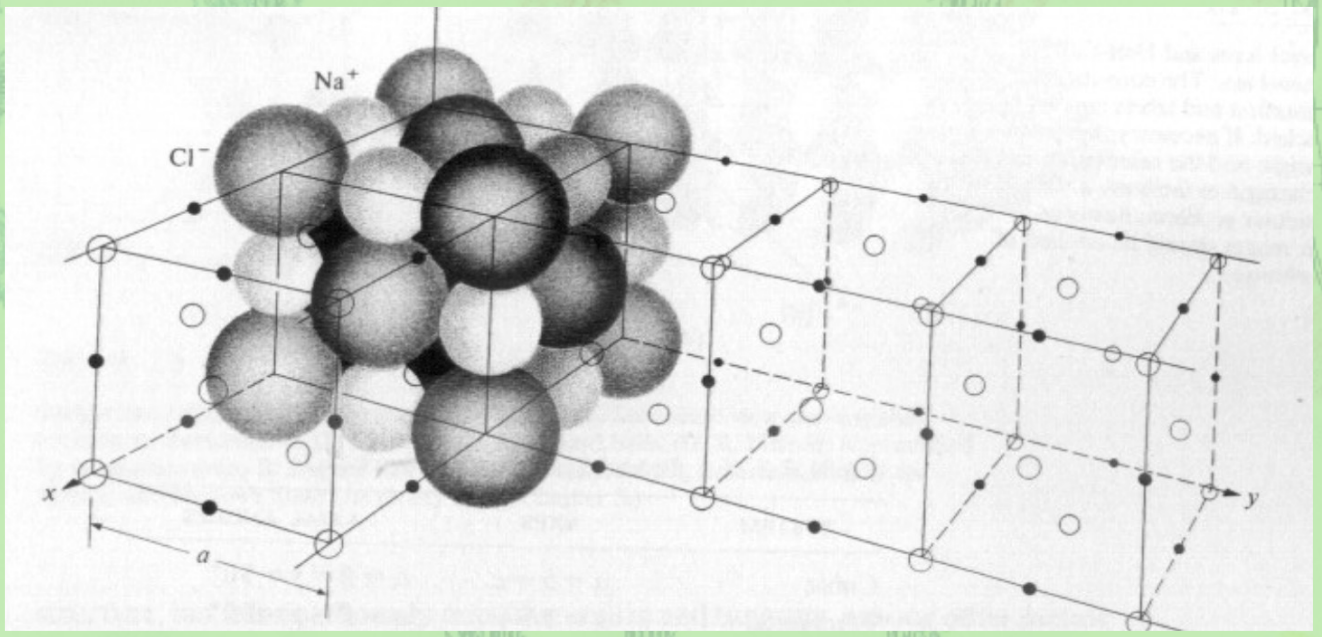
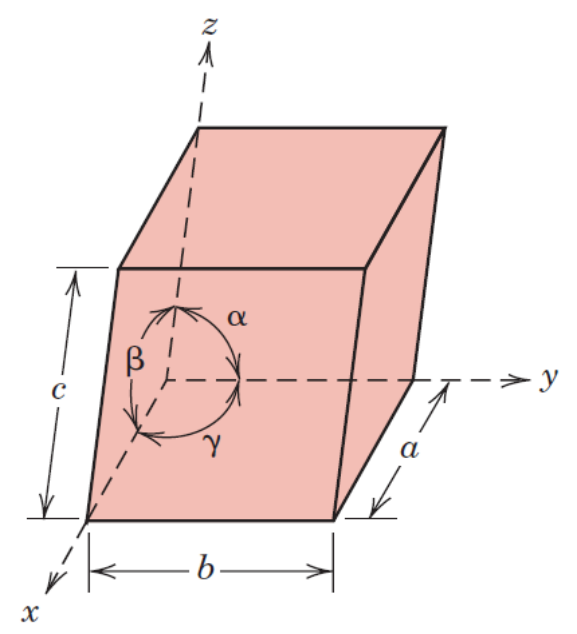
III. Kristalno stanje



- Ćelija je strukturni motiv čijim se ponavljanjem može opisati kristalno uređenje.
  - primitivna – najmanji
  - jedinična – najzorniji
- Posljedice:
  - susjed
  - daljina
  - smjer

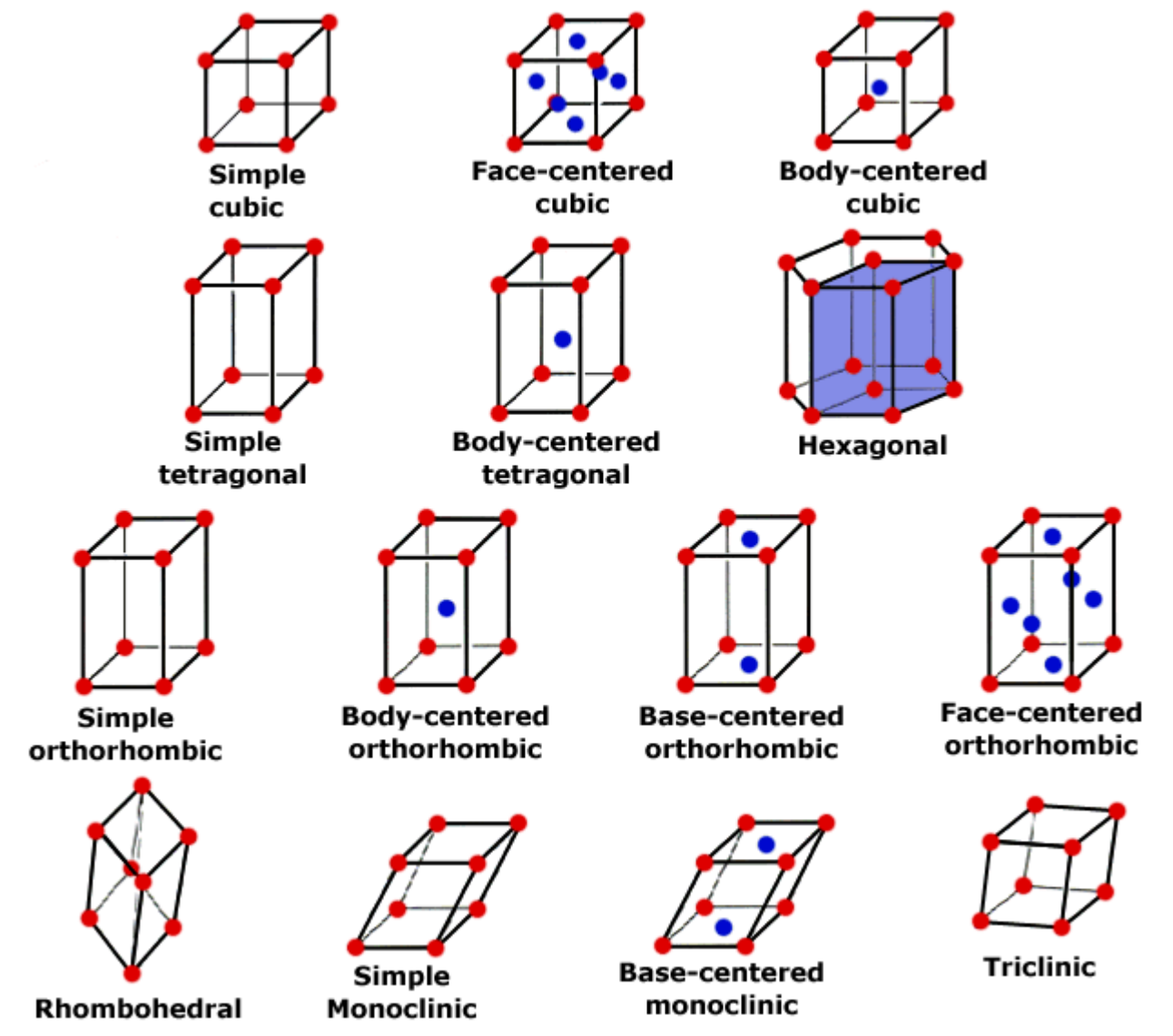
A. Opis kristalnog uređenja

- 7 (i samo 7) kristalnih sustava:



- kubni
- tetragonski
- ortorombski
- monoklinski
- triklinski
- heksagonski
- romboedarski

