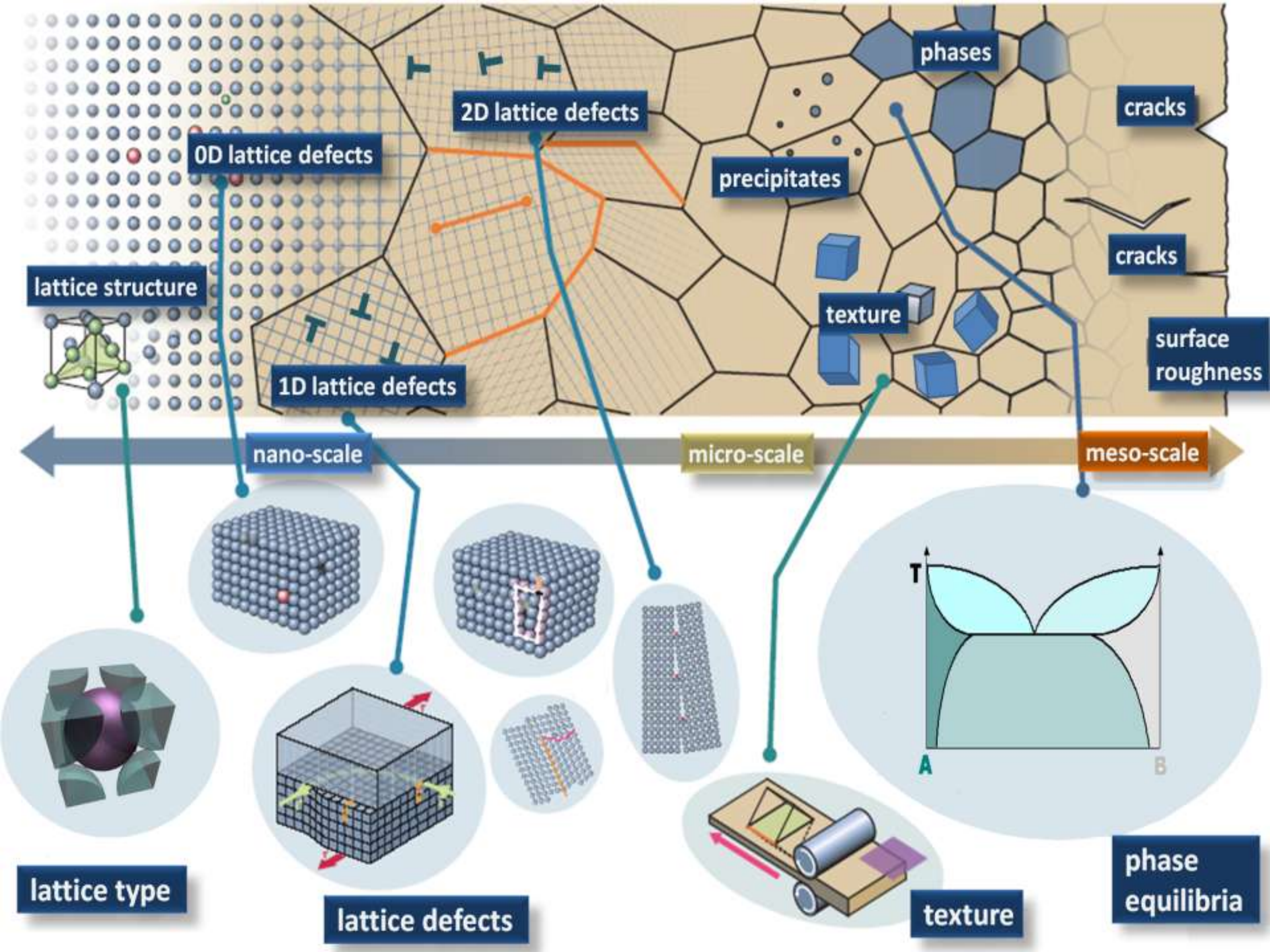
The crystalline structure of metals: why does it matter for crystal plasticity?

Professor Dierk Raabe

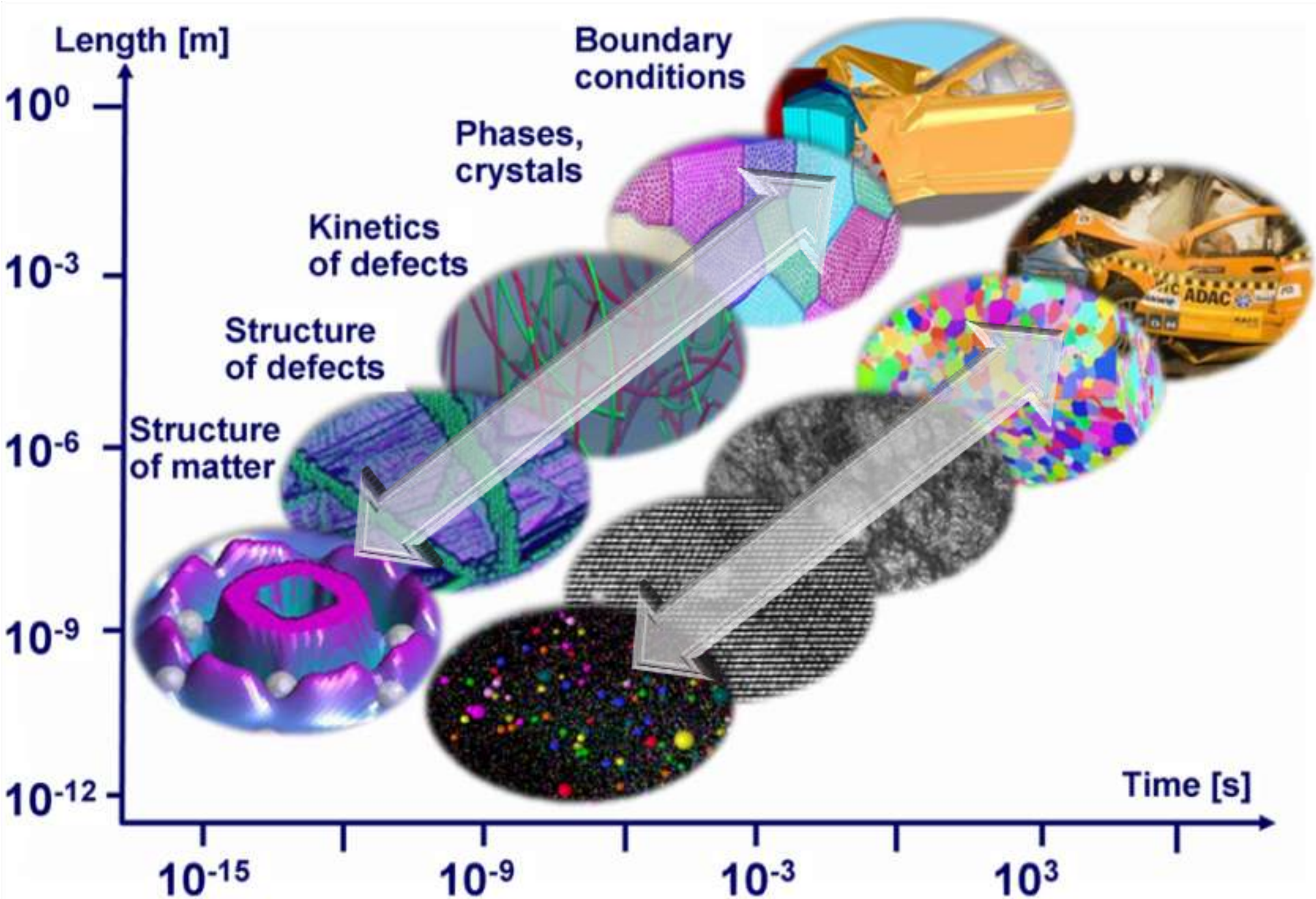
Max-Planck-Institut für Eisenforschung GmbH
Düsseldorf, Germany
WWW.MPIE.DE
d.raabe@mpie.de

Class 2013

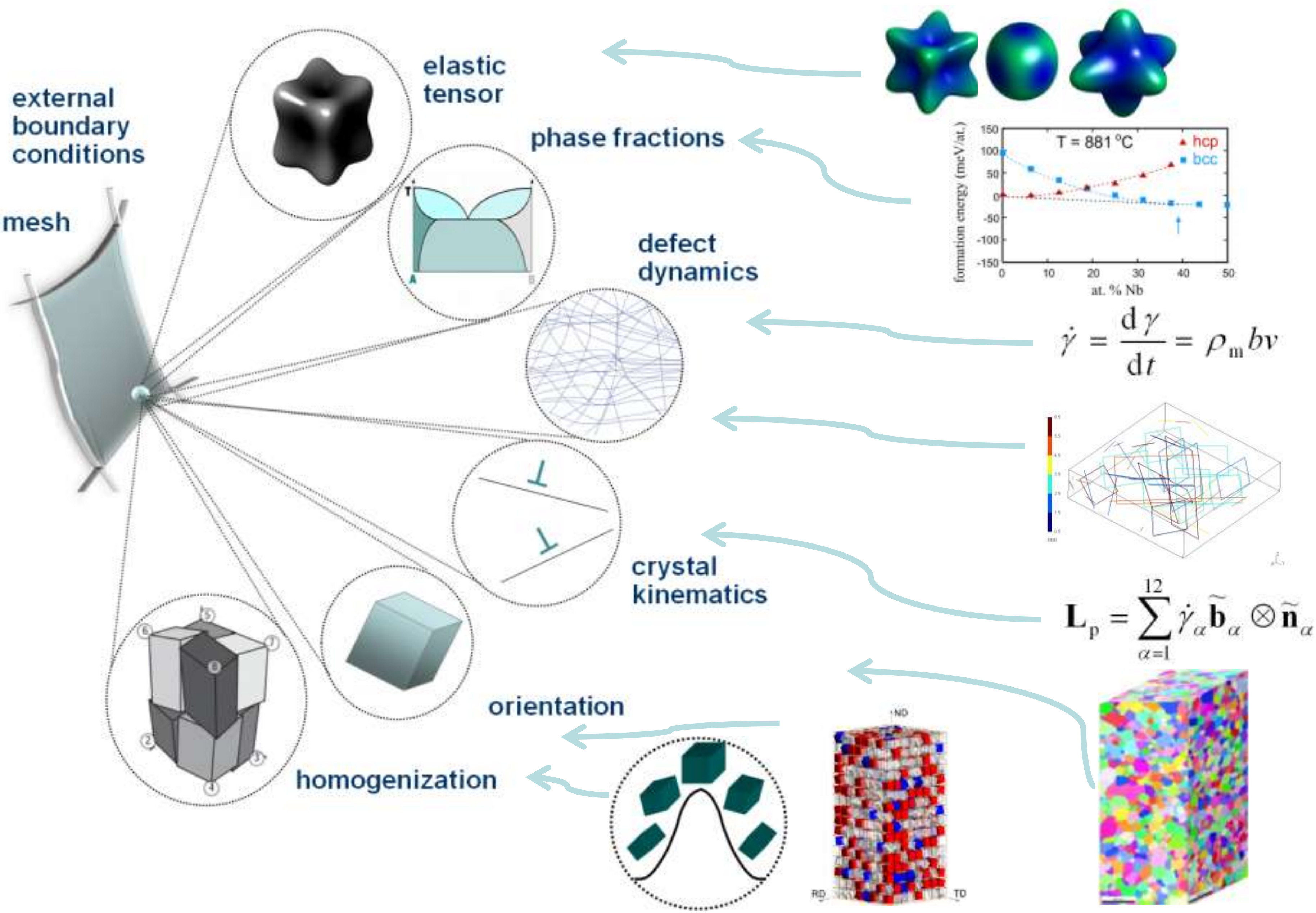


phases
cracks
2D lattice defects
0D lattice defects
precipitates
cracks
lattice structure
texture
surface roughness
1D lattice defects
nano-scale
micro-scale
meso-scale
T
A
B
lattice type
lattice defects
texture
phase equilibria

