متالورژی فیزیکی
جلسه پنجم : ترکیبات بین فلزی

علی اشرفی

دانشکده مهندسی مواد

دانشگاه صنعتی اصفهان

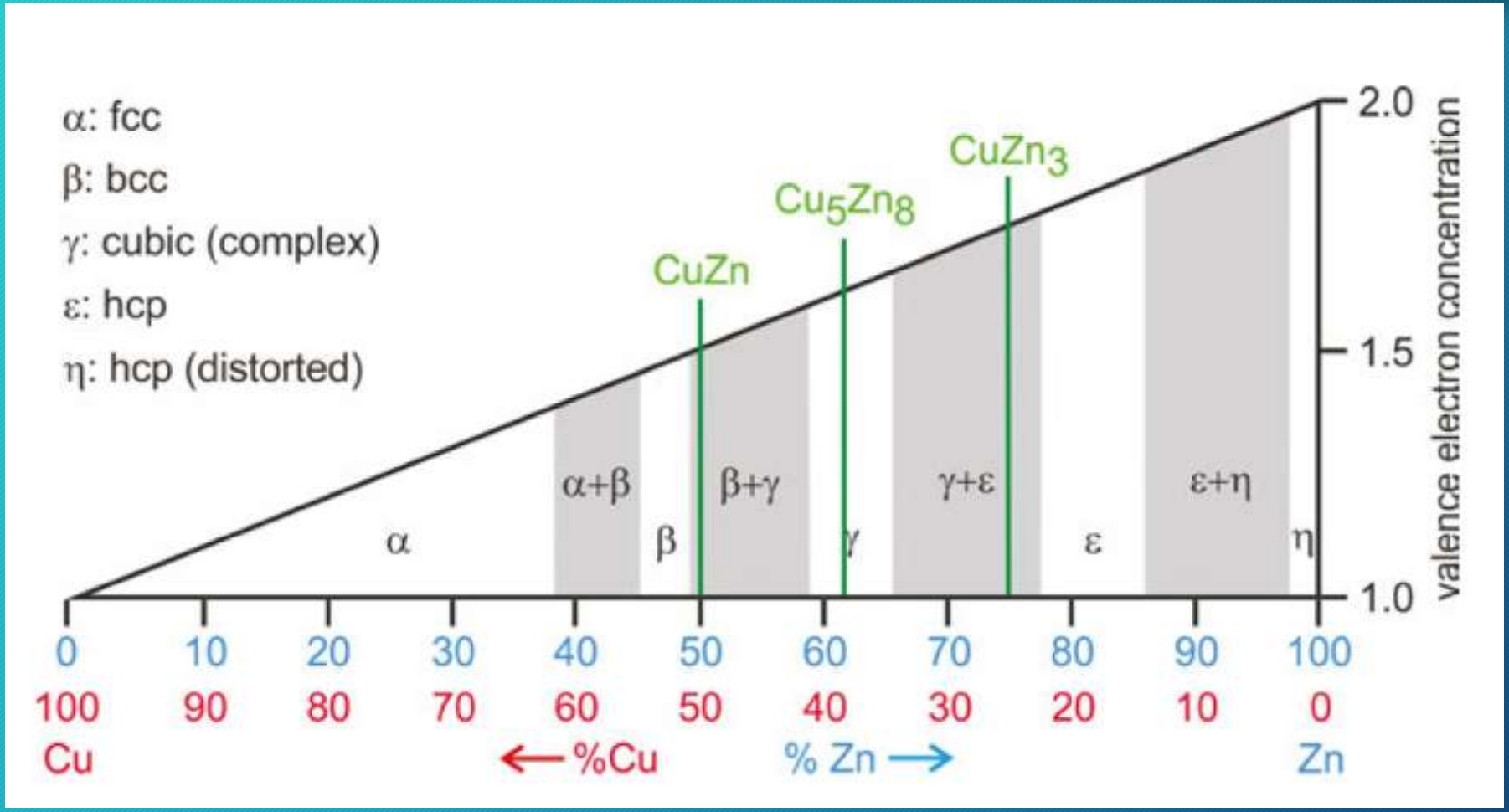
انواع ترکیبات بین فلزی

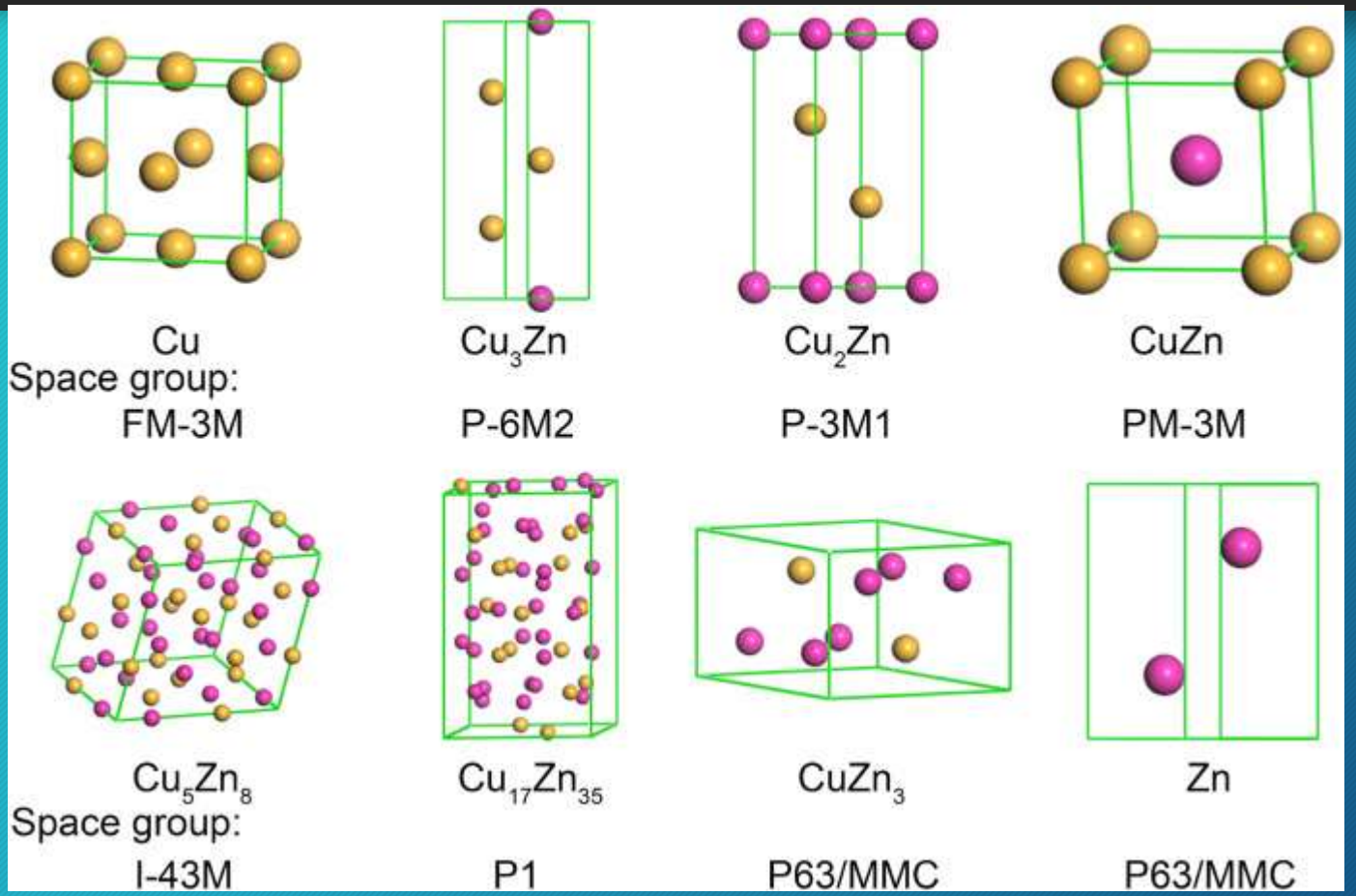
- فازهای هیوم روتری (Hume Rothery)
- فازهای لاوه (Laves)
- فازهای زینتل (Zintl)
- بورایدها (Borides)
- آلومینایدها (Aluminides)
- کاربیدها
- سیلیسیدها
- نیتریدها
- فسفیدها
- هیدریدها
- ...

Hume-Rothery phases

- *a large number of intermetallic compounds whose structures solely depend on the valence electron concentration, not on the composition of a given phase.*

