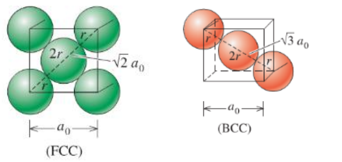
1. Odrediti zapreminu jedinične ćelije za BCC, FCC strukturu.



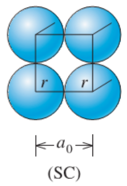
BCC

$$V_{\acute{c}} = a^3 = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

FCC

$$V_{\acute{c}} = a^3 = \left(2\sqrt{2}R\right)^3 = 16\sqrt{2}R^3$$

2. Odrediti zapreminu jedinične ćelije za SC, HCP strukturu.



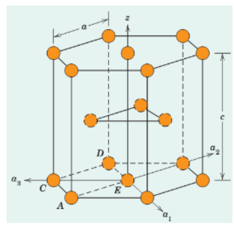
SC

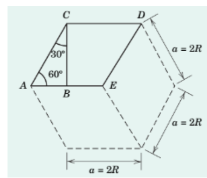
$$V_{\acute{c}} = a^3 = (2R)^3 = 8R^3$$

HCP

$$V_{\acute{c}} = B \cdot H)$$

(površina Bazisa (B=3 x površina romba ACDE) puta visina(c))





$$B = 3 \cdot (\overline{AE} \times \overline{CB}) = 3 \cdot \left(a \times \frac{a\sqrt{3}}{2}\right) = \frac{3\sqrt{3}}{2}a^2$$

$$\overline{AE} = a = 2R$$

$$\overline{CB} = a \cdot \cos 30^\circ = \frac{a\sqrt{3}}{2} = 2R\frac{\sqrt{3}}{2} = R\sqrt{3}$$

$$V_{\acute{c}} = \frac{3\sqrt{3}}{2}a^2 c = 6R^2 c\sqrt{3}$$

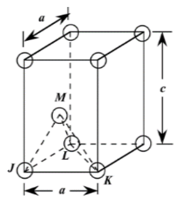
3. Pokazati da je kod HCP rešetke idealan odnos c/a = 1,633.

(Šta podrazumeva idealan odnos? Podrazumeva se da su atomi međusobno pakovani tako da je udeo slobodnog prostora najoptimalniji.)

(Analiza se može jednostavno izvesti na jednoj trećini HEP jedinice ćelije.)

(Atom (sfera) (M) nalazi se na pola visine (c), jer se na taj način postiže najgušće pakovanje → ($\overline{MH} = \frac{c}{2}$))

(Tačka (H) je projekcija tačke (M) na bazis)

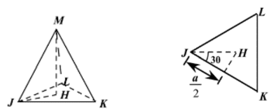


$$\overline{JM} = \overline{JK} = 2R = a$$

Iz trougla ΔJHM sledi:

$$(\overline{JM})^2 = (\overline{JH})^2 + (\overline{MH})^2$$

$$a^2 = (\overline{JH})^2 + \left(\frac{c}{2}\right)^2 \qquad (1)$$



Nepoznato je $\overline{JH}$.

(Njega možemo dobiti iz ΔJLK)

$$\cos 30^\circ = \frac{\overline{JH'}}{\overline{JH}} = \frac{\frac{a}{2}}{\overline{JH}}; \ \overline{JH} = \frac{\frac{a}{2}}{\cos 30^\circ} = \frac{\frac{a}{2}}{\frac{\sqrt{3}}{2}} = \frac{a}{\sqrt{3}};$$

Kada primenimo u jednačini (1)

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = \frac{a^2}{3} + \frac{c^2}{4};$$

Nama je potreban odnos $\frac{c}{a}$.