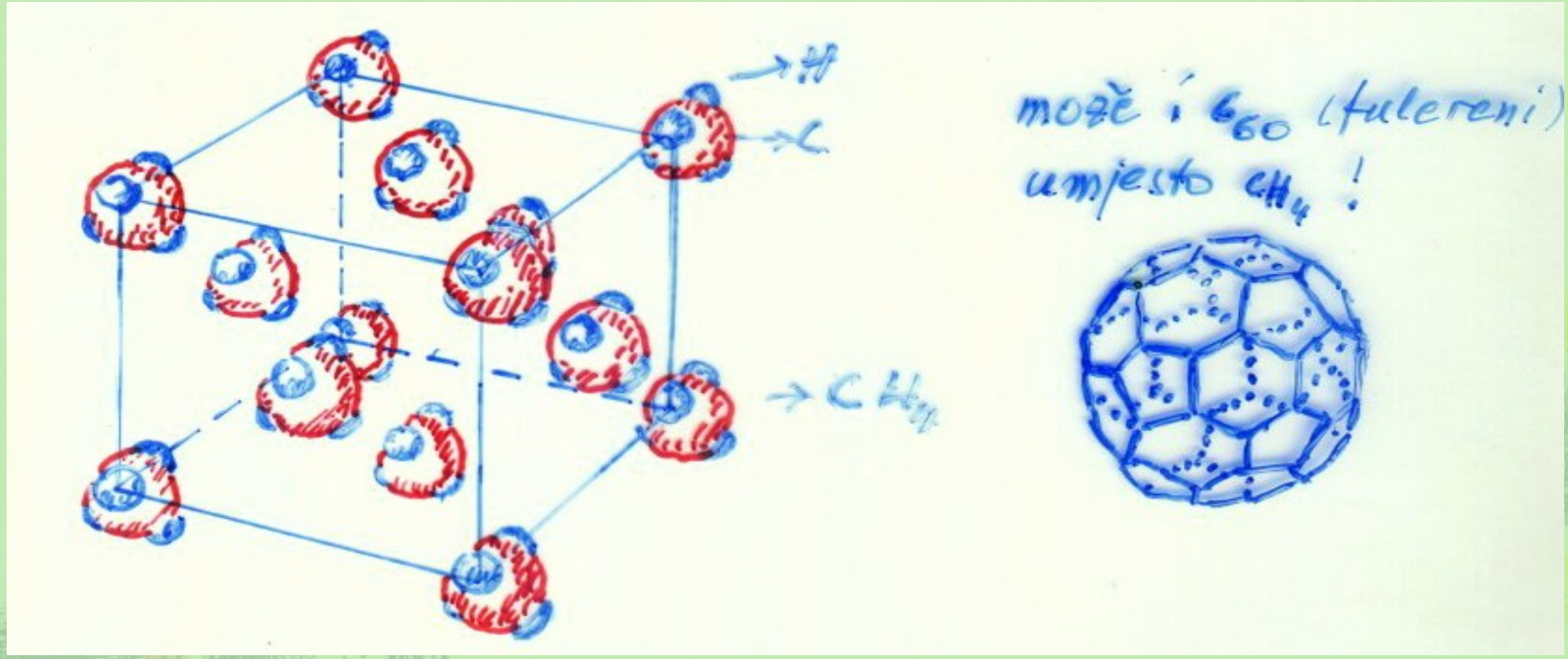
14 Bravaisovih rešetki:



- Kristalni sustavi
  - 7 geometrija koje svojim periodičnim ponavljanjem popune cijeli prostor
- Uzorci s točkama (prostorne rešetke, Bravais)
  - 14 načina ugradnje "atoma", koji čuvaju translacijsku simetriju
- Točkaste grupe
  - 32 elementa simetrije
- Prostorne grupe
  - 230 prostornih grupa

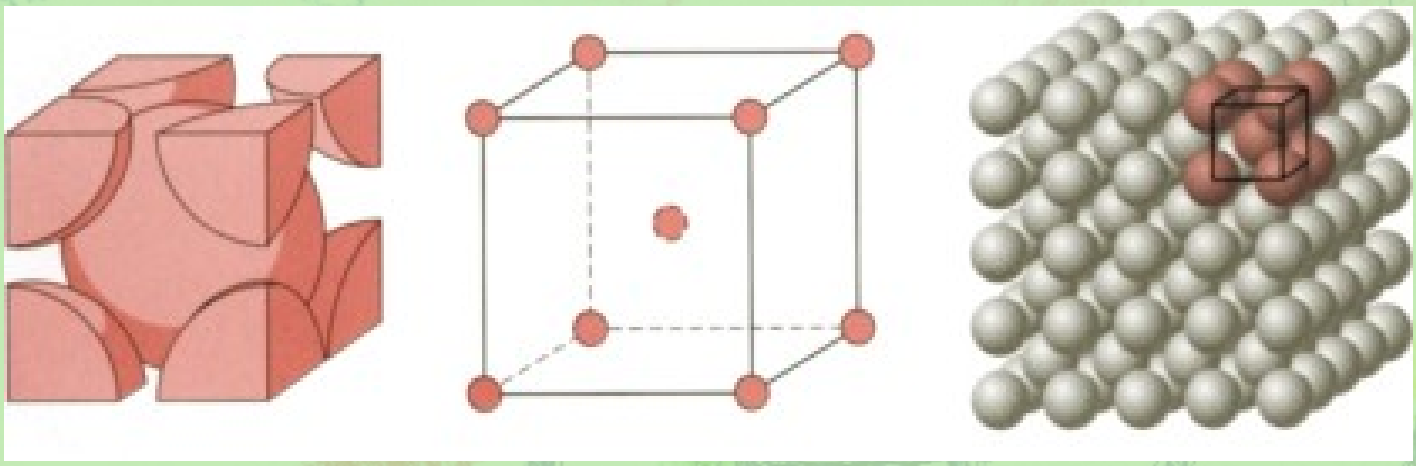
Crystal family	Crystal system	Required symmetries of point group	Point groups	Space groups	Bravais lattices	Lattice system
Triclinic		None	2	2	1	Triclinic
Monoclinic		1 twofold axis of rotation or 1 mirror plane	3	13	2	Monoclinic
Orthorhombic		3 twofold axes of rotation or 1 twofold axis of rotation and two mirror planes.	3	59	4	Orthorhombic
Tetragonal		1 fourfold axis of rotation	7	68	2	Tetragonal
Hexagonal	Trigonal	1 threefold axis of rotation	5	7	1	Rhombohedral
				18	1	Hexagonal
	Hexagonal	1 sixfold axis of rotation	7	27		
Cubic		4 threefold axes of rotation	5	36	3	Cubic
Total: 6	7		32	230	14	7

- Gradnja kristala: smještamo atome ili skupine atoma u točke rešetke

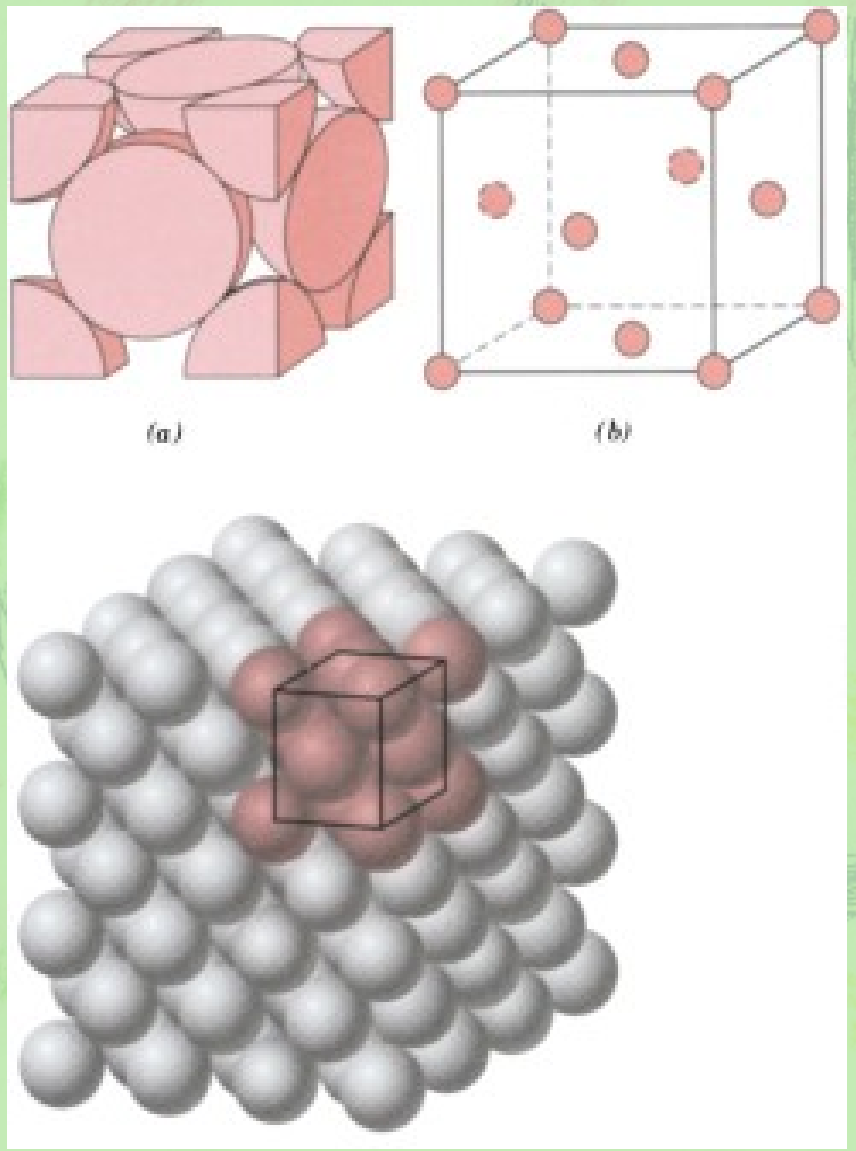


Primjeri:

