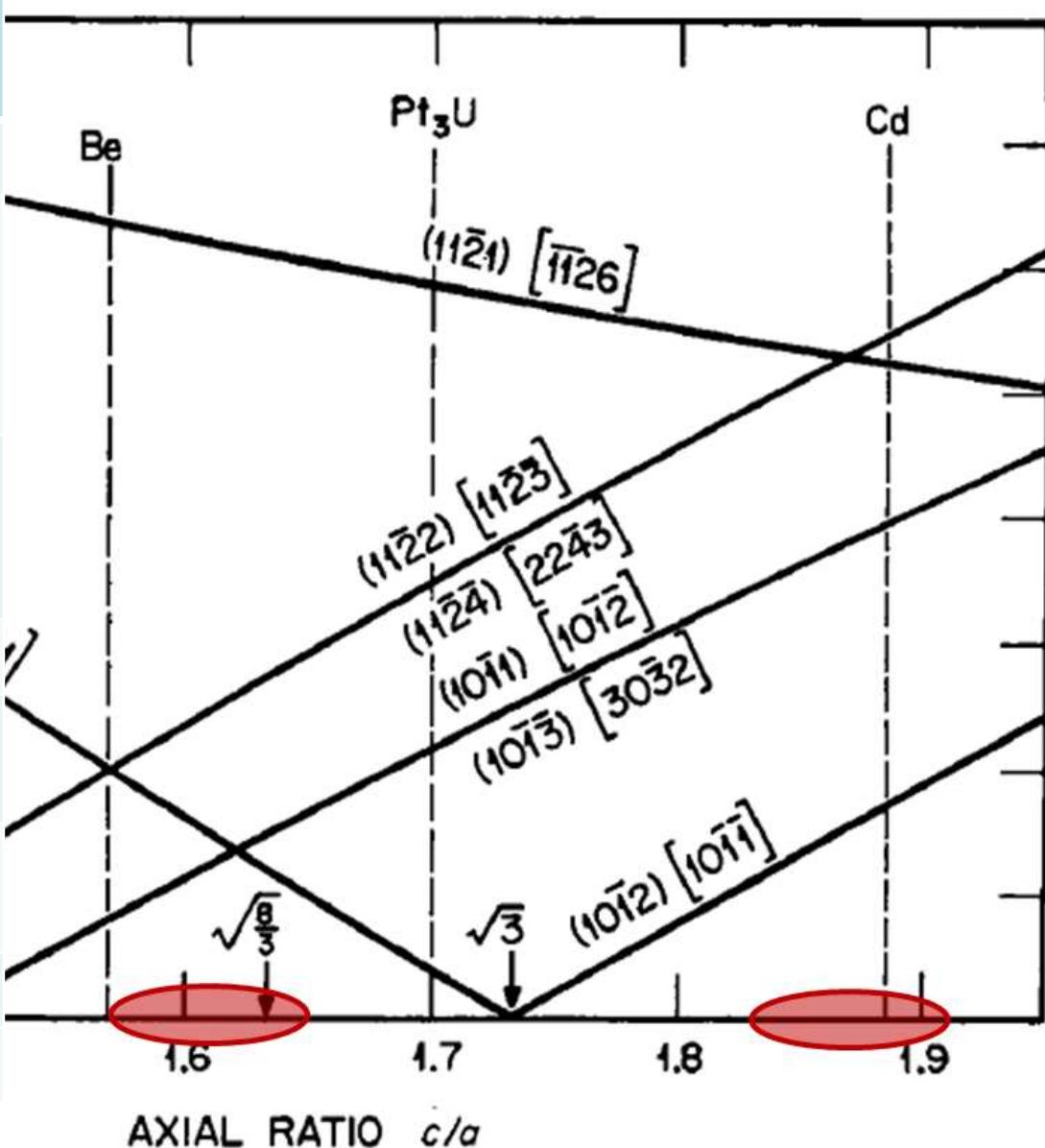
# Twinning in hexagonal metals



Yoo, 1981

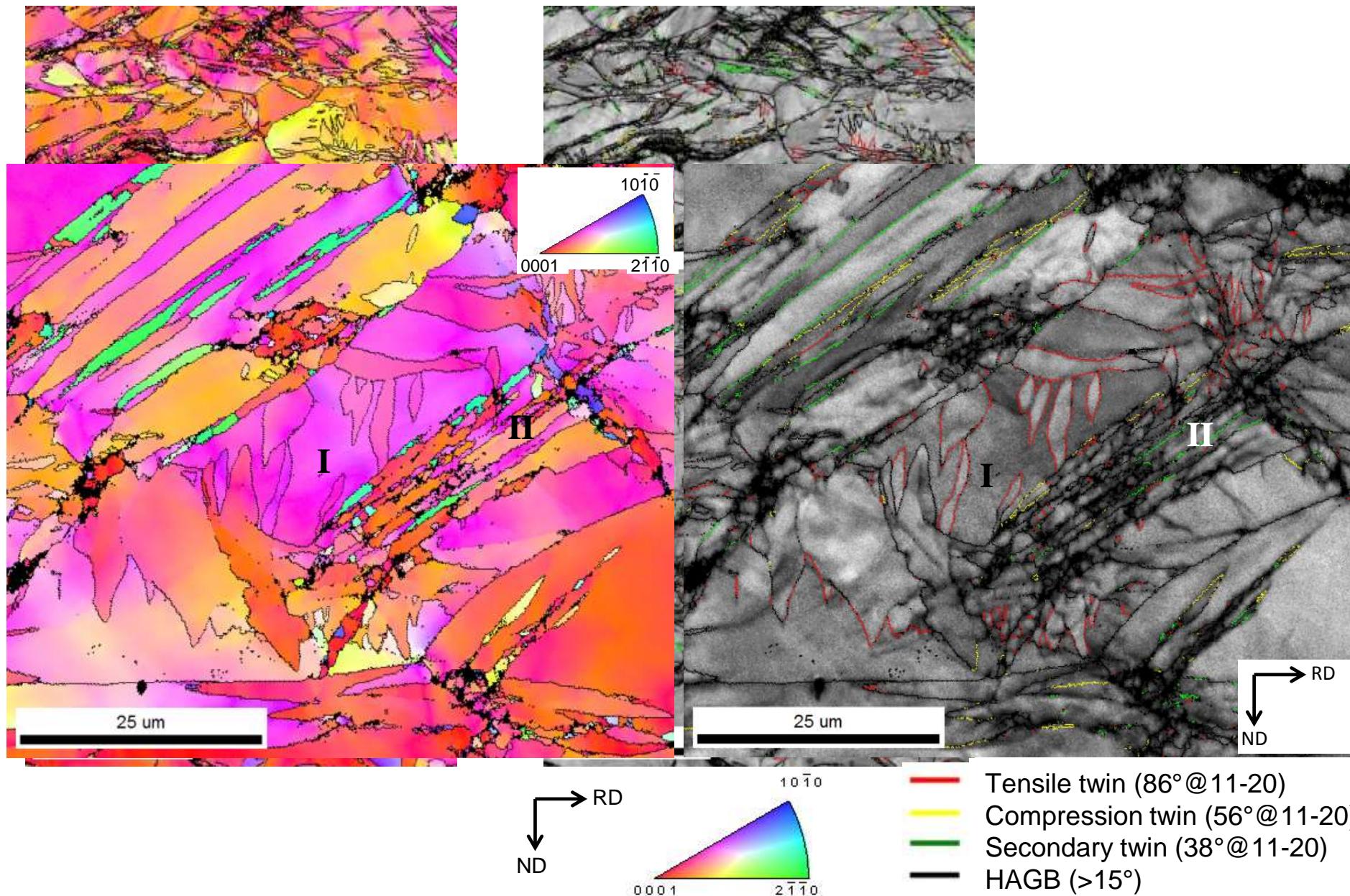
# Twinning in hexagonal metals

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



# 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?

# Structure

- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink banding
- Twinning in hexagonal metals
- Stacking faults in hexagonal metals
- Texture components in hexagonal metals
- Anisotropy of precipitation strengthening
- Phase transformations; dual- / multiphase systems
- Damage, fracture in hexagonal metals
- Characterization of plasticity carriers in hexagonal metals

# Stacking faults in hexagonal metals

Basal stacking faults in hex metals:

I<sub>1</sub>- stacking sequence ...ABABCBCB...

I<sub>2</sub> - 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 faults in hexagonal metals

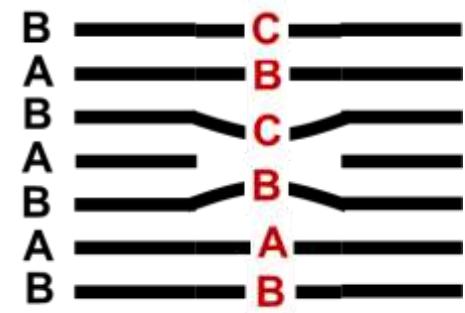
Basal stacking faults in hex metals:

I<sub>1</sub>- stacking sequence ...ABABCBCBC...

Shockley-type basal  $\langle a \rangle$  partial and

Frank-type  $\frac{1}{2}\langle c+a \rangle$  partial

→ sessile, proposed as Frank-Read source  $\langle c+a \rangle$



# Stacking faults in hexagonal metals

Basal stacking faults in hex metals:

I<sub>1</sub>- stacking sequence ...ABABCBCB...

Shockley-type basal  $\langle a \rangle$  partial and Frank-type  $\frac{1}{2}\langle c+a \rangle$  partial

→ sessile, proposed as Frank-Read source  $\langle c+a \rangle$

I<sub>2</sub> - 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 ...ABABCBCB...

Shockley-type basal  $\langle a \rangle$  partial and Frank-type  $\frac{1}{2}\langle c+a \rangle$  partial

→ sessile, proposed as Frank-Read source  $\langle c+a \rangle$

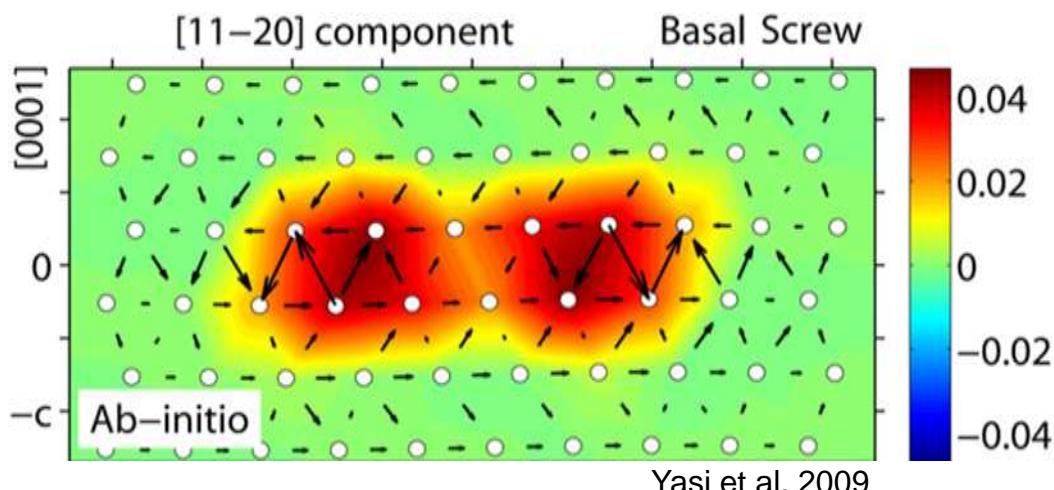
$I_2$  - stacking sequence ...ABCACAC...

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



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

# Stacking faults in hexagonal metals

Basal stacking faults in hex metals:

I<sub>1</sub>- stacking sequence ...ABABCBCB...

Shockley-type basal partial and Frank-type  $\frac{1}{2}\langle c+a \rangle$  partial

→ sessile, proposed as Frank-Read source  $\langle c+a \rangle$

I<sub>2</sub> - stacking sequence ...ABCACAC...

2 Shockley-type basal partials :

$$\frac{1}{3}[\bar{1}2\bar{1}0] \rightarrow \frac{1}{3}[01\bar{1}0] + \frac{1}{3}[\bar{1}100]$$

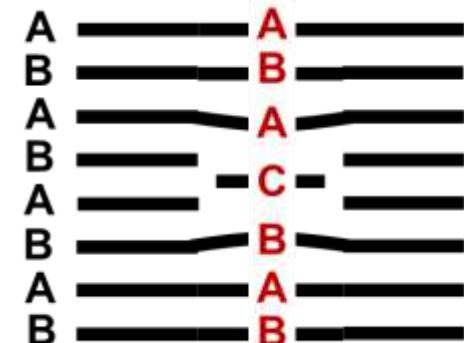
“equivalent” to ISF in fcc

proposed as measure for cross-slip probability

E - stacking sequence ...ABABCABAB...

energetically unfavorable

experimentally not observed



# Stacking faults in hexagonal metals

(I<sub>2</sub>-type) GSFEs for hexagonal metals

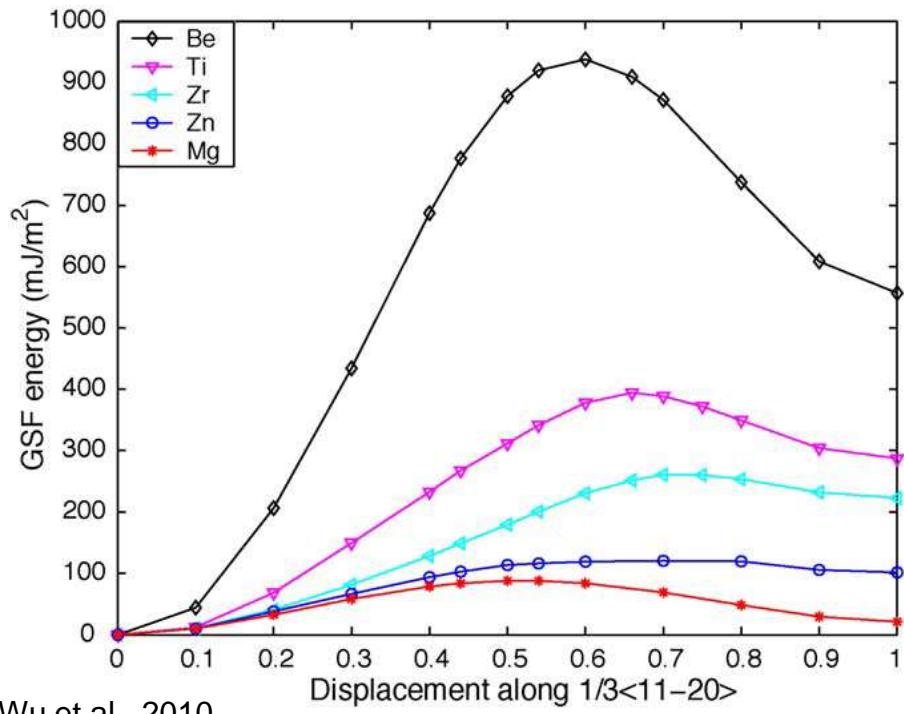
SFE:

Dissociation and formation of SFI2 on basal plane?

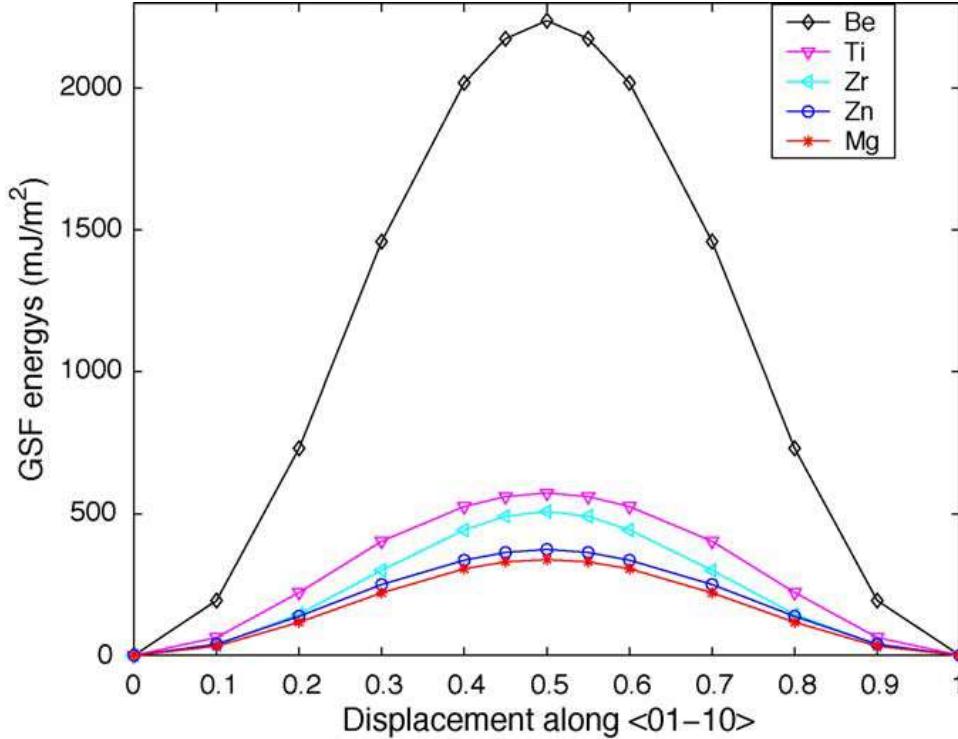
Cross-slip on prismatic planes?

USFE:

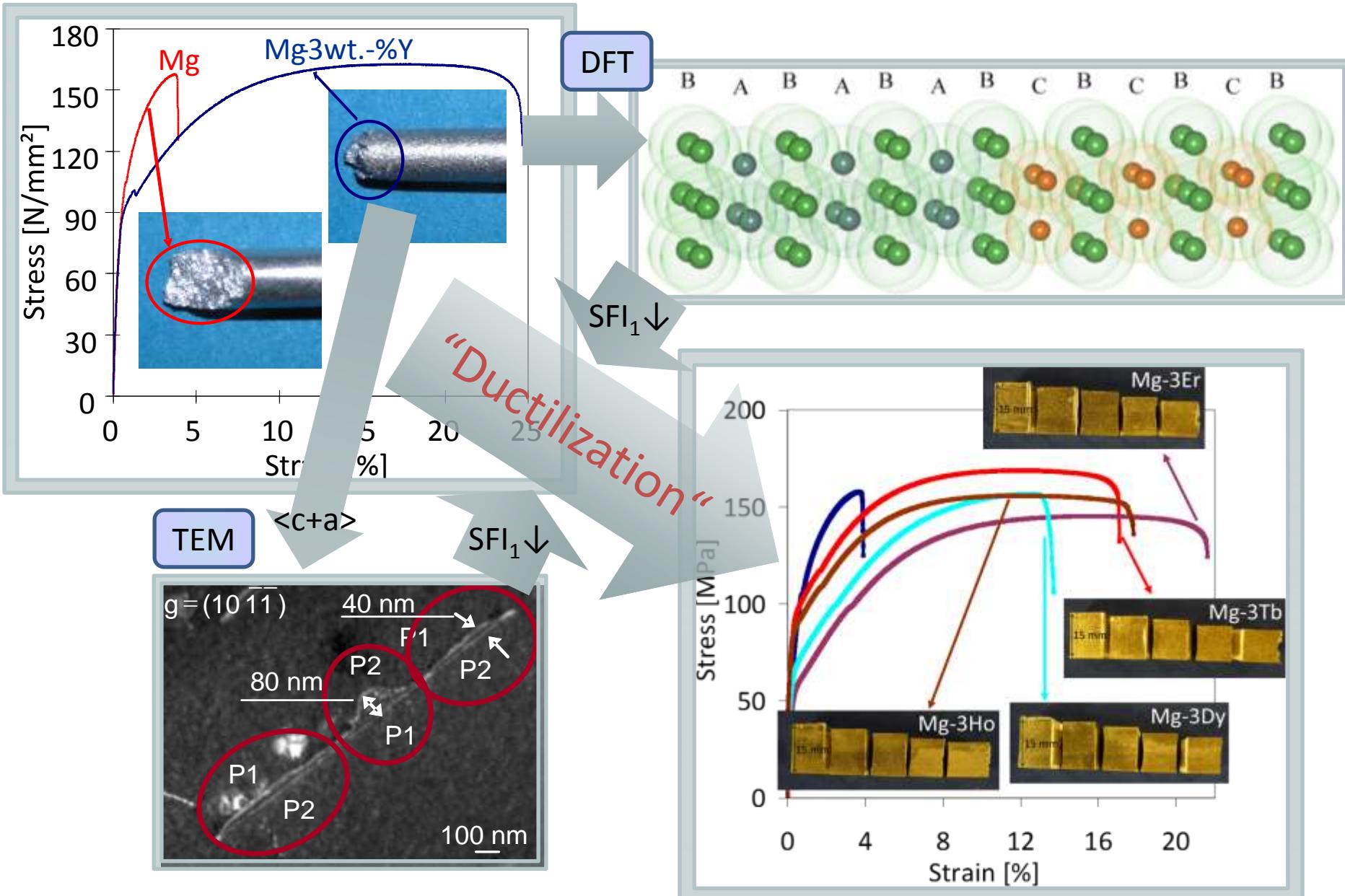
Nucleation of  $\langle a \rangle$  dislocations?