$$\frac{c^2}{a^2} = \frac{8}{3}; \frac{c}{a} = \sqrt{\frac{8}{3}} = 1{,}633$$

4. Odrediti faktor atomskog pakovanja za: FCC; BCC i HCP.

FCC; 4 atoma po ćeliji

$$APF = \frac{zapremina\ atoma\ u\ jednoj\ ćeliji}{zapremina\ jedne\ ćelije} = \frac{V_a}{V_ć}$$

$$V_a = 4 \times \frac{4}{3} R^3 \pi = \frac{16}{3} R^3 \pi \qquad APF = \frac{V_a}{V_ć} = \frac{\frac{16}{3} R^3 \pi}{16\sqrt{2} R^3} = 0{,}74$$

$$V_ć = a^3 = \left(2\sqrt{2}R\right)^3 = 16\sqrt{2}R^3$$

BCC; 2 atoma po ćeliji

$$V_a = 2 \times \frac{4}{3} R^3 \pi = \frac{8}{3} R^3 \pi \qquad APF = \frac{V_a}{V_ć} = \frac{\frac{8}{3} R^3 \pi}{\frac{64}{3\sqrt{3}} R^3} = 0{,}68$$

$$V_ć = a^3 = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

HCP; 6 atoma po ćeliji

$$V_a = 6 \times \frac{4}{3} R^3 \pi = \frac{24}{3} R^3 \pi = 8R^3 \pi \qquad APF = \frac{V_a}{V_ć} = \frac{8R^3 \pi}{19{,}596 R^3 \sqrt{3}} = 0{,}74$$

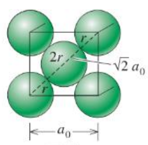
$$V_ć = 6R^2 c\sqrt{3} = 6(1{,}633 \cdot 2 \cdot R)R^2\sqrt{3} = 19{,}596 R^3 \sqrt{3}$$

$$\frac{c}{a} = 1{,}633; c = 1{,}633 \cdot a = 1{,}633 \cdot 2R$$

5. Rodijum ima atomski radijus od 0,1245[nm] i gustinu od 12,41[g/cm^3]. Odrediti da li on ima FCC ili BCC kristalnu strukturu?

(Da bi proverili koju strukturu ima, potrebno je da odredimo gustinu za FCC i BCC strukturu)

- kod FCC strukture; n = 4 atoma po ćeliji
- $V_ć = 16\sqrt{2}R^3$
- $\bar{A}_{Rh} = 102{,}91\ g/mol$



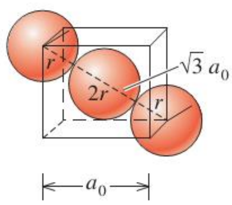
(FCC)

$$\rho = \frac{n \cdot \bar{A}_{Rh}}{V_ć \cdot N_A} = \frac{4\ atom/ćel. \cdot 102{,}91\ g/mol}{16\sqrt{2} \cdot \left(\frac{(1{,}345 \times 10^{-8} cm)^3}{1\ ćel.}\right)\left(6{,}022 \times 10^{23} \frac{atom}{mol}\right)} = 12{,}41\ g/cm^3$$

(Odatle sledi da Rh ima FCC strukturu)

6. Sračunati poluprečnik atoma vanadijuma ako on gradi BCC kristalnu strukturu i ima gustinu 5,96[g/cm^3], i ima atomsku težinu 50,9 [g/mol].

$$\rho = \frac{n \cdot \bar{A}_V}{V_ć \cdot N_A}$$



(BCC)

- n =2 atom/ćeliji

- $V_ć = \frac{64R^3}{3\sqrt{3}}$

- $\bar{A}_V = 50{,}96\ g/mol$

- $\rho = 5{,}96\ g/cm^3$

$$\rho = \frac{n \cdot \bar{A}_V}{V_ć \cdot N_A} = \frac{n \cdot \bar{A}_V}{\frac{64R^3}{3\sqrt{3}} \cdot N_A}$$

$$R = \left(\frac{3\sqrt{3} \cdot n \cdot \bar{A}_V}{64 \cdot \rho \cdot N_A}\right)^{\frac{1}{3}}$$

$$R = \left(\frac{3\sqrt{3} \cdot 2\,\frac{atom}{ćel} \cdot 50{,}96\ g/mol}{64 \cdot 5{,}95\ g/cm^3 \cdot 6{,}022 \times 10^{23}\,\frac{atom}{mol}}\right)^{\frac{1}{3}} = 1{,}32 \times 10^{-8} = 0{,}132\ nm$$

7. Neki hipotetički metal ima prostu kubnu kristalnu rešetku. Ako je njegova atomska težina 70,4[g/mol], I atomski radijus 0,126[nm], sračunati njegovu gustinu.