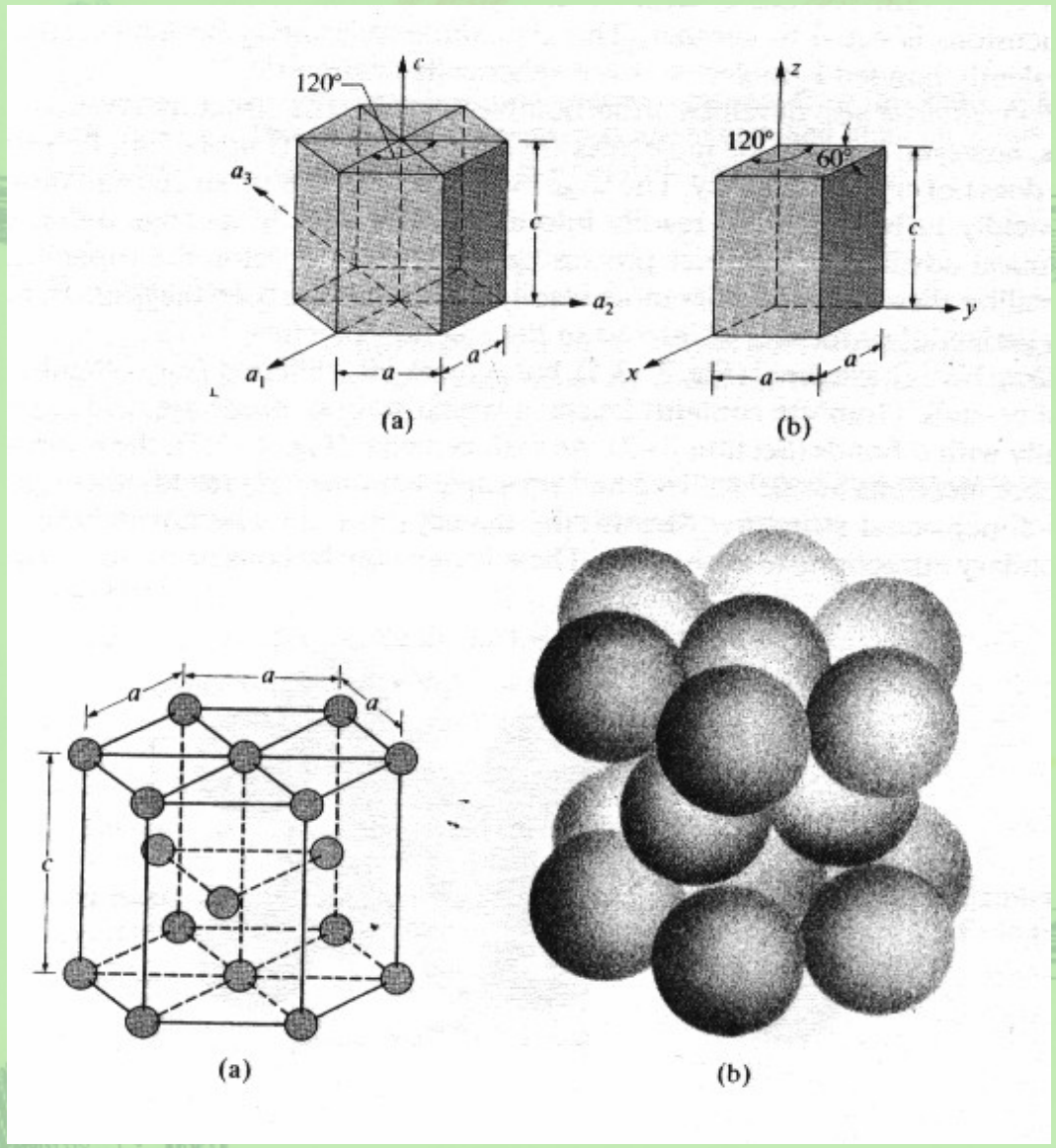
- BCC

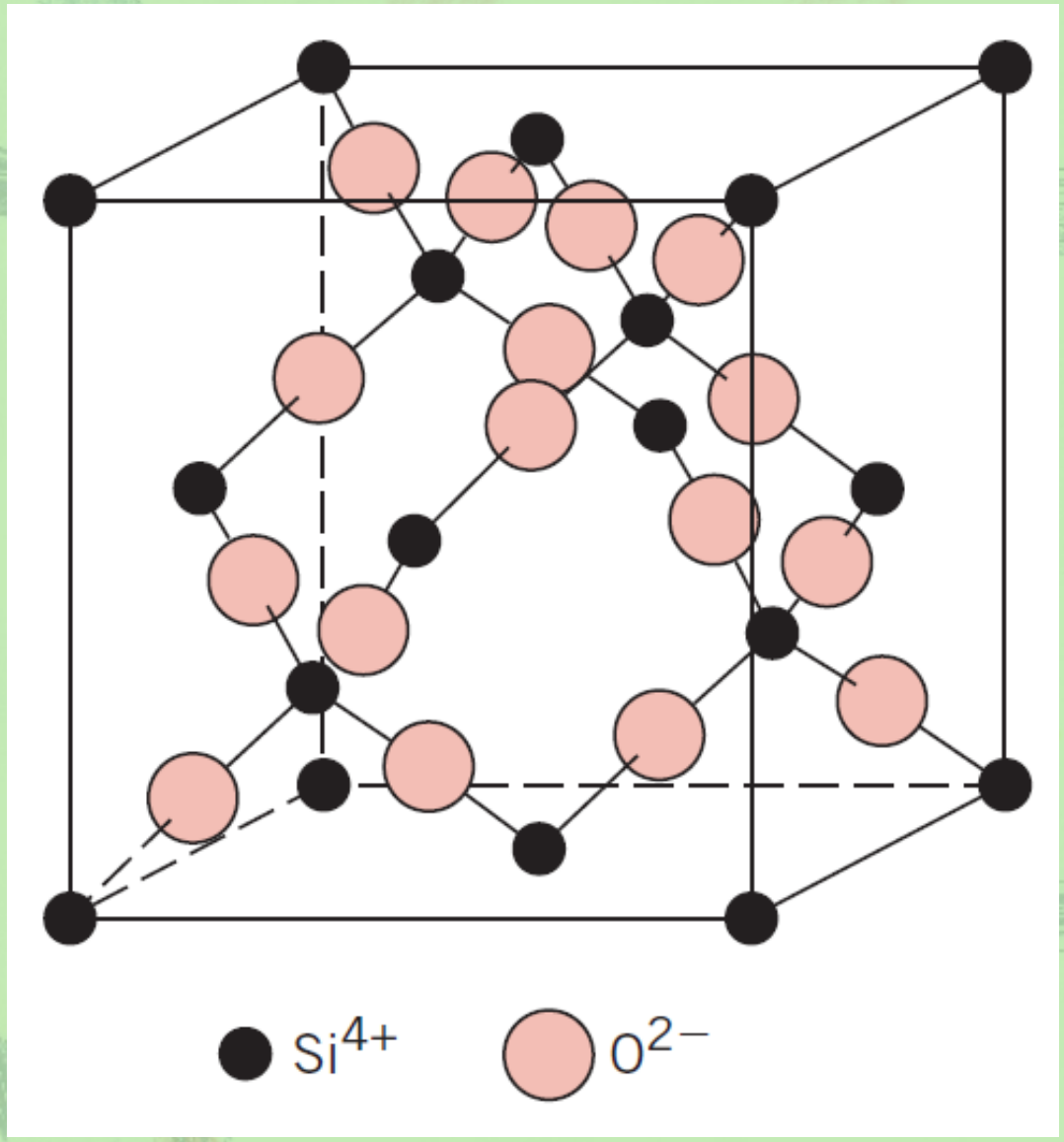


- FCC



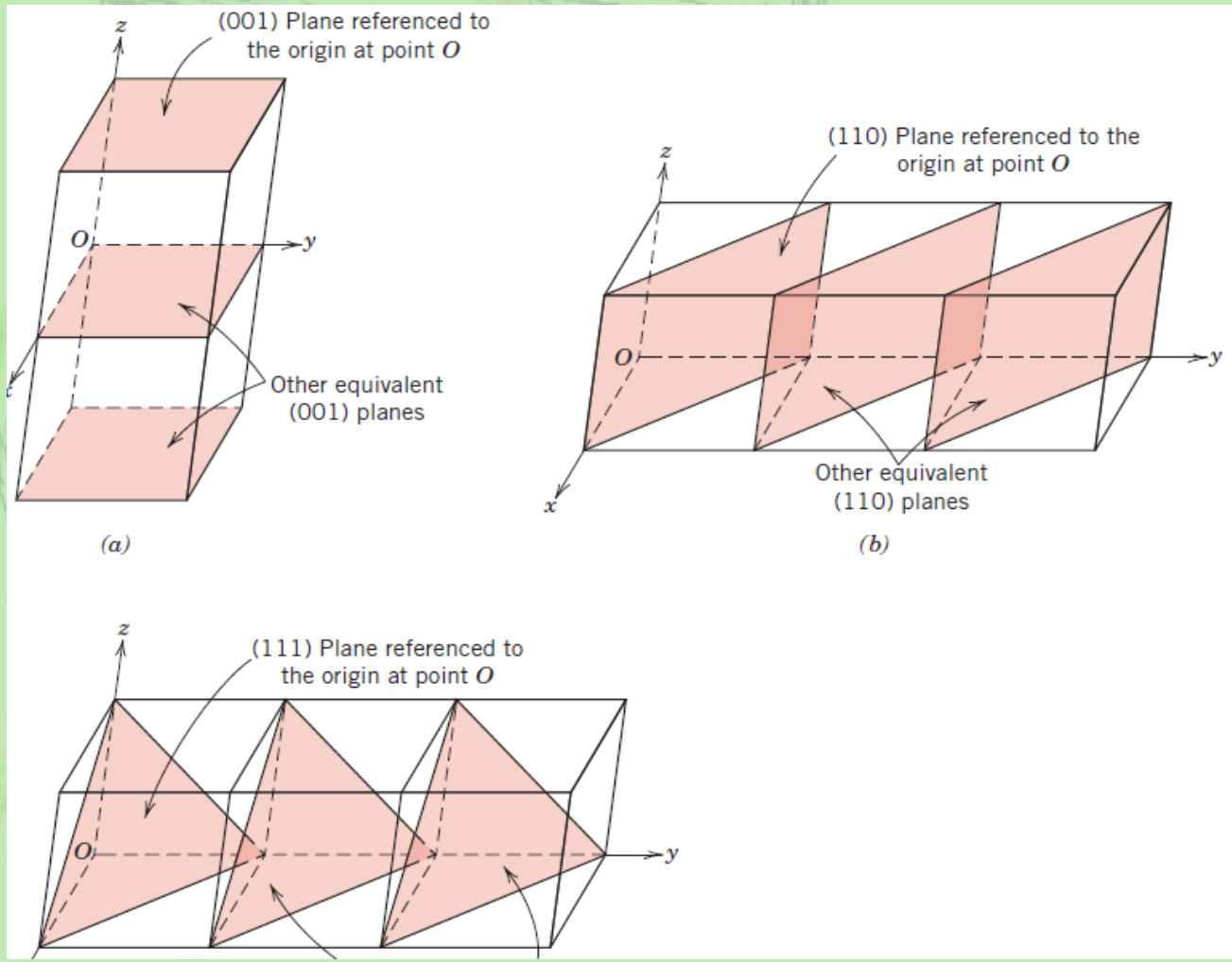
- HCP




Si^{4+}
O^{2-}

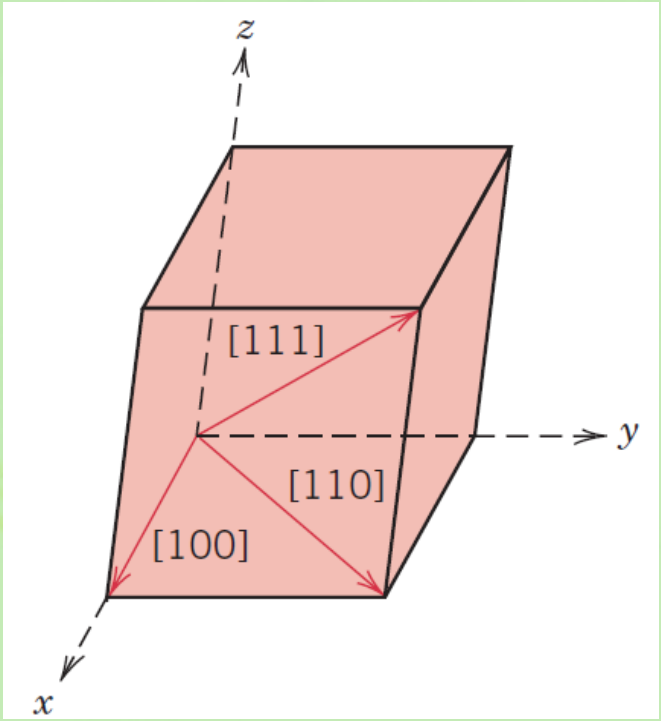
B. Plošna struktura

- Eksperimentalno se određuju udaljenosti među ravninama
- Millerovi indeksi (hkl)
- Porodice ravnina, npr. {100}

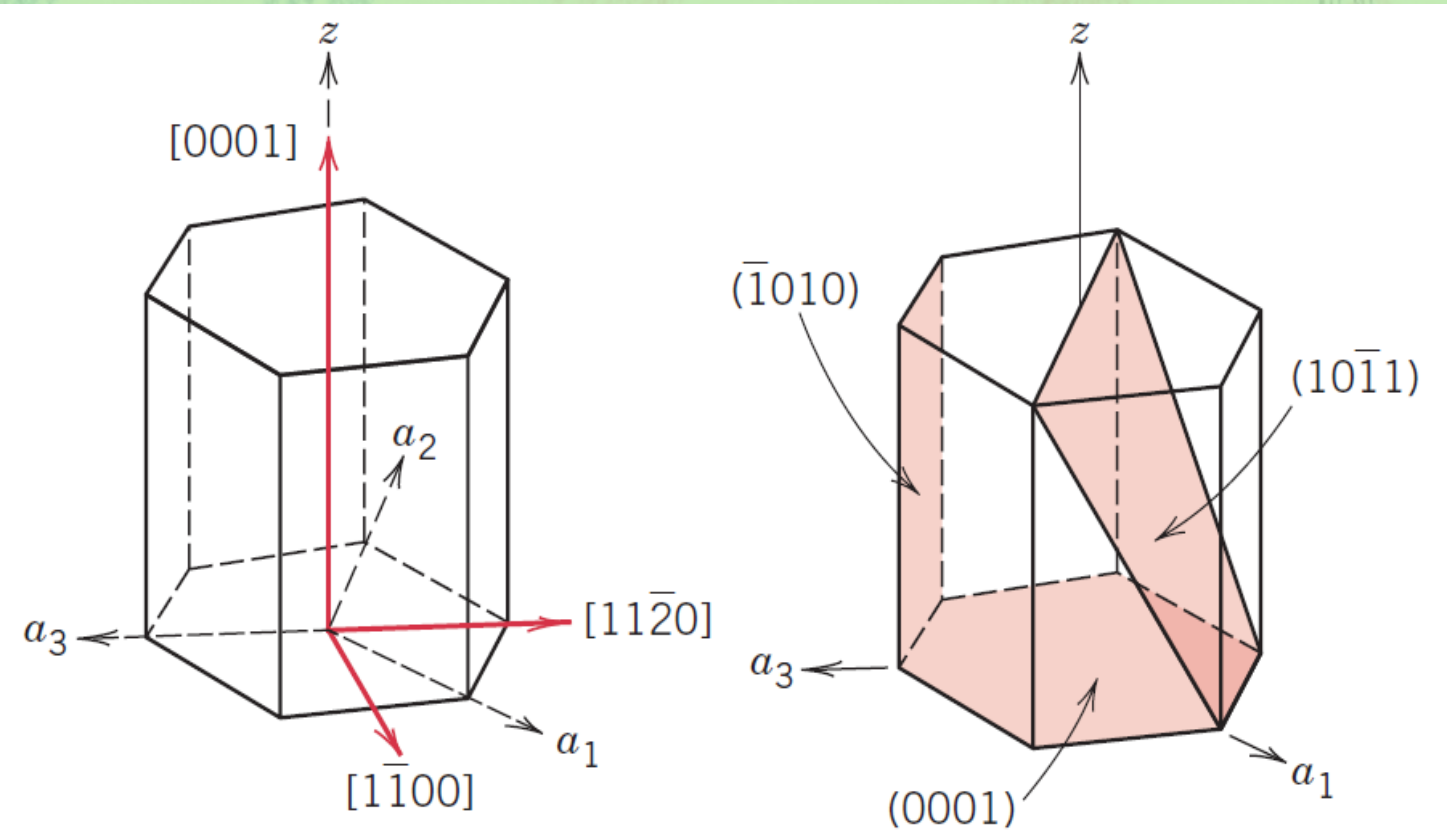


C. Smjerovi

- Osim koordinata atoma, važno je označiti i ravnine i smjerove, jer svojstva