Multiscale Modeling and Experimentation

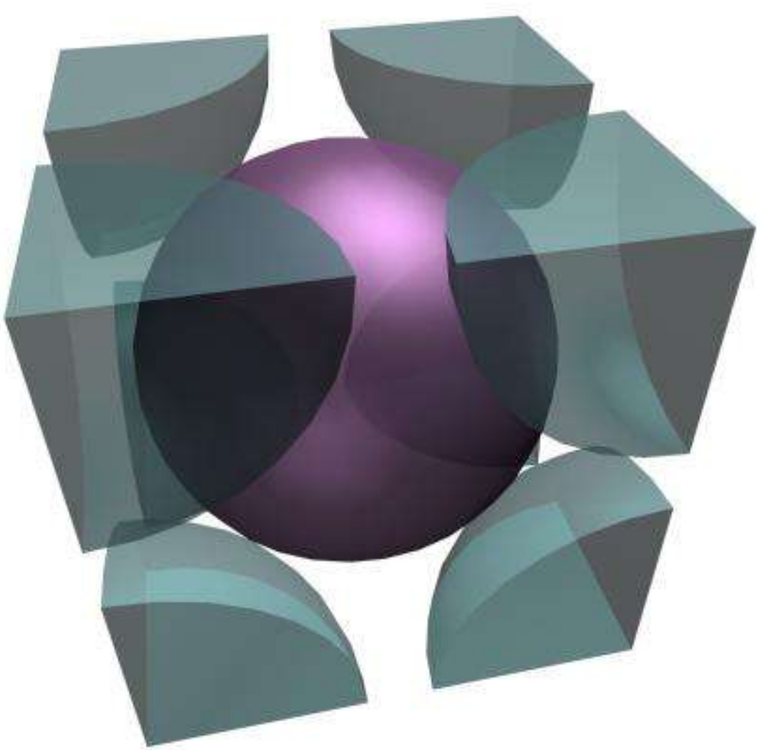


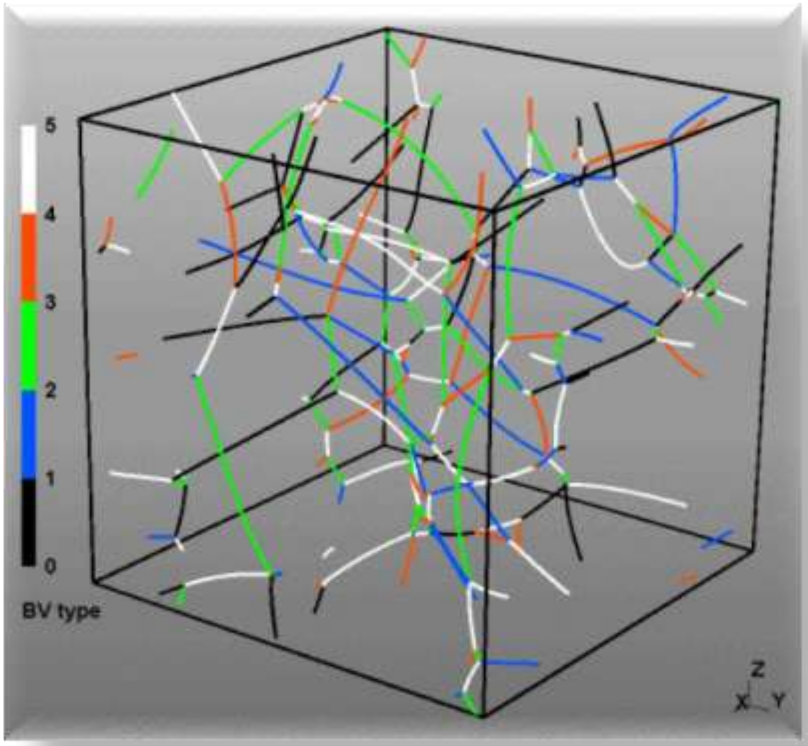
Multiscale crystal plasticity FEM



Crystal dislocations: Relationship between lattice and defects

Why is the crystal lattice relevant for understanding complex dislocation structures?





Body centered cubic (bcc) lattice structure

Why is the crystal lattice relevant for understanding complex dislocation structures?

Densely packed planes: glide planes; densely packed translation shear vectors: Burgers vectors

Twinning systems

Stacking fault energy: cross slip, recovery, annihilation, Suzuki effect, twinning, strain hardening, stair rod dislocations, reactions

Shockley partial dislocations (*b* = a/6<112>)

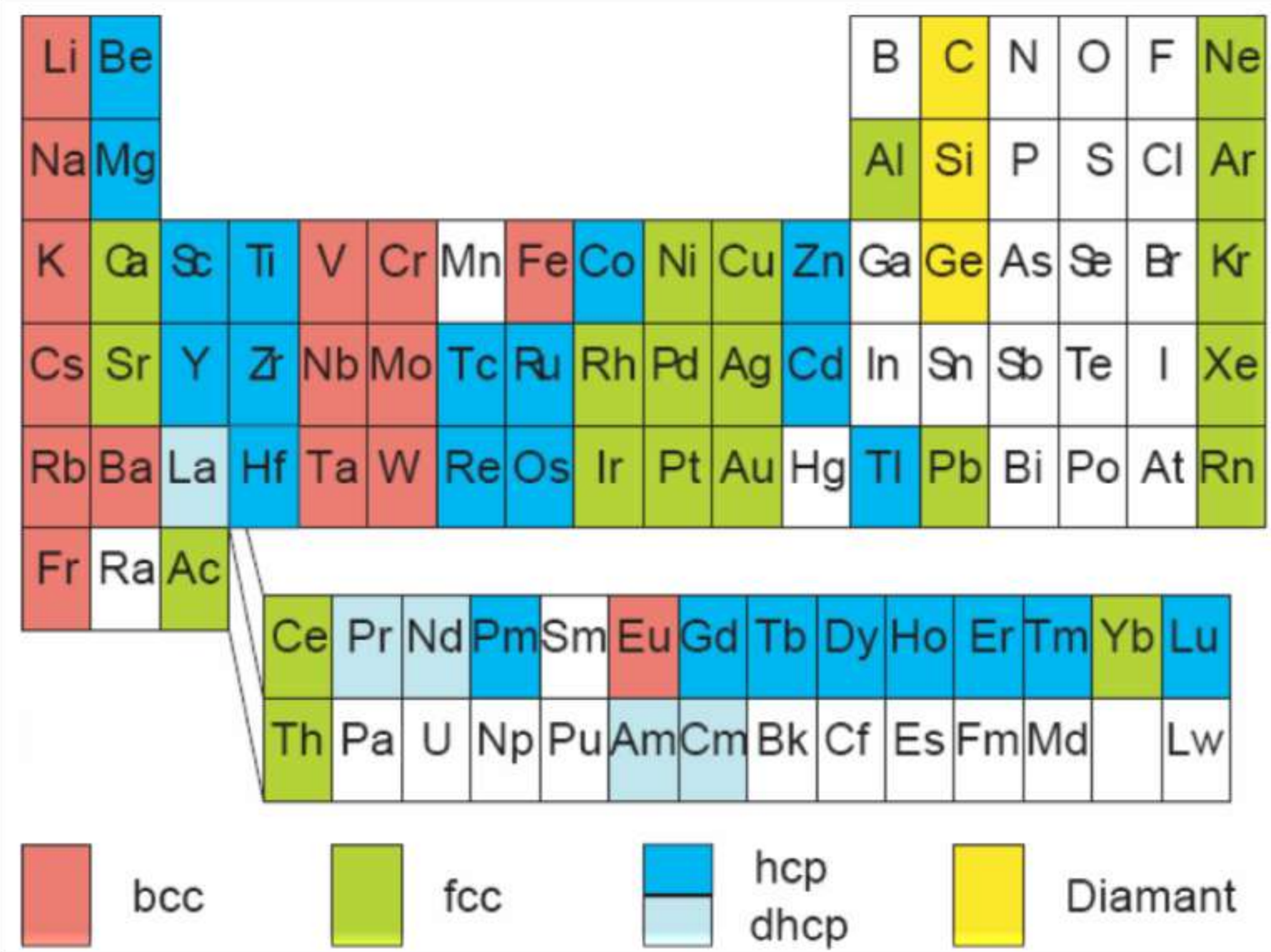
Special properties of the 3 main lattice types regarding plasticity defects

FCC: stacking fault energy can vary from very low values (α-Brass- 0 wt% Zn in Cu; TWIP steels: ≈ 20 m J / m2) to very high values (Al : ≈ 180 m J / m2): Regarding lattice defects in plasticity FCC is not a 'homogeneous' structure

Hex: hcp or hex?; c/a ratio determines slip systems and twinning: some hex metals are very brittle (Mg) and some are very ductile (Ti)

BCC: non-close packed planes: pencile glide behavior; multiple slip systems: {110}; {112}; {123}; complex core of dislocation; twinnign vs. anti-twinning glide sense

How frequently do certain crystal structures occur in the PSE?



Lattice parameters

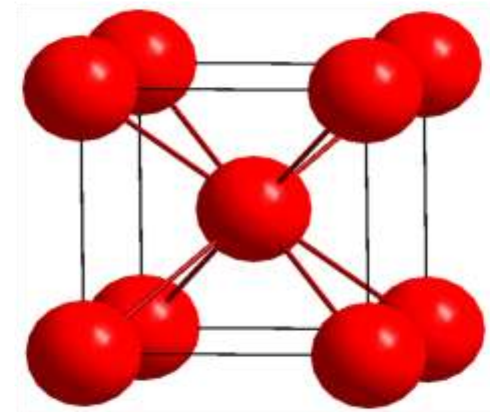
FCC: Face centered cubic close packed, (a)	Hexagonal close packed (a, c)	BCC: Body centered cubic (a)
Cu (3.6147)	Be (2.2856, 3.5832)	Fe (2.8664)
Ag (4.0857)	Mg (3.2094, 5.2105)	Cr (2.8846)
Au (4.0783)	Zn (2.6649, 4.9468)	Mo (3.1469)
Al (4.0495)	Cd (2.9788, 5.6167)	W (3.1650)
Ni (3.5240)	Ti (2.506, 4.6788)	Ta (3.3026)
Pd (3.8907)	Zr (3.312, 5.1477)	Ba (5.019)
Pt (3.9239)	Ru (2.7058, 4.2816)	
Pb (4.9502)	Os (2.7353, 4.3191)	
	Re (2.760, 4.458)	