- n =1 atom/ćeliji
- $V_ć = 8R^3$
- $\bar{A}_ć = 70{,}4\ g/mol$
- $R = 0{,}126\ nm = 1{,}26 \times 10^{-8}\ cm$

$$\rho = \frac{n \cdot \bar{A}_ć}{V_ć \cdot N_A} = \frac{1\,\frac{atom}{ćel} \cdot 70{,}4\ g/mol}{\left(2 \cdot (1{,}26 \times 10^{-8} cm)\right)^3 \cdot 6{,}022 \times 10^{23}\,\frac{atom}{mol}}$$

$\rho = 7{,}31\ g/cm^3$

8. Odrediti poluprečnik atoma iridijuma ako on gradi FCC strukturu, ima gustinu 22,4 [g/cm^3], i atomsku težinu 192,2 [g/mol].

- kod FCC strukture; n = 4 atoma po ćeliji
- $V_ć = 16\sqrt{2}R^3$

$$\rho = \frac{n \cdot \bar{A}_{Rh}}{V_ć \cdot N_A} = \frac{n \cdot \bar{A}_{Rh}}{16\sqrt{2}R^3 \cdot N_A}$$

$$R = \left(\frac{n \cdot \bar{A}_V}{16\sqrt{2} \cdot \rho \cdot N_A}\right)^{\frac{1}{3}} = \left(\frac{4\,\frac{atom}{ćel} \cdot 192{,}2\ g/mol}{16 \cdot 22{,}4\ g/cm^3 \cdot \sqrt{2} \cdot 6{,}022 \times 10^{23}\,\frac{atom}{mol}}\right)^{\frac{1}{3}} = 0{,}136\ nm$$

9. Ukoliko je radijus atoma aluminijuma 0,143[nm] odrediti zapreminu njegove jedinične ćelije u kubnim metrima.

Al ima FCC strukturu

$$V_ć = 16\sqrt{2}R^3 = 16 \cdot (0{,}143 \times 10^{-9} m)^3 \cdot \sqrt{2} = 6.62 \times 10^{-29} m^3$$

10. Gvožđe ima BCC kristalnu strukturu, atomski radijus od 0,124[nm], i atomsku težinu od 55,85[g/mol]. Odrediti teorijsku gustinu gvožđa.

$$\rho = \frac{n \cdot \bar{A}_{Rh}}{V_ć \cdot N_A}$$

BCC struktura; n=2 atoma/ćeliji

$$V_ć = a^3 = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}$$

$$N_A = 6{,}022 \times 10^{23}\,\frac{atom}{mol}$$

$$R = 0{,}124\text{ nm} = 0{,}124 \times 10^{-7}\,cm$$

$$\rho = \frac{n \cdot \bar{A}_{Rh}}{V_ć \cdot N_A} = \frac{2 \cdot 55{,}85\,g/mol}{\frac{64}{3\sqrt{3}} \cdot (0{,}124 \times 10^{-7}cm)^3 \cdot 6{,}022 \times 10^{23}\,\frac{atom}{mol}} = 7{,}9\,g/cm^3$$

11. Zironijum ima HCP kristalnu strukturu i gustinu od 6,51 g/cm^3. a) Kolika je zapremina njegove jedne ćelije u kubnim metrima? b) Koliko je c/a odnos 1,593 odrediti vrednosti c i a.

a)