- *Copper with a valence electron concentration (VEC) of 1.0 adopts a fcc structure and zinc with VEC = 2.0 crystallizes with the hexagonal-closest packing*


α: fcc
β: bcc
γ: cubic (complex)
ε: hcp
η: hcp (distorted)
CuZn
Cu5Zn8
CuZn3
α
α+β
β
β+γ
γ
γ+ε
ε
ε+η
η
2.0
1.5
1.0
valence electron concentration
0 10 20 30 40 50 60 70 80 90 100
100 90 80 70 60 50 40 30 20 10 0
Cu
←%Cu
% Zn→
Zn

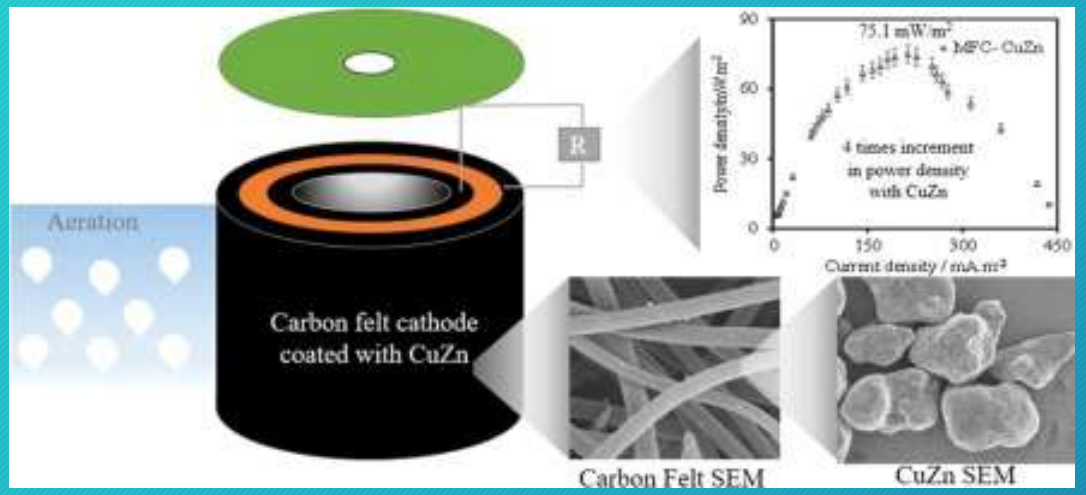

Cu
Space group:
FM-3M
Cu3Zn
P-6M2
Cu2Zn
P-3M1
CuZn
PM-3M
Cu5Zn8
Space group:
I-43M
Cu17Zn35
P1
CuZn3
P63/MMC
Zn
P63/MMC