mogu ovisiti o njima (u Fe_{bcc} modul elastičnosti najveći duž dijagonale, a os najlakšeg magnetiziranja duž brida)
- [u,v,w]
- najmanji skup brojeva
- porodica smjerova, npr. <111>



- iznimka: heksagonski sustav



D. Položaji atoma

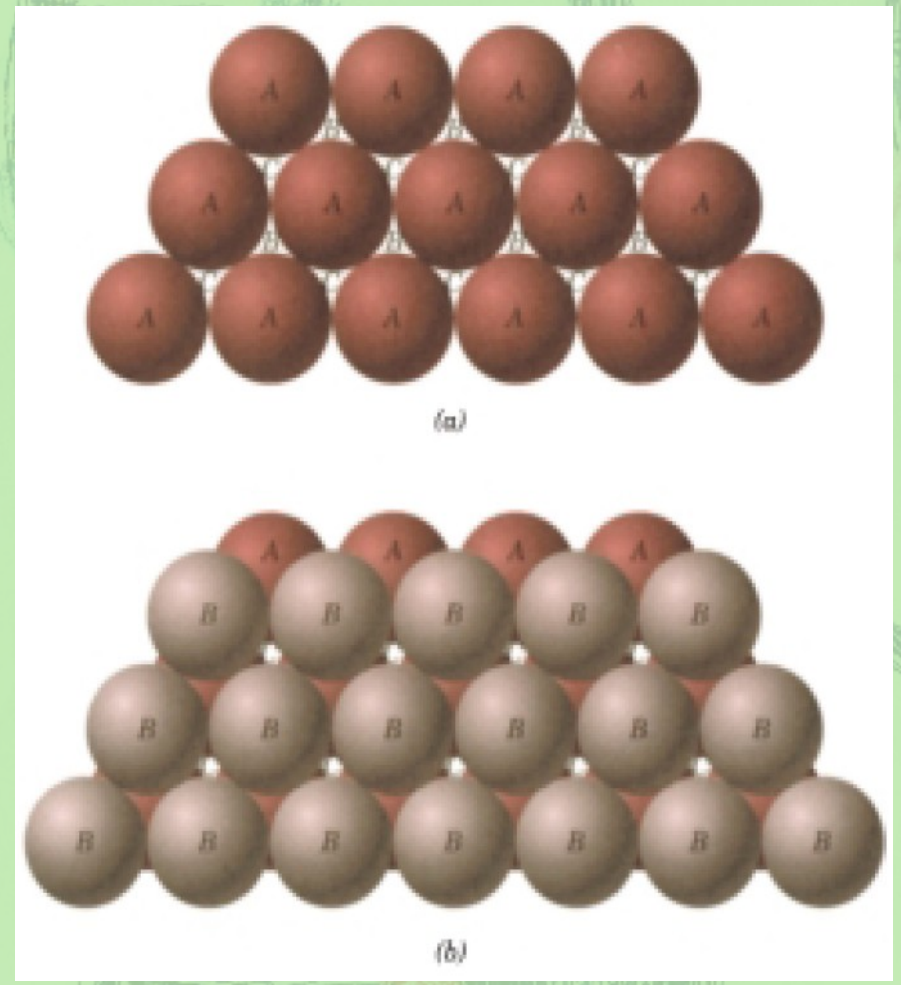
- npr. središte jedinične ćelije kubne strukture je na koordinati (a/2, b/2, c/2), to se označava kao 1/2,1/2,1/2
- u slučaju okomitih osi, udaljenosti se računaju preko korijena zbroja kvadrata