Wu et al., 2010



# Stacking faults in hexagonal metals



# Quiz

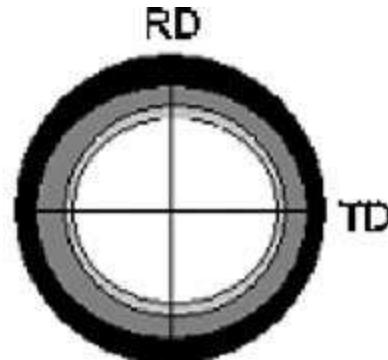
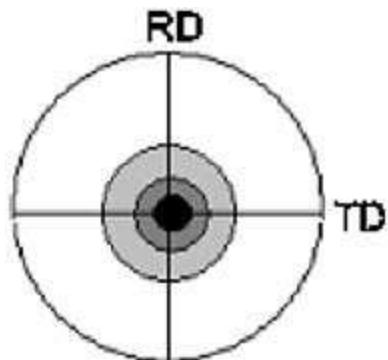
- Which stacking faults in hexagonal metals do you remember?
- How do the stacking fault energy(s) influence the deformation behavior of hexagonal metals?

# Structure

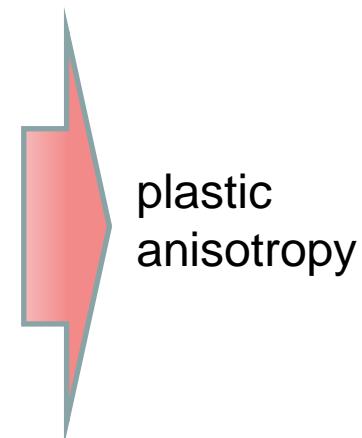
- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink banding
- Twinning in hexagonal metals
- Stacking faults in hexagonal metals
- Texture components in hexagonal metals
- Anisotropy of precipitation strengthening
- Phase transformations; dual- / multiphase systems
- Damage, fracture in hexagonal metals
- Characterization of plasticity carriers in hexagonal metals

# Texture components in hexagonal metals

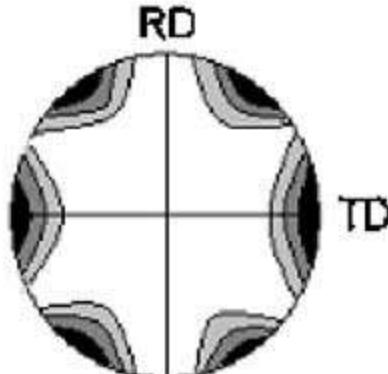
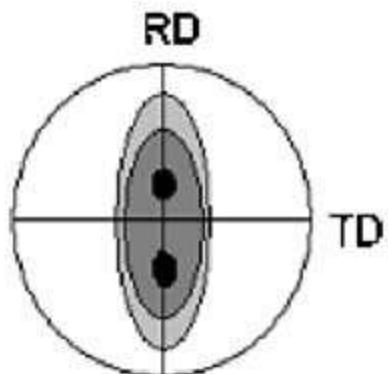
$c/a \approx 1.633$



Basal  $\langle a \rangle$  slip +  
tension twinning

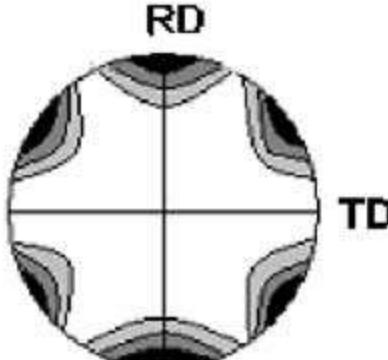
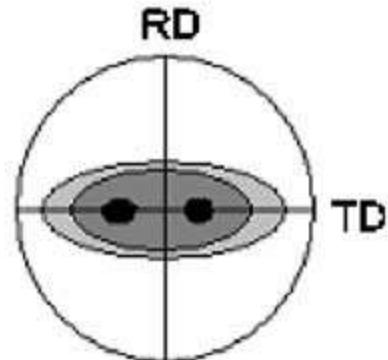


$c/a > 1.633$



Basal  $\langle a \rangle$  slip +  
pyramidal slip

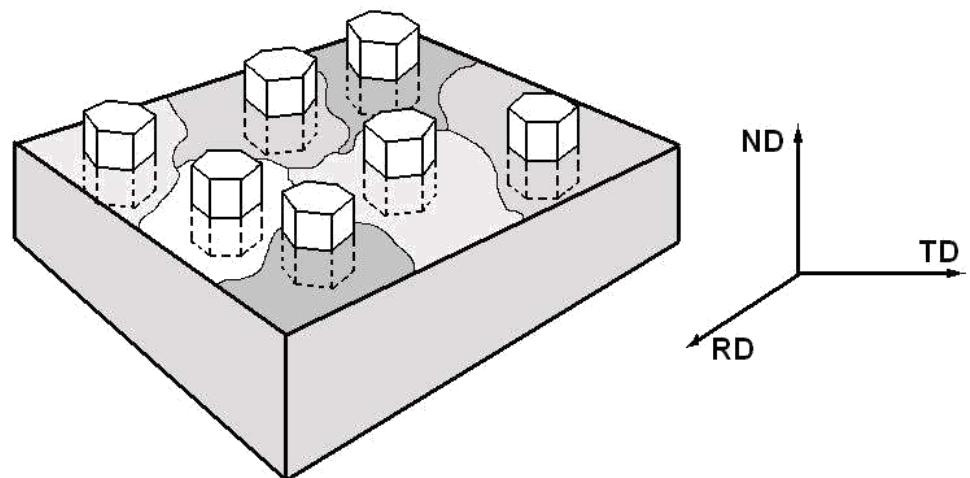
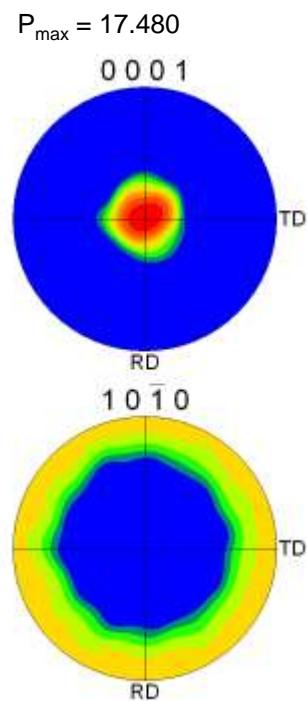
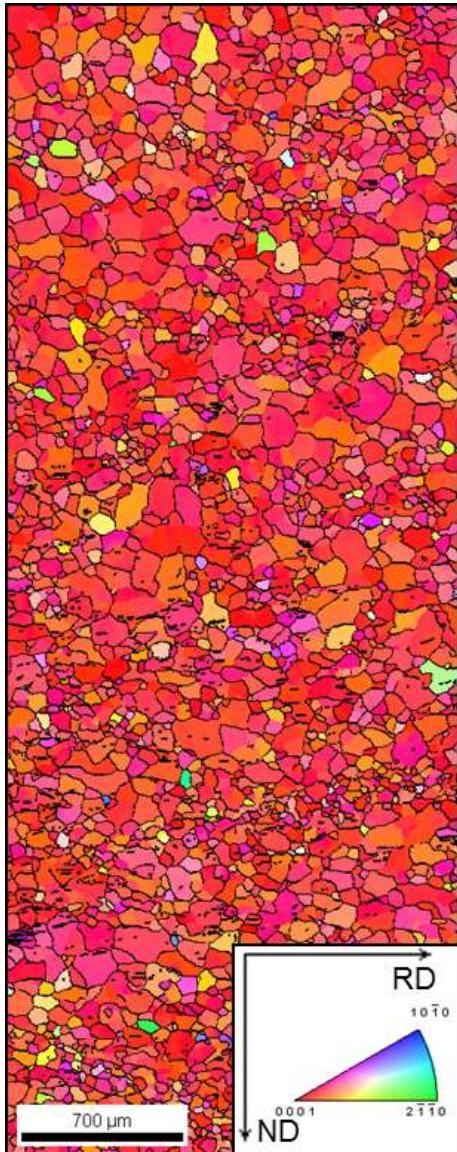
$c/a < 1.633$



Prismatic  $\langle a \rangle$  slip +  
basal  $\langle a \rangle$  slip

Wang et al., 2003

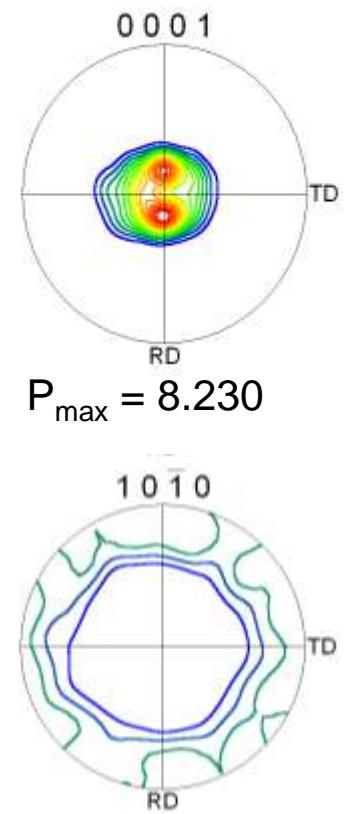
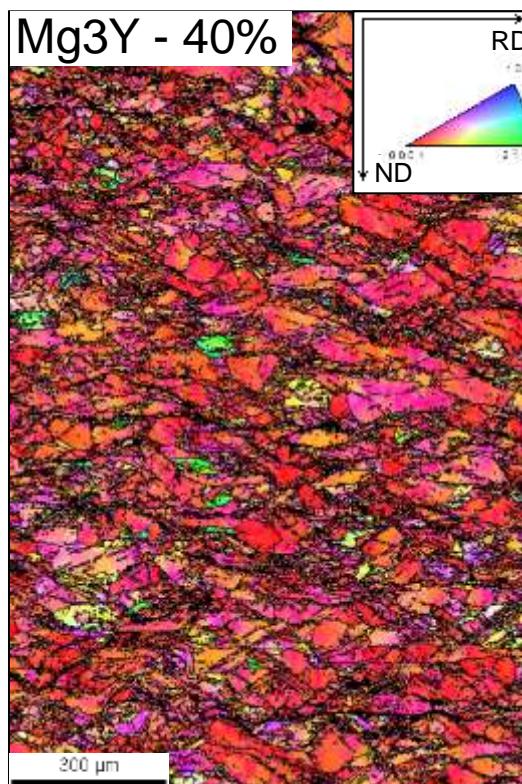
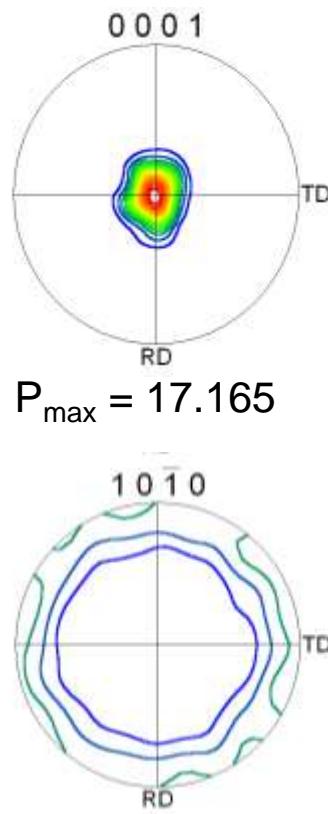
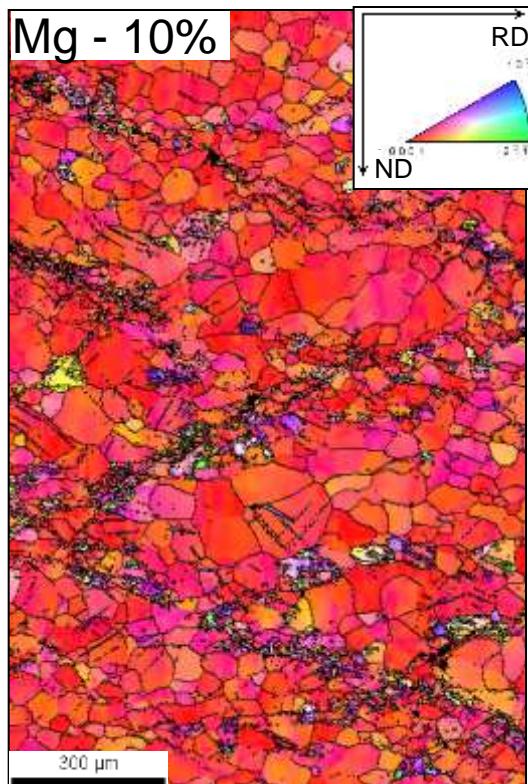
# Texture components in hexagonal metals



Example for strong basal texturing: Mg

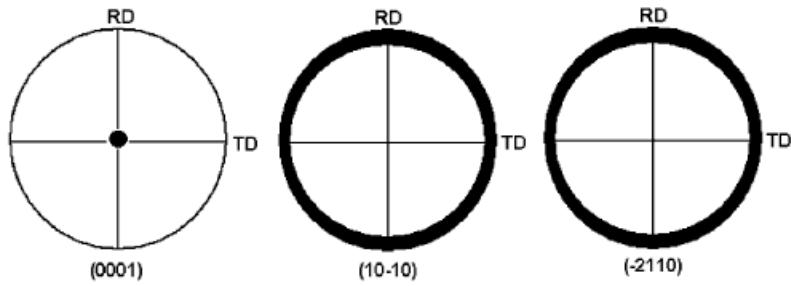
# Texture components in hexagonal metals

Deformation texture at fracture begin

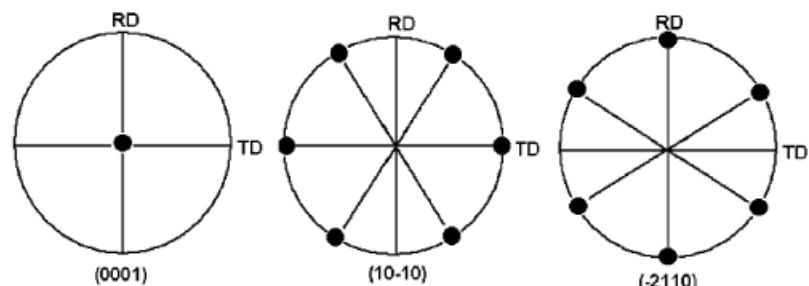


- Strong basal type texture
- Matrix grains (0001)||ND
- Basal slip and tensile twinning
- Weaker (0.5) basal texture intensity
- r-type texture ((0001) 15° tow. RD)
- non-basal deformation mechanisms

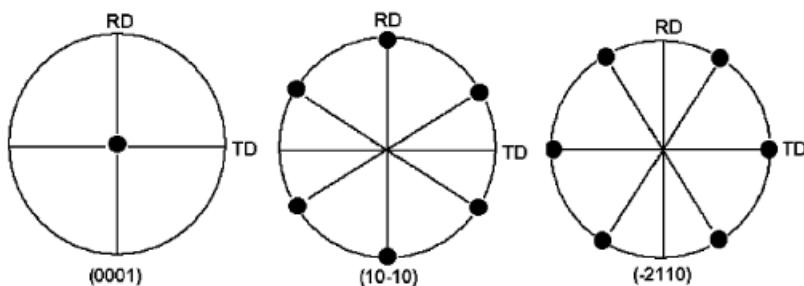
# Texture components in hexagonal metals