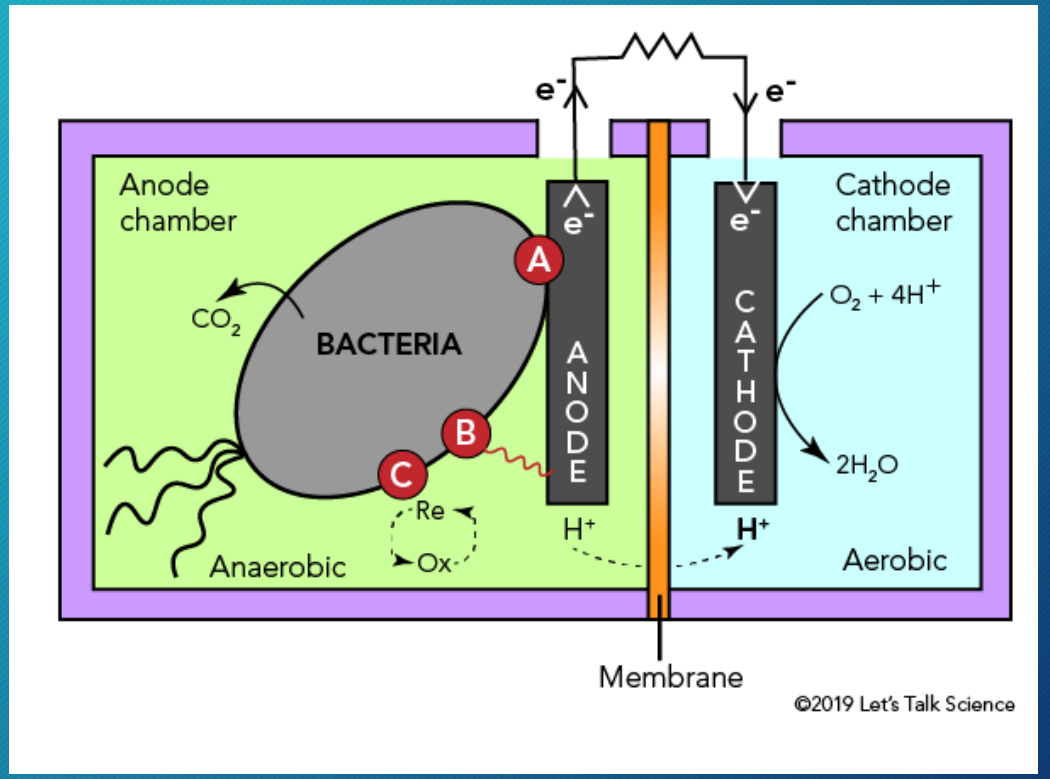
نحوه محاسبه VEC (Valence Electron Concentration)

Composition	No. VE	No. Atoms	VEC
β phase			
CuZn	1 + 2	2	3:2 = 21/14
Cu_3Al	3 + 3	4	6:4 = 21/14
γ phase			
Cu_5Zn_8	5 + 16	13	21/13
Cu_9Al_4	9 + 12	13	21/13
ε phase			
$CuZn_3$	1 + 6	4	7:4 = 21/12
Au_5Al_3	5 + 9	8	14:8 = 21/12

کاربرد

- *CuZn in Microbial Fuel cell*



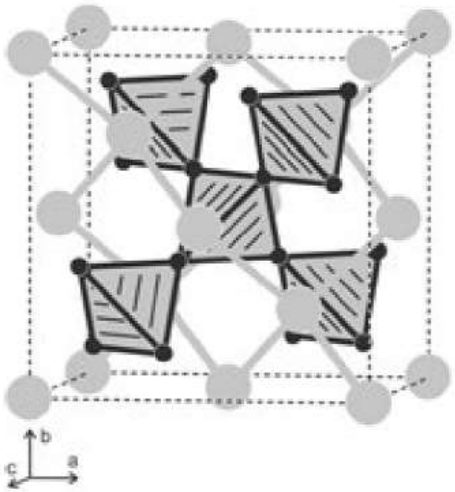


https://doi.org/10.1016/j.cplett.2020.137536

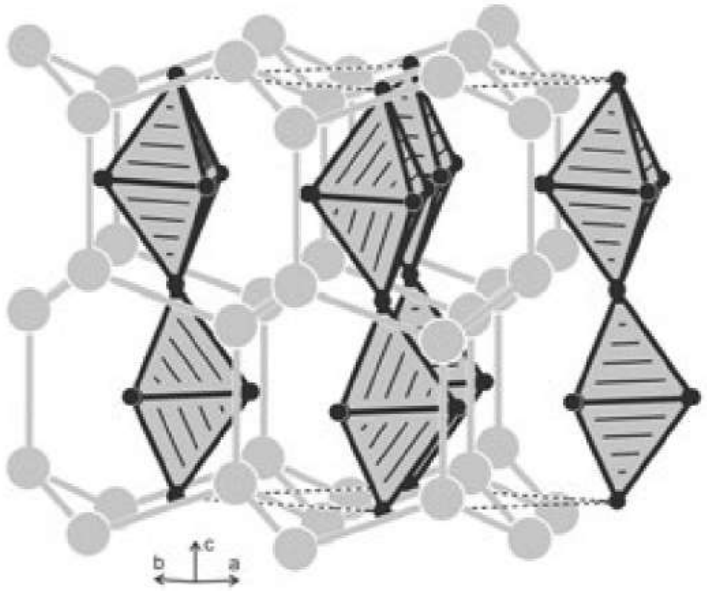
فازهای لاوه

- *The Laves phases have the general composition AB2 and they can be considered as line-compounds without noticeable homogeneity ranges, in contrast to the Hume- Rothery phases*

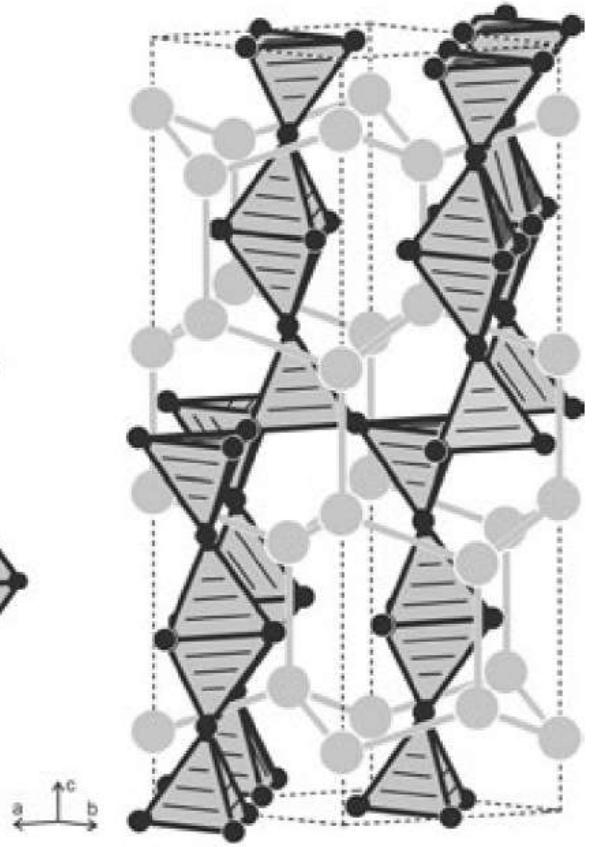
- *The structures are closely packed and they form with a typical ratio of the atomic radii of rA/rB = ≈ 1.225*



$MgCu_2$ ($Fd\bar{3}m$)



$MgZn_2$ ($P6_3/mmc$)