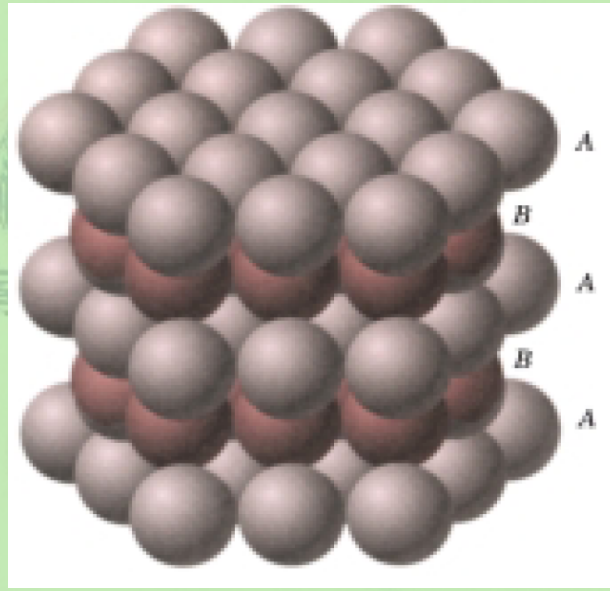
- Olakšanja uvođenjem smjerova i ravnina
  - presjecišta ravnina: $(hkl)_x(h'k'l')=[uvw]$
  - smjerovi unutar ravnina: $(hkl)\cdot[uvw]=0$
  - međuravninske udaljenosti $d_{hkl}=a/\mathrm{sqrt}(h^2+k^2+l^2)$
  - volumne, planarne i linearne gustoće

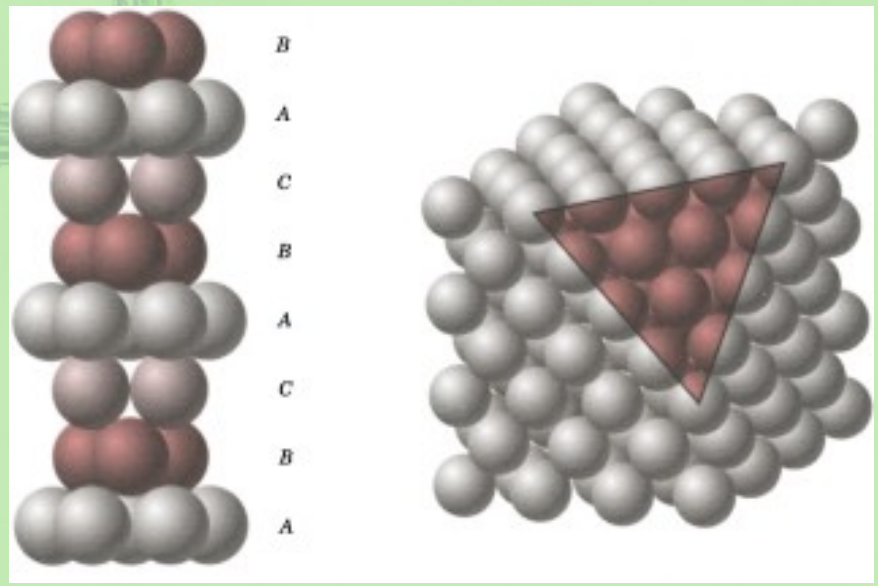
E. Neke prototipne kristalne strukture

- i) FCC (CCP)
- ii) BCC
- iii) HCP
- iv) dijamantna
- v) ZnS
- vi) CsCl
- vii) NaCl
- viii) CaF_2
- ix) $CaTiO_3$ (perovskiti)

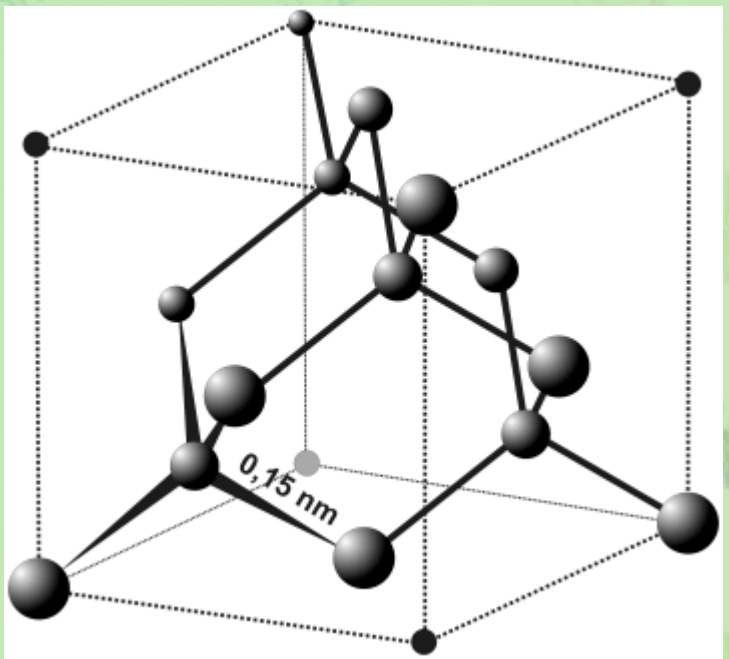
- Gusto pakirani kristali





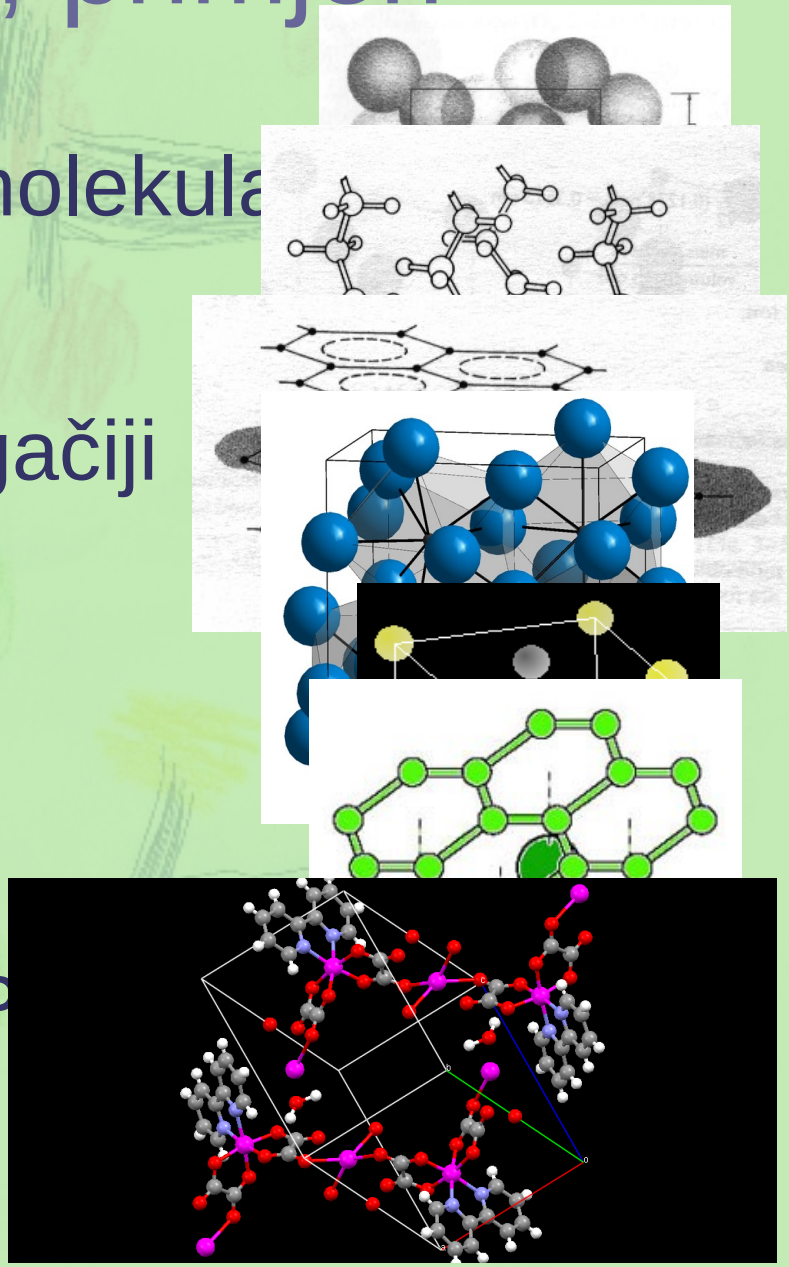


- dijamant



Nekubne strukture, primjeri

- i) jod, ortorombski, nesferna molekula
- ii) polietilen, ortorombski
- iii) grafit, heksagonski, ali drugačiji
- iv) cementit, ortorombski
- v) $BaTiO_3$, tetragonski
- vi) MgB_2, heksagonski
- vii) više nego BCC+FCC+HCP naravno!