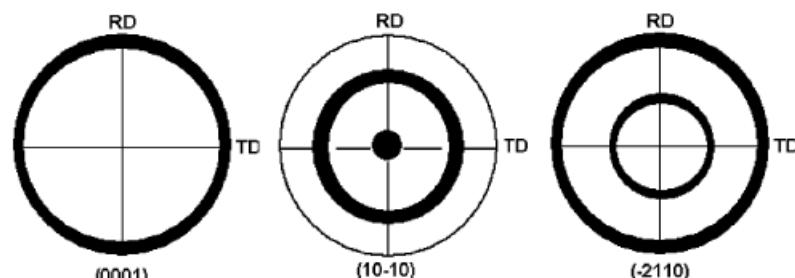
{0001} basal



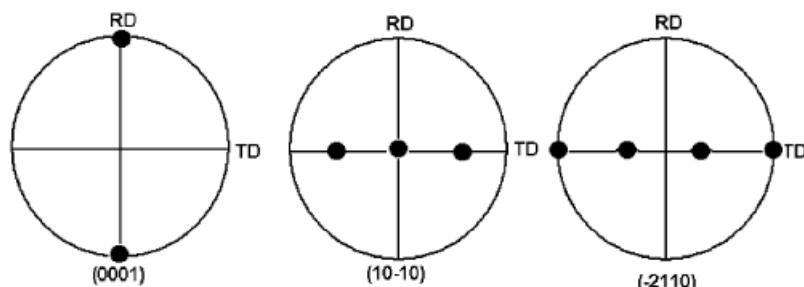
{0001}<11\bar{2}0>



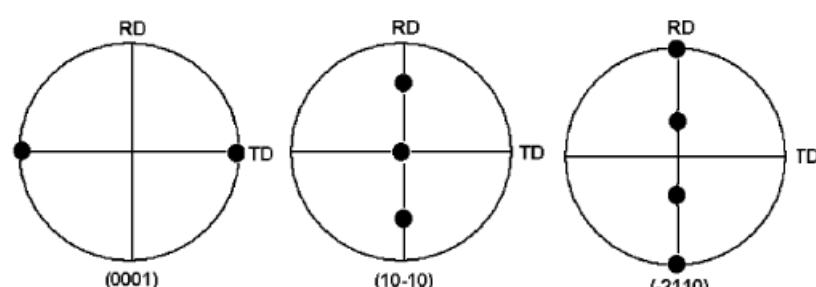
{0001}<10\bar{1}0>



{10\bar{1}0} fiber



[10\bar{1}0]<0001>

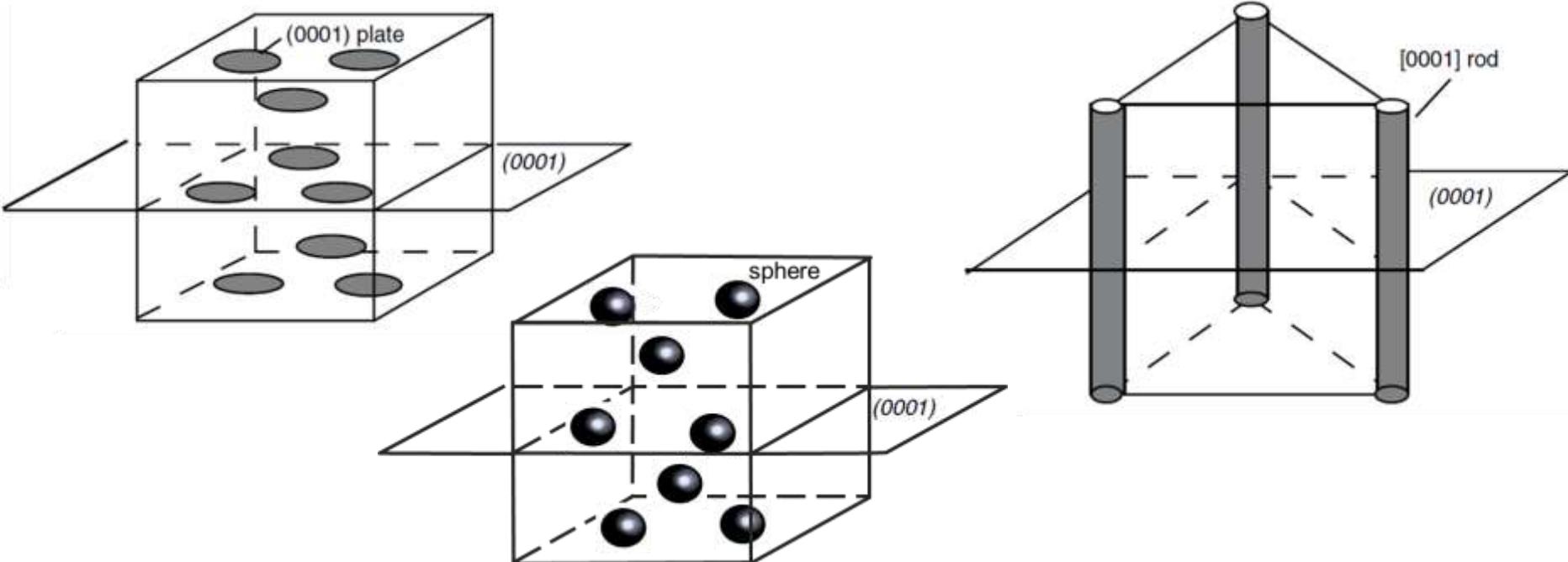


{10\bar{1}0}<11\bar{2}0>

# Structure

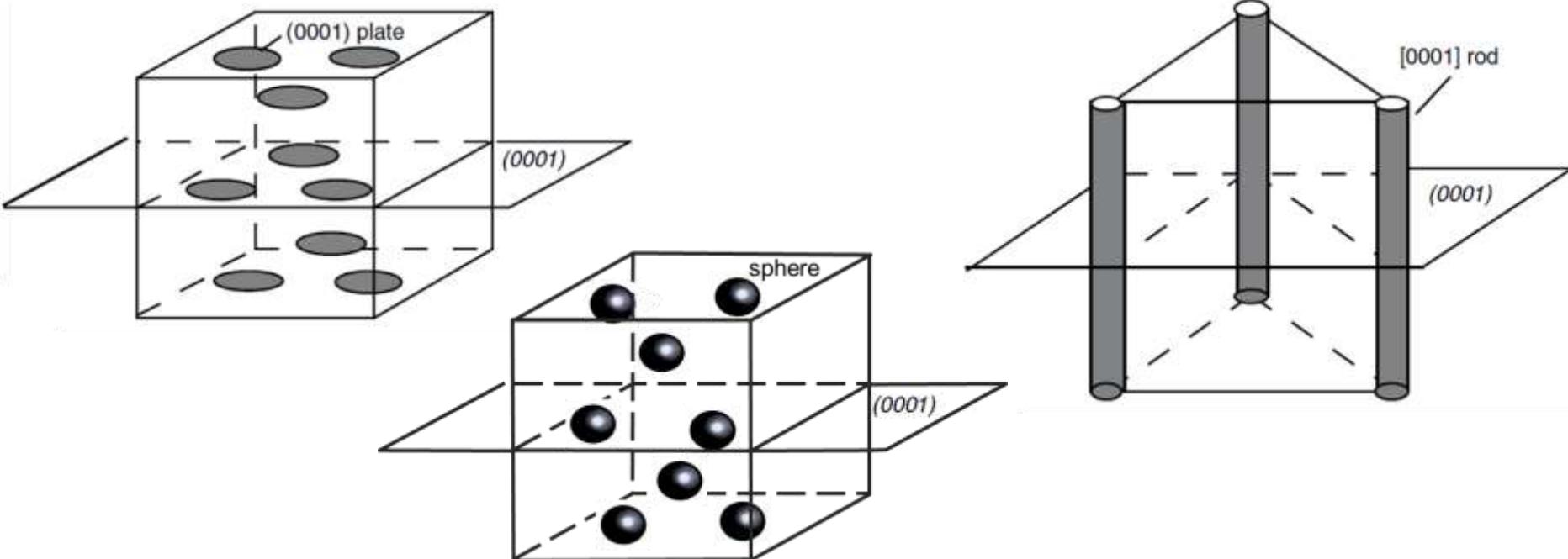
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# Anisotropy of precipitation strengthening

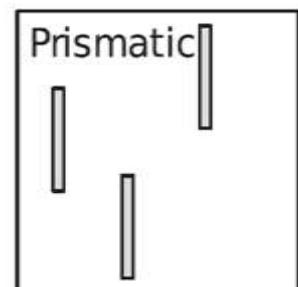
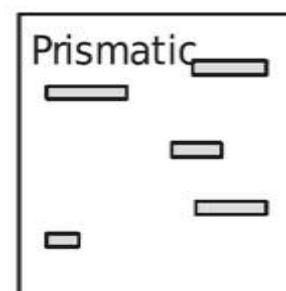
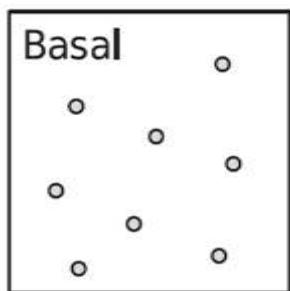
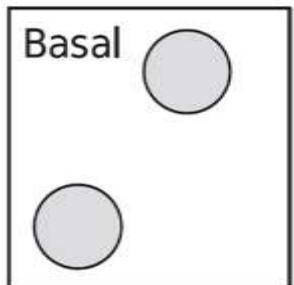


Which is most effective?

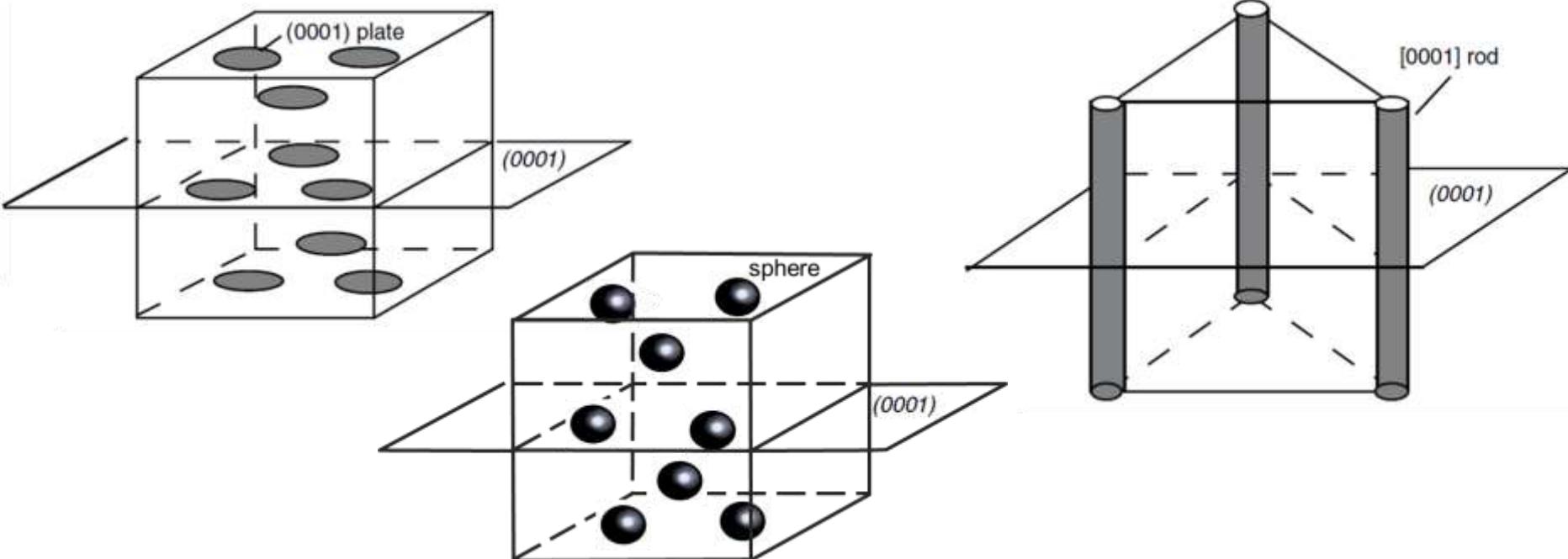
# Anisotropy of precipitation strengthening



Which is most effective?



# Anisotropy of precipitation strengthening



$$\text{Orowan Looping: } \Delta\tau = \frac{Gb}{2\pi\lambda\sqrt{1-\nu}} \ln \frac{d_p}{r_0}$$

G: shear modulus

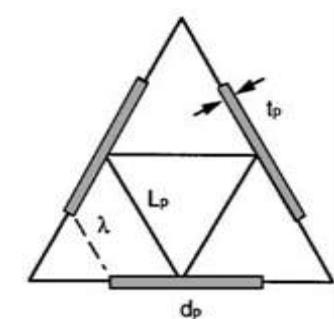
b: Burgers vector

$\nu$ : Poisson's ratio

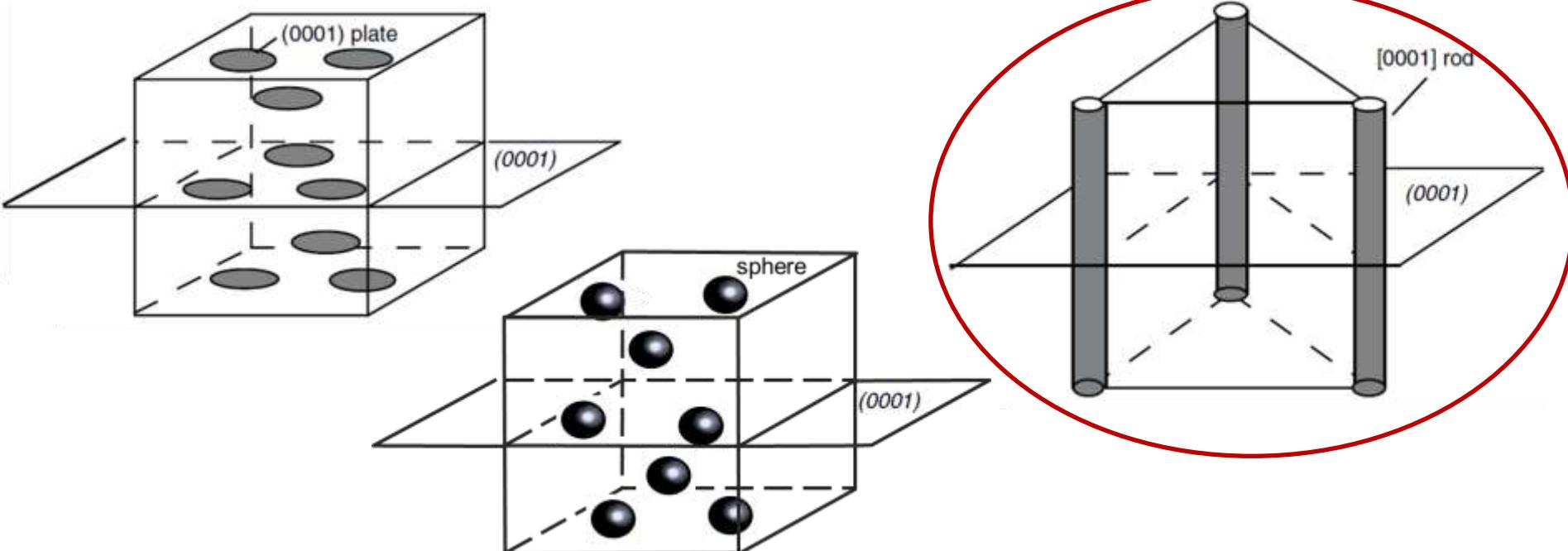
$\lambda$ : planar interobstacle distance

$d_p$ : planar precipitate diameter

$r_0$ : dislocation core radius



# Anisotropy of precipitation strengthening



Orowan Looping:  $\Delta\tau = \frac{Gb}{2\pi\lambda\sqrt{1-\nu}} \ln \frac{d_p}{r_0}$

G: shear modulus

b: Burgers vector

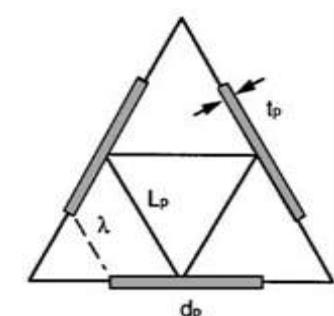
$\nu$ : Poisson's ratio

$\lambda$ : planar interobstacle distance

$d_p$ : planar precipitate diameter

$r_0$ : dislocation core radius

A: aspect ratio



$$\frac{d(\text{plate})}{d(\text{sphere})} = \left(\frac{2A}{3}\right)^{\frac{1}{3}}$$

$$\frac{d(\text{rod})}{d(\text{sphere})} = \left(\frac{2}{3A}\right)^{\frac{1}{3}}$$

# Structure

- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink banding
- Twinning in hexagonal metals
- Stacking faults in hexagonal metals
- Texture components in hexagonal metals
- Anisotropy of precipitation strengthening
- Phase transformations; dual- / multiphase systems
- Damage, fracture in hexagonal metals
- Characterization of plasticity carriers in hexagonal metals

# Phase transformations

Co: high temperature fcc phase

strain-induced (martensitic) phase transformation: fcc → hcp

Zr: high temperature bcc phase

rarely reported strain induced phase transformation

Ti: high temperature bcc phase

several martensitic phases

stress-induced martensitic transformation

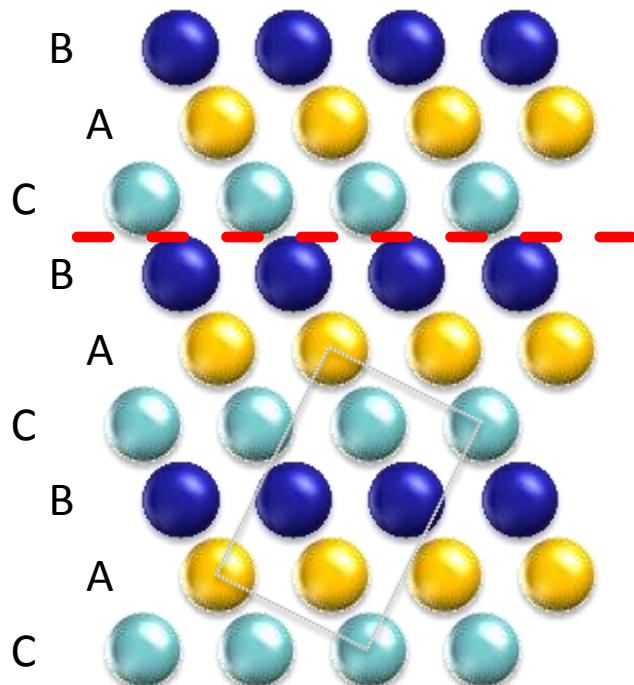
*Reminder:*

*Martensitic transformation is a diffusionless solid-state phase transformation which occurs either by quenching from HAT phase or strain-induced.*

# Phase transformations – fcc → hcp

Co: high temperature fcc phase

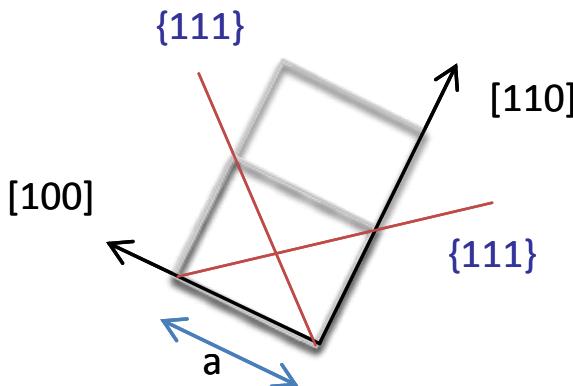
strain-induced (martensitic) phase transformation: fcc → hcp



perfect fcc lattice in  $<110>$  projection

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

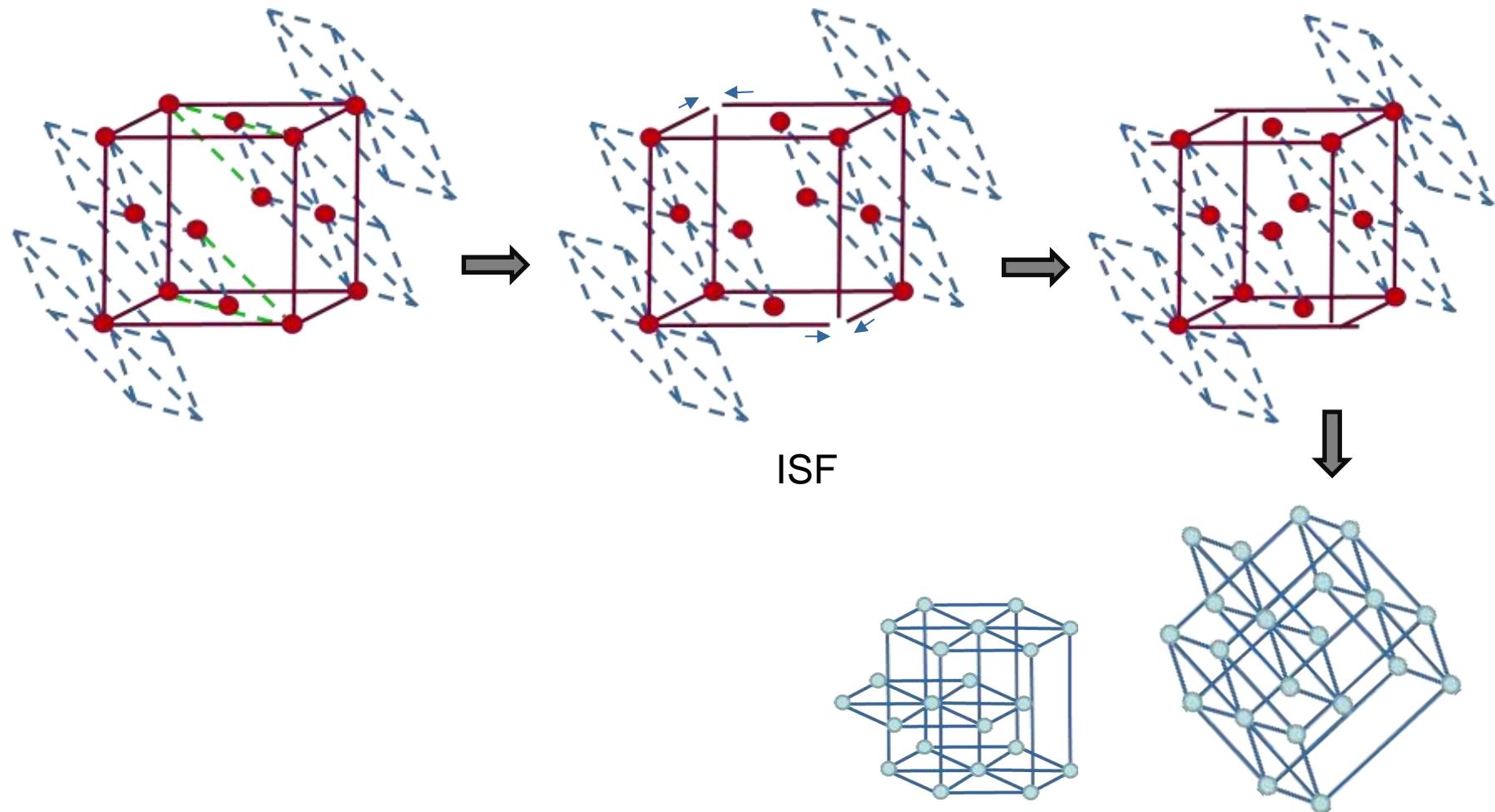
locally hexagonal stacking  
-> accumulation of SFs leads to hcp stacking  
(Co fcc (HT) → hcp (LT))