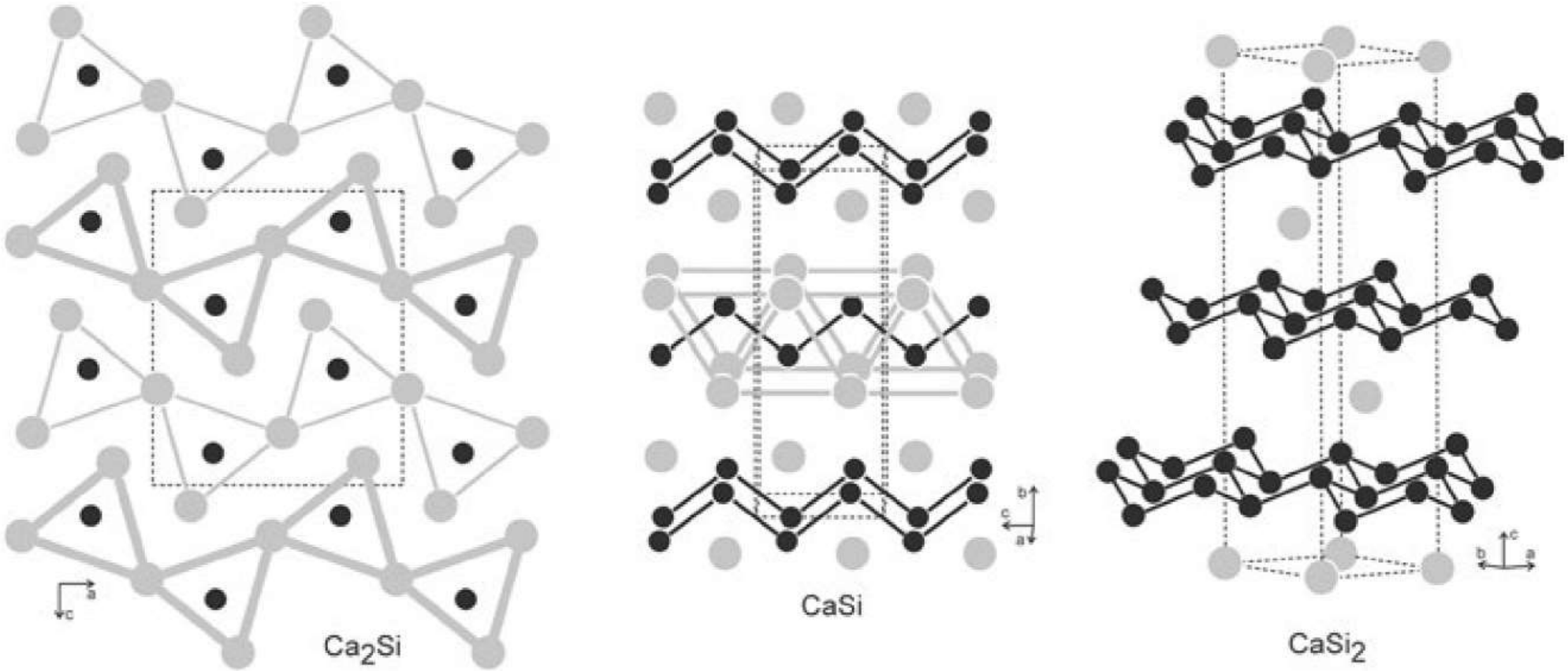
$MgNi_2$ ($P6_3/mmc$)

مثال هایی از فازهای لاوه

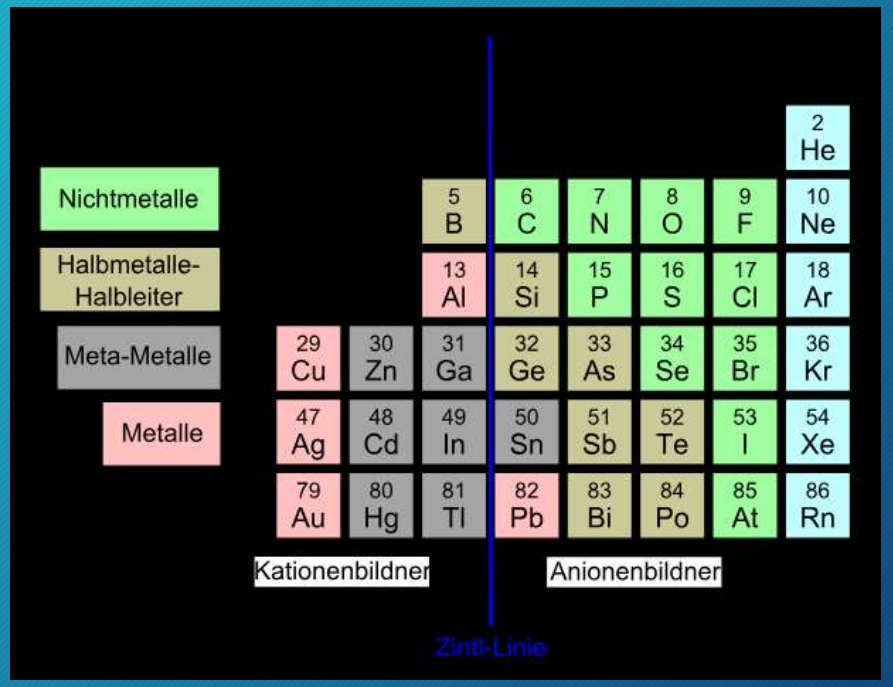
$MgCu_2$ type	$MgZn_2$ type	$MgNi_2$ type
$CaAl_2$	$CaLi_2$	$TaCo_2$
$CaIr_2$	$TaFe_2$	$ScFe_2$
$CeCo_2$	$CeMn_2$	$HfMo_2$
$ZrMo_2$	$ZrRe_2$	$TaZn_2$