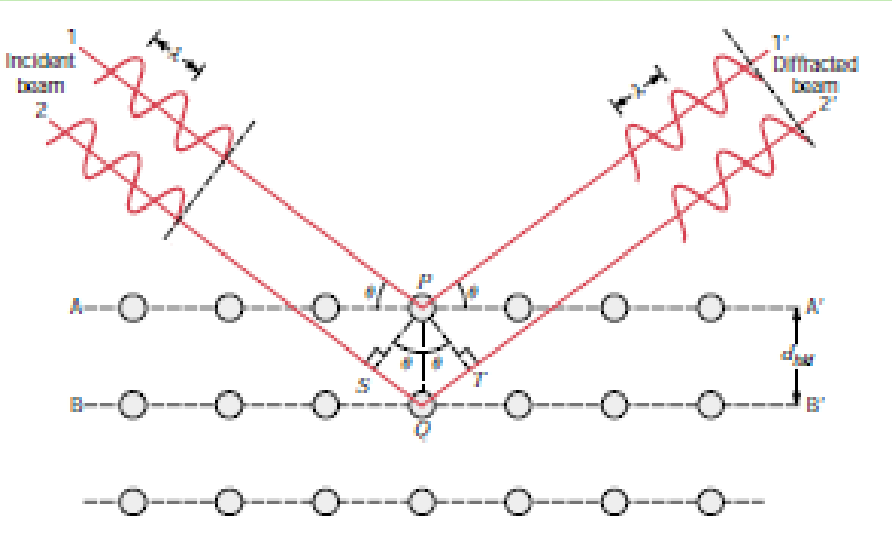


F. Polimorfizam

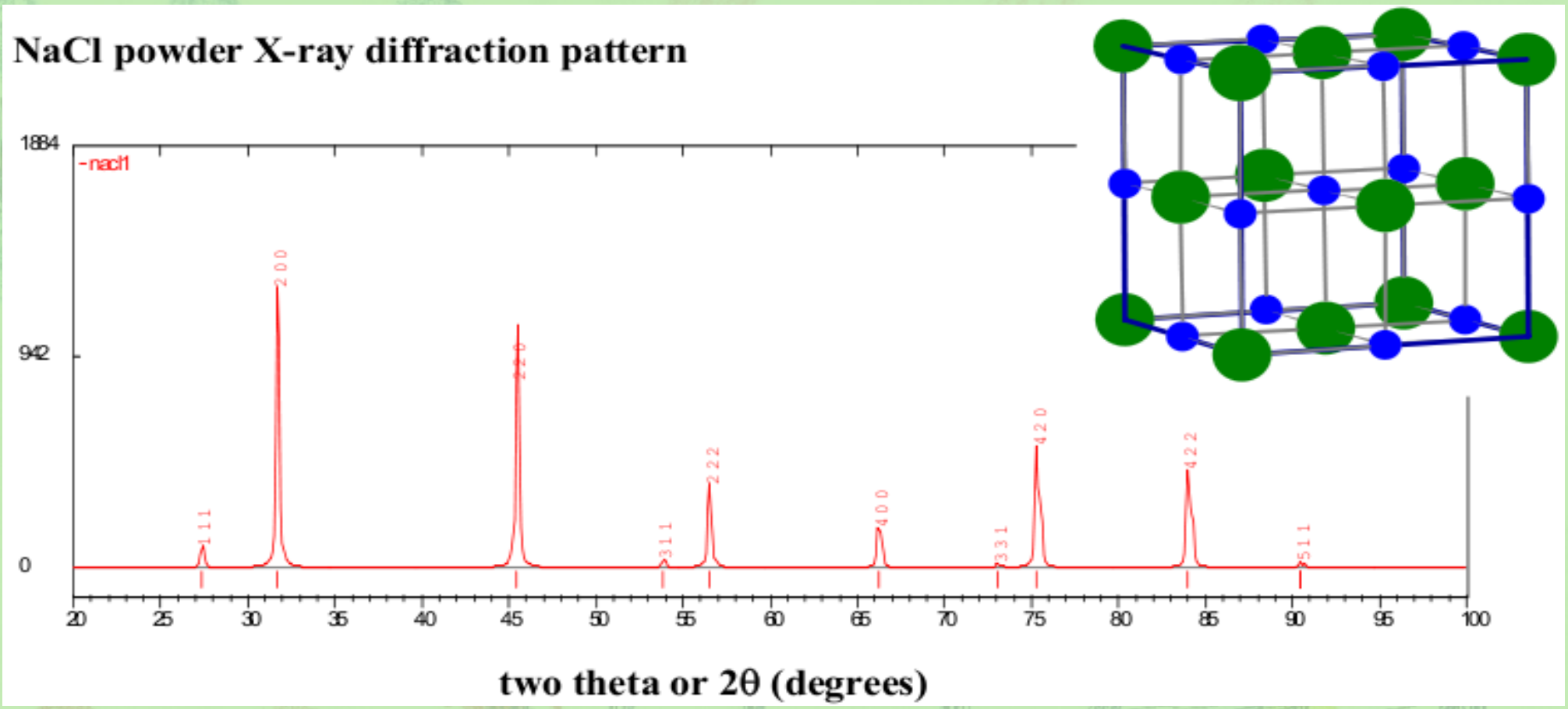
- Polimorfizam je pojava da neka tvar u različitim vanjskim uvjetima (p,T,...) ima različite kristalne strukture

G. Istraživanje kristalne strukture

- Difrakcija rentgenskih zraka



- kutevi
- intenziteti
- velika točnost (preciznost)



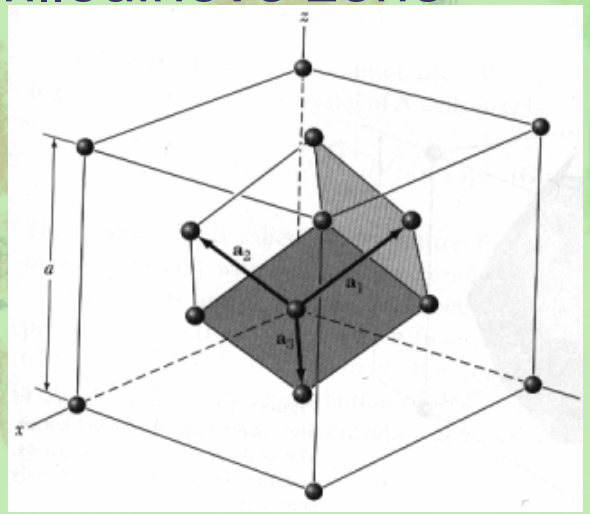
- ćelija
- ravnine
- atomi

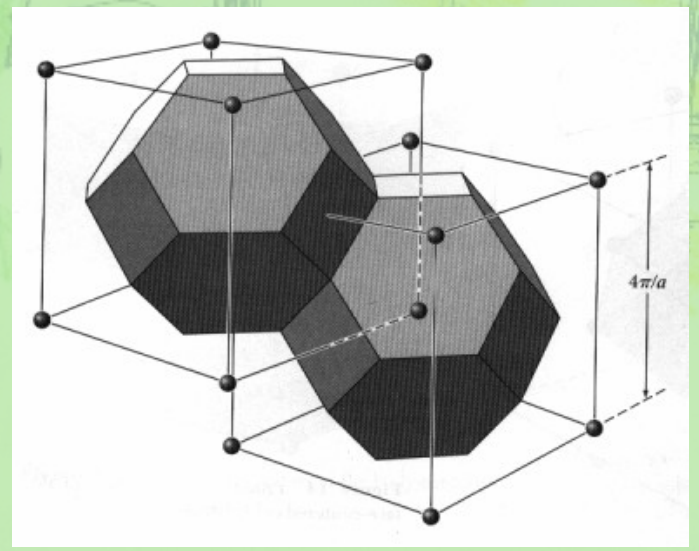
H. Recipročna rešetka

Periodičnu strukturu može se predstaviti Fourierovim razvojem. Zadatak je pronaći vektore recipročne rešetke. Iz primitivnih vektora kristalne rešetke izračunaju se primitivni vektori recipročne rešetke.