Crystal structure: BCC

atoms per cell $= (8 \times 1/8) + 1 = 2$

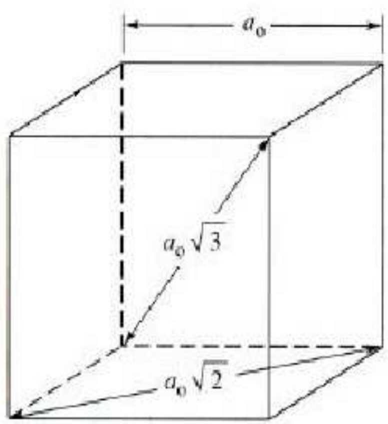
coordination number $= 4 + 4 = 8$

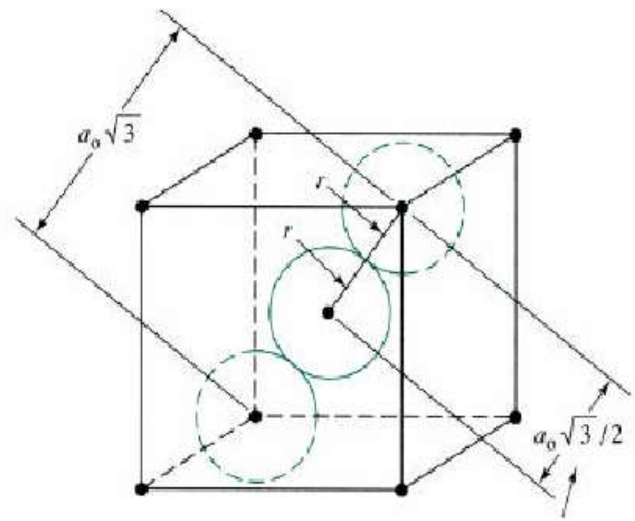
atomic packaging $= 0.68$



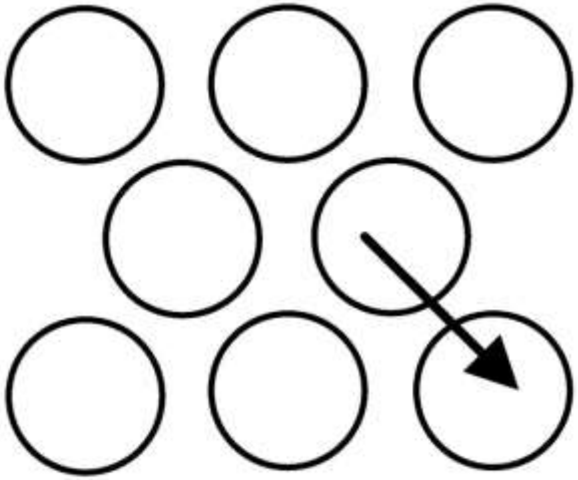
$$4r = \sqrt{3}a$$

$$\boxed{a = \frac{4}{\sqrt{3}} r}$$

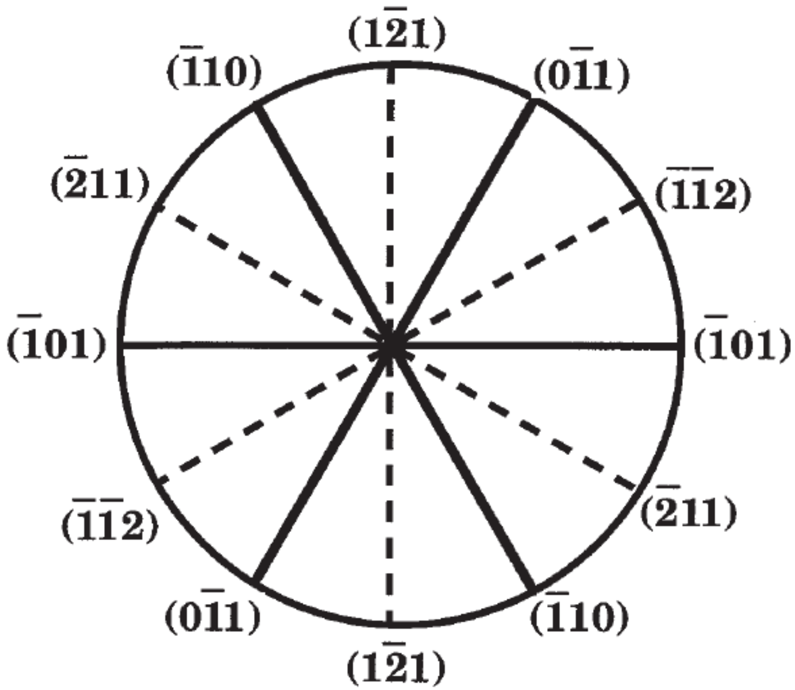




Glide plane: BCC

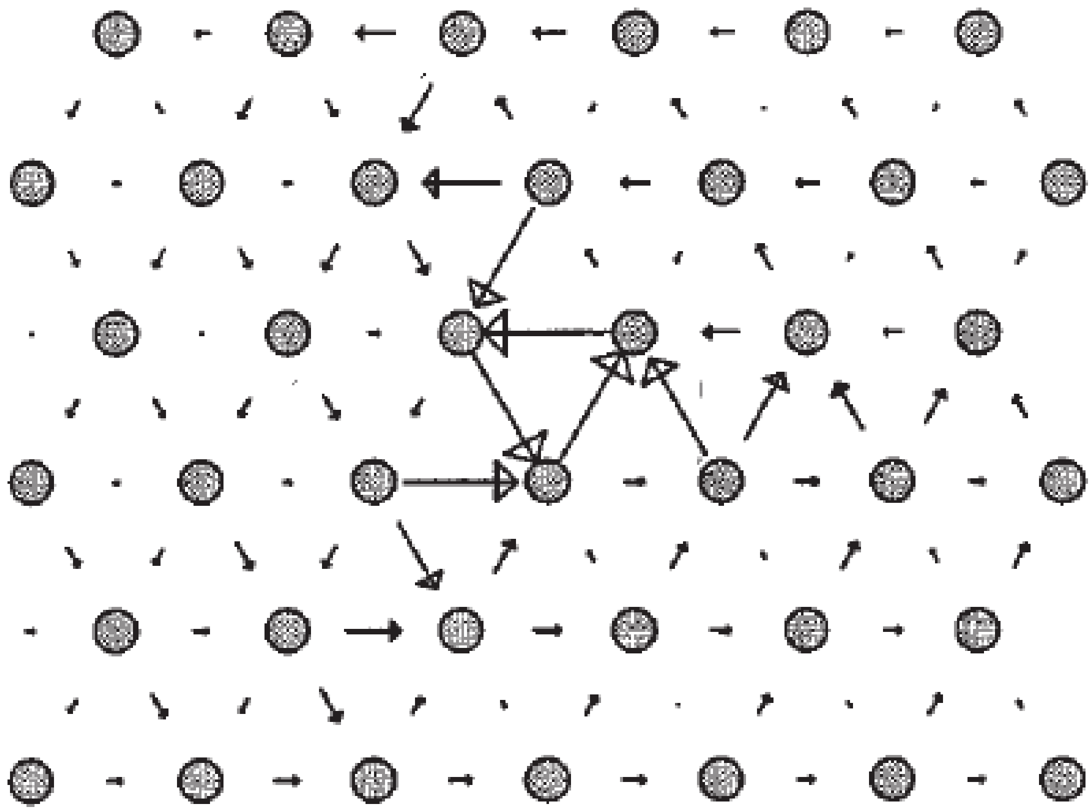


Glide plane: BCC



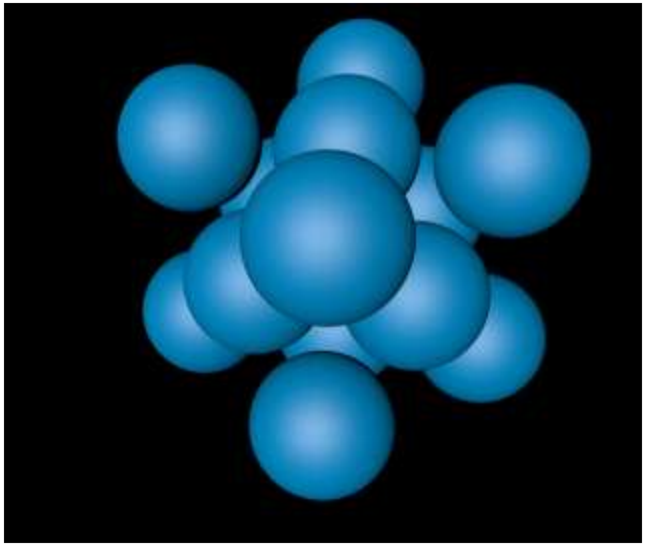
[111] stereographic projection showing orientations of all {110} and {112} planes belonging to the [111] zone.

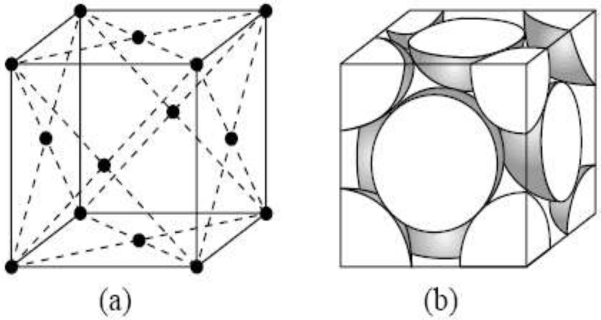
Glide plane: dislocation core structure in BCC