فازهای زینتل

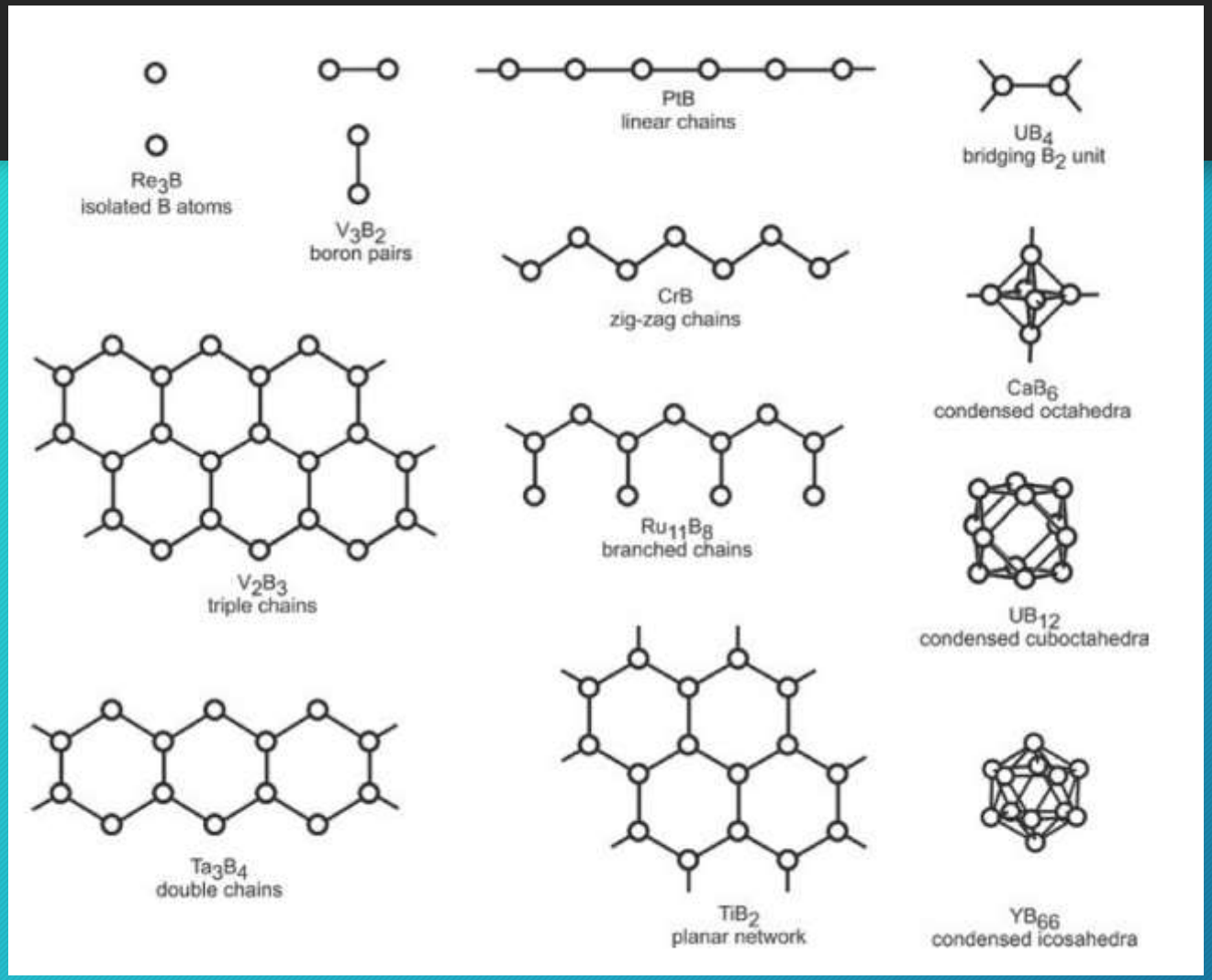
- *Zintl phases form with a weak electronegative metal (alkali, alkaline earth, or rare earth element) and a half-metal of the p block*
- *Zintl-line runs in between the third and fourth main group of the Periodic Table*
- *Such compounds generally form with elements that are on the left- and right-hand part of the so-called Zintl-line*

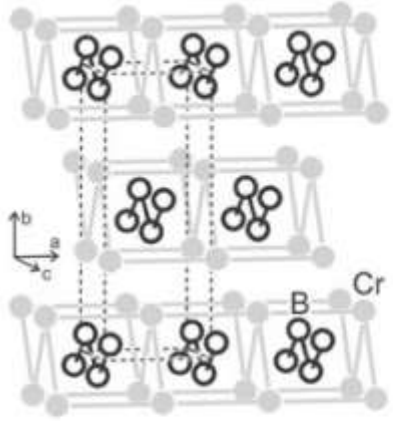

Ca2Si
CaSi
CaSi2

Compound	No. VE	Formal charge	Connectedness	Anionic substructure
isolated Zintl anions				
Ca_2Si	4	4–	0	Si^{4-}
Na_3As	5	3–	0	As^{3-}
pairs				
Ca_5Si_3	4/3	4–/3–	0/1	Si^{4-} and Si_2^{6-} pairs
Yb_2MgSi_2	3	3–	1	Si_2^{6-} pairs
clusters				
Na_4Si_4	4	1–	3	Si_4^{4-} tetrahedra
chains				
CaSi	4	2–	2	zig-zag-chains
LiAs	5	1–	2	spiral chains
rings				
InP_3	5	1–	2	P_6^{6-} chairs
layers				
$CaSi_2$	4	1–	3	puckered hexagons
networks				
NaTl	3	1–	4	diamond network
$BaGa_2$	3	1–	3	graphite network

