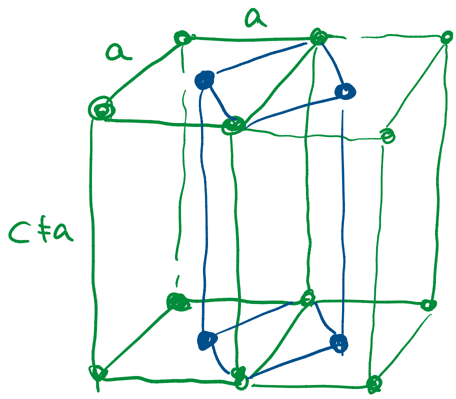
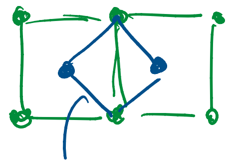
Übungen 1-5

Freitag, 29. September 2023 07:46

Afg 1

tetragonal basiszentriertes Bravaisgitter



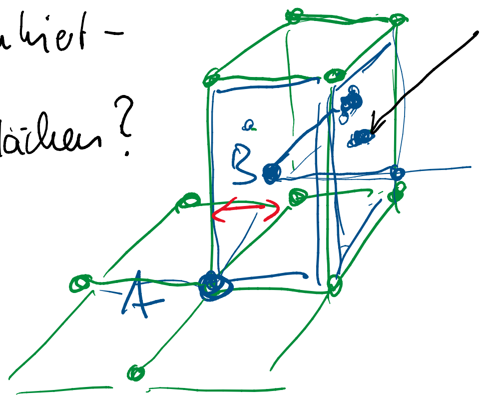


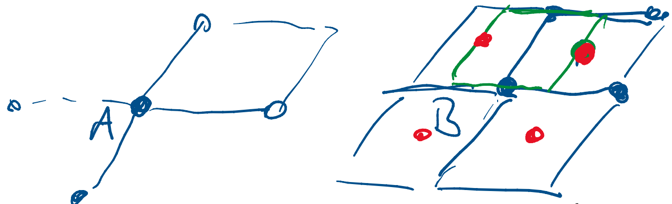
tetragonal primitive

primitives Gitter zeigt dieselben Symmetrien

basiszentriert - andere Seitenflächen?

4 Seitenflächen! Symmetrie!





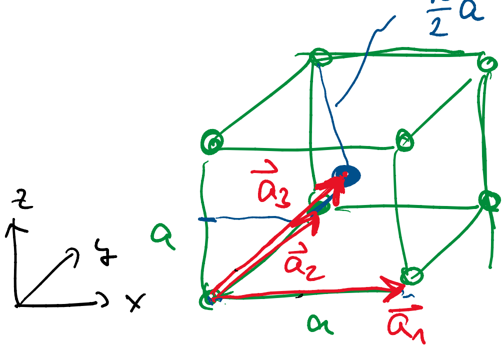
kein Bravaisgitter!

Afg 2:

Kubisch innenzentriertes Gitter

bcc (body-centered cubic) (fcc in Klammern)

primitive 3 Gittervektoren



- Volumen der EZ: $V_{EZ} = a^3$ (a^3)

(4) 2 Atome $\hat{=}$ 2 primitive EZ

- Volumen der EZ: $V_{EZ} = a$ (...)
- # primitive Gitterpunkte in EZ 2 Atome $\hat{=}$ 2 primitive EZ (4)
- Volumen der primitiven EZ $V_{prim} = \frac{V_{EZ}}{2}$ $\left(\frac{V_{EZ}}{4}\right)$

prim. Gittervektoren $\vec{a}_1, \vec{a}_2, \vec{a}_3$

Volumen = Spatprodukt $= (\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3 = V_{prim}$

$$\vec{a}_1 = a \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \vec{a}_2 = a \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \vec{a}_3 = \cancel{\sqrt{3}} \frac{a}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\cancel{\sqrt{3}}} = \frac{a}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$V_{prim} = \frac{a^3}{2}.$$

- Koordinationszahl 8 im Abstand $d_{NN} = \frac{\sqrt{3}}{2} a$

(fcc: 8 $d_{NN} = \frac{\sqrt{2}}{2} a$)

- Packungsdichte (filling factor)

1 Kugel pro primitiven Gitterpunkt: 2 Punkte

$$R = \frac{d_{NN}}{2} = \frac{\sqrt{3}}{4} a$$

$$2 \, \frac{4\pi}{3} R^3 = \frac{8\pi}{3} a^3 \left(\frac{\sqrt{3}}{4}\right)^3 = 0.68 a^3$$

Packungsdichte 68 %

(fcc 4 Kugel pro EZ $\Rightarrow$ $V_{AF} = 0.74 a^3 \Rightarrow 74\%$)