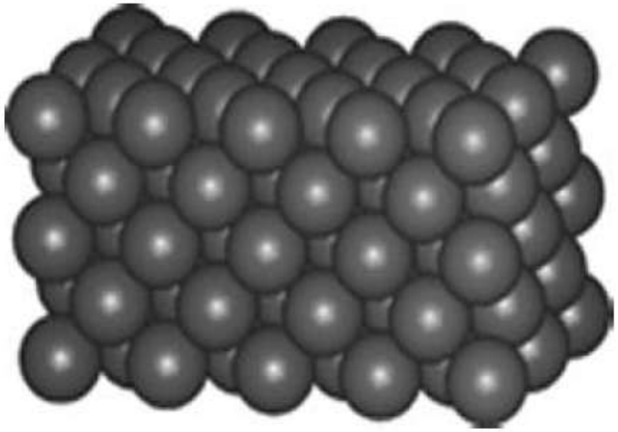


courtesy of V. Vitek

Fe (γ), Al, Cu, Au

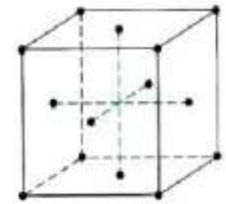


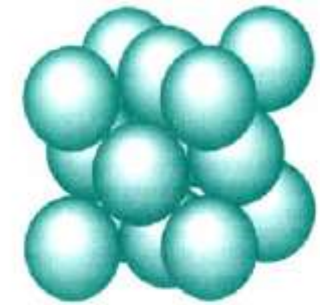




Crystal structure: FCC

atoms per cell = (8 x 1/8) + (6 x ½) = 4



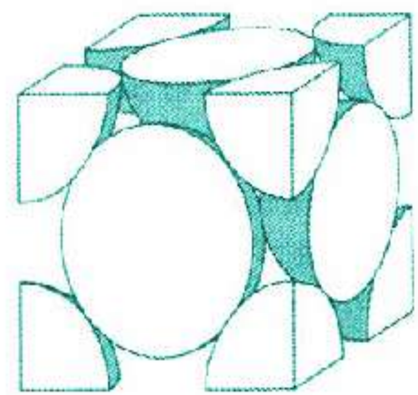


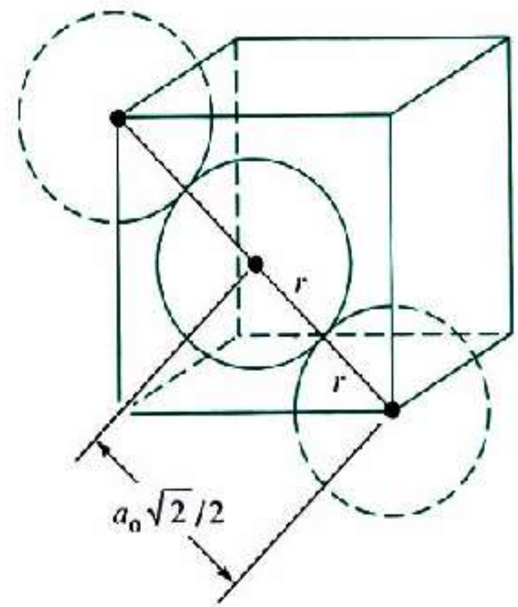
coordination number = 4 + 4 + 4 = 12

atomic packaging = 0.74

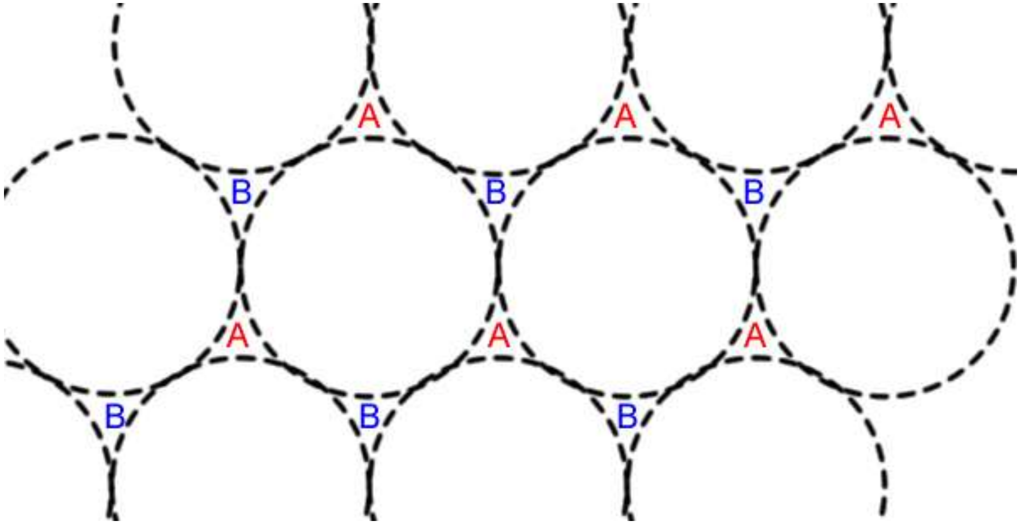
$$4r = \sqrt{2}a$$

$$\boxed{a = 2\sqrt{2}r}$$

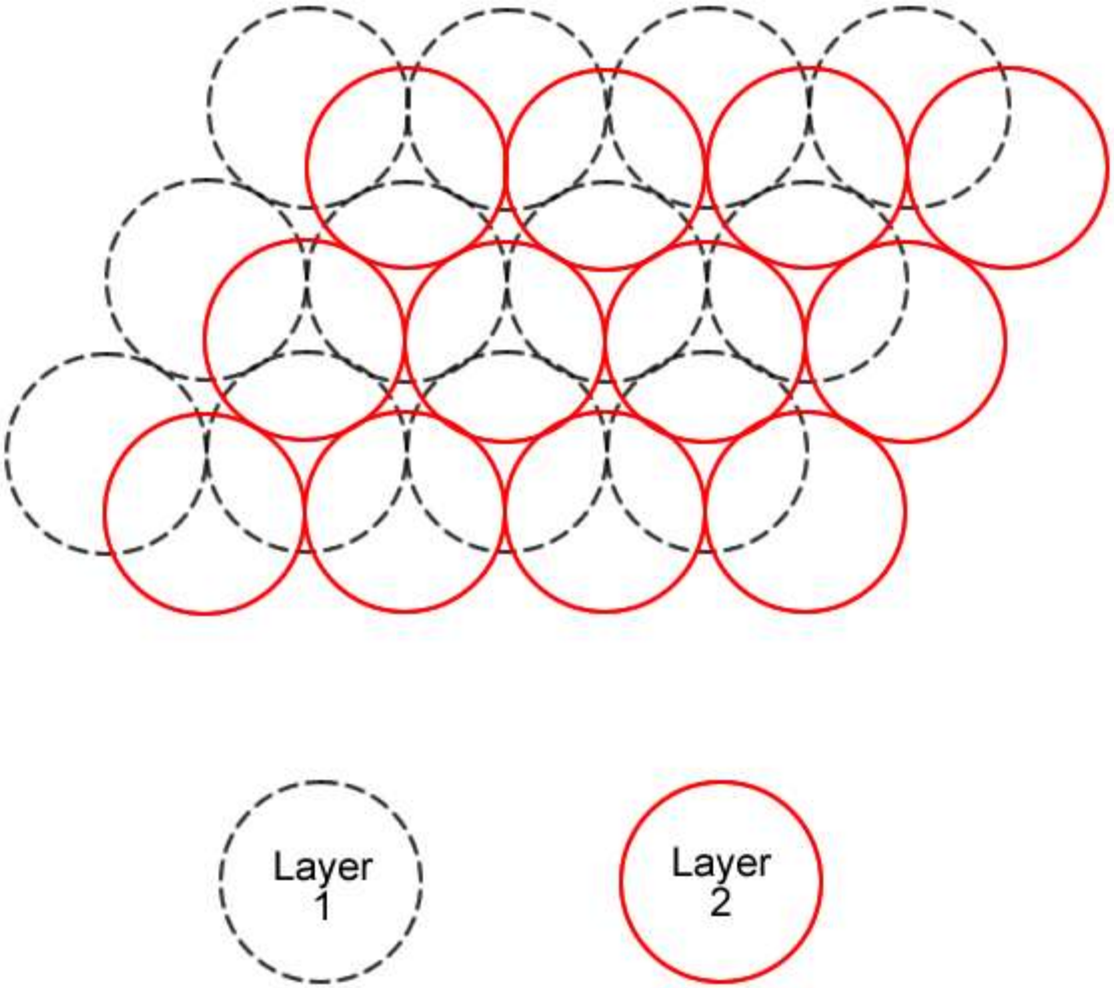




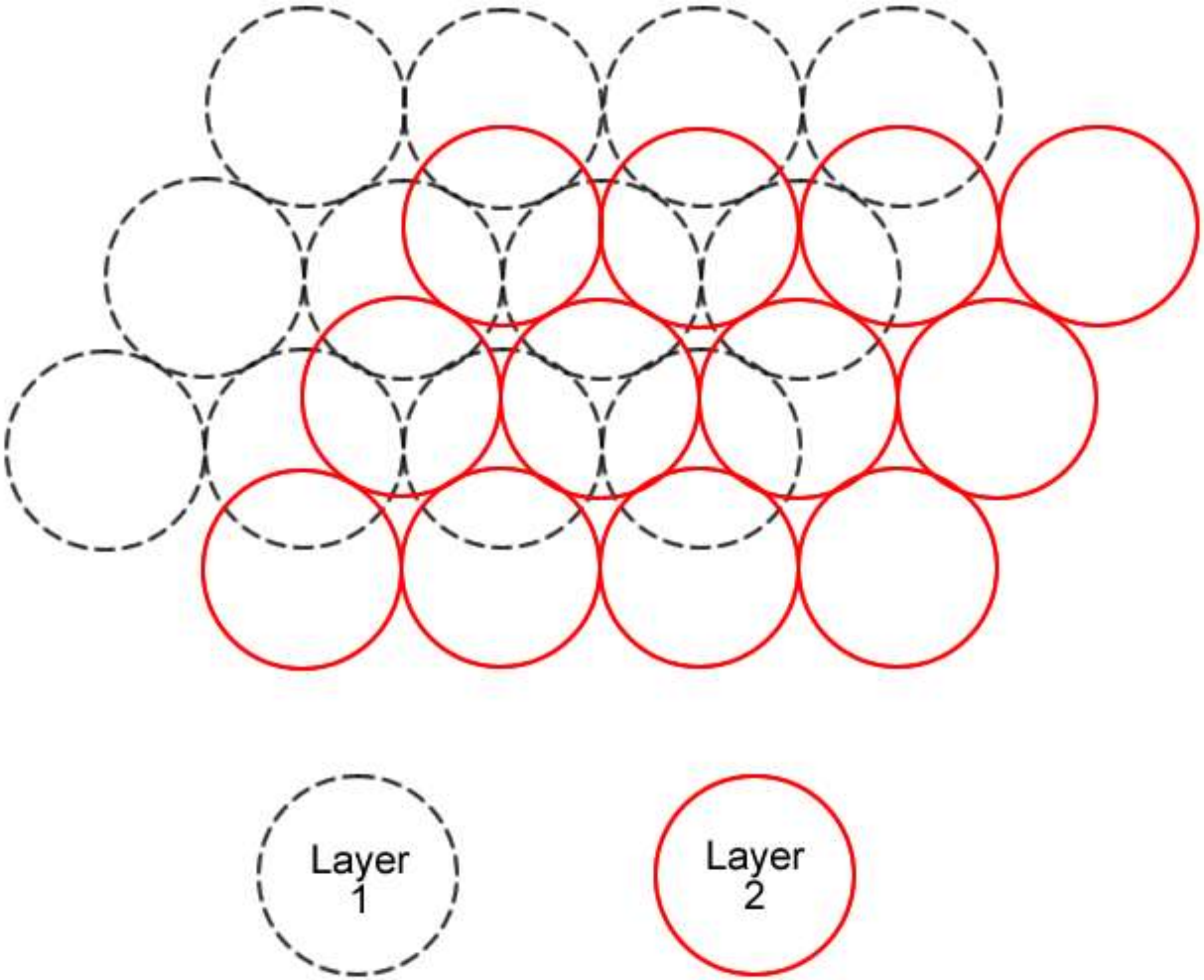
FCC – stacking sequence of dense (111) planes



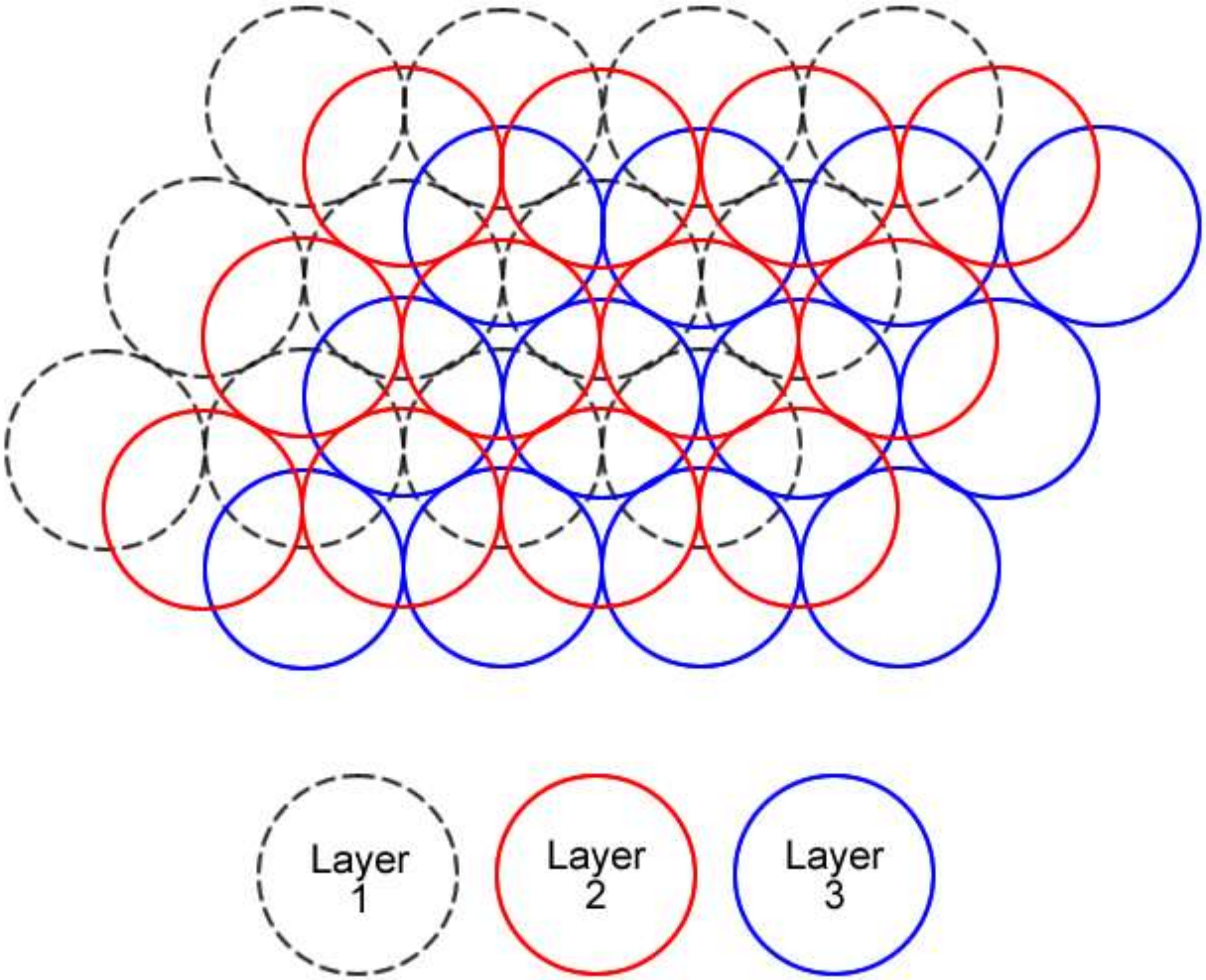
FCC – stacking sequence of dense (111) planes



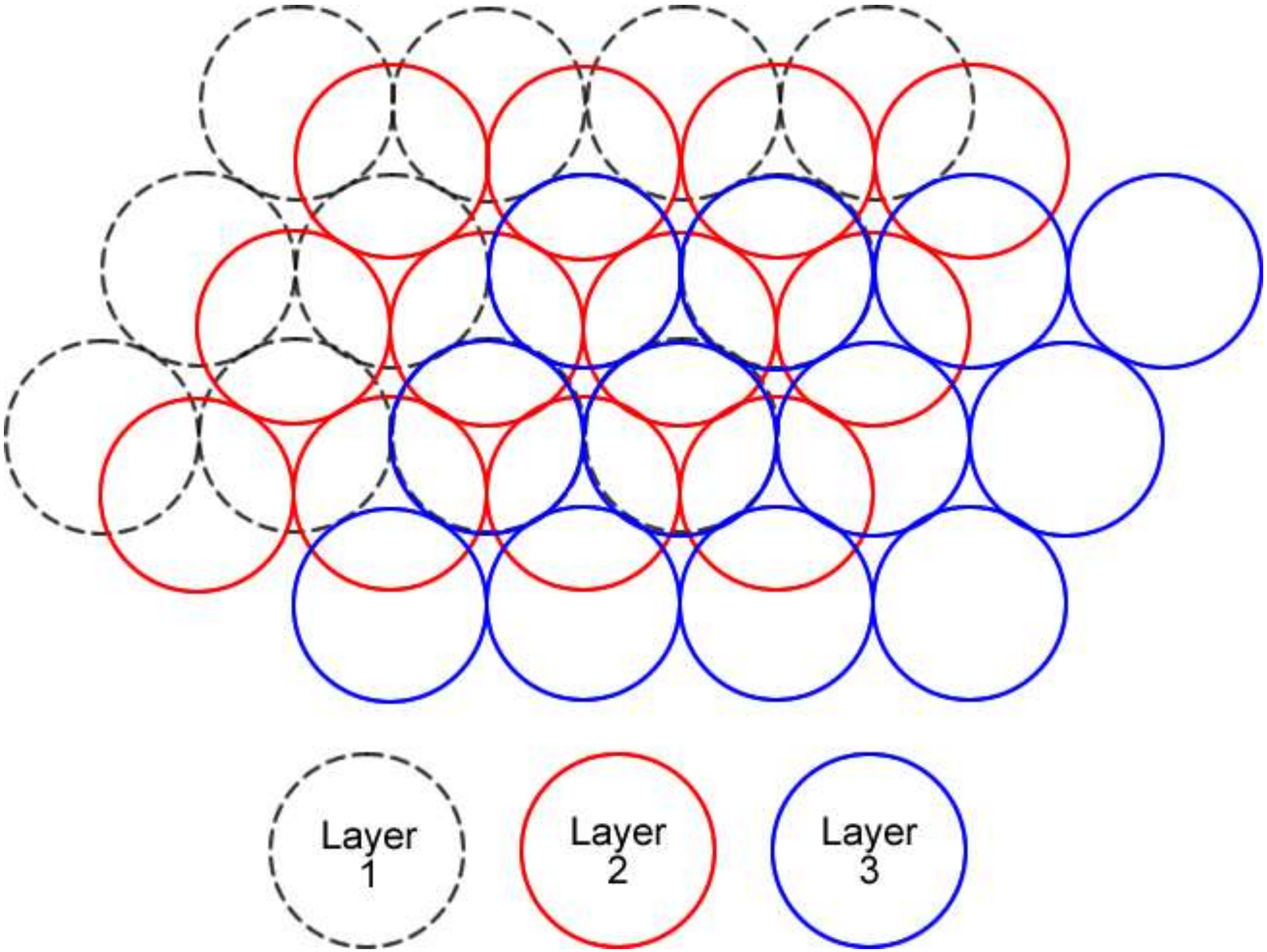
FCC – stacking sequence of dense (111) planes