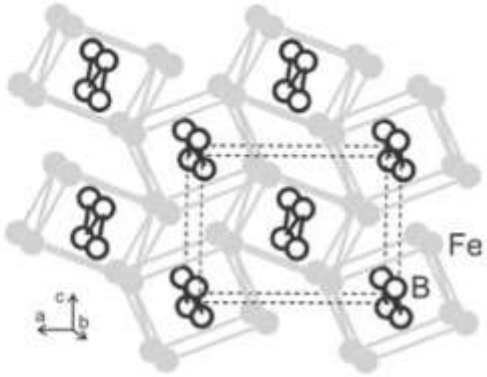


بورایدها

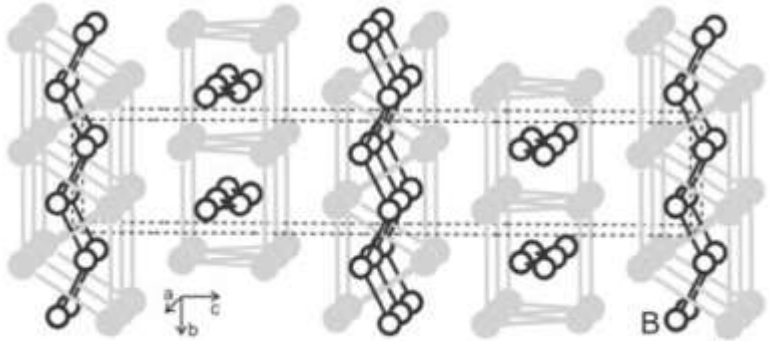

Re_3B
isolated B atoms
V_3B_2
boron pairs
PtB
linear chains
UB_4
bridging B_2 unit
CrB
zig-zag chains
CaB_6
condensed octahedra
V_2B_3
triple chains
$Ru_{11}B_8$
branched chains
UB_{12}
condensed cuboctahedra
Ta_3B_4
double chains
TiB_2
planar network
YB_{66}
condensed icosahedra



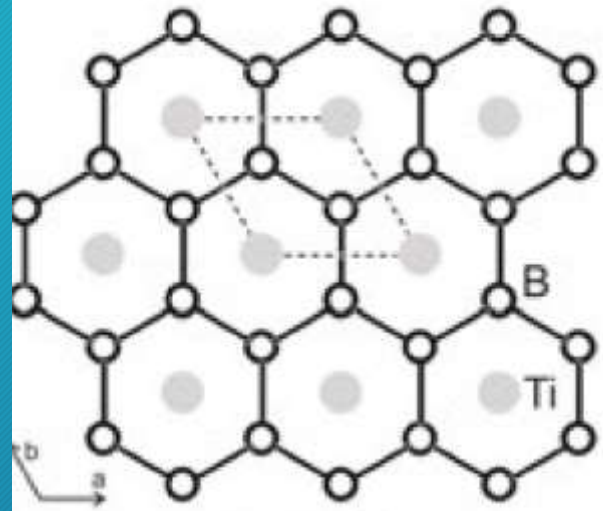
CrB (*Cmcm*)



FeB (*Pnma*)



α-MoB ($I4_1/amd$)



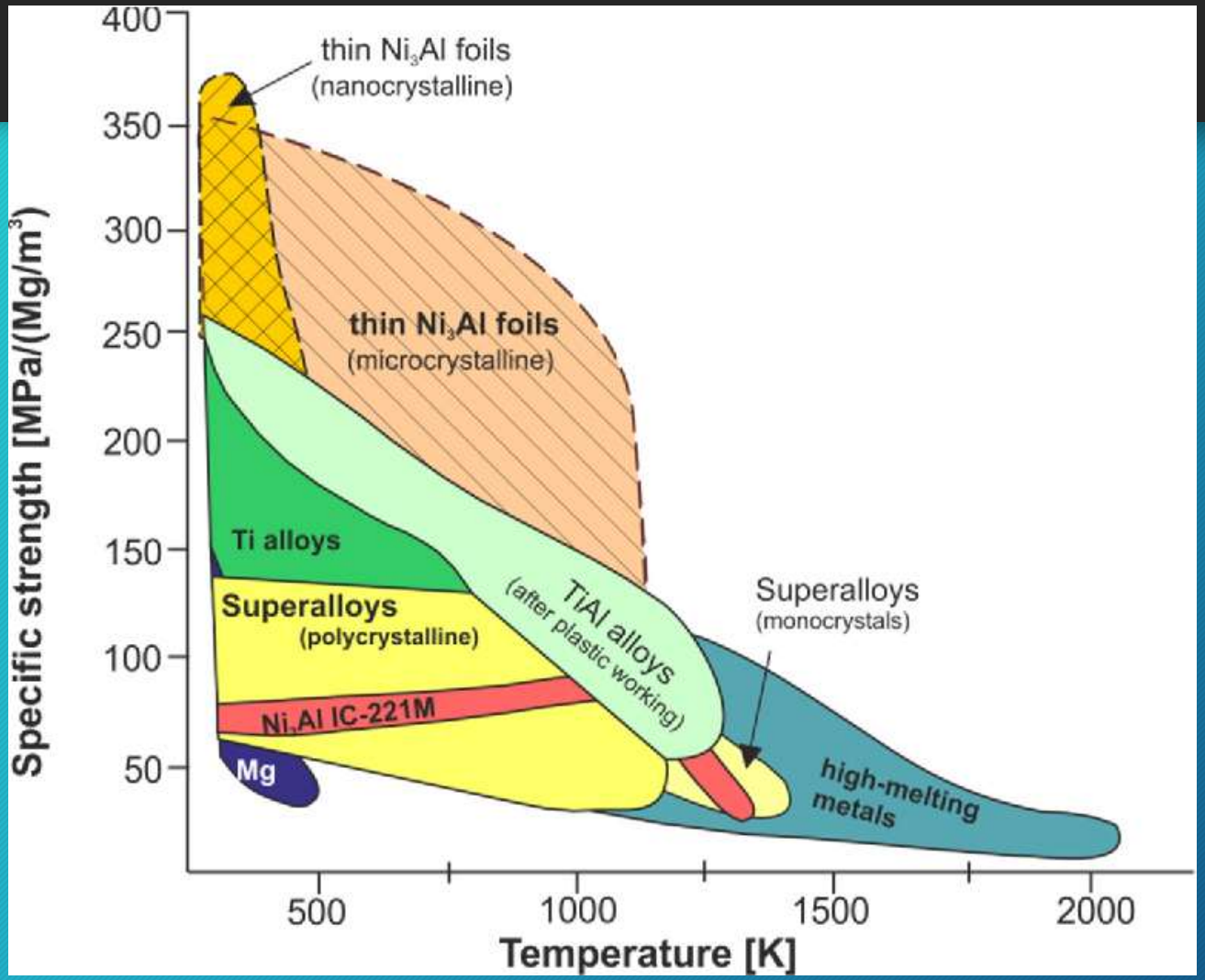
TiB_2 ($P6/mmm$)

آلومینایدها

- *calcium (Ca8Al3, Ca13Al14, CaAl2, CaAl4), strontium (Sr8Al7, SrAl, Sr5Al9, SrAl2, SrAl4), and barium (Ba3Al5, Ba4Al5, Ba7Al13, Ba21Al40, BaAl2, BaAl4) aluminides*