- HCP;n=6 atoma po ćeliji
- $\bar{A}_{Zr} = 91{,}22\,g/mol$

$\rho = \frac{n \cdot \bar{A}_{Zr}}{V_ć \cdot N_A}$; $V_ć = \frac{n \cdot \bar{A}_{Zr}}{\rho \cdot N_A}$

$$V_ć = \frac{n \cdot \bar{A}_{Zr}}{\rho \cdot N_A} = \frac{6\,\frac{atom}{ćel} \cdot 91{,}22\,\frac{g}{mol}}{6{,}51\,\frac{g}{cm^3} \cdot 6{,}022 \times 10^{23}\,\frac{atom}{mol}} = 1{,}396 \times 10^{-22}\,\frac{cm^3}{ćel} = 1{,}396 \times 10^{-28}\,\frac{cm^3}{ćel}$$

b)

Zapremina HEP je: $V_ć = 6R^2 c\sqrt{3}$

Takođe → a=2R → $V_ć = 6\left(\frac{a}{2}\right)^2 c\sqrt{3} = \frac{3\sqrt{3}}{2}a^2 c$

$\frac{c}{a} = 1{,}593 \rightarrow c = 1{,}593 \cdot a$

$$V_ć = \frac{3\sqrt{3}}{2}a^2 c = \frac{3\sqrt{3}}{2} \cdot 1{,}593 \cdot a^3 = 1{,}396 \times 10^{-28}\,\frac{m^3}{ćel}$$

$$a = 3{,}23 \times 10^{-8}\,cm = 0{,}323\,nm$$

$$c = 1{,}593 \cdot 0{,}323 = 0{,}515\,nm$$

12. Kalaj gradi tetragonalnu jediničnu ćeliju sledećih parametara: a=0,583 nm i c=0,318 nm. Ukoliko su vrednosti gustine $\rho = 7{,}3\,\frac{g}{cm^3}$, atomske težine $n = 118{,}69\,\frac{g}{mol}$ i radijusa $R = 0{,}151\,nm$, odrediti APF.

(Da bi se odredio APF potrebno je najpre utvrditi broj atoma u jednoj ćeliji)

$a = 0{,}583\,nm = 5{,}83 \times 10^{-8}\,cm$

$V_ć = a^2 \cdot c$

$\rho = \frac{n \cdot \bar{A}_{Sn}}{V_ć \cdot N_A} \rightarrow n = \frac{\rho \cdot V_ć \cdot N_A}{\bar{A}_{Sn}}$

$$n = \frac{\rho \cdot V_ć \cdot N_A}{\bar{A}_{Sn}} = \frac{7{,}3\,\frac{g}{cm^3} \cdot (5{,}83)^2 \cdot (3{,}18) \times 10^{-24}\,\frac{cm^3}{ćel} \cdot 6{,}022 \times 10^{23}\,\frac{atom}{mol}}{118{,}69\,g/mol} = 4\,\frac{atom}{ćel}$$

$$APF = \frac{V_a}{V_ć} = \frac{4 \cdot \left(\frac{4}{3} R^3 \pi\right)}{a^2 \cdot c} = \frac{4 \cdot \left(\frac{4}{3}(1{,}51 \times 10^{-8}\ cm)^3 \pi\right)}{(5{,}83 \times 10^{-8} cm)^2 \cdot (3{,}18 \times 10^{-8} cm)}$$

$$APF = 0{,}534$$

13. Jod ima ortogonalnu jediničnu ćeliju koja ima sledeće parametre rešetke: a=0,479 nm i b=0,725 mn c=0,978 nm.
    a) Ukoliko je APF=0,547 i atomski radijus R=0,177 nm. Odrediti broj atoma u jednoj ćeliji.
    b) Atomska težina joda je 126,91 g/mol. Odrediti teorijsku gustinu

a)