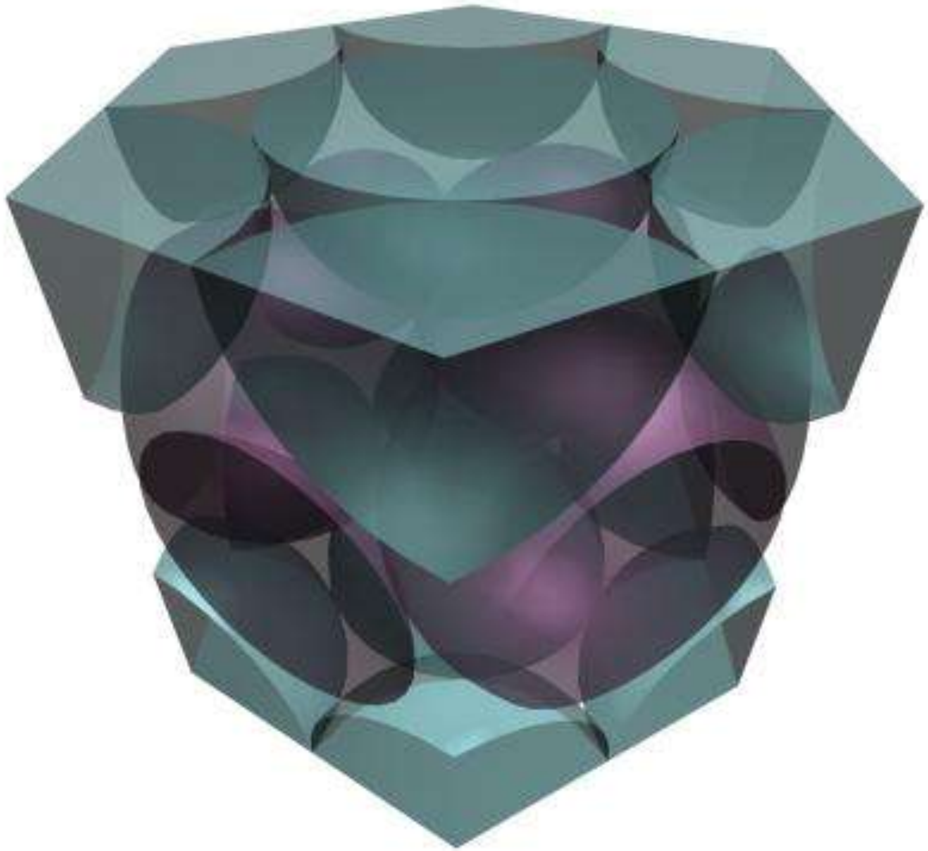
FCC – stacking sequence of dense (111) planes



FCC – stacking sequence of dense (111) planes

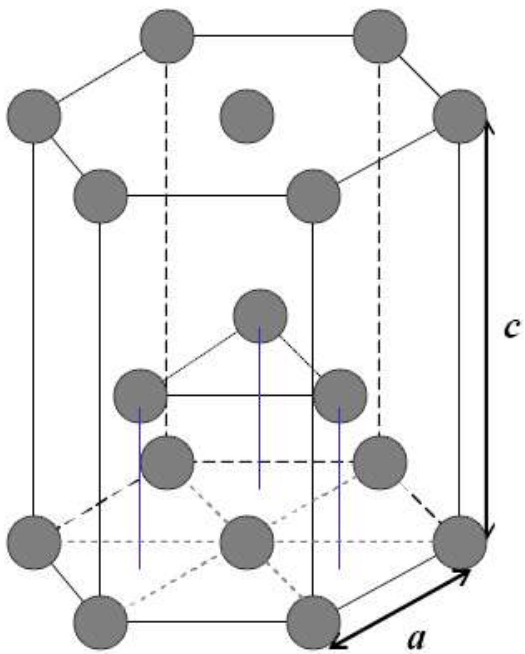


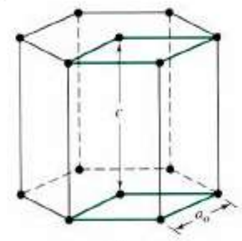
Crystal structure: Hexagonal

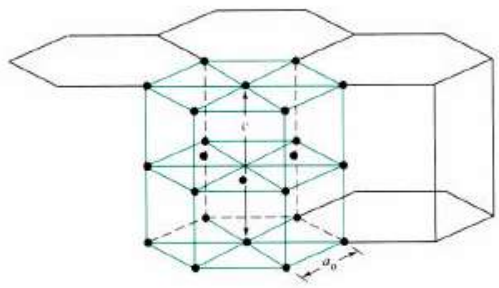


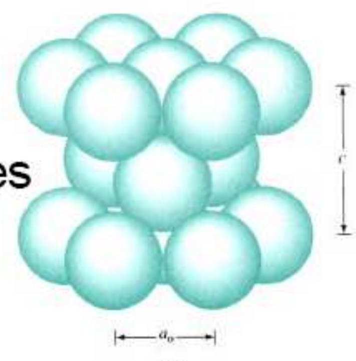
3. HCP: hexagonal close-packed

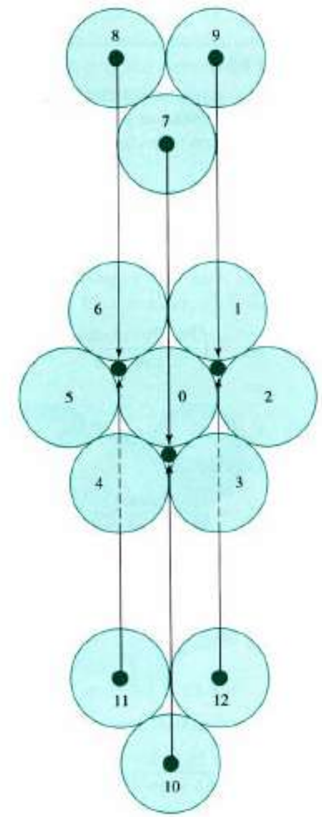
(Mg, Be, Co, Ti, Zn)




(a)


(b)



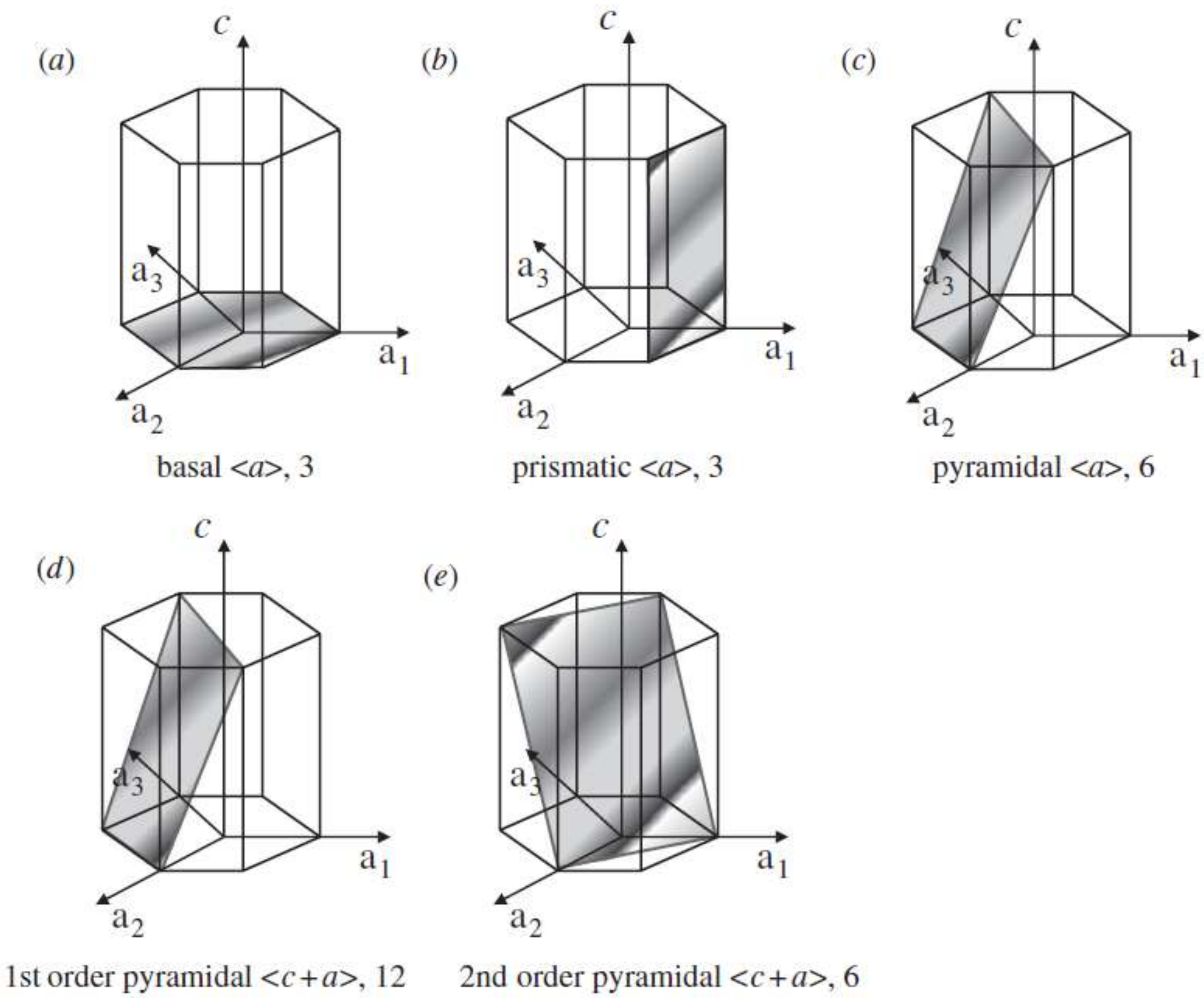


(d)

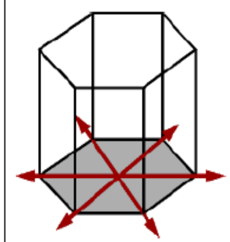
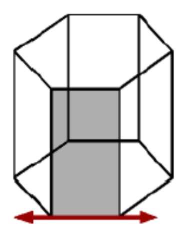
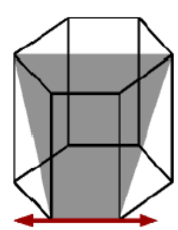
noncubic symmetry: ***a*** and ***c*** axes

c/a ~ 1.633

Crystal structure: Hexagonal

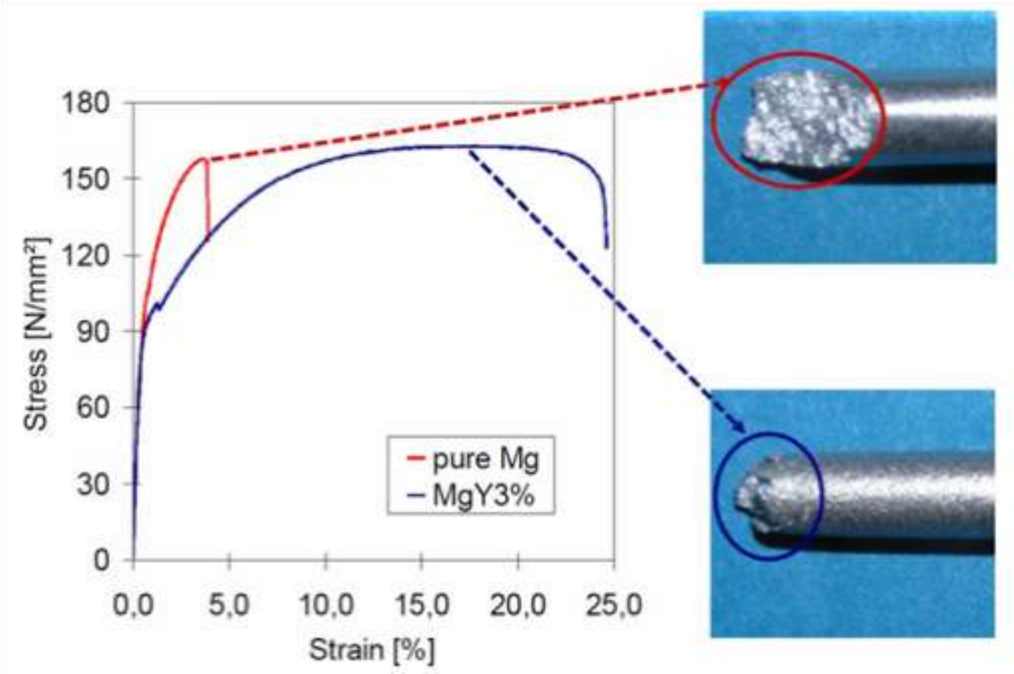


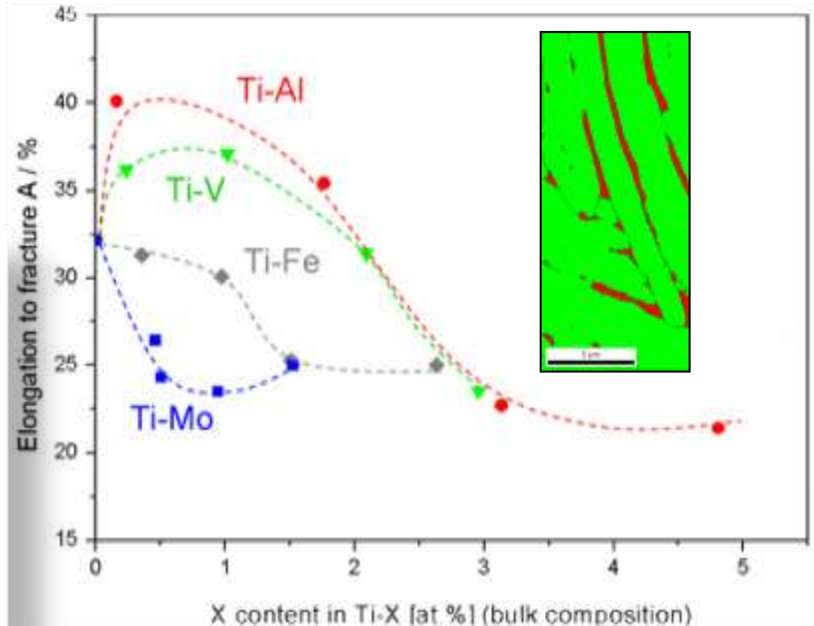
vectors and planes for hexagonal materials