- uvjet za difrakciju
- Brillouinove zone

Primjer: FCC





rompski dodekaedar

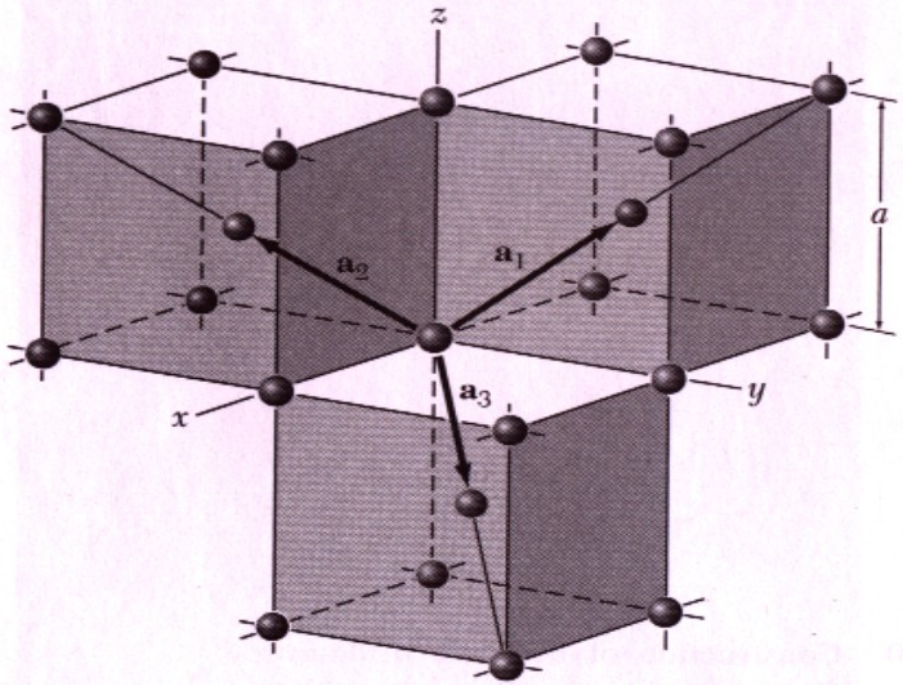


Figure 12 Primitive basis vectors of the body-centered cubic lattice.

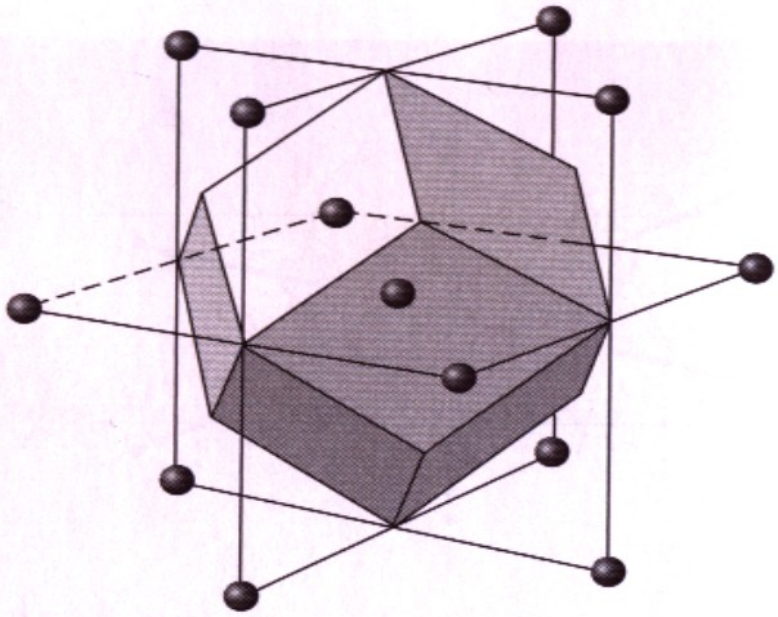
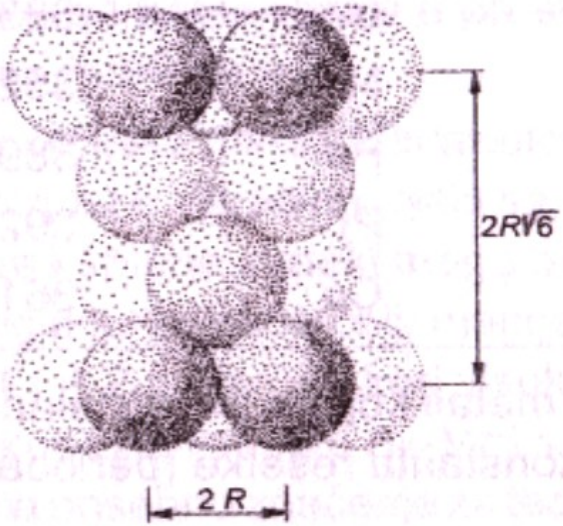
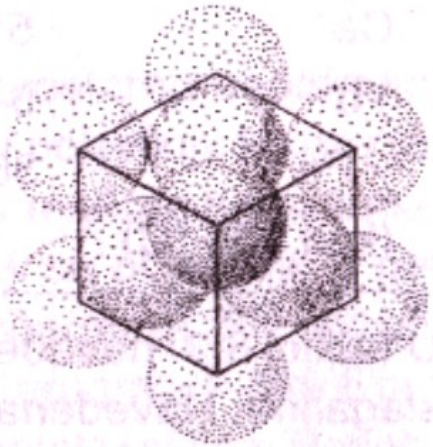


Figure 13 First Brillouin zone of the body-centered cubic lattice. The figure is a regular rhombic dodecahedron.

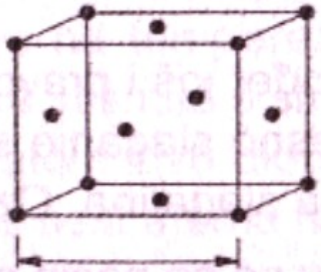
kuboktaedar



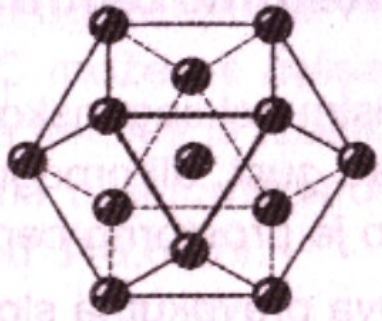
a)



b)



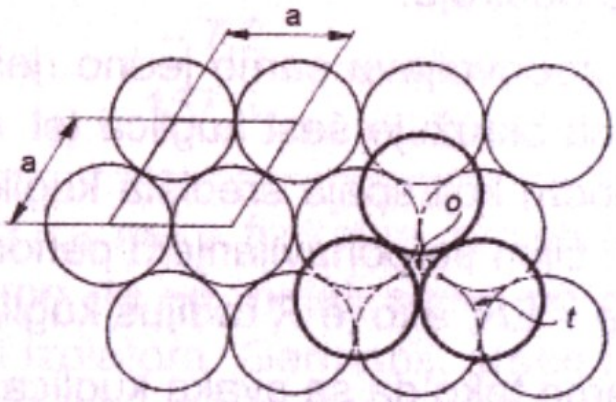
c)



d)

Sl. 8.2. Gusta kubična slagalina. **a)** Gusto slaganje slojeva u kubičnu slagalinu. **b)** Kuglice u gustoj kubičnoj slagalini razmještene su u plošnocentriranoj kocki s dijagonalom okomitom na slojeve. **c)** Plošnocentrirana kocka kao jedinična ćelija guste kubične slagaline. **d)** Kubooktaedar kao koordinacijski poliedar svake kuglice u kubičnoj gustoj slagalini.

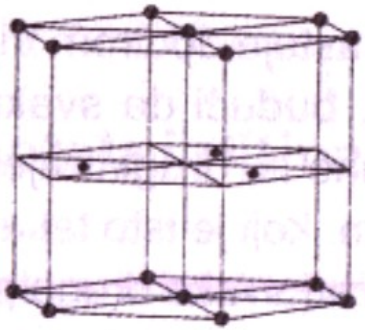
heksagonski kuboktaedar



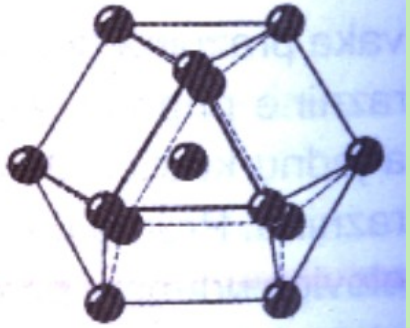
a)

b)

Sl. 8.1. Gusta heksagonska slagalina: **a)** gusti sloj kuglica, **b)** gusto slaganje slojeva u heksagonsku slagalinu, **c)** jedinična ćelija heksagonske slagaline, **d)** heksagonski kubooktaedar kao koordinacijski poliedar svake kuglice u heksagonskoj gustoj slagalini.