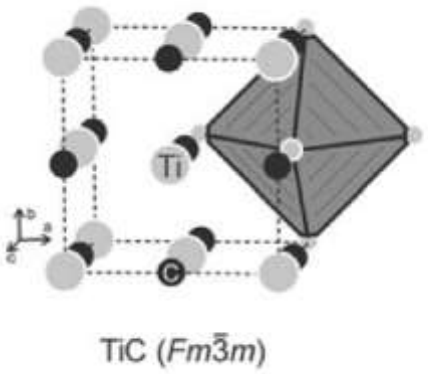
- *Mg17Al12, Mg23Al30, Mg32Al49, Mg3Al5, Mg2Al3, Mg28Al45, Mg9Al11, and MgAl2.*

- *Ti3Al, Zr3Al, Fe3Al, Ni3Al,*

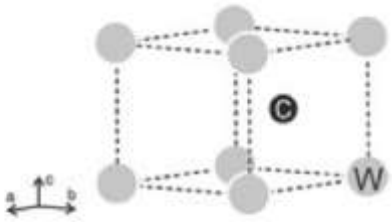

Specific strength [MPa/(Mg/m³)]
400
350
300
250
200
150
100
50
thin Ni₃Al foils
(nanocrystalline)
thin Ni₃Al foils
(microcrystalline)
Ti alloys
Superalloys
(polycrystalline)
Ni₃Al IC-221M
Mg
TiAl alloys
(after plastic working)
Superalloys
(monocrystals)
high-melting
metals
500
1000
1500
2000
Temperature [K]

کاربیدها

- کاربیدهای شبه نمک نظیر Li2C2, CaC2, و Al4C3
- کاربیدهای با پیوند کوالانسی نظیر B4C و SiC
- کاربیدهای فلزی نظیر TiC ، WC ، Cr3C2, Cr23C6, Mo2C, HfC, ZrC, NbC, VC، Fe3C ,Cr7C3,