Gitter	Beispiel		Gleitebenen G Typ	Gleitebenen G Zahl	Gleitrichtung g Typ	Gleitrichtung g Zahl	Gesamtzahl der Gleitsysteme
hex	Cd Zn Mg Ti_{α} Be		(0001)	1	[1120]	3	3
	Cd Zn Mg Ti_{α} Be Zr_{α}		(1010)	3	[1120]	1	3
	Mg Ti_{α}		(1011)	6	[1120]	1	6

hexagonal alloy systems: crystal structure and plasticity: examples

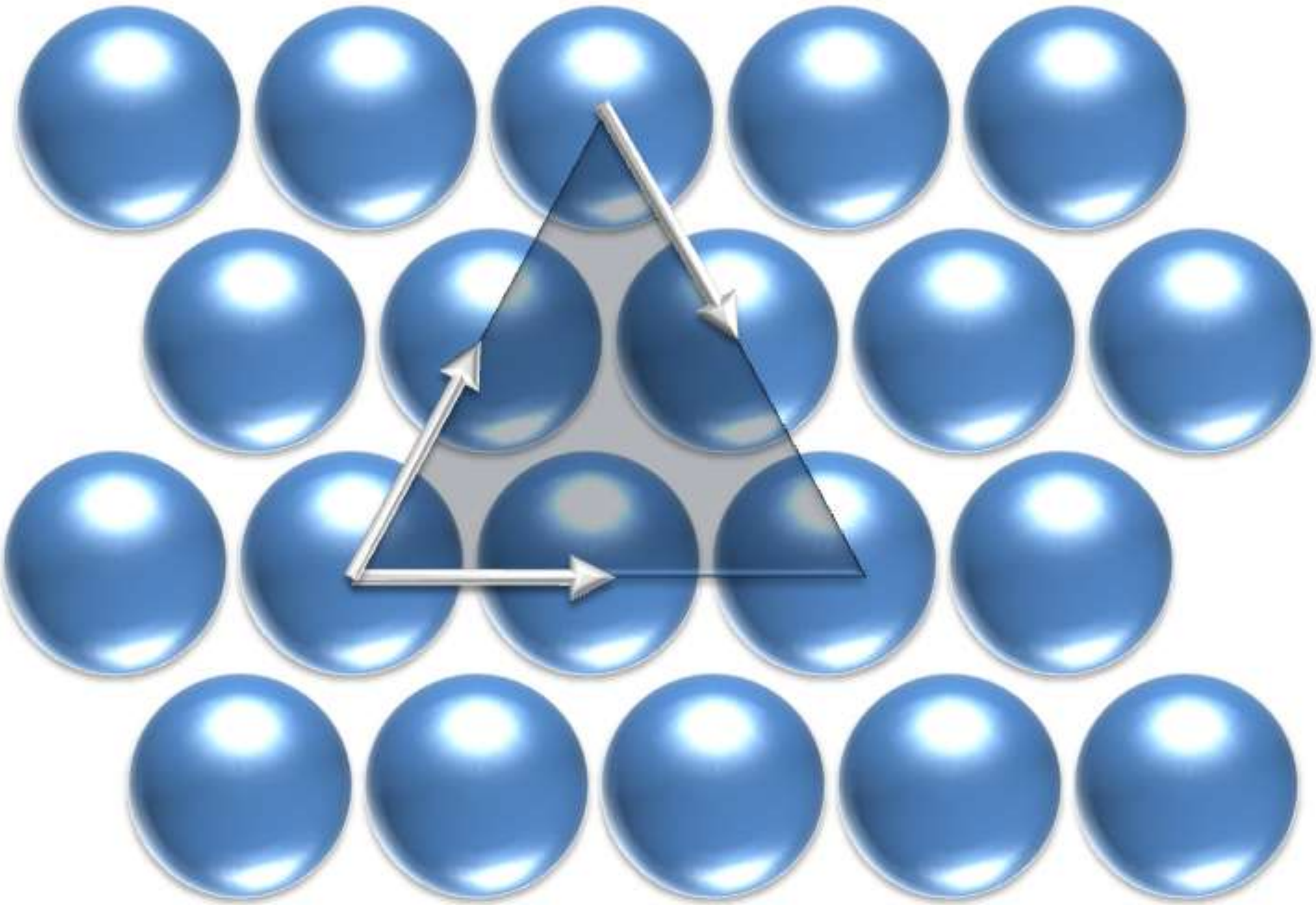
Mg - RE

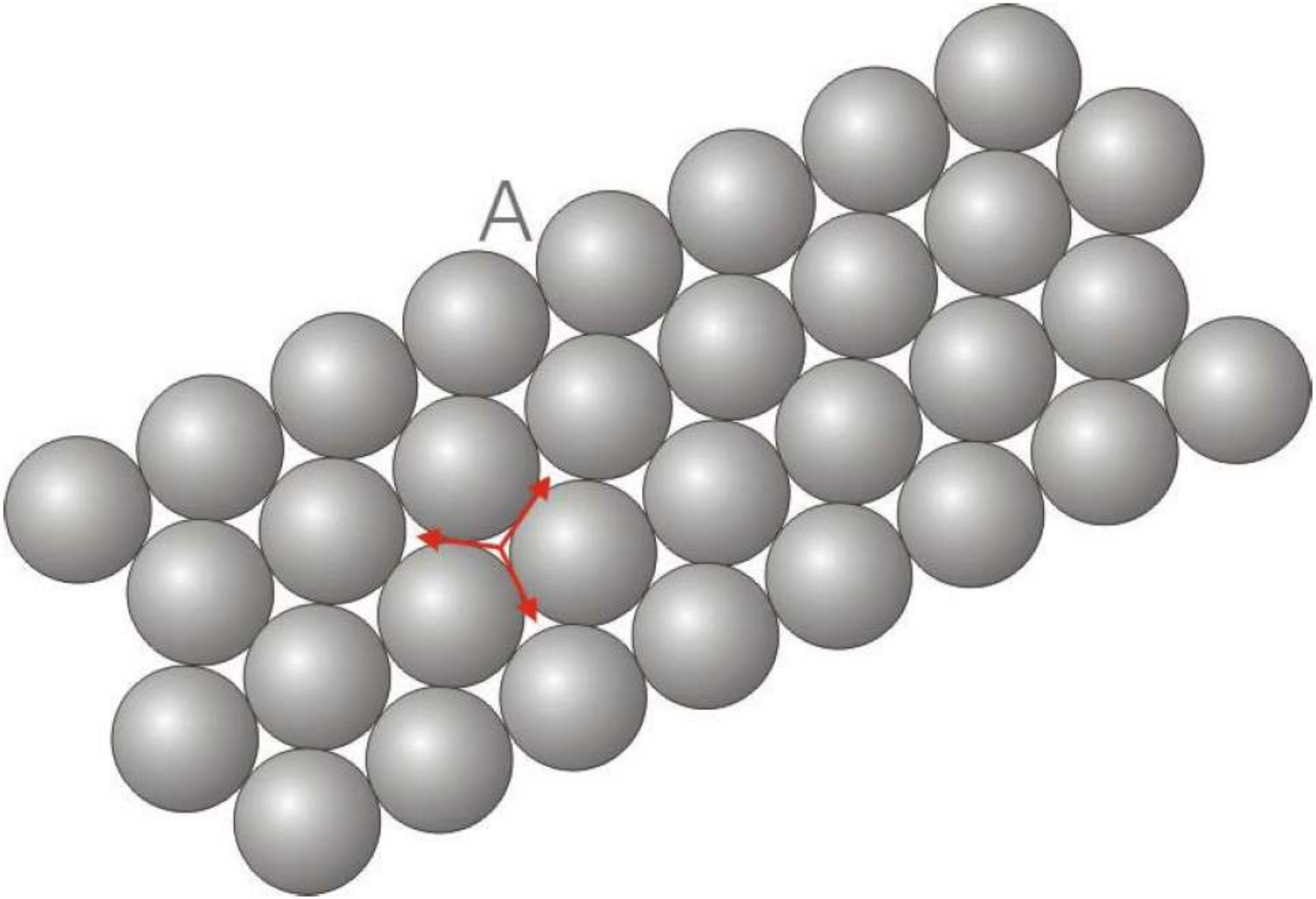




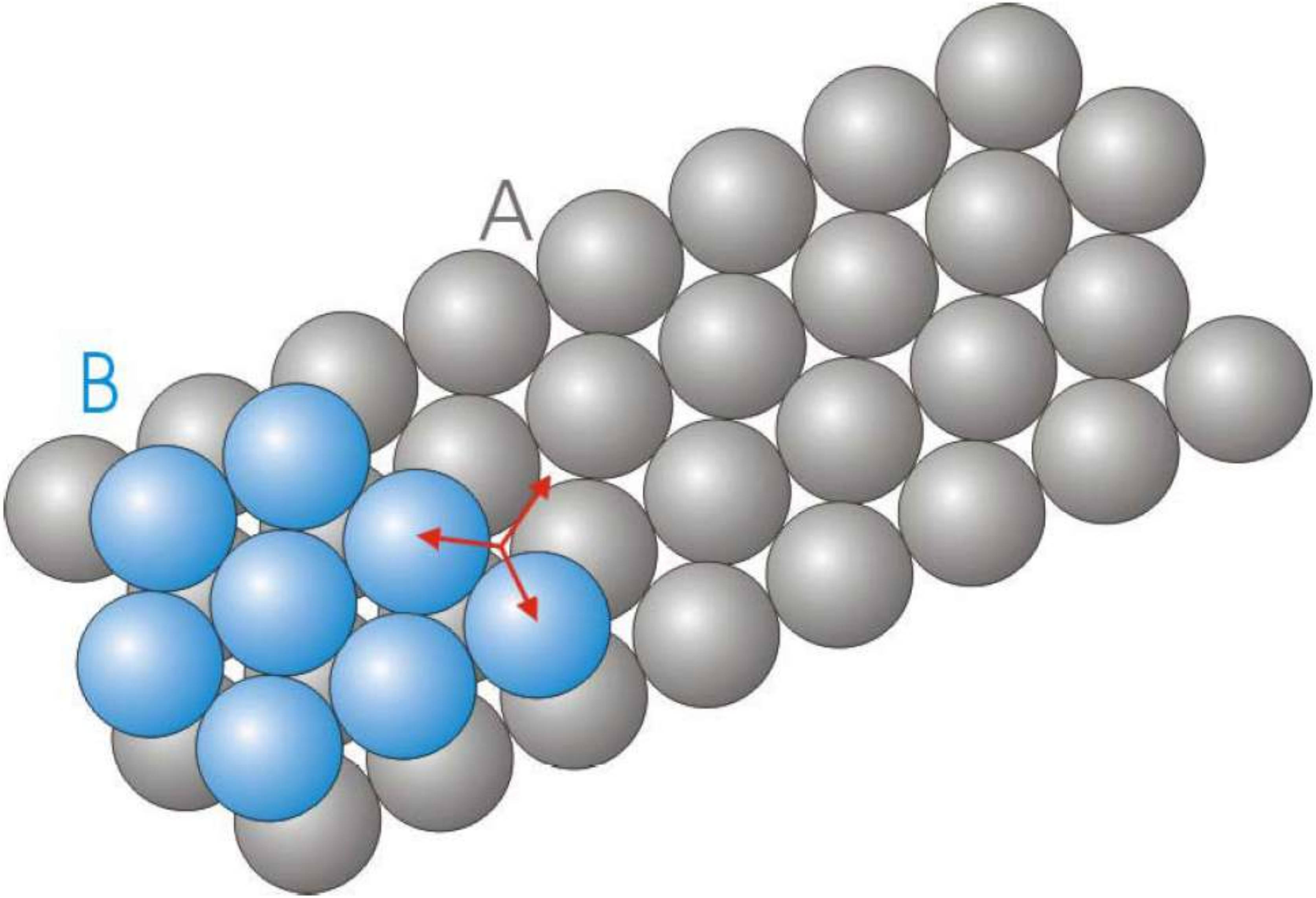
Mg - Li

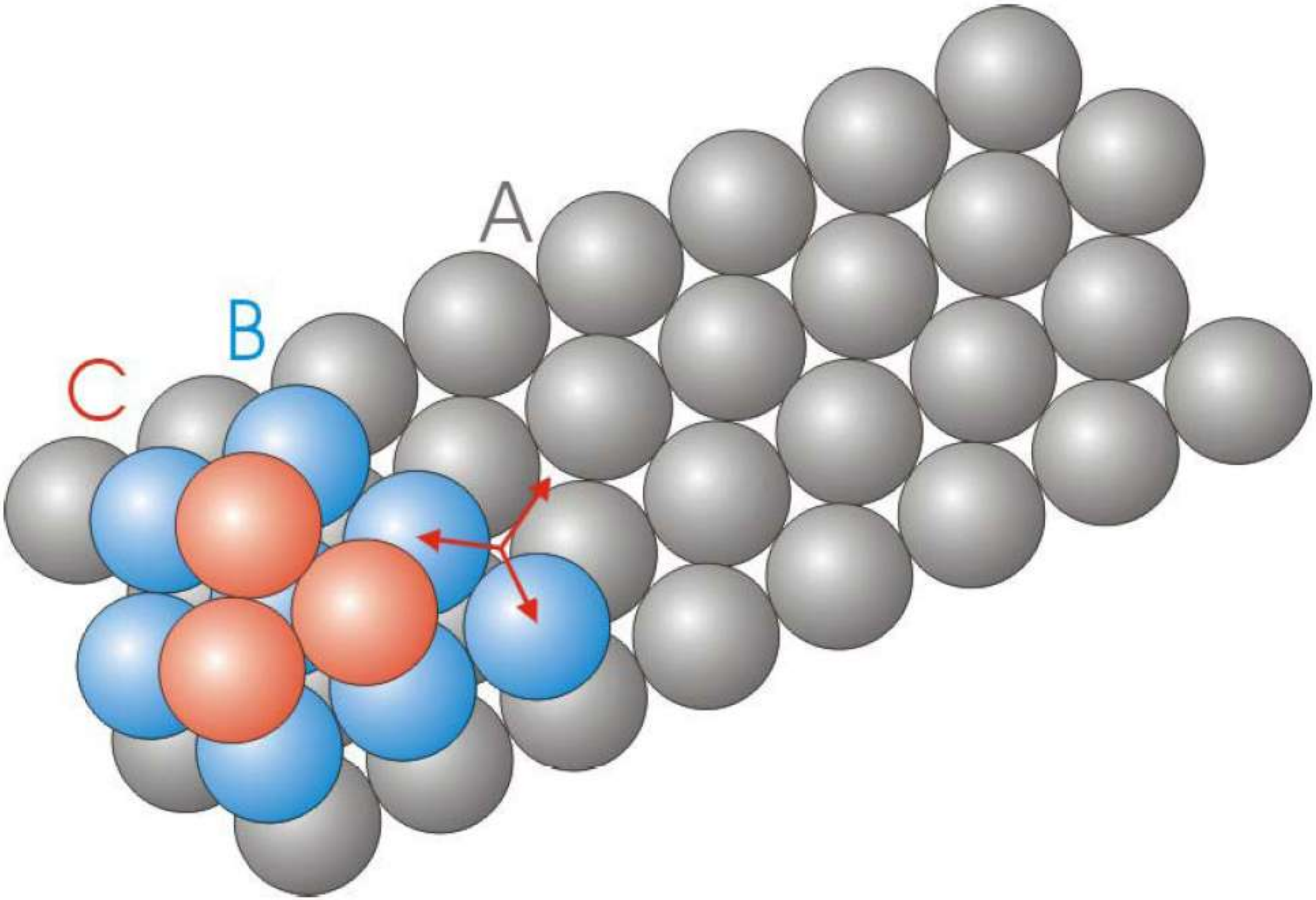