# Phase transformations

Co: high temperature fcc phase

strain-induced (martensitic) phase transformation: fcc  $\rightarrow$  hcp

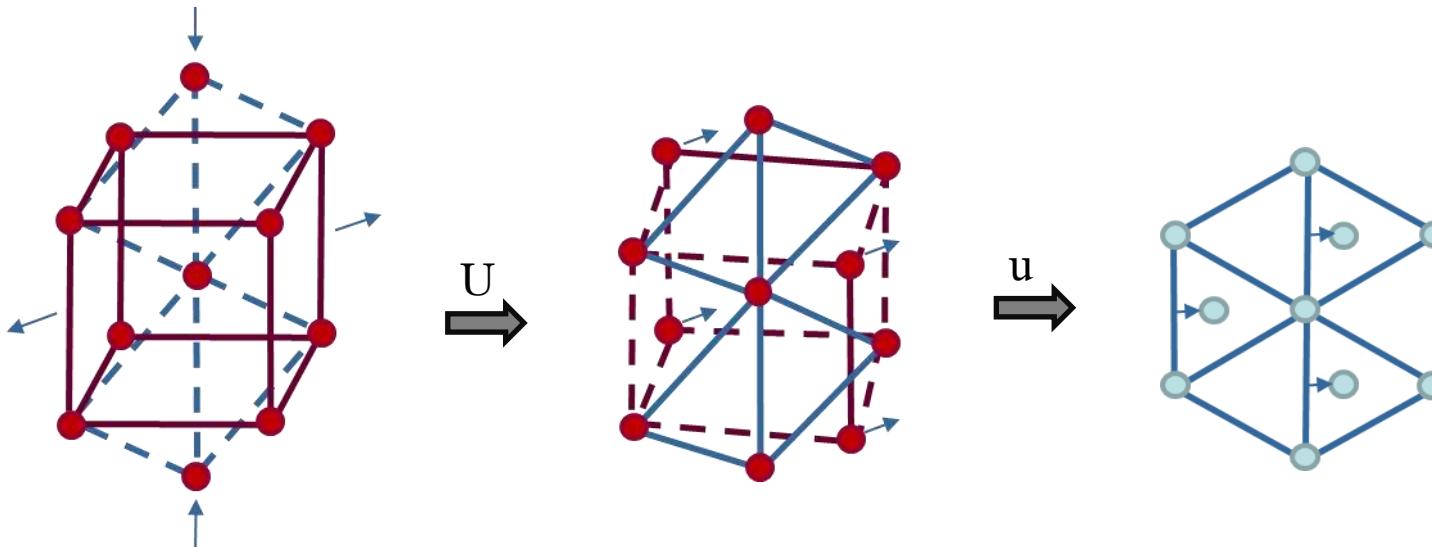


# Phase transformations

Zr, Ti: high temperature bcc phase

martensitic phase transformation: bcc  $\rightarrow$  hcp

Burgers Path / Burgers Orientation Relationship (BOR)



U: hcp deformation  
u: atomic shuffle

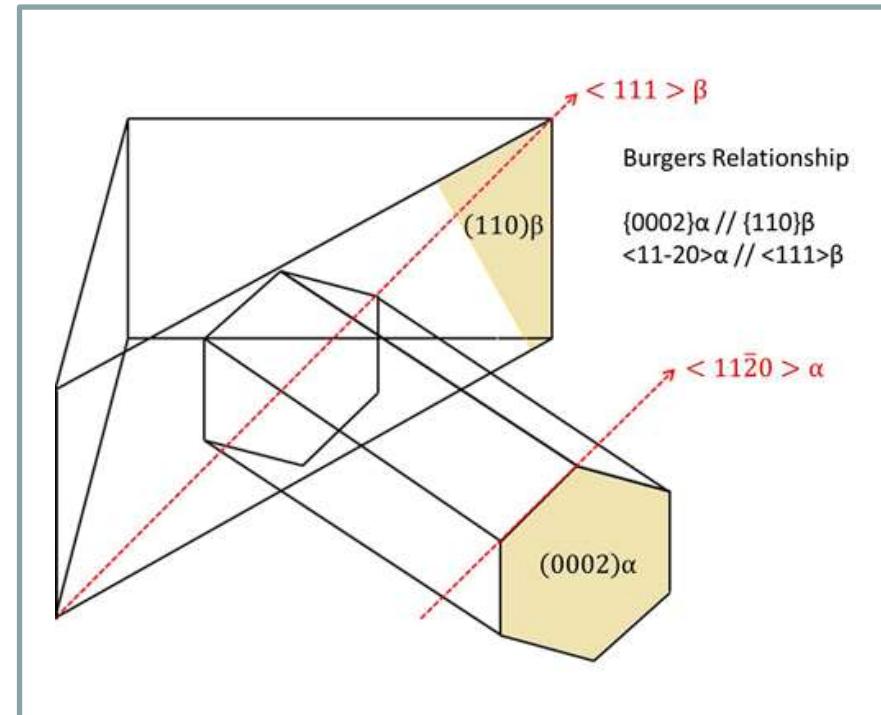
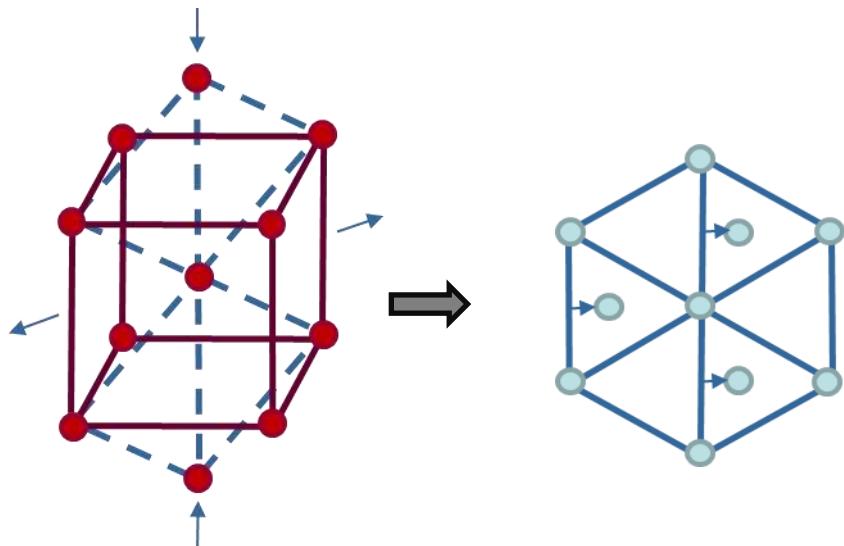
$$\mathbf{U}(V) = \begin{pmatrix} \frac{\alpha(V)}{2} + \frac{3}{4\sqrt{2}} & \frac{\alpha(V)}{2} - \frac{3}{4\sqrt{2}} & 0 \\ \frac{\alpha(V)}{2} - \frac{3}{4\sqrt{2}} & \frac{\alpha(V)}{2} + \frac{3}{4\sqrt{2}} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} \end{pmatrix} \quad \mathbf{u} = \begin{pmatrix} \frac{1}{4\sqrt{2}} \\ \frac{-1}{4\sqrt{2}} \\ 0 \end{pmatrix} \quad \alpha(V) = \sqrt{\frac{3}{8}} \left(\frac{c}{a}\right)_V$$

# Phase transformations

Zr, Ti: high temperature bcc phase

martensitic phase transformation: bcc  $\rightarrow$  hcp

Burgers Path / Burgers Orientation Relationship (BOR)



# Phase transformations

Co: high temperature fcc phase

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rarely reported strain induced phase transformation

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several martensitic phases

stress-induced martensitic transformation



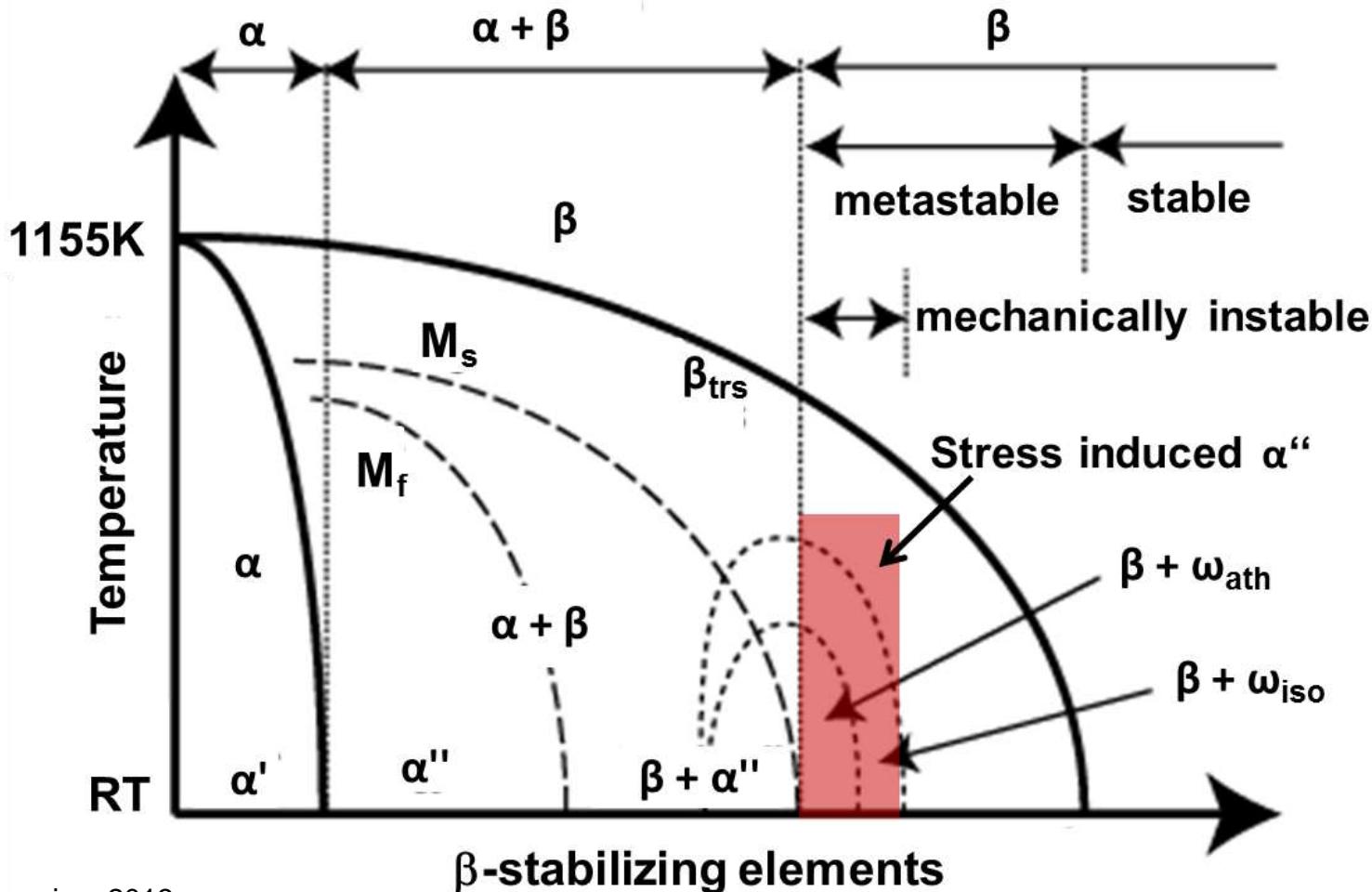
Technologically relevant dual- and multiphase alloys

# Dual- / multiphase systems

Ti - alloying elements:

$\beta$ -stabilizing elements : V, Nb, Ta, Mo, W, Fe, Co, Ni, H

$\alpha$ -stabilizing elements: Al, Ga, In, Sn, N, O



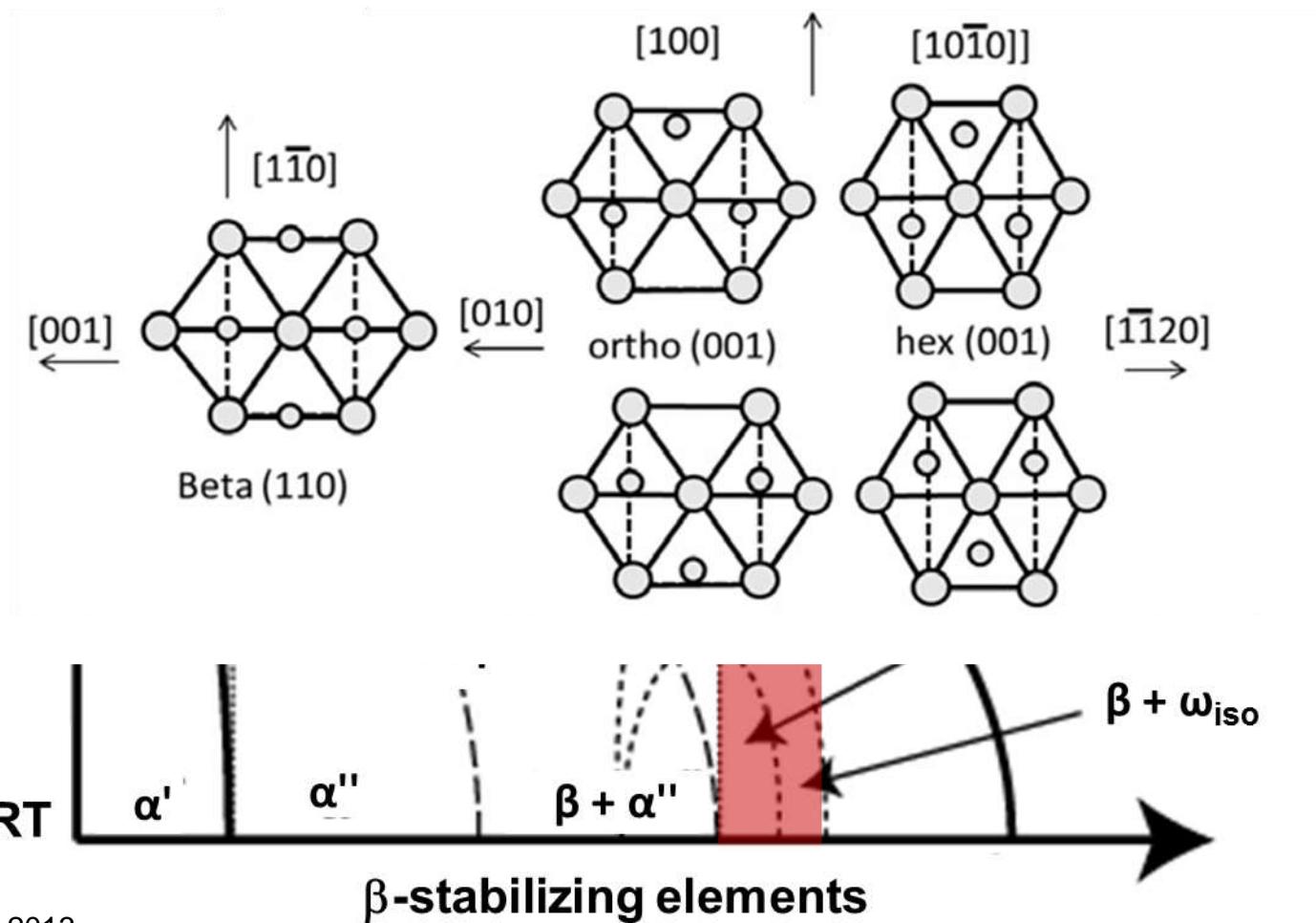
- $\alpha$ : hex
- $\beta$ : bcc
- $\omega$ : hex
- $\alpha'$ : distorted hex
- $\alpha''$ : orthorhombic

# Dual- / multiphase systems

Ti - alloying elements:

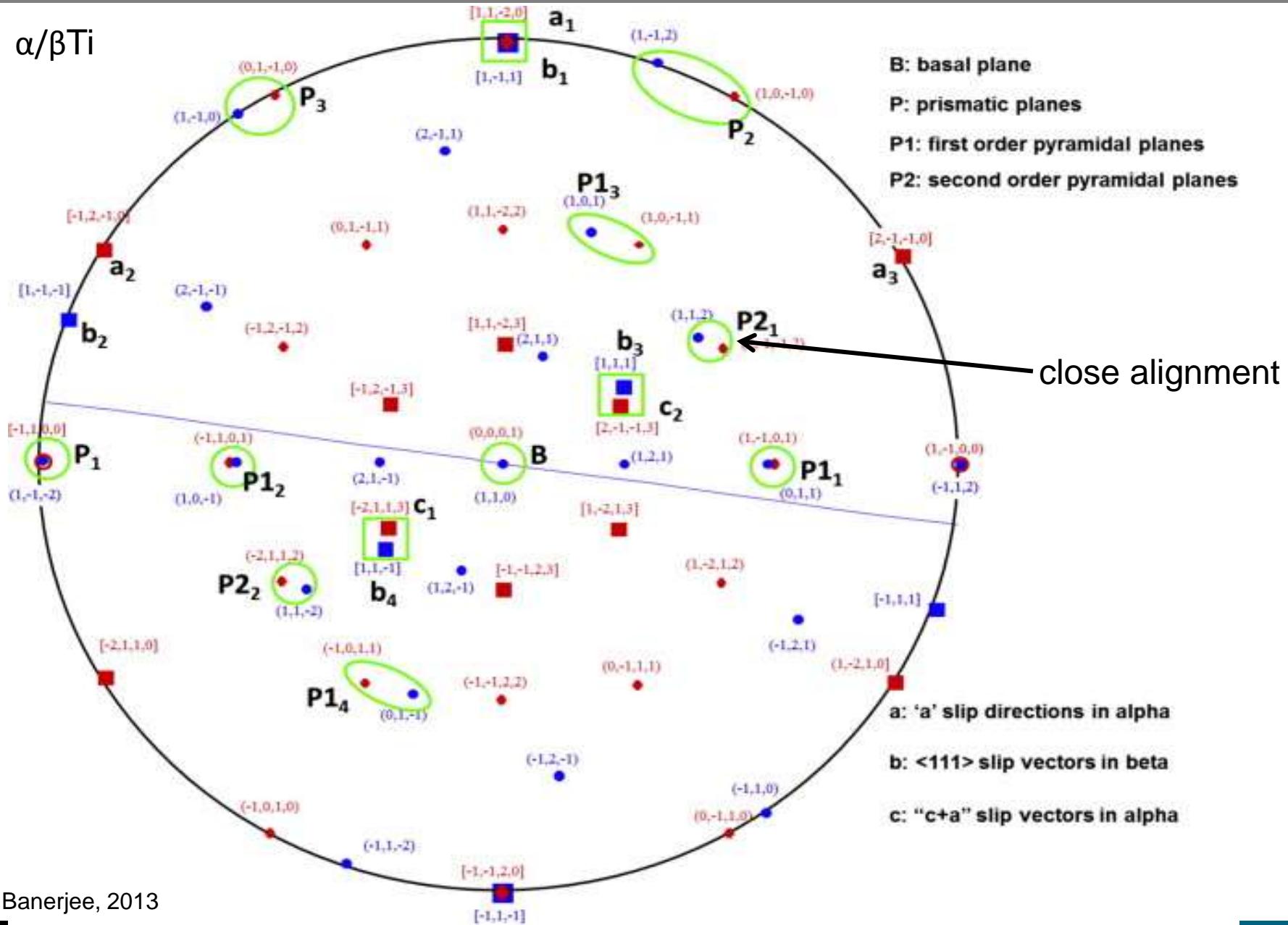
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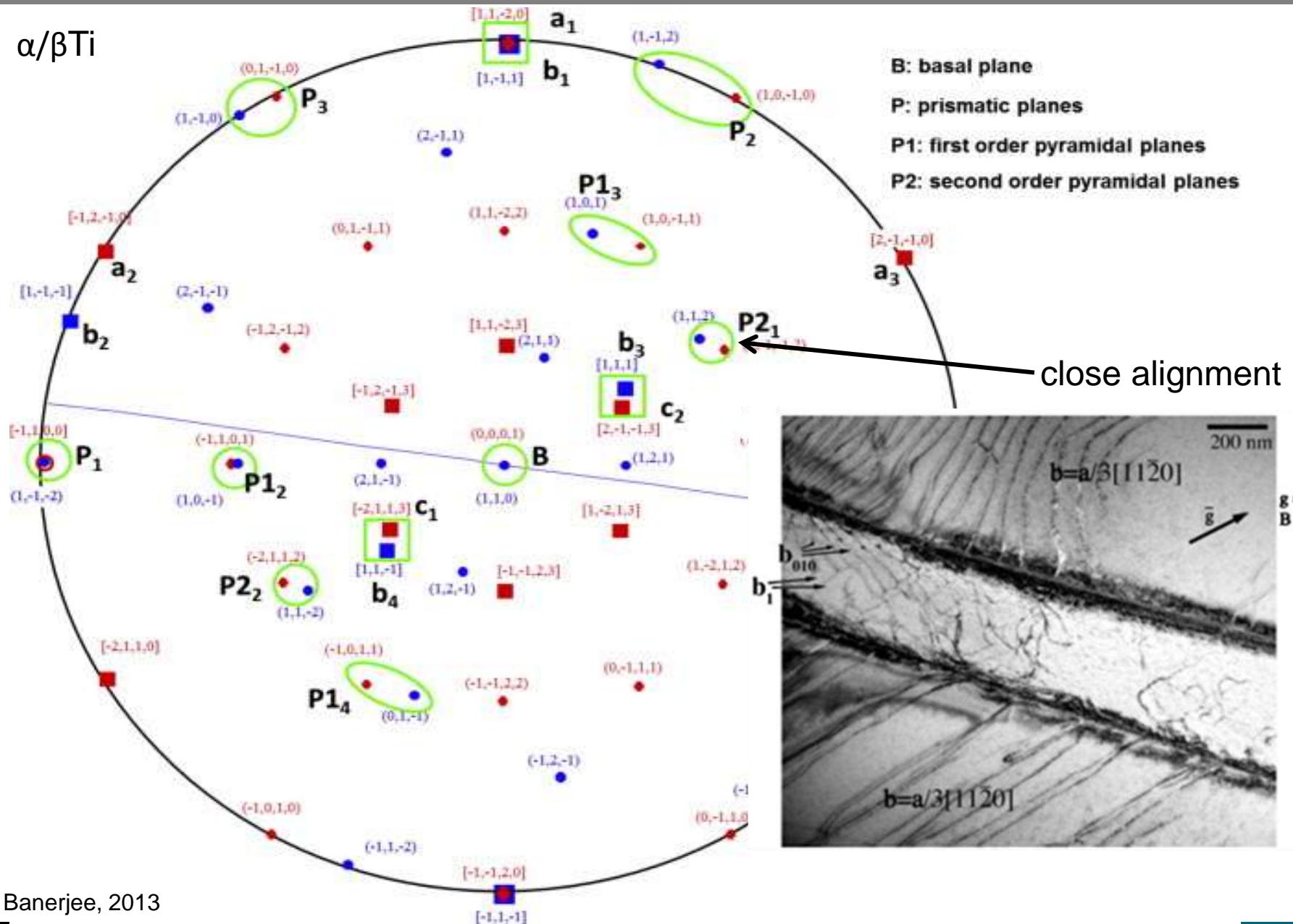
# Dual- / multiphase systems