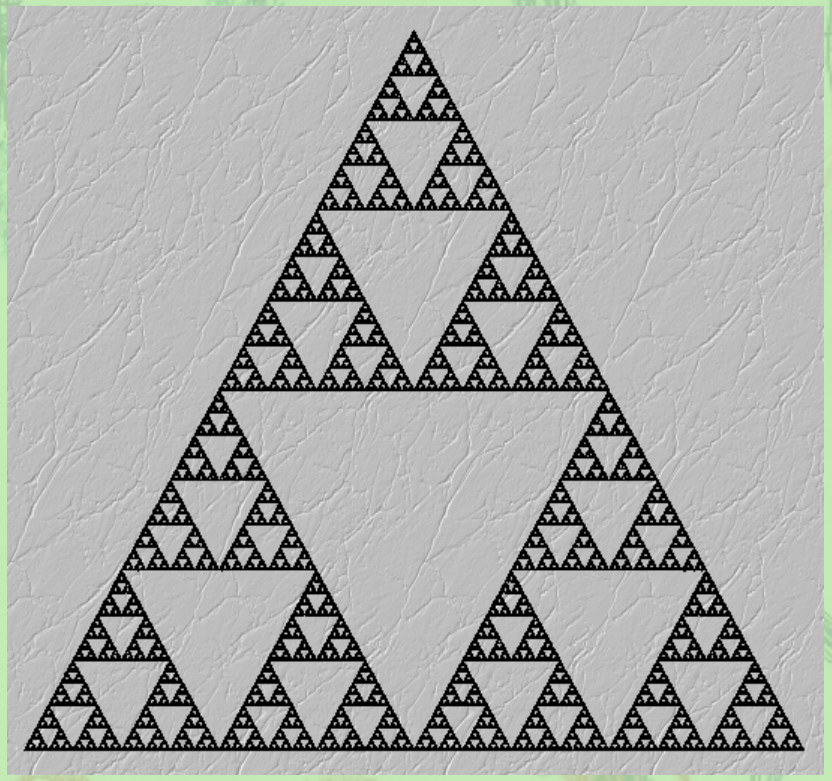


c)



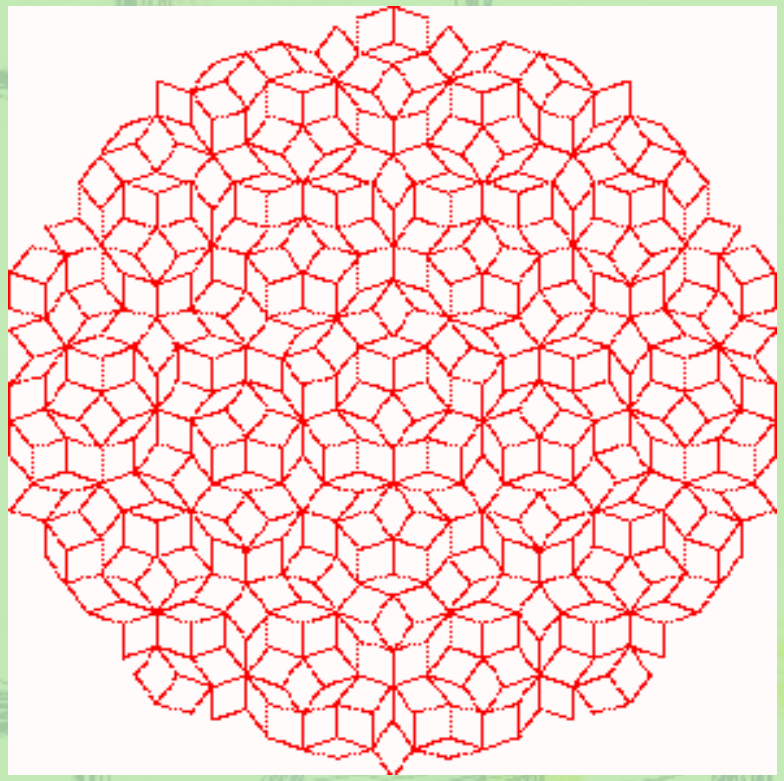
d)

I: Fraktali i kvazikristali



Trokut Sierpinskog

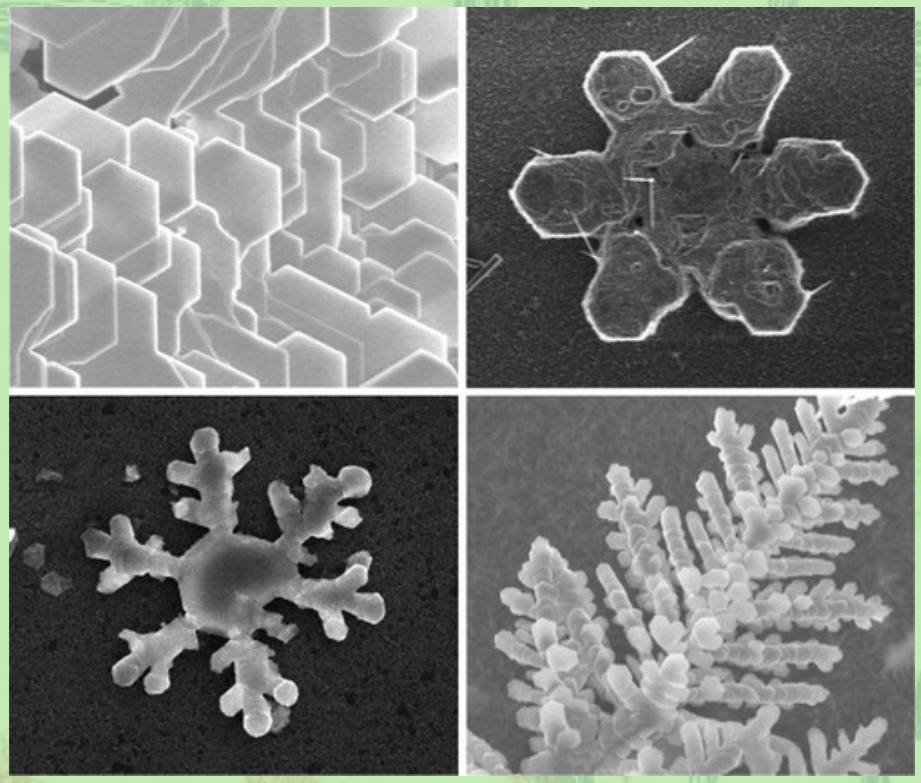
ponavlja se u sitnijim dijelovima



Penroseovo popločavanje

uređeno, bez periodičnosti

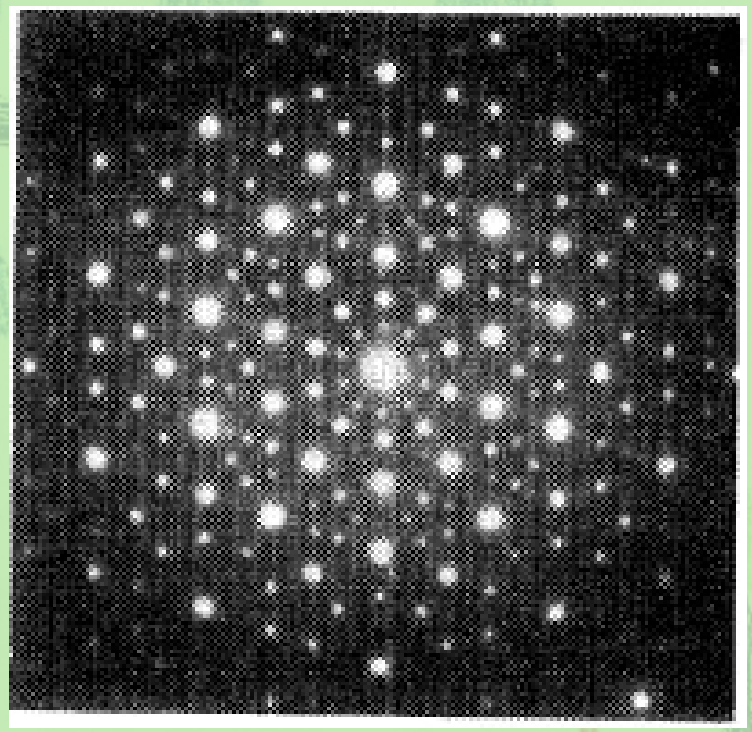
"Fraktalni kristali"



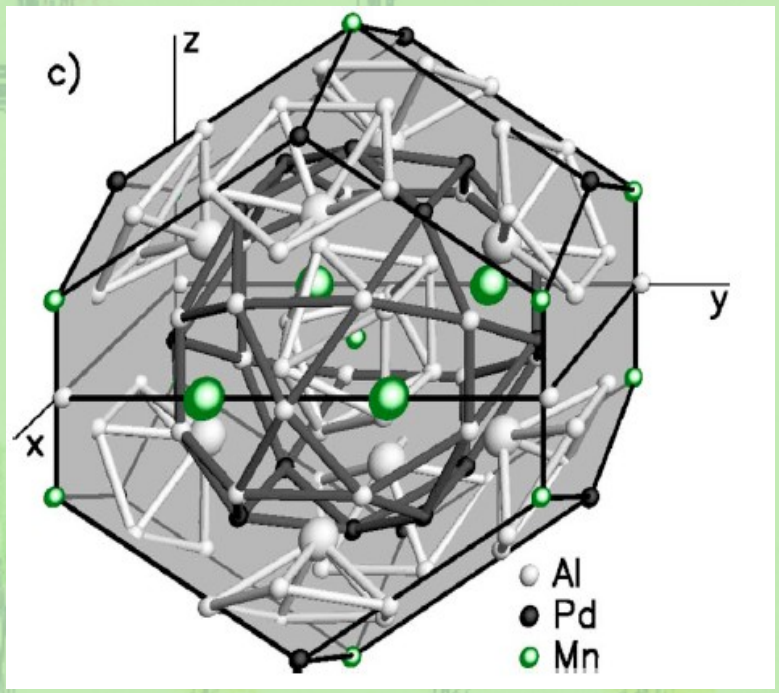
Langmuir, **25** (2009) 10223

- Zn
- Kochoida

Kvazikristal



Phys.Rev.Lett. **53** (1984) 1951



Phys.Rev.B **72** (2005) 174206

- Al s 10-14at% Mn, Fe ili Cr,
- Zn-Mg-Ho
- i-$Al_{64}Cu_{23}Fe_{13}$
- općenito: dobro vode struju, slabo vode toplinu