Crystal structure: Hexagonal / FCC



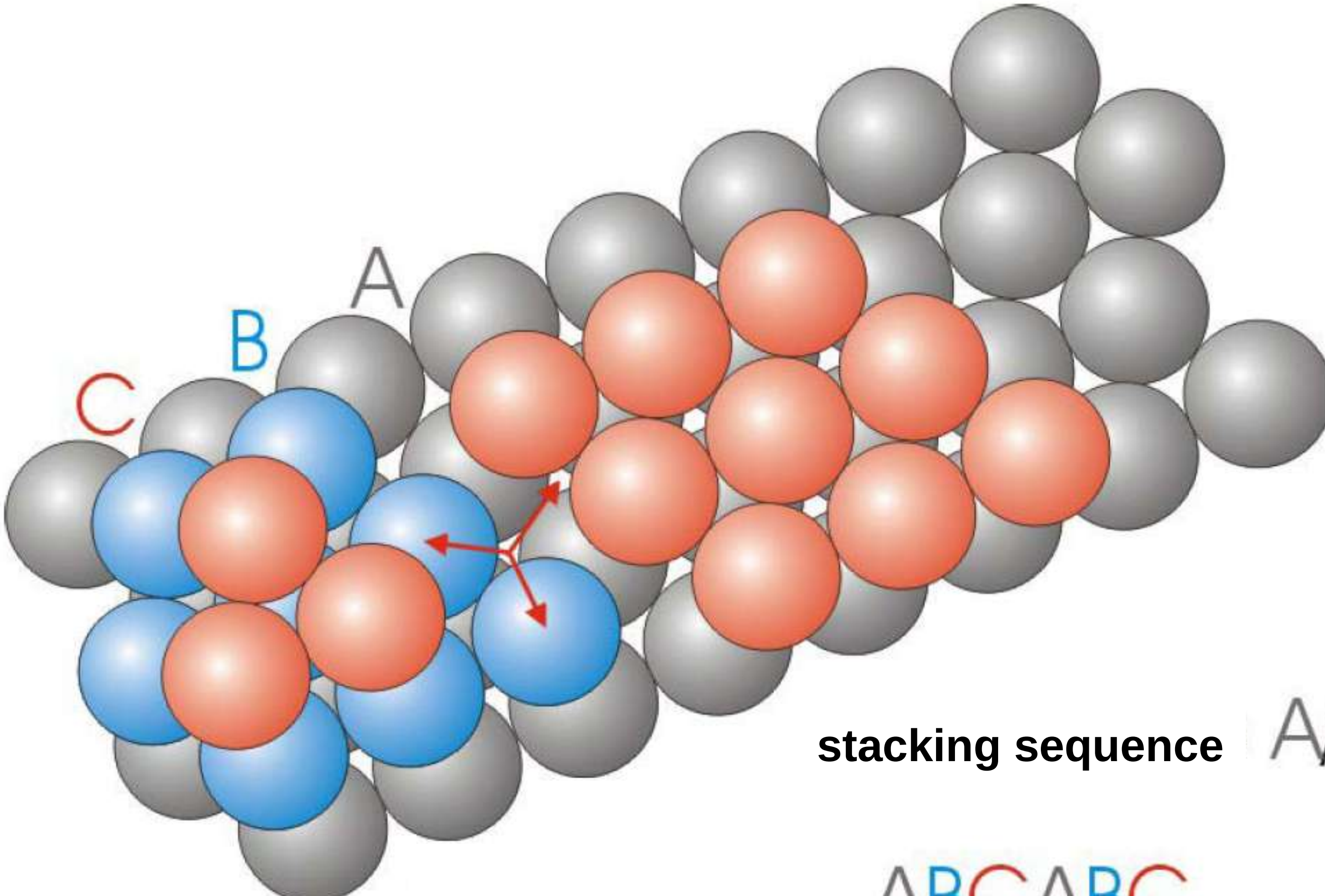

A

Crystal structure: Hexagonal / FCC



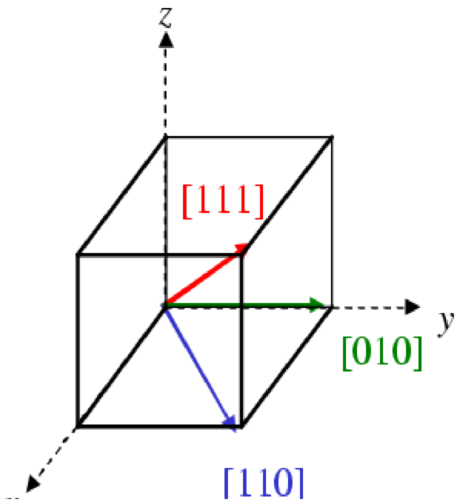

A
B
C

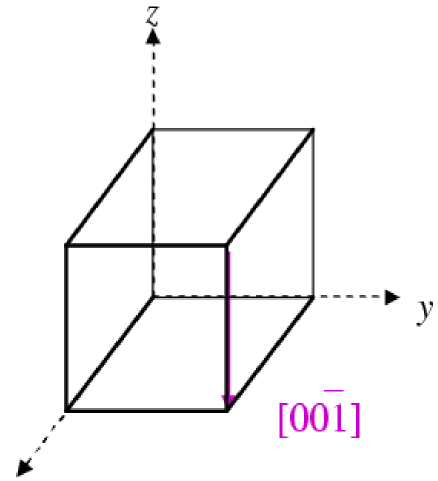
Crystal structure: Hexagonal / FCC

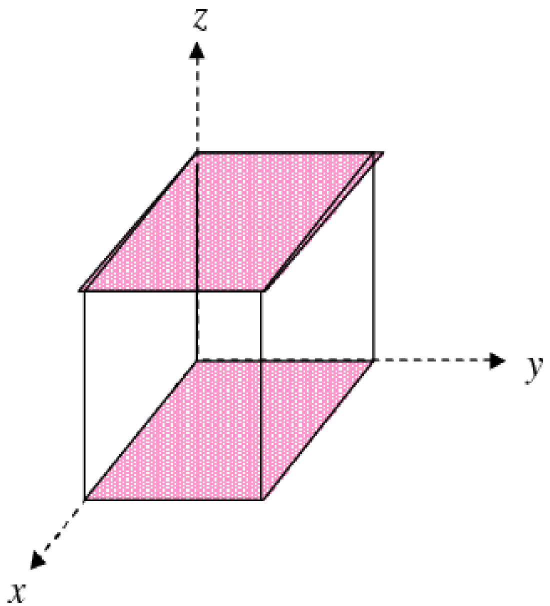


stacking sequence A/CABC

stacking sequence ABCABC

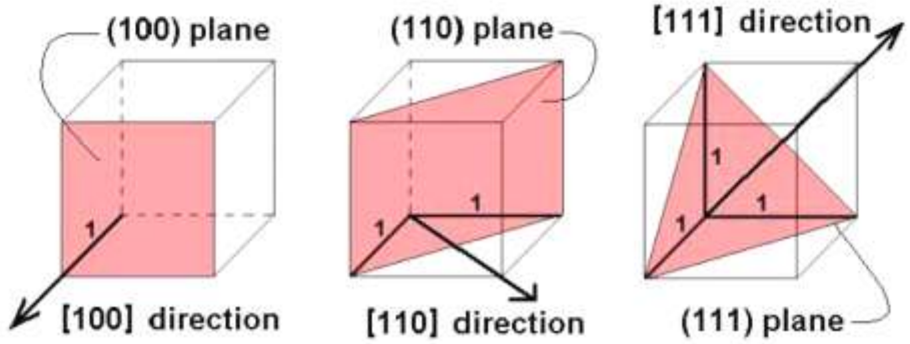


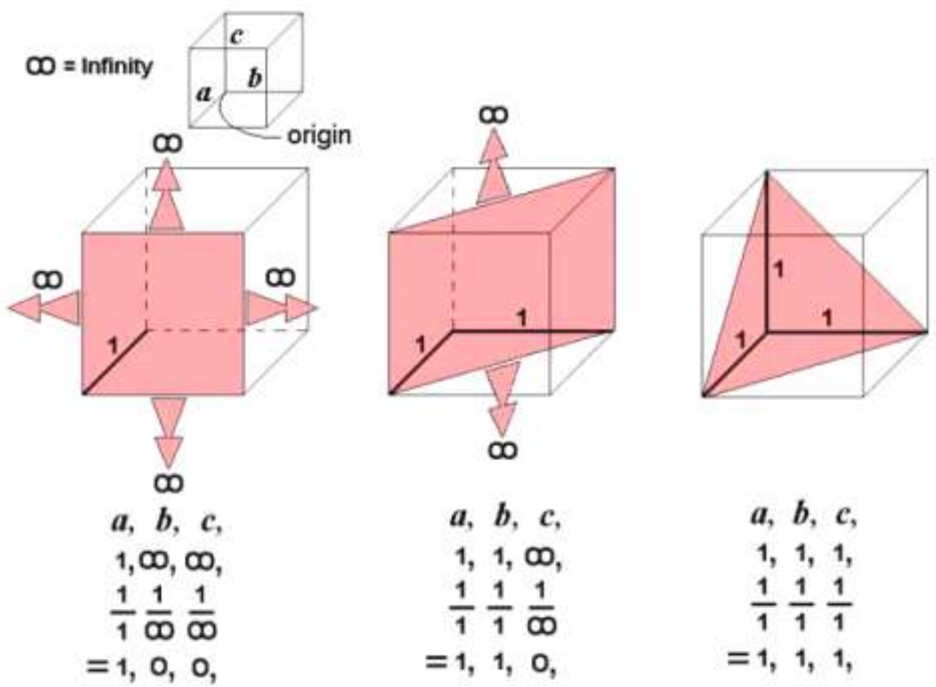




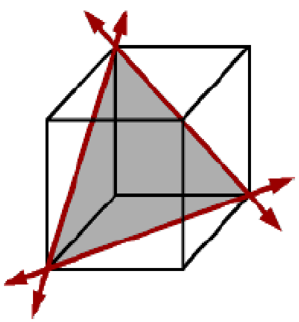
	x	y	z
Intercepts	∞	∞	1
reciprocals	0	0	1
Indices		(001)	