$\alpha/\beta\text{Ti}$

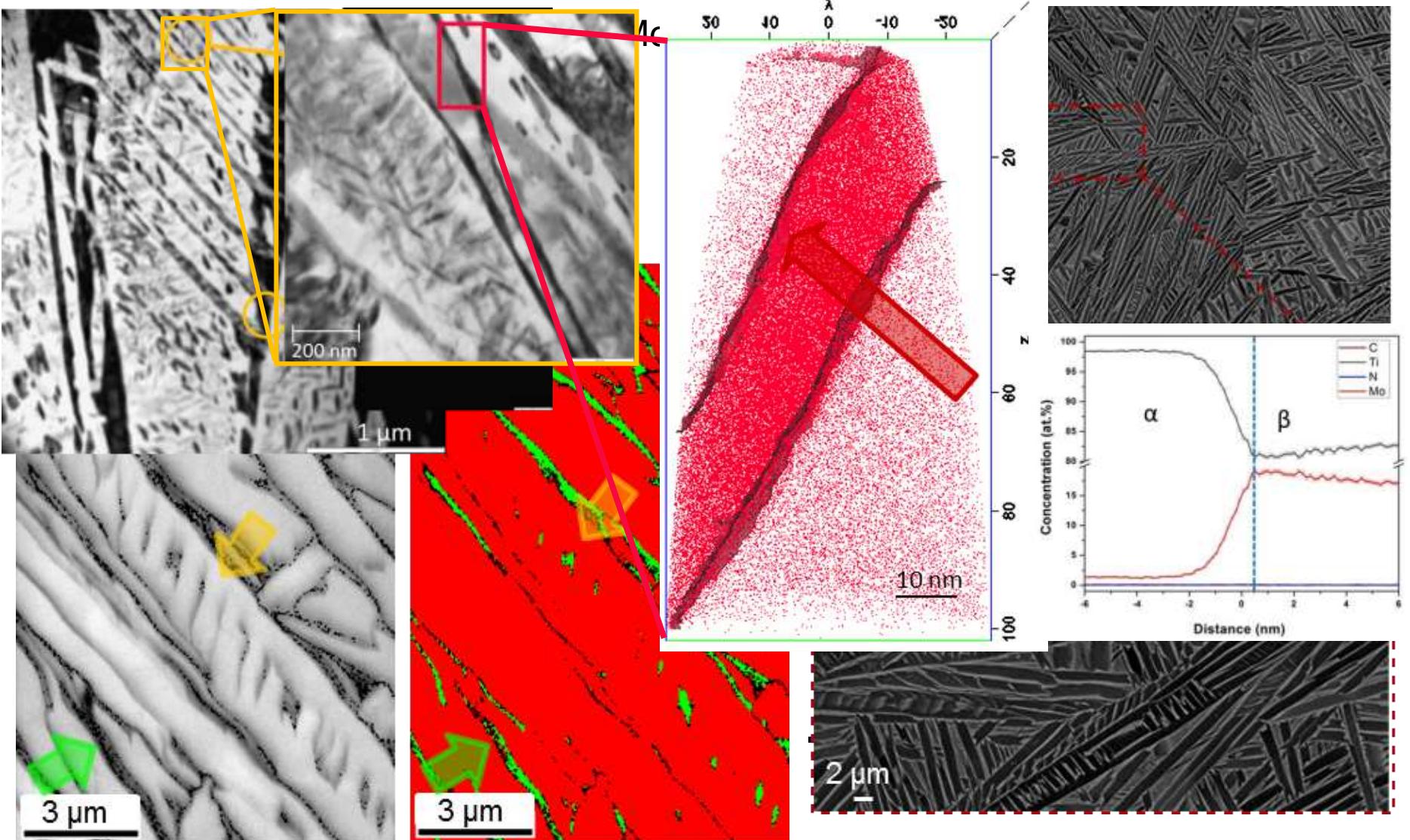


# Dual- / multiphase systems

$\alpha/\beta\text{Ti}$



# Dual- / multiphase systems



# Quiz

- Why is precipitation strengthening anisotropic in hexagonal metals?
- Which precipitate shape is most effective?
- Which hexagonal metals have a high temperature cubic phase?
  - Which cubic phase?
- What is the effect on the deformation behavior?

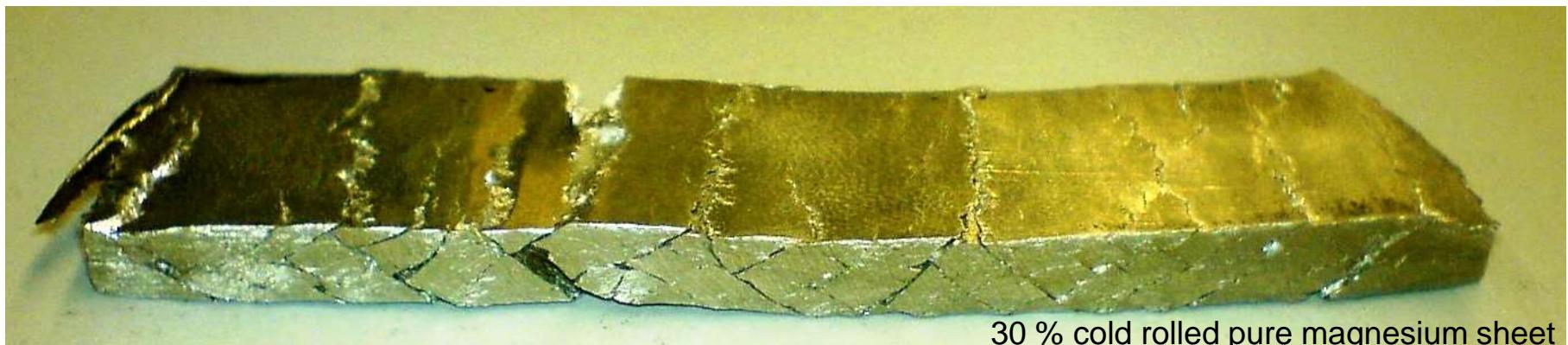
# Structure

- Crystal structure and Miller-Bravais indices
- Dislocations in hexagonal metals
  - Special case: kink banding
- Twinning in hexagonal metals
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- Damage, fracture in hexagonal metals
- Characterization of plasticity carriers in hexagonal metals

# Damage, fracture in hexagonal metals

„Conventional“ failure:

- Stress concentration (e.g. grain or phase boundaries, twin tips)
  - Accommodation of shape change by twinning
  - Stress-corrosion
- 
- Additional failure mode in hex metals: shear banding



Highly localized deformation  
Independent of microstructure



„Emergency exit“

# Damage, fracture in hexagonal metals

Slip system type	Burgers vector type	Slip direction	Slip plane	Independent slip systems
basal	$\vec{a}$	$<11\bar{2}0>$	(0002)	2
prismatic	$\vec{a}$	$<11\bar{2}0>$	{1010}	2
pyramidal $\langle a \rangle$	$\vec{a}$	$<11\bar{2}0>$	{1011}	4
pyramidal $\langle c+a \rangle$	$\vec{c} + \vec{a}$	$<11\bar{2}3>$	{1011}	5
pyramidal $\langle c+a \rangle$	$\vec{c} + \vec{a}$	$<11\bar{2}3>$	{1122}	5
twinning				0.5 (polar)

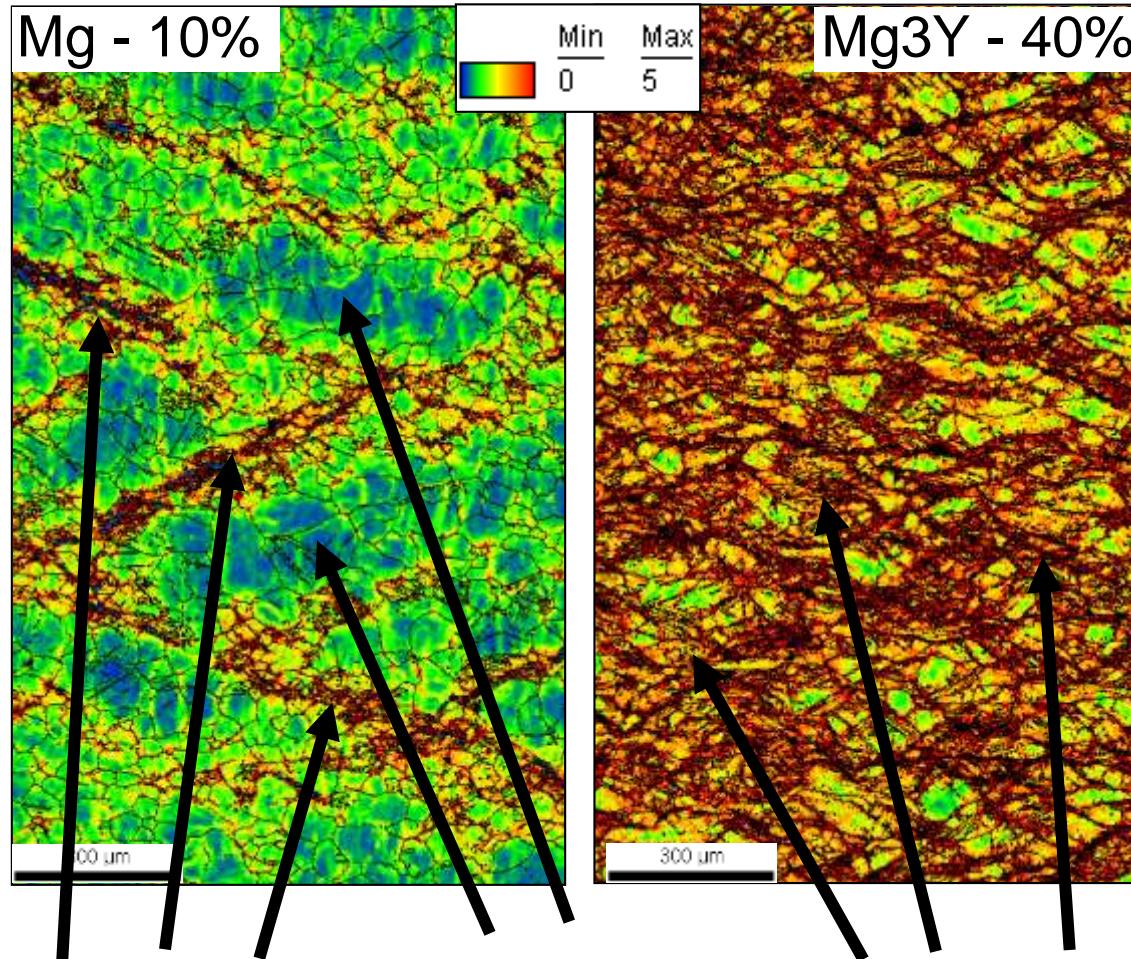
## von Mises criterion

Compatible polycrystalline deformation:  $\geq 5$  independent slip (deformation) systems:

- Case 1: basal  $\langle a \rangle$  + twinning                                  2.5 independent systems
  - Case 2: prismatic  $\langle a \rangle$  + twinning                                  2.5 independent systems
  - Case 3: basal  $\langle a \rangle$  + prismatic  $\langle a \rangle$  + twinning          4.5 independent systems
- Pyramidal slip systems necessary to reach 5 independent deformation systems

# Damage, fracture in hexagonal metals

Deformation microstructure at fracture begin – KAM\* maps



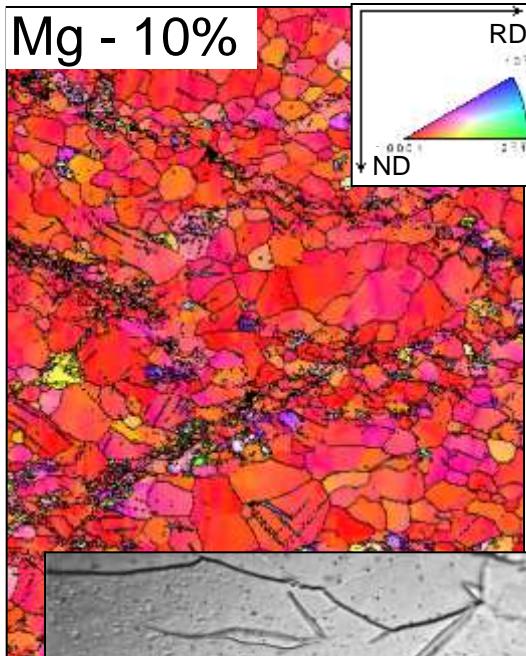
- Pure Mg
  - Strongly localized strain in few shear bands
  - Low internal misorientations in matrix grains
  
- Mg<sub>3</sub>Y
  - High amount of shear bands
  - Homogeneously distributed strain

\*KAM: Kernel average misorientation, calculated as the average over all misorientation angles determined between the centre and all edge pixels in a kernel of pixels in an orientation map

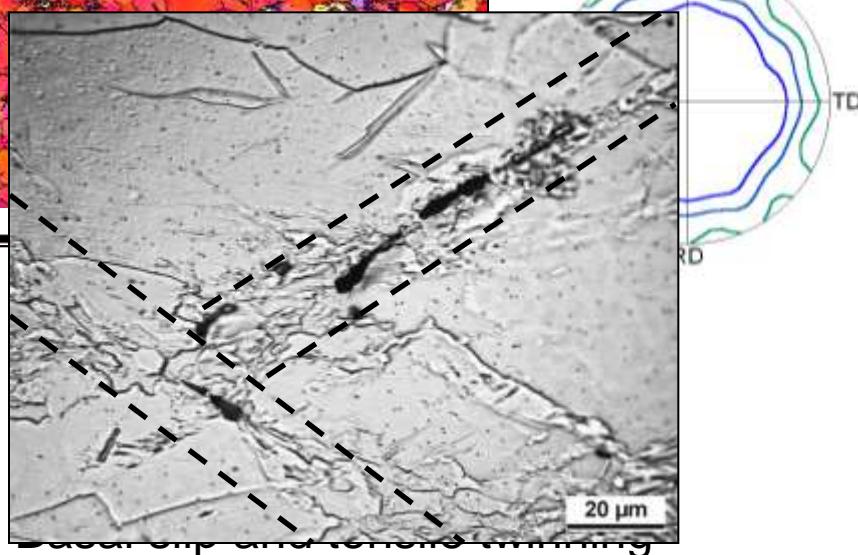
# Damage, fracture in hexagonal metals

Deformation texture at fracture begin

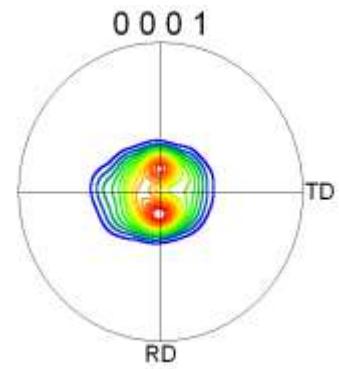
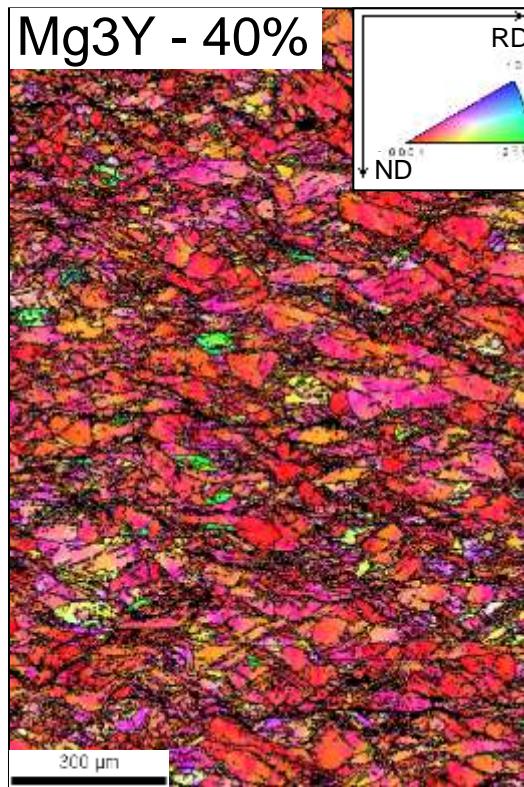
Mg - 10%