$$APF = \frac{n \cdot V_a}{V_ć}$$

$$n = \frac{APF \cdot V_ć}{V_a} = \frac{APF \cdot abc}{\frac{4}{3} R^3 \pi}$$

$$V_a = \frac{4}{3} R^3 \pi$$

$$V_ć = abc$$

$$n = \frac{APF \cdot abc}{\frac{4}{3} R^3 \pi} = \frac{(0{,}547) \cdot (4{,}79 \times 10^{-8}\ cm) \cdot (7{,}25 \times 10^{-8}\ cm) \cdot (9{,}78 \times 10^{-8}\ cm)}{\frac{4}{3}(1{,}77 \times 10^{-8}\ cm)^3 \pi} = 8$$

b)

$$\rho = \frac{n \cdot \bar{A}_I}{V_ć \cdot N_A}$$

$$\rho = \frac{8 \frac{atoma}{ćel} \cdot 126{,}91 \frac{g}{mol}}{(4{,}79 \times 10^{-8}\ cm) \cdot (7{,}25 \times 10^{-8}\ cm) \cdot (9{,}78 \times 10^{-8}\ cm) \cdot 6{,}022 \times 10^{23} \frac{atom}{mol}} = 4{,}96 \frac{g}{cm^3}$$

14. Titanijum ima HCP jediničnu ćeliju koja ima sledeće parametre rešetke: a=2R i c/a=1,58. Ako je radijus Ti atoma 0,1445 nm. a) Odrediti zapreminu jedne ćelije. b) Sračunati gustinu Ti.

a)

$$V_ć = 6R^2 c\sqrt{3}$$

kod Ti; $c = 1{,}58 \cdot a = 2 \cdot 1{,}58 \cdot R = 3{,}16 \cdot R$

$$V_ć = 6R^2 c\sqrt{3} = 6 \cdot (3{,}16) R^3 \sqrt{3}$$

$$V_ć = 6 \cdot (1{,}445 \times 10^{-8}\ cm)^3 \cdot (3{,}16)\sqrt{3} = 9{,}91 \times 10^{-23} \frac{cm^3}{ćel}$$

b)

Teorijska gustina za Ti je:

$$\rho = \frac{n \cdot \bar{A}_{Ti}}{V_ć \cdot N_A}$$

n=6

$$\rho = \frac{6\,\frac{atoma}{ćel} \cdot 47{,}87\,\frac{g}{mol}}{9{,}91 \times 10^{-23}\,\frac{cm^3}{ćel} \cdot 6{,}022 \times 10^{23}\,\frac{atom}{mol}} = 4{,}81\,\frac{g}{cm^3}$$

15. Cink ima HEP strukturu sa c/a odnosom c/a=1,856 i gustinom od 7,13 g/cm^3. Odrediti radijus za Zn.

HEP:

$$\mathrm{V}_{ć} = 6R^2c\sqrt{3}$$

$$\mathrm{c} = 1{,}856 \cdot \mathrm{a} = 2 \cdot 1{,}856 \cdot \mathrm{R} = 3{,}712 \cdot \mathrm{R}$$

$$\mathrm{V}_{ć} = 6R^2c\sqrt{3} = 6 \cdot (3{,}712) \cdot R^3\sqrt{3} = 22{,}272 \cdot R^3\sqrt{3}$$

$$\rho = \frac{n \cdot \bar{A}_{Zn}}{\mathrm{V}_{ć} \cdot N_A} = \frac{6 \cdot 65{,}41\,\frac{g}{mol}}{22{,}272 \cdot R^3\sqrt{3} \cdot 6{,}022 \times 10^{23}\,\frac{atom}{mol}}$$

$$R = \left(\frac{n \cdot \bar{A}_{Zn}}{22{,}272 \cdot \sqrt{3} \cdot \rho \cdot N_A}\right)^{\frac{1}{3}} = \left(\frac{6 \cdot 65{,}41\,\frac{g}{mol}}{22{,}272 \cdot \sqrt{3} \cdot 7{,}13\,\frac{g}{cm^3} \cdot 6{,}022 \times 10^{23}\,\frac{atom}{mol}}\right)^{\frac{1}{3}}$$

$$R = 1{,}333 \times 10^{-8}cm = 0{,}1333\ nm$$