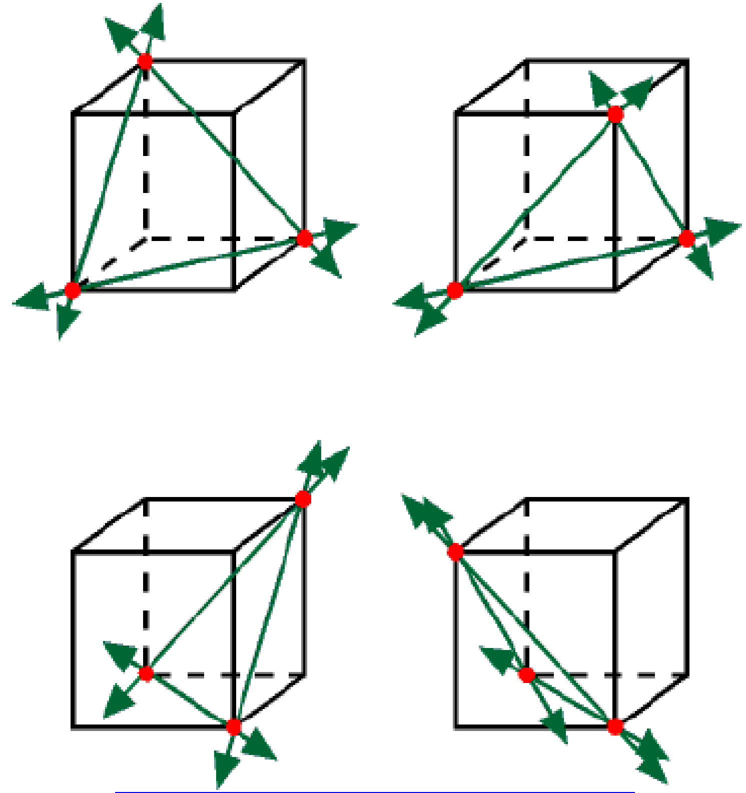
Deriving Miller indices: the description of lattice vectors





Miller Indices of typical planes and directions in FCC metals

Gitter	Beispiel		Gleitebenen G Typ	Gleitebenen G Zahl	Gleitrichtung g Typ	Gleitrichtung g Zahl	Gesamtzahl der Gleitsysteme
kfz	Al Cu Ni Ag Au		(111)	4	[110]	3	12

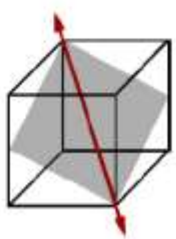
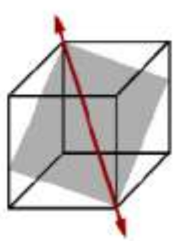


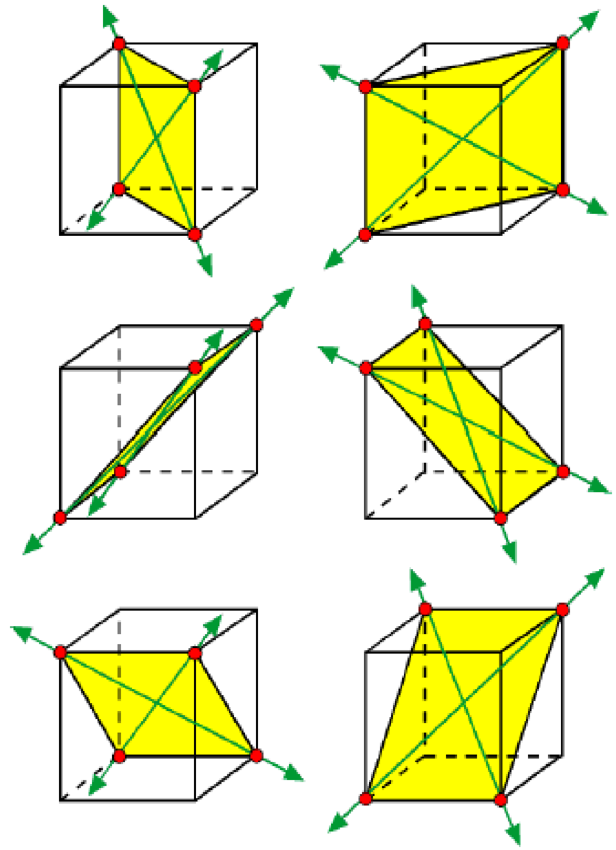
kfz

4E x 3R = 12

(111) [110]

Miller Indices of typical planes and directions in BCC metals

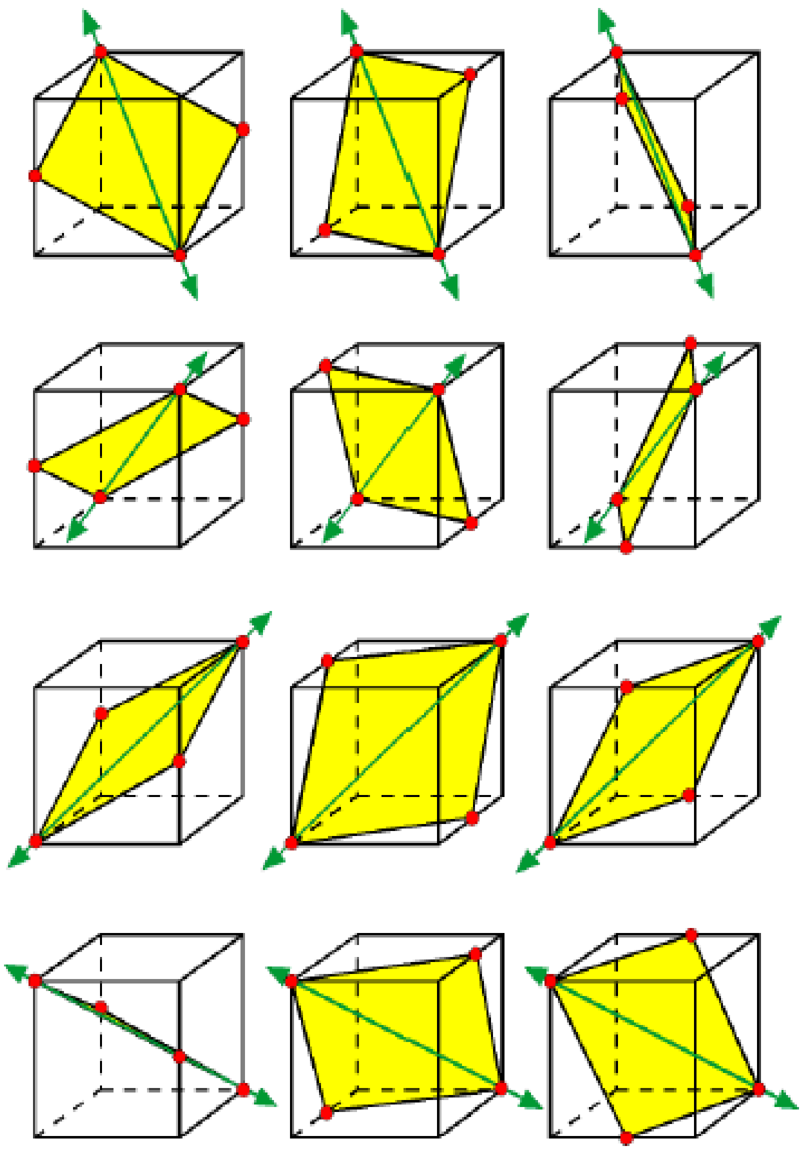
Gitter	Beispiel		Gleitebenen G		Gleitrichtung g		Gesamtzahl der Gleitsysteme
			Typ	Zahl	Typ	Zahl	
krz	$Fe_{\alpha\delta}$ W Mo Nb Ta		(110)	6	[111]	2	12
	$Fe_{\alpha\delta}$ W Mo Nb		(112)	12	[111]	1	12
	$Fe_{\alpha\delta}$ W_a Mo		(123)	24	[111]	1	24



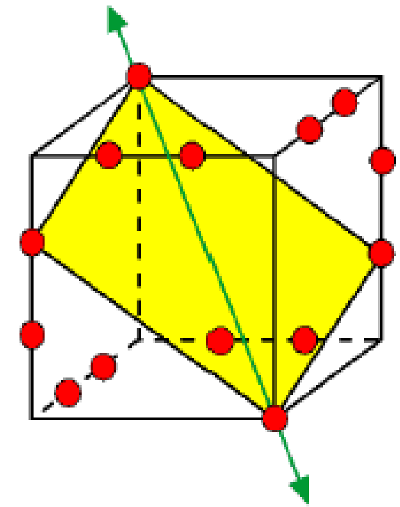
krz

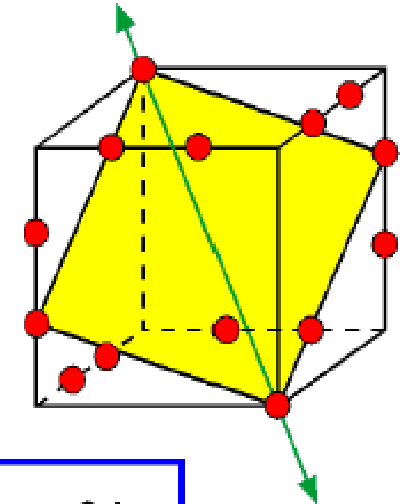
6E	x	2R	= 12
(110)		[111]	

Miller Indices of typical planes and directions in BCC metals



12E x 1R = 12
(112) [111]





24E x 1R = 24
(123) [111]

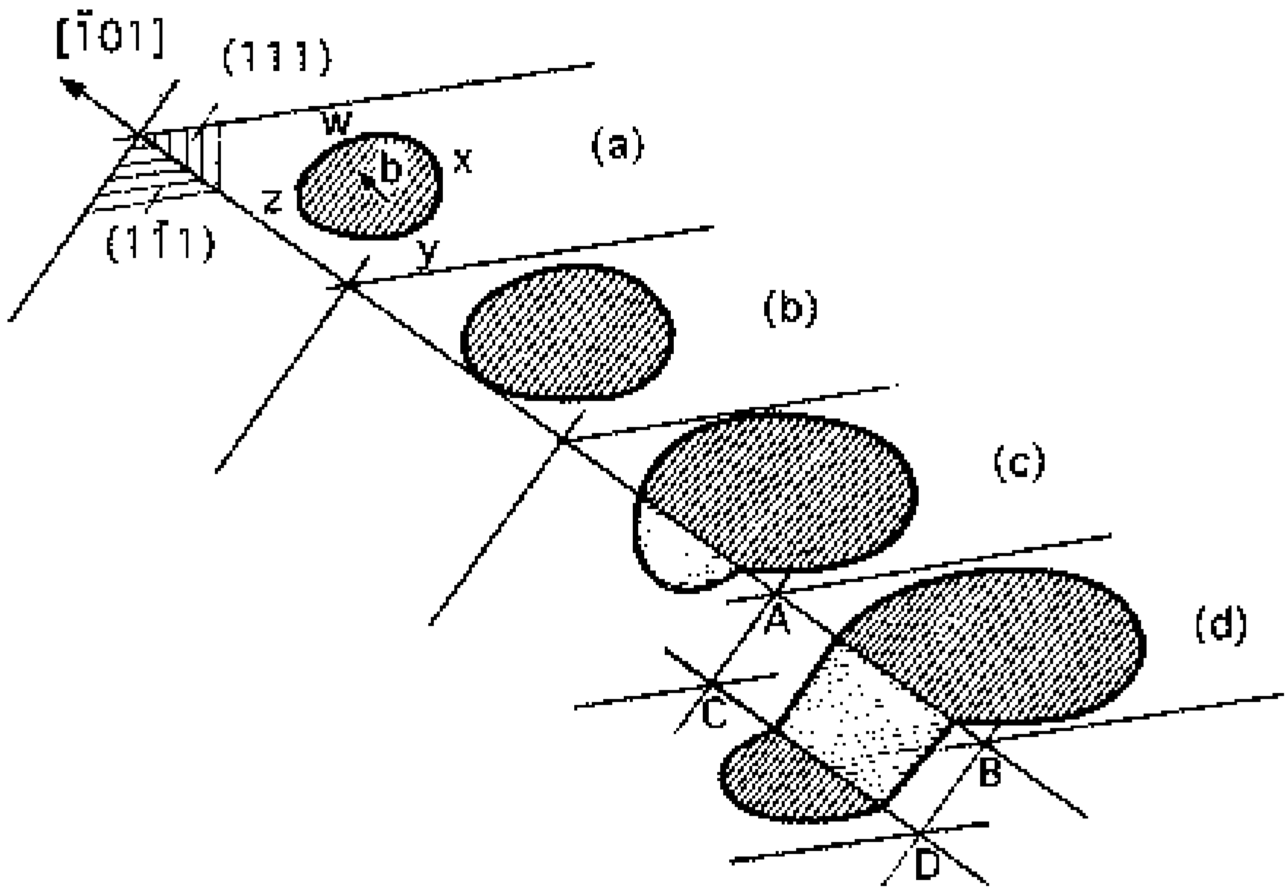
Miller Indices

$$<100> = [1,0,0],[\bar{1},0,0],[0,1,0],[0,\bar{1},0],[0,0,1],[0,0,\bar{1}]$$

$$<110> = [1,1,0],[\bar{1},1,0],[1,\bar{1},0],[\bar{1},\bar{1},0],[1,0,1],[\bar{1},0,\bar{1}],\ldots\ldots$$

	specific	general
direction	[ ]	< >
plane	( )	{ }

vectors and planes


[1̄01]
(111)
(11̄1)
w
x
y
z
b
(a)
(b)
(c)
(d)
A
B
C
D