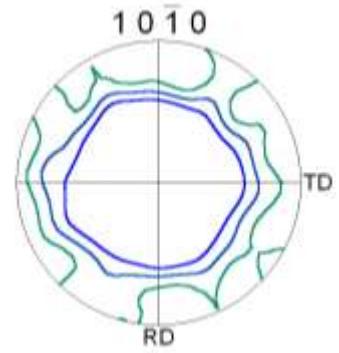
$$P_{\max} = 17.165$$



Mg<sub>3</sub>Y - 40%

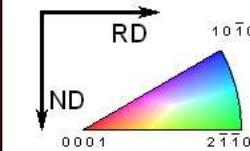
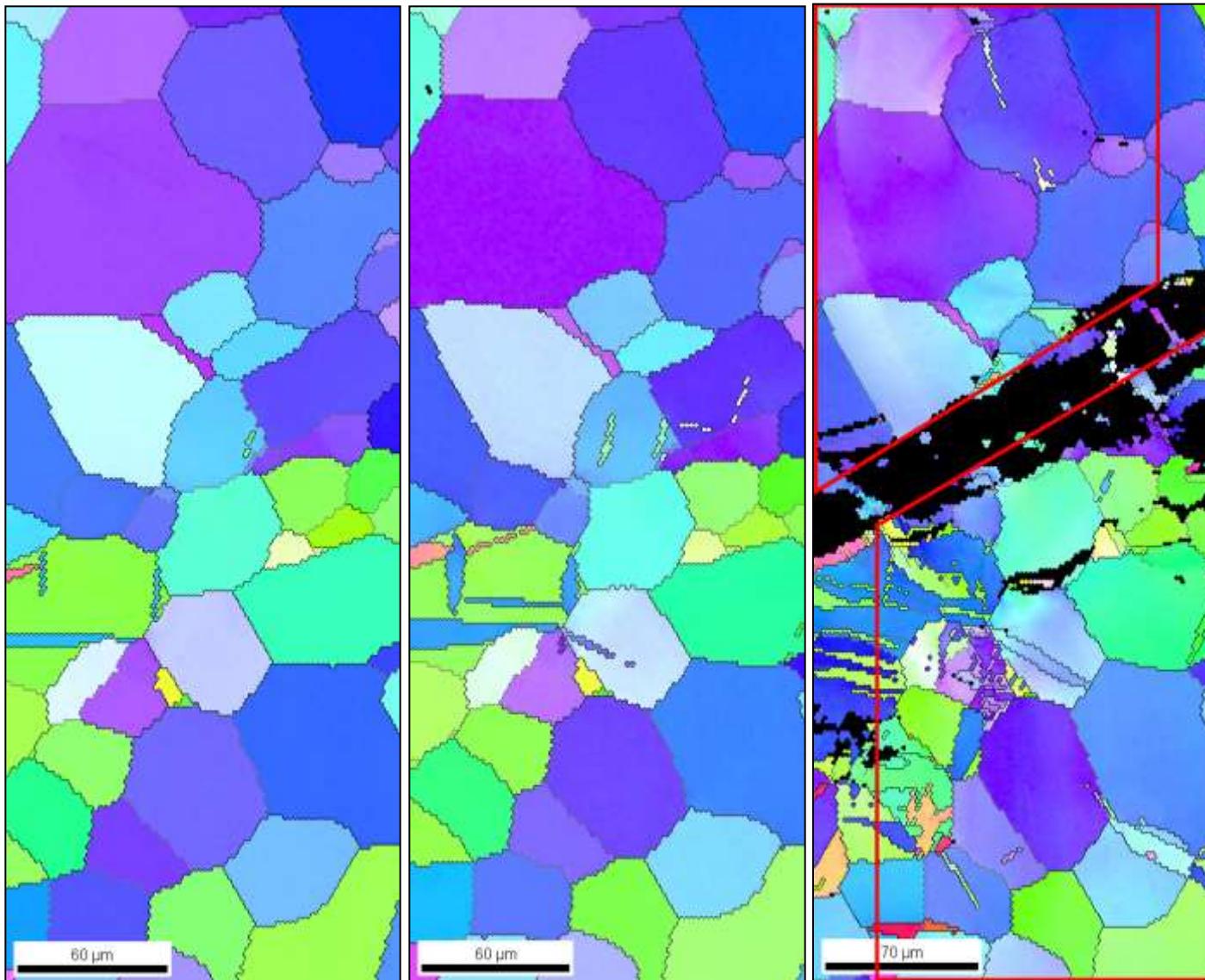


$$P_{\max} = 8.230$$



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

# Damage, fracture in hexagonal metals

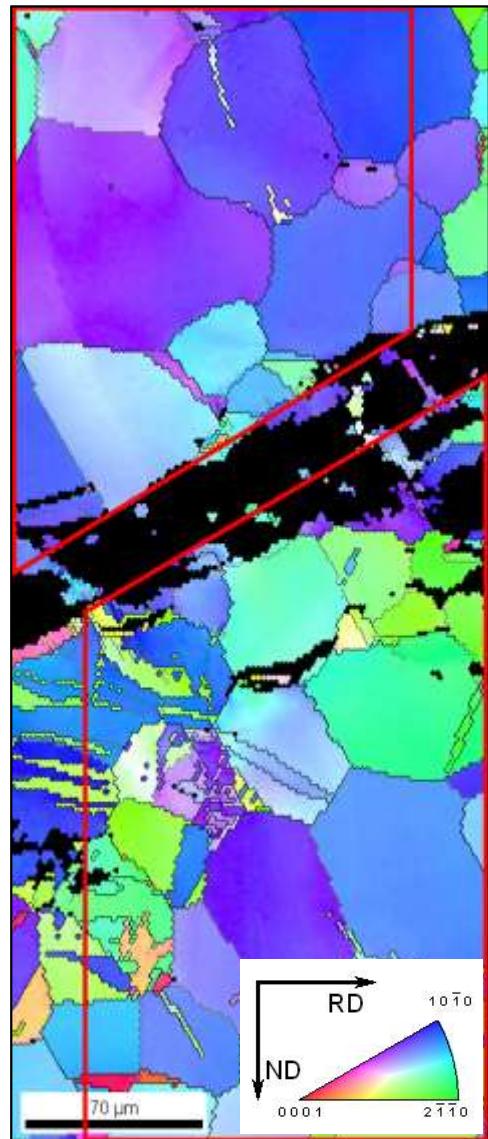


RX

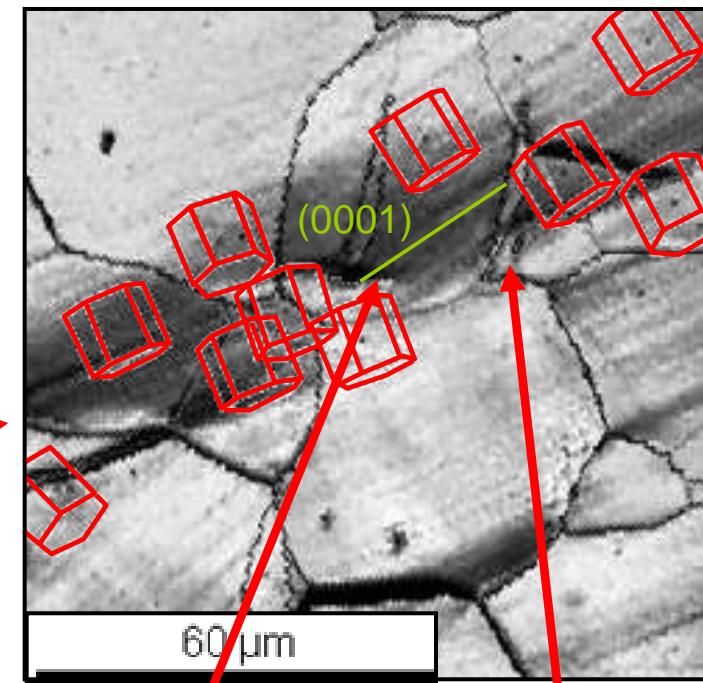
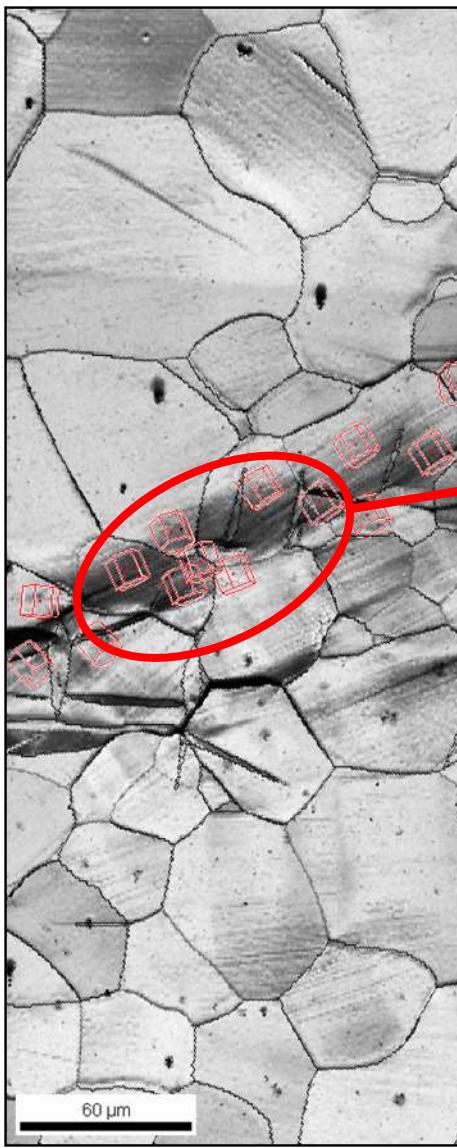
4% compression

8% compression

# Damage, fracture in hexagonal metals



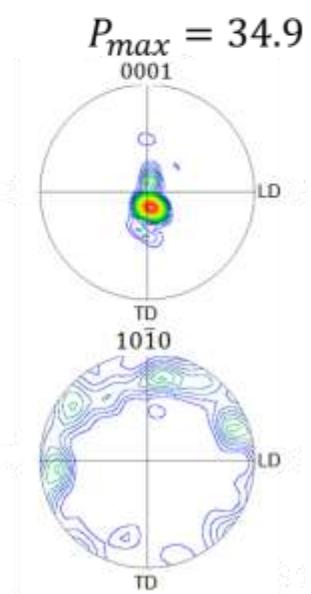
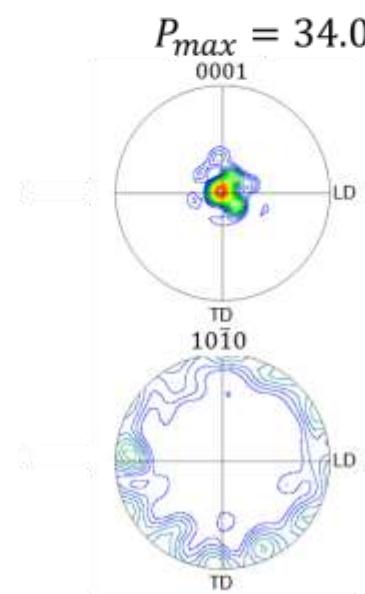
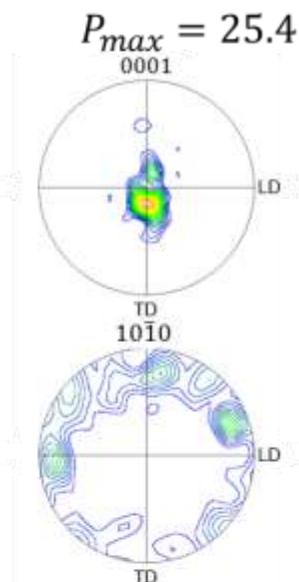
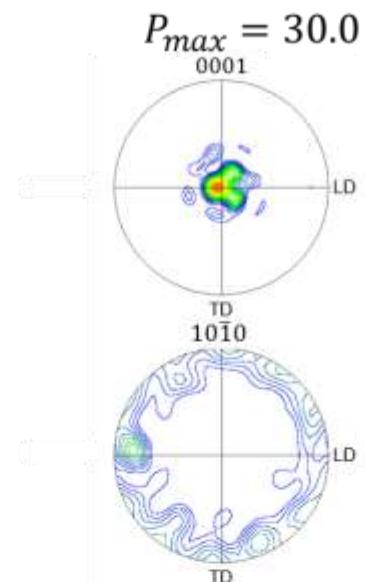
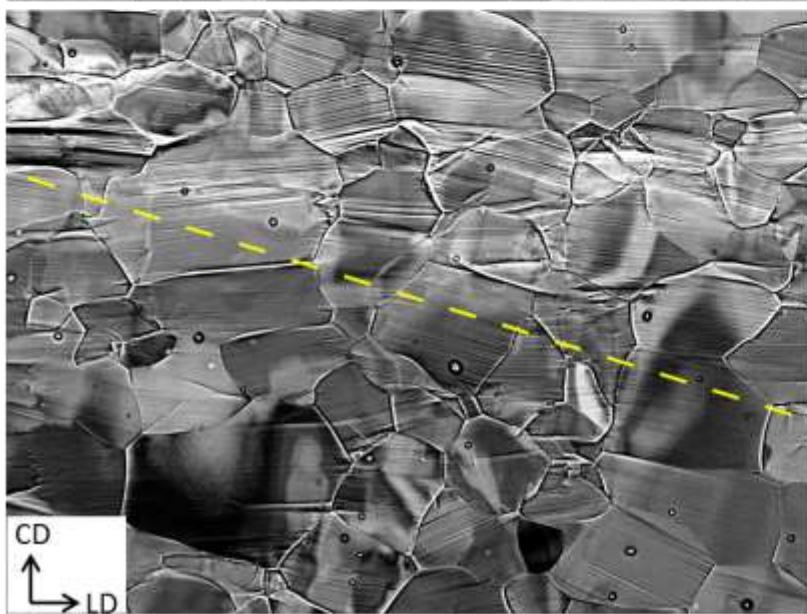
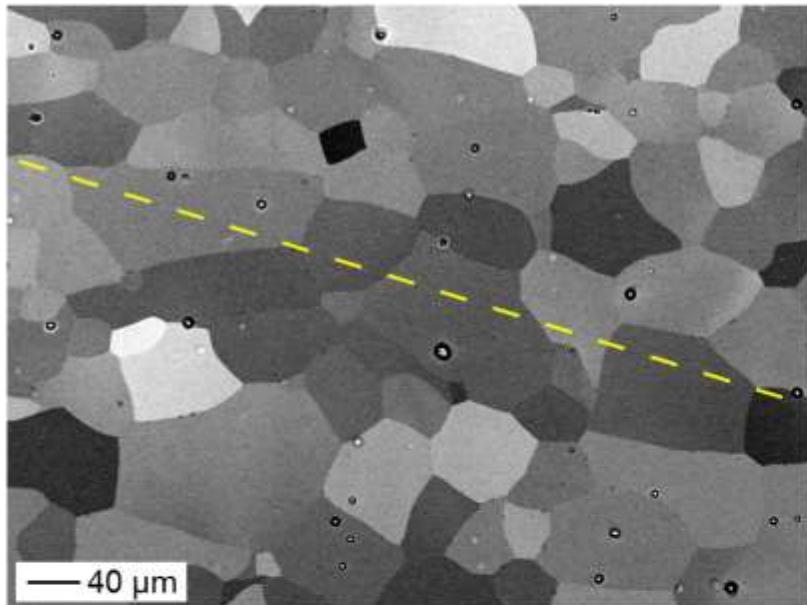
8% compression



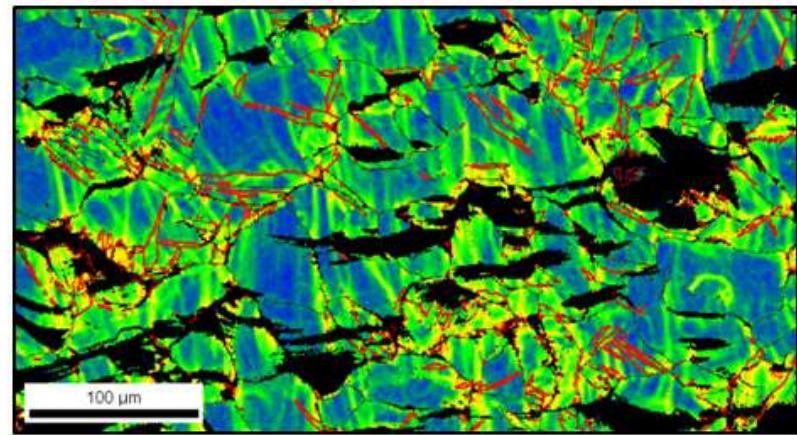
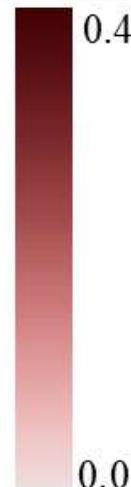
Shear band

Basal slip

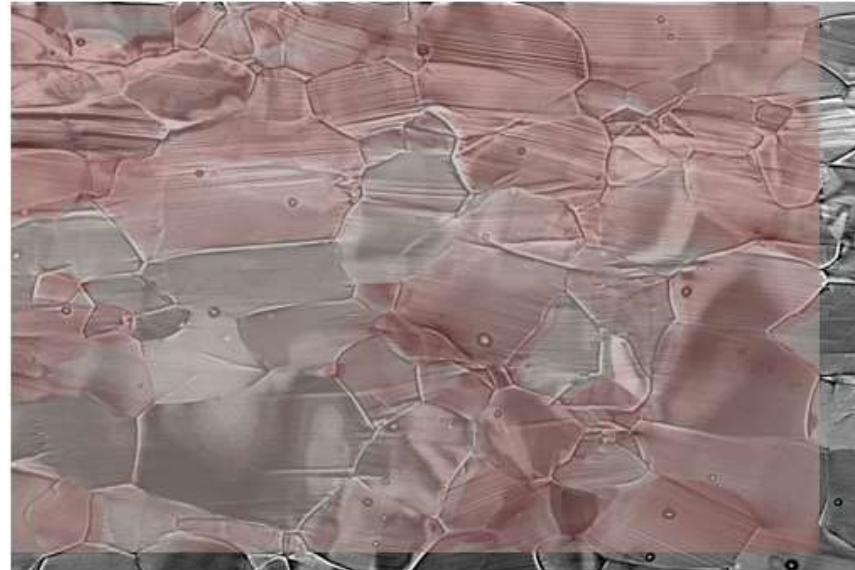
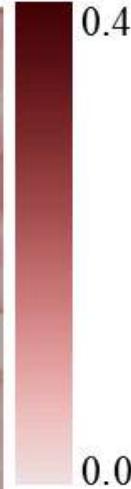
# Damage, fracture in hexagonal metals



# Damage, fracture in hexagonal metals



Plane strain compression

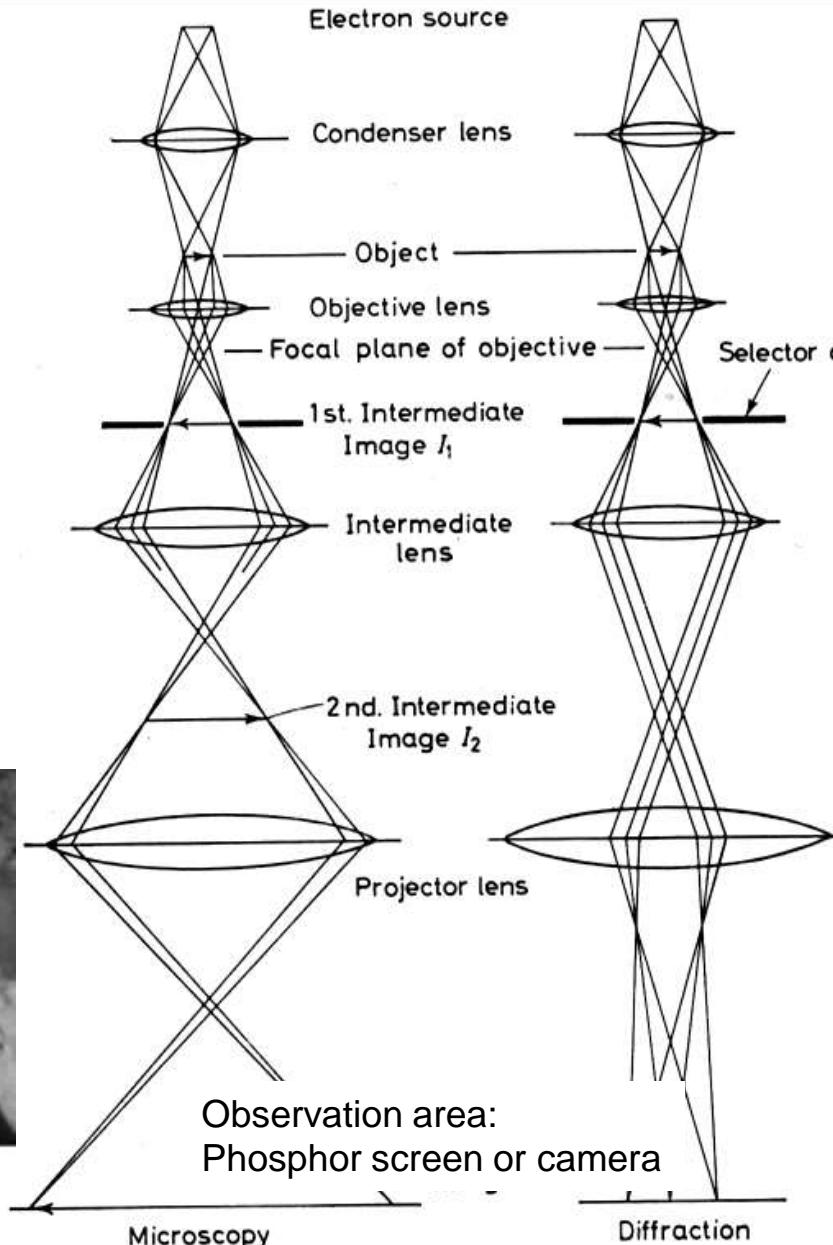
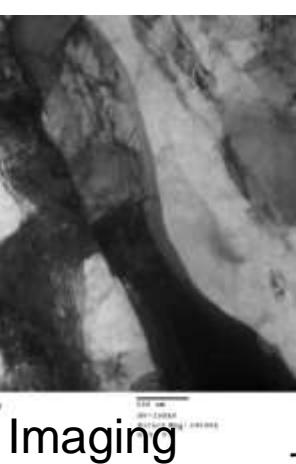