"dichteste Kugelpackung"

Afg 3: Gitterkonstante Au (fcc)

$$S_m = 19.3 \, g/cm^3$$

aus Afg 2: $d_{NN} = \frac{\sqrt{2}}{2} a$ $\quad R = \frac{d_{NN}}{2}$ atomic mass units

Periodensystem Au $M = 197 \, g/mol$ (amu)

Periodensystem Au $M = 197\ g/mol$ (amu)

$\rho_m = 19.3\ g/cm^3 \Rightarrow \rho = \frac{19.3\ g/cm^3}{197\ g/mol} \cdot N_A = 5.9 \times 10^{22}\ cm^{-3}$
Anzahldichte

$V_{1\,Atom} = \rho^{-1} = 1.695 \times 10^{-23}\ cm^3 = 16.95\ Å^3$

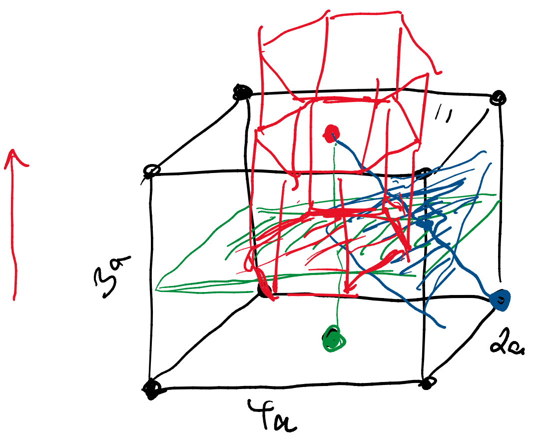
$V_{EZ} = 4 V_1 = 67.79\ Å^3 \underset{fcc}{=} a^3$

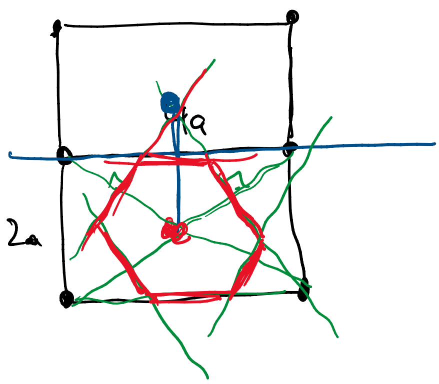
$\Rightarrow a = \sqrt[3]{4V_1} = \underline{\underline{4.08\ Å}}$

$d_{NN} = \frac{\sqrt{2}}{2} a = 2.88\ Å$ $R = 1.44\ Å = 144\ pm$

(Wikipedia: Au-Atom 166 pm
kovalente Radius 136 pm)

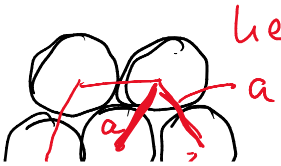
<u>Afg 4:</u> Wigner-Seitz-Zelle orthor. Basisvekn.
$a_1 : a_2 : a_3 = 4 : 2 : 3$



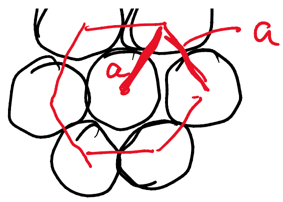


<u>Afg 5:</u> Dichteste Kugelpackungen

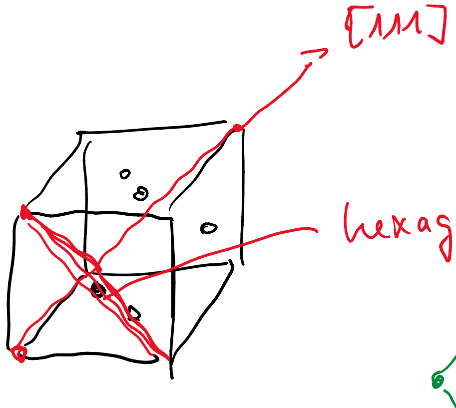
in 2D:



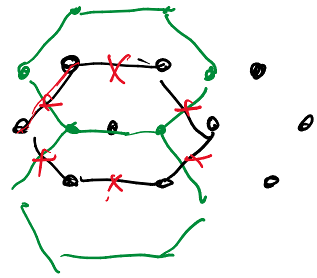
hexagonal
überall gleiche Abstände



überall gleiche Abstände



hexagonale Ebenen



Stapelfolge A - B - C → fcc

A - B - A - B hcp

hexagonal close packed

Problem: Abstand zweier Ebenen

$$c = \frac{2\sqrt{2}}{\sqrt{3}} a = 1.633\, a \quad \text{für hcp und fcc}$$

→ Füllfaktor $\frac{\pi}{6}\sqrt{2} = \underline{\underline{74\%}}$.