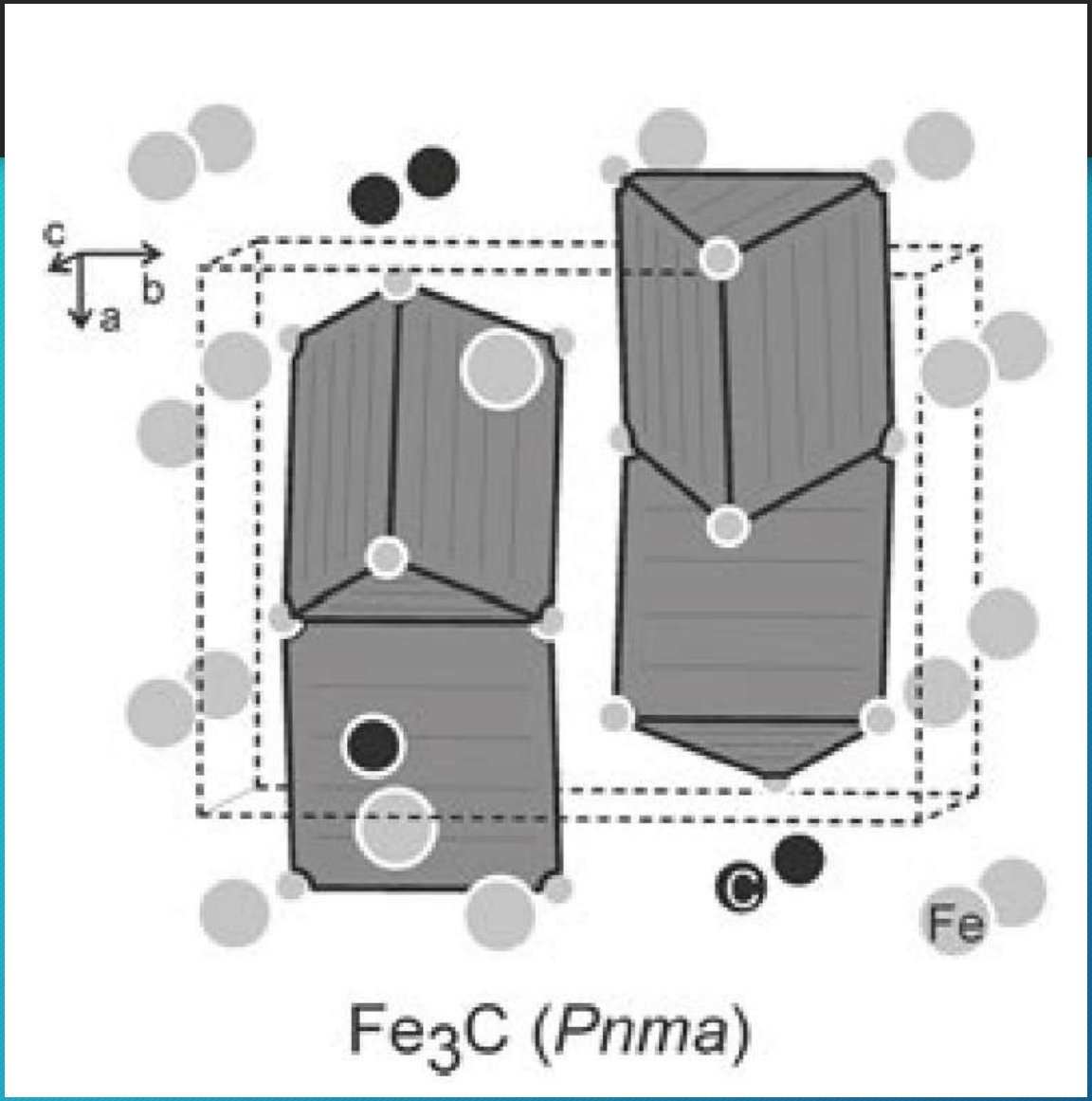


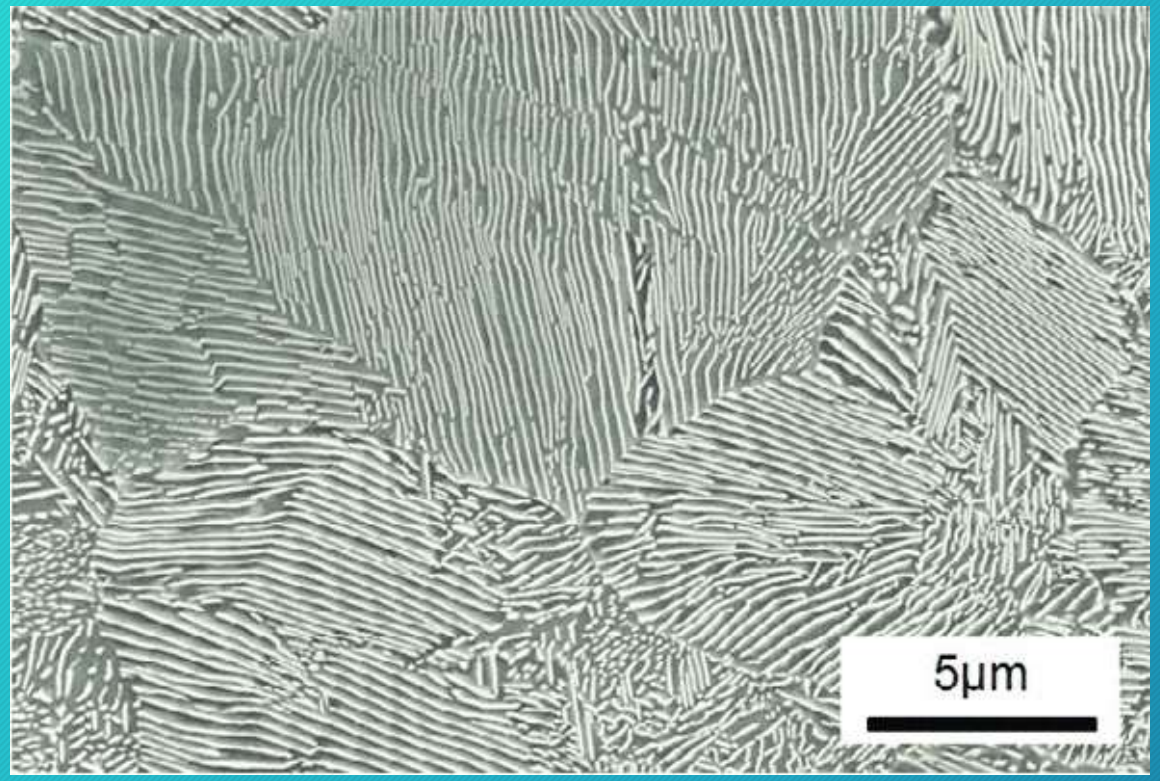
TiC ($Fm\bar{3}m$)

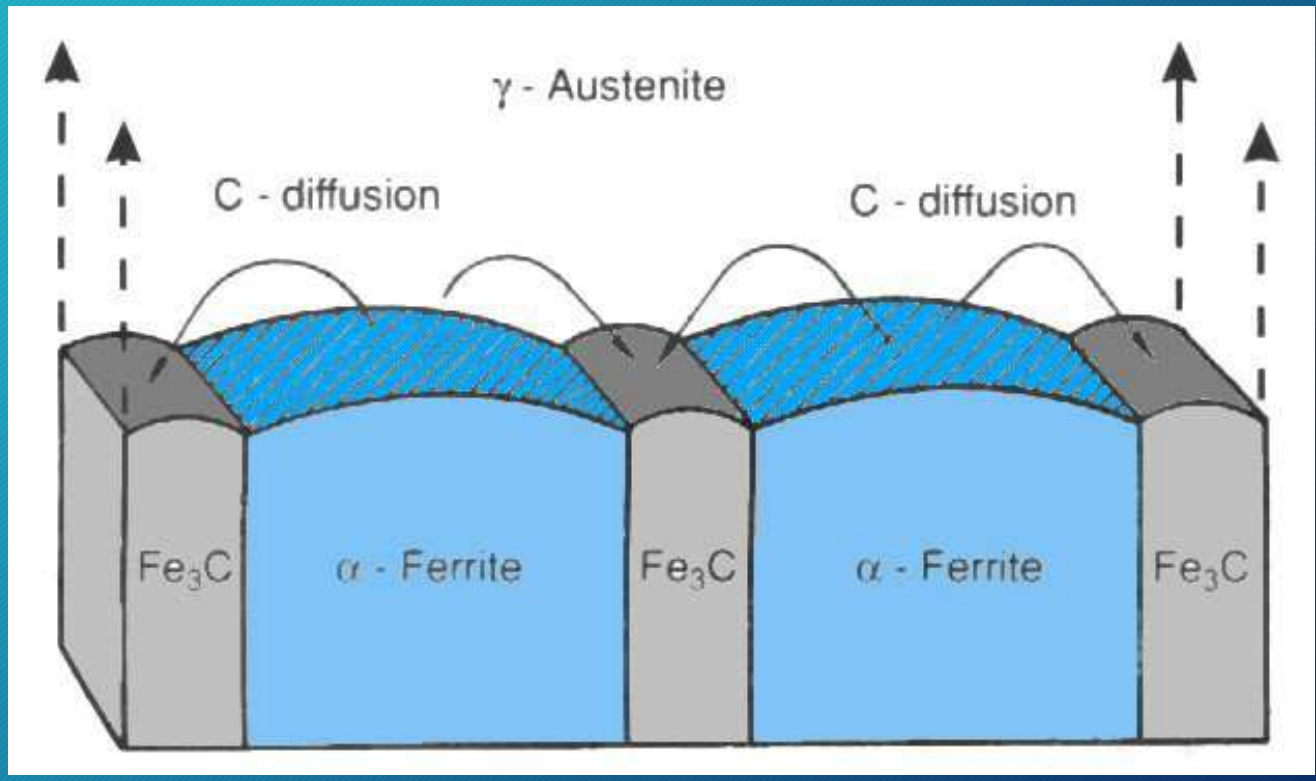


WC ($P\bar{6}m2$)

DOI: 10.1007/s40145-021-0484-z


c
b
a
C
Fe
Fe3C (Pnma)


5μm


γ - Austenite
C - diffusion
C - diffusion
Fe3C
α - Ferrite
Fe3C
α - Ferrite
Fe3C