Plane strain compression  
+ out-of-plane shear

# Structure

- Crystal structure and Miller-Bravais indices
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- Texture components in hexagonal metals
- Anisotropy of precipitation strengthening
- Phase transformations; dual- / multiphase systems
- Damage, fracture in hexagonal metals
- Characterization of plasticity carriers in hexagonal metals

# Characterization of plasticity carriers in hexagonal metals

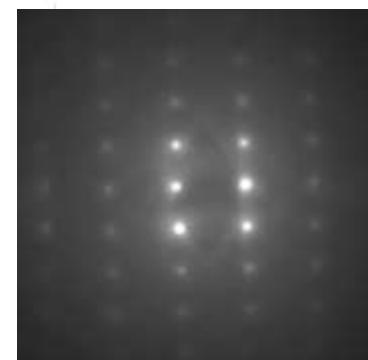


**Illumination system:**  
parallel or convergent illumination

**Objective lens:**  
creates image of sample

**Intermediate lens:**  
focused either on  
diffraction plane  
or on image plane

**projector lens:**  
creates final magnification

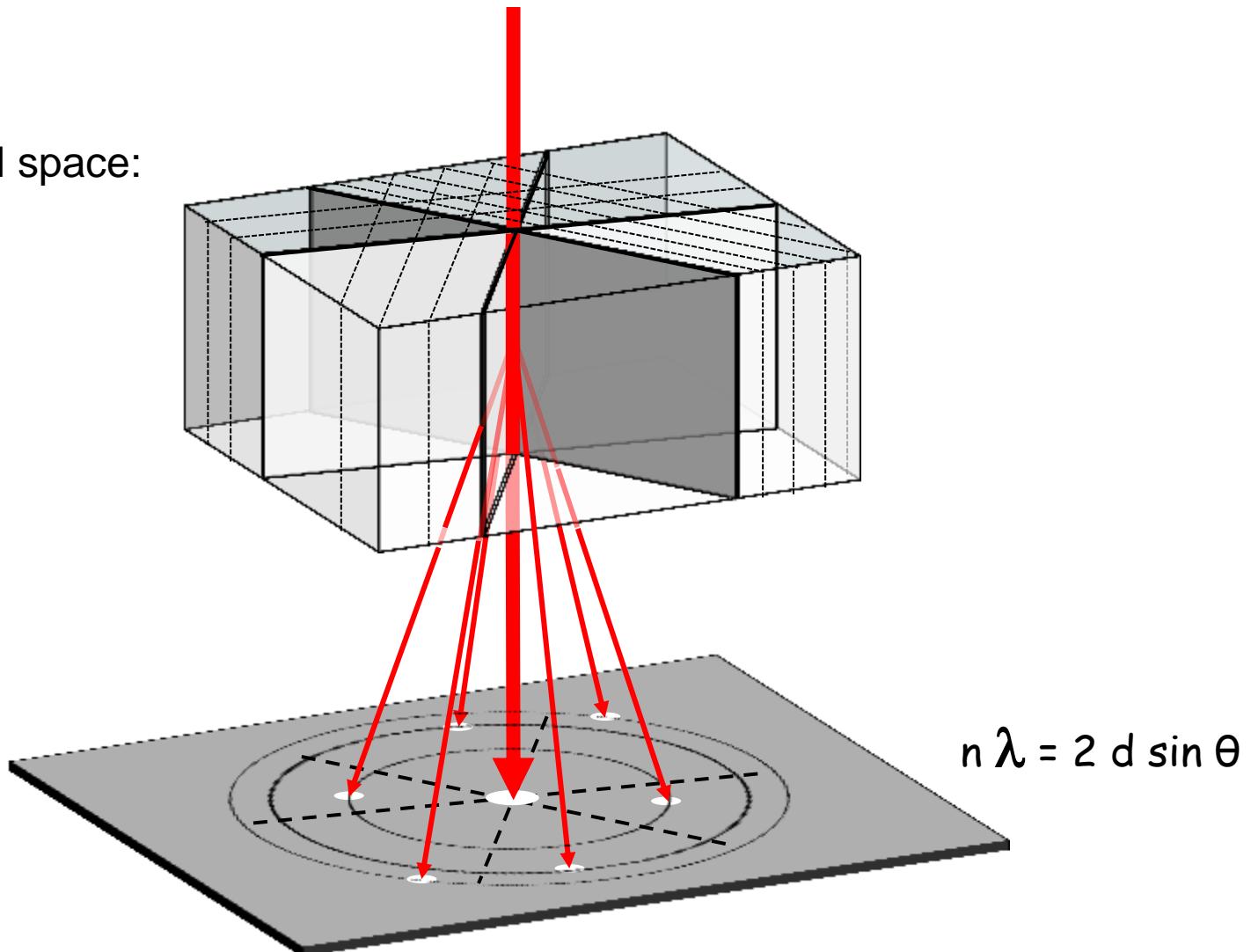


Diffraction

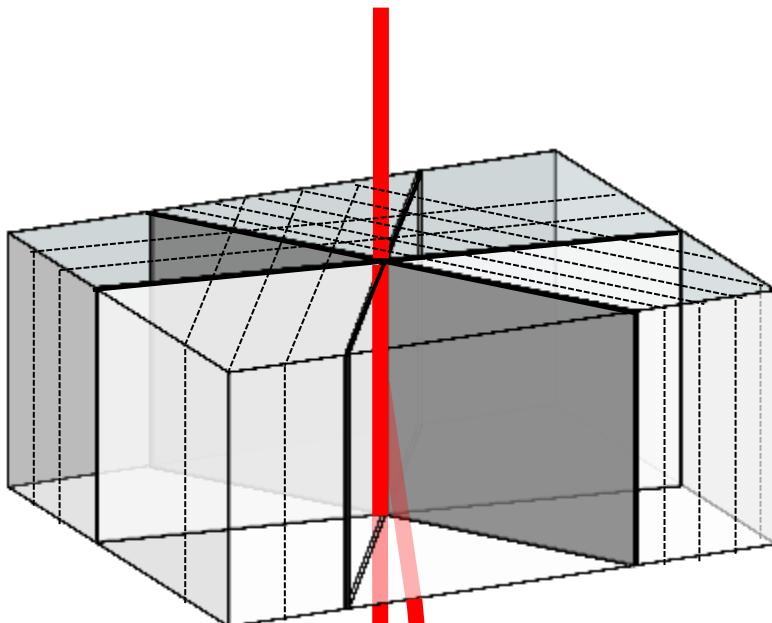
© Zaefferer

Diffraction: „multi-beam“ conditions  
multiple sets of lattice planes are in Bragg condition

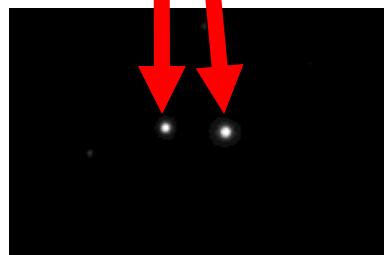
Reciprocal space:  
Inverse



Diffraction: „multi-beam“ conditions  
only one set of lattice planes is in Bragg condition



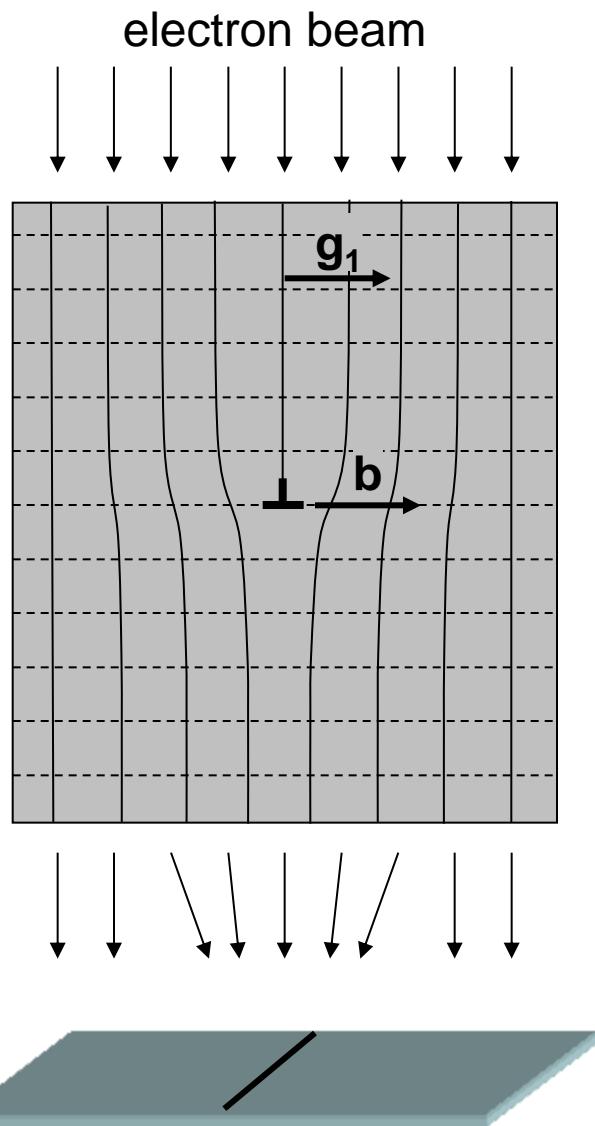
Identification of defect types and Burgers vectors



# Characterization of plasticity carriers in hexagonal metals

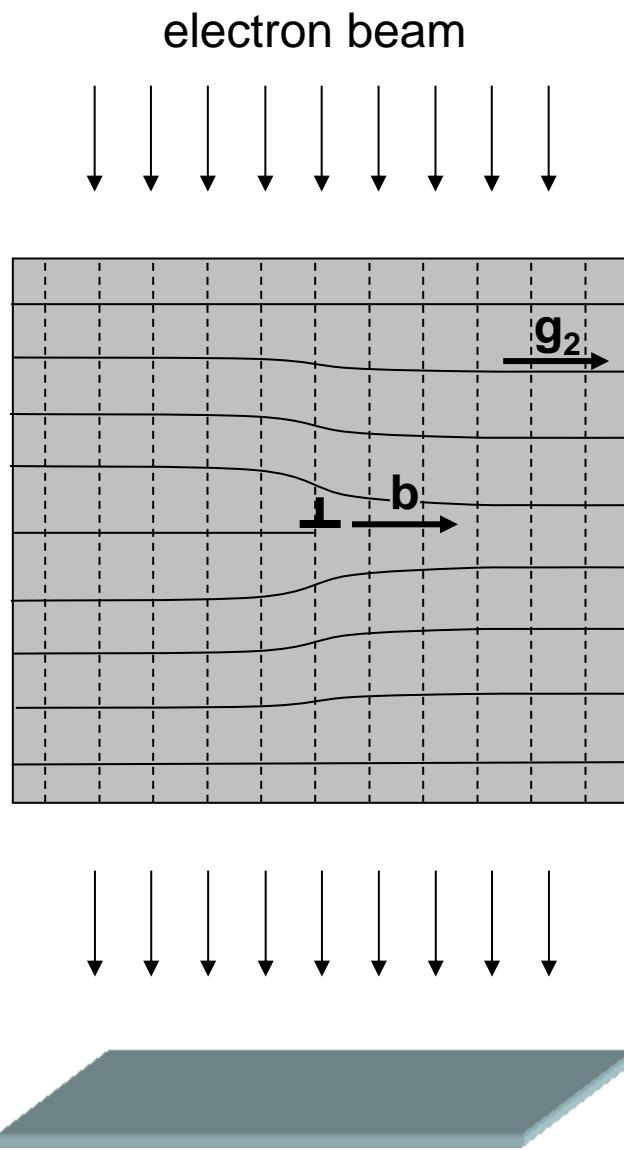


2-beam condition  $g_1$



$g_1 \cdot b \neq 0$   
dislocation  
visible

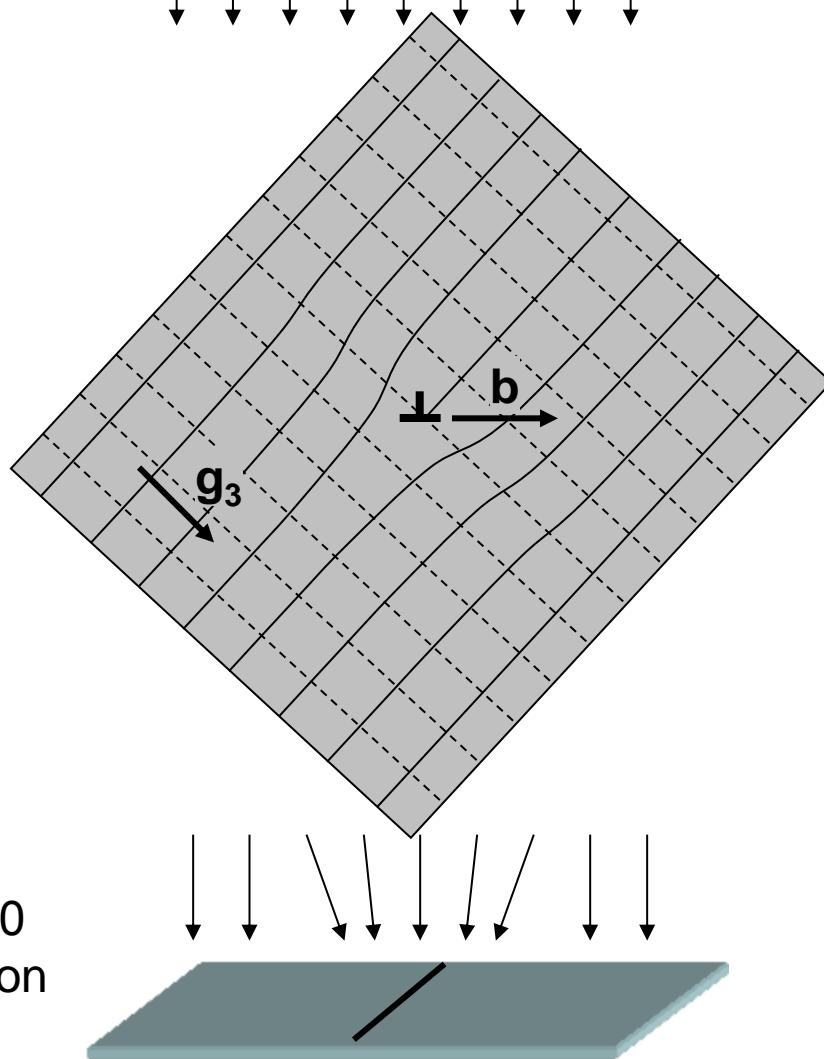
2-beam condition  $g_2$



# Characterization of plasticity carriers in hexagonal metals

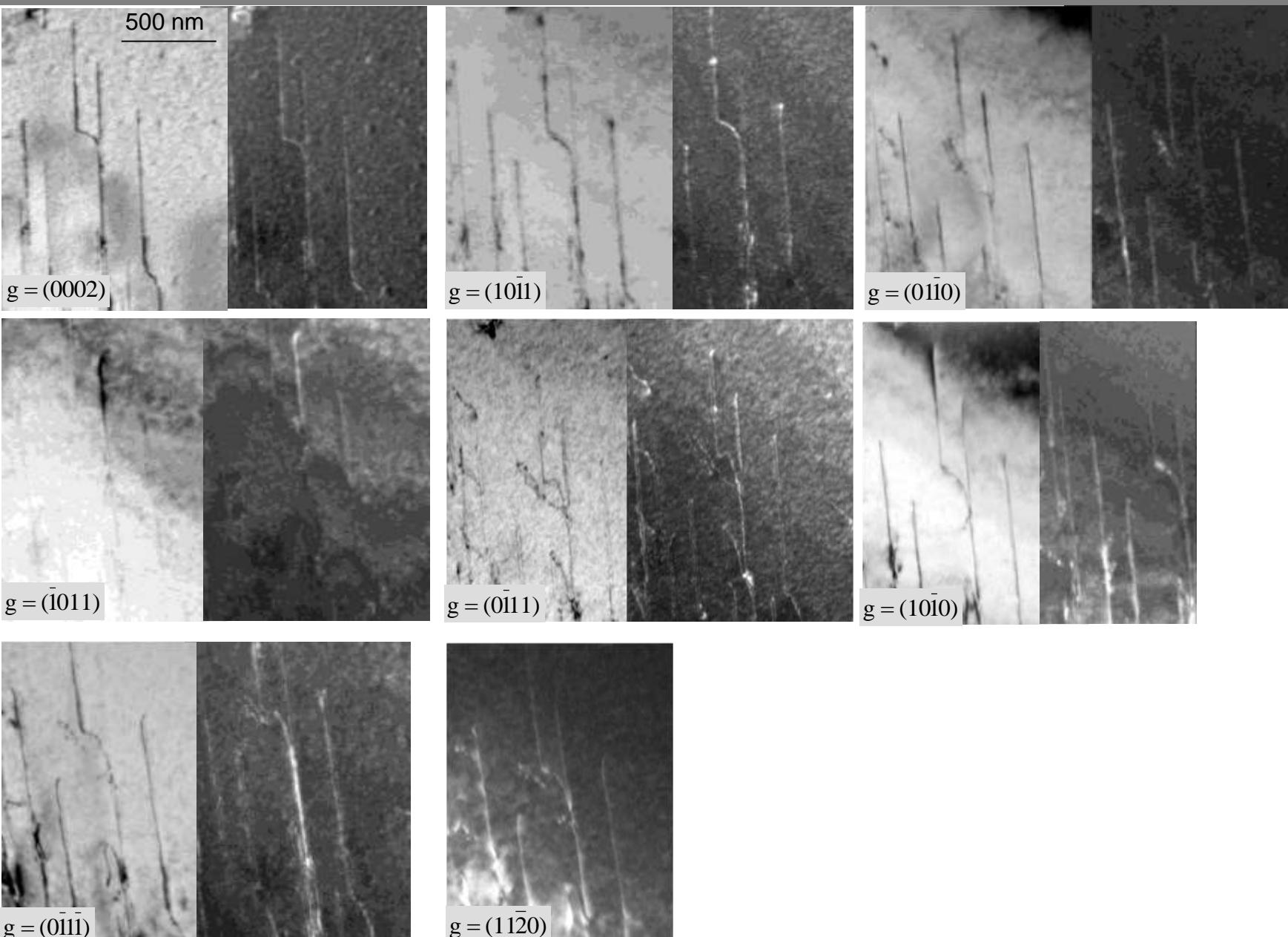
2-beam condition  $g_3$

electron beam

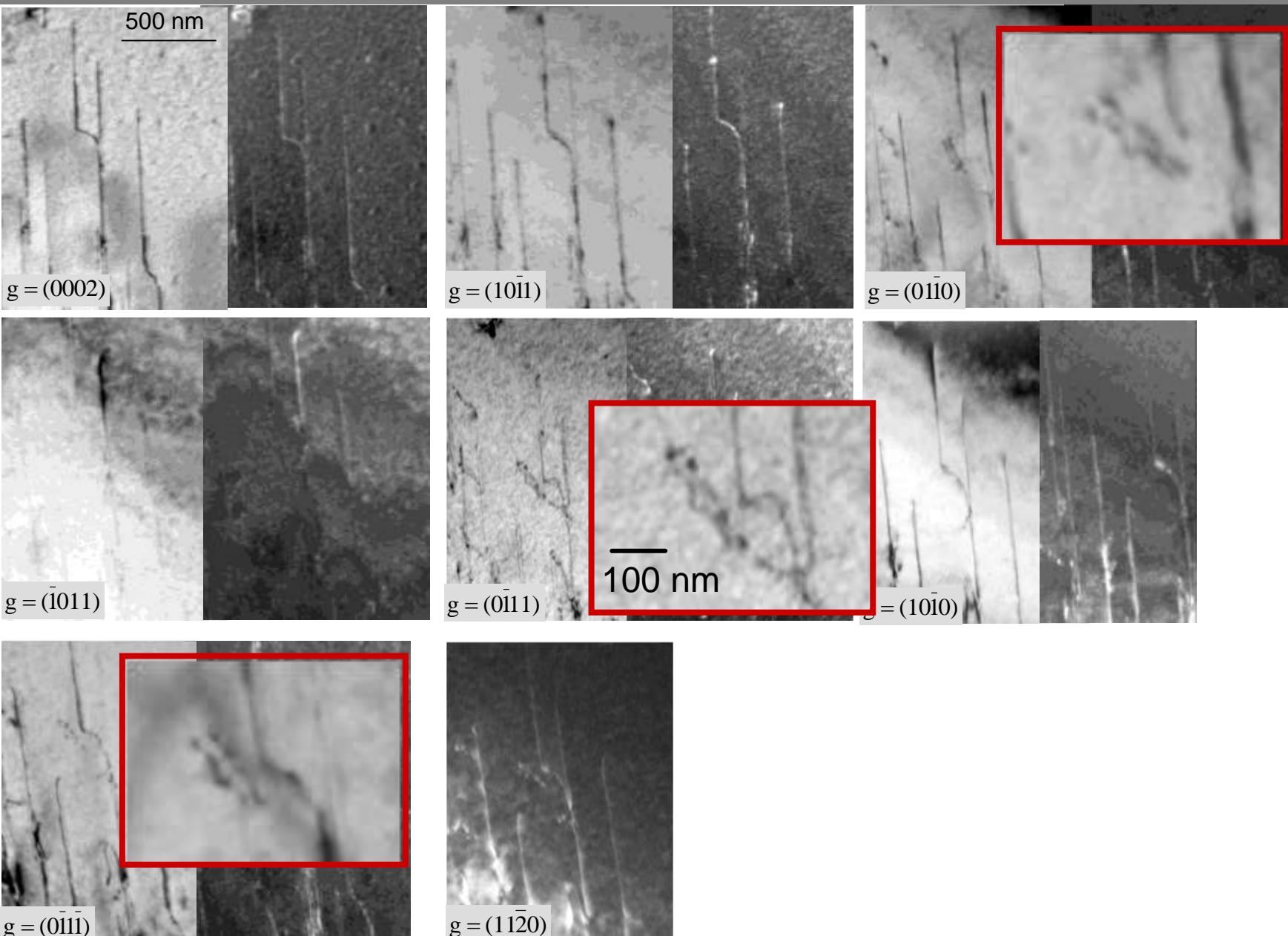


$\mathbf{g}_3 \cdot \mathbf{b} \neq 0$   
dislocation  
visible

# Characterization of plasticity carriers in hexagonal metals



# Characterization of plasticity carriers in hexagonal metals



# Characterization of plasticity carriers in hexagonal metals



		Diffraction vector						
Burgers vector		0002	-1011	10-10	10-11	0-11-1	0-111	01-10
perfect	$\frac{1}{3} [11-20]$	0,00	-1,00	1,00	1,00	-1,00	-1,00	1,00
perfect	$\frac{1}{3} [1-210]$	0,00	0,00	0,00	0,00	1,00	1,00	-1,00
perfect	$\frac{1}{3} [-2110]$	0,00	1,00	-1,00	-1,00	0,00	0,00	0,00
perfect	[0001]	2,00	1,00	0,00	1,00	-1,00	1,00	0,00
perfect	$\frac{1}{3} [11-23]$	2,00	0,00	1,00	2,00	-2,00	0,00	1,00
perfect	$\frac{1}{3} [1-213]$	2,00	1,00	0,00	1,00	0,00	2,00	-1,00
perfect	$\frac{1}{3} [-2113]$	2,00	2,00	-1,00	0,00	-1,00	1,00	0,00
perfect	$\frac{1}{3} [11-2-3]$	-2,00	-2,00	1,00	0,00	0,00	-2,00	1,00
perfect	$\frac{1}{3} [1-21-3]$	-2,00	-1,00	0,00	-1,00	2,00	0,00	-1,00
perfect	$\frac{1}{3} [-211-3]$	-2,00	0,00	-1,00	-2,00	1,00	-1,00	0,00
partial	$\frac{1}{3} [10-10]$	0,00	-0,67	0,67	0,67	-0,33	-0,33	0,33
partial	$\frac{1}{3} [1-100]$	0,00	-0,33	0,33	0,33	0,33	0,33	-0,33
partial	$\frac{1}{3} [01-10]$	0,00	-0,33	0,33	0,33	-0,67	-0,67	0,67
partial	$\frac{1}{2} [0001]$	1,00	0,50	0,00	0,50	-0,50	0,50	0,00
partial	$\frac{1}{6} [20-23]$	1,00	-0,17	0,67	1,17	-0,83	0,17	0,33
partial	$\frac{1}{6} [2-20-3]$	-1,00	-0,83	0,33	-0,17	0,83	-0,17	-0,33
partial	$\frac{1}{6} [02-2-3]$	-1,00	-0,83	0,33	-0,17	-0,17	-1,17	0,67
partial	$\frac{1}{6} [-2023]$	1,00	1,17	-0,67	-0,17	-0,17	0,83	-0,33
partial	$\frac{1}{6} [02-23]$	1,00	0,17	0,33	0,83	-1,17	-0,17	0,67
partial	$\frac{1}{6} [20-2-3]$	-1,00	-1,17	0,67	0,17	0,17	-0,83	0,33
partial	$\frac{1}{6} [11-21]$	0,33	-0,33	0,50	0,67	-0,67	-0,33	0,50
partial	$\frac{1}{6} [11-2-1]$	-0,33	-0,67	0,50	0,33	-0,33	-0,67	0,50

$g \cdot b = 0$  invisible

$g \cdot b \neq 0$  visible

$g \cdot b \leq 0.5$  weak contrast

# Characterization of plasticity carriers in hexagonal metals



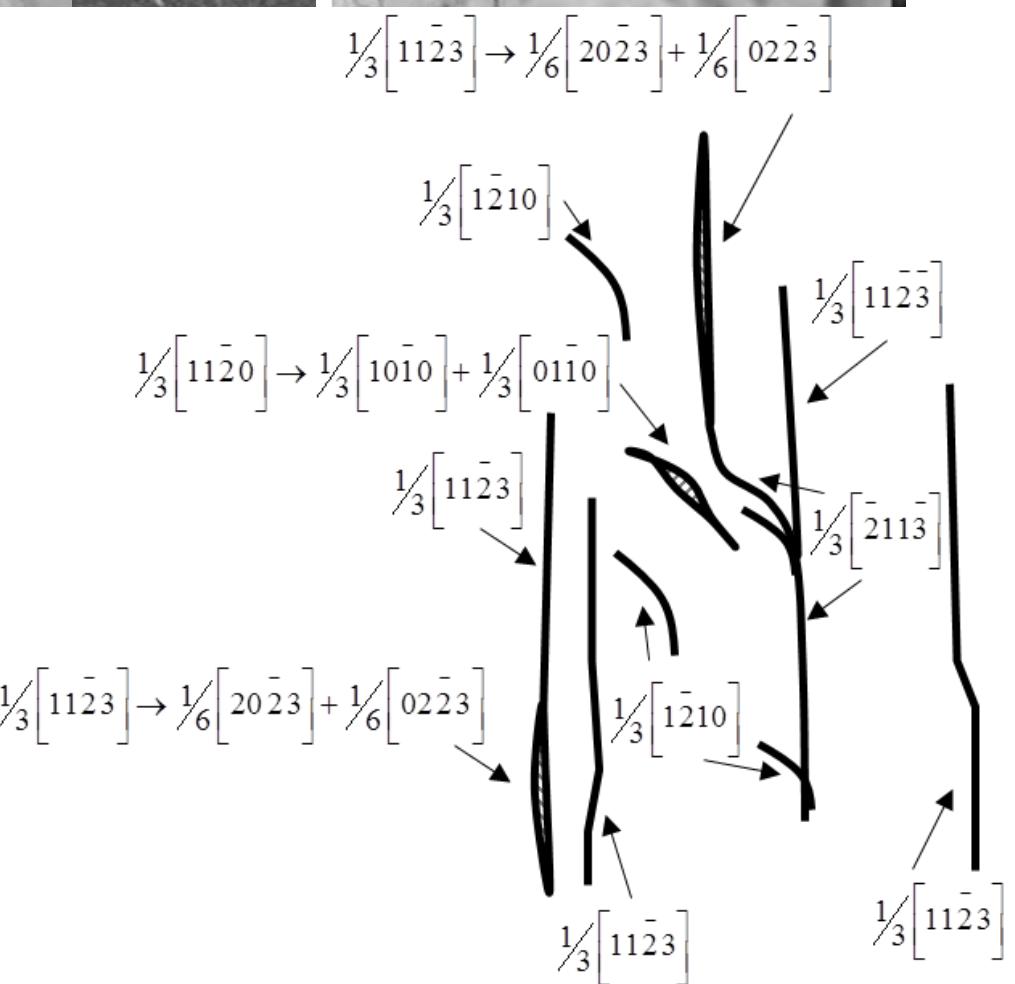
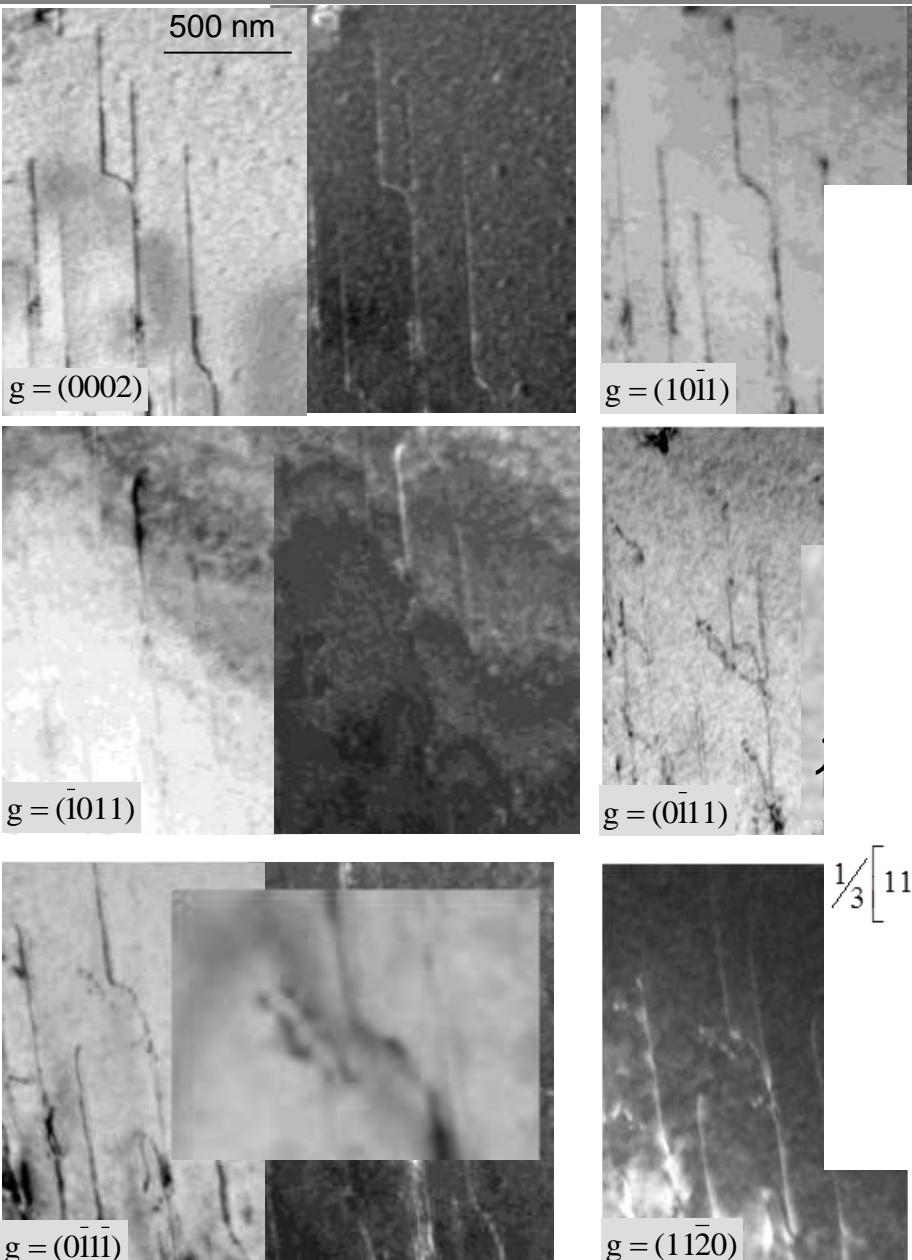
		Diffraction vector						
Burgers vector		0002	-1011	10-10	10-11	0-11-1	0-111	01-10
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perfect	$\frac{1}{3} [1-210]$	0,00	0,00	0,00	0,00	1,00	1,00	-1,00
perfect	$\frac{1}{3} [-2110]$	0,00	1,00	-1,00	-1,00	0,00	0,00	0,00
perfect	[0001]	2,00	1,00	0,00	1,00	-1,00	1,00	0,00
perfect	$\frac{1}{3} [11-23]$	2,00	0,00	1,00	2,00	-2,00	0,00	1,00
perfect	$\frac{1}{3} [1-213]$	2,00	1,00	0,00	1,00	0,00	2,00	-1,00
perfect	$\frac{1}{3} [-2113]$	2,00	2,00	-1,00	0,00	-1,00	1,00	0,00
perfect	$\frac{1}{3} [11-2-3]$	-2,00	-2,00	1,00	0,00	0,00	-2,00	1,00
perfect	$\frac{1}{3} [1-21-3]$	-2,00	-1,00	0,00	-1,00	2,00	0,00	-1,00
perfect	$\frac{1}{3} [-211-3]$	-2,00	0,00	-1,00	-2,00	1,00	-1,00	0,00
partial	$\frac{1}{3} [10-10]$	0,00	-0,67	0,67	0,67	-0,33	-0,33	0,33
partial	$\frac{1}{3} [1-100]$	0,00	-0,33	0,33	0,33	0,33	0,33	-0,33
partial	$\frac{1}{3} [01-10]$	0,00	-0,33	0,33	0,33	-0,67	-0,67	0,67
partial	$\frac{1}{2} [0001]$	1,00	0,50	0,00	0,50	-0,50	0,50	0,00
partial	$\frac{1}{6} [20-23]$	1,00	-0,17	0,67	1,17	-0,83	0,17	0,33
partial	$\frac{1}{6} [2-20-3]$	-1,00	-0,83	0,33	-0,17	0,83	-0,17	-0,33
partial	$\frac{1}{6} [02-2-3]$	-1,00	-0,83	0,33	-0,17	-0,17	-1,17	0,67
partial	$\frac{1}{6} [-2023]$	1,00	1,17	-0,67	-0,17	-0,17	0,83	-0,33
partial	$\frac{1}{6} [02-23]$	1,00	0,17	0,33	0,83	-1,17	-0,17	0,67
partial	$\frac{1}{6} [20-2-3]$	-1,00	-1,17	0,67	0,17	0,17	-0,83	0,33
partial	$\frac{1}{6} [11-21]$	0,33	-0,33	0,50	0,67	-0,67	-0,33	0,50
partial	$\frac{1}{6} [11-2-1]$	-0,33	-0,67	0,50	0,33	-0,33	-0,67	0,50

$g \cdot b = 0$  invisible

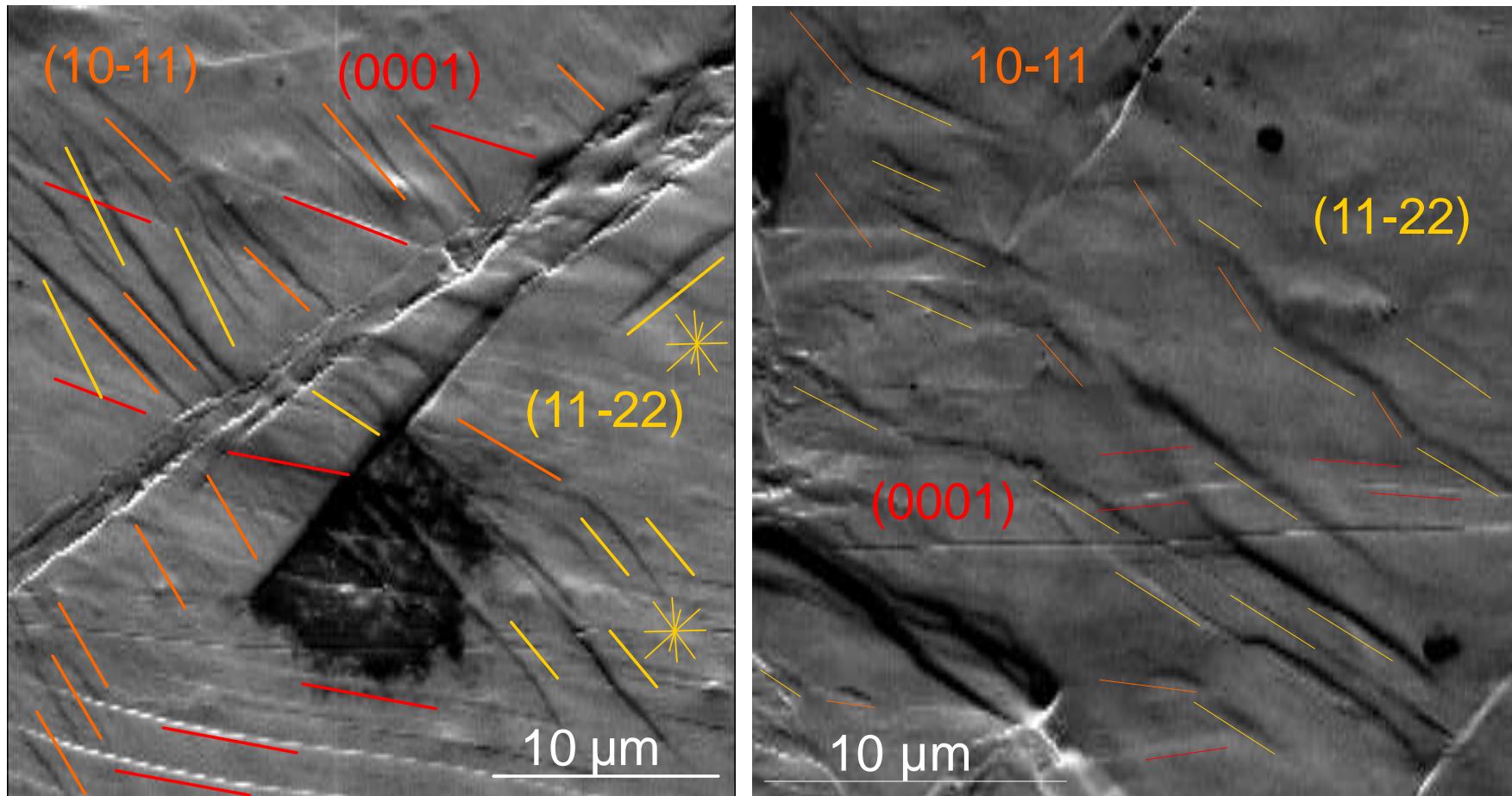
$g \cdot b \neq 0$  visible

$g \cdot b \leq 0.5$  weak contrast

# Characterization of plasticity carriers in hexagonal metals



# Characterization of plasticity carriers in hexagonal metals



- TEM: only GNDs and “debris” of active dislocations
- Confirmation of slip system activity (slip band analysis, texture) necessary

# Quiz

- Which method can be used to characterize dislocations?
- Do you remember how dislocations are characterized?

# Interest? - Important literature



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Thank you for your  
kind attention!