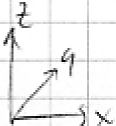
A1

a) bcc: $\vec{a}_1 = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} a$, $\vec{a}_2 = \begin{pmatrix} 1/2 \\ -1/2 \\ -1/2 \end{pmatrix} a$, $\vec{a}_3 = \begin{pmatrix} 1/2 \\ 1/2 \\ -1/2 \end{pmatrix} a$



$$\vec{b}_1 = \frac{2\pi}{V_{EZ}} \vec{a}_2 \times \vec{a}_3 \quad , \quad V_{EZ} = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$$

$$= \begin{pmatrix} 1/2 \\ 1/2 \\ +1/2 \end{pmatrix} \cdot \begin{pmatrix} 1/2 \\ 1/2 - 1/2 \\ 1/2 \end{pmatrix} = \frac{1}{2} a^3$$

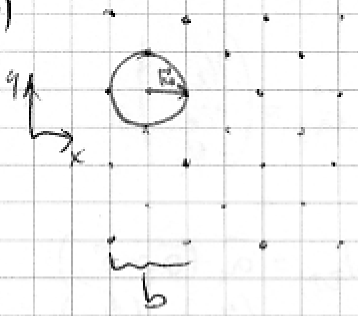
$$\rightarrow \vec{b}_1 = \frac{4\pi}{a^3} \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix} a^2 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

$$\vec{b}_2 = \frac{4\pi}{a^3} \vec{a}_3 \times \vec{a}_1 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

$$\vec{b}_3 = \frac{4\pi}{a^2} \vec{a}_1 \times \vec{a}_2 = \frac{2\pi}{a} \begin{pmatrix} 0 \\ -1 \\ -1 \end{pmatrix}$$

→ fcc-Gitter im rez. Raum

b)



$\cancel{k_{0,min} = \frac{b}{2} = \frac{\sqrt{2}\,2\pi}{2a} = \frac{\sqrt{2}\pi}{a}}$

$\cancel{b = \sqrt{2}\,\frac{2\pi}{a}}$

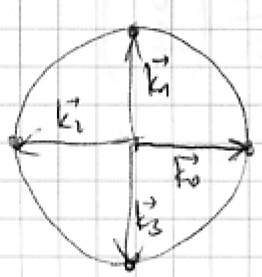
$\cancel{b = \frac{2\pi}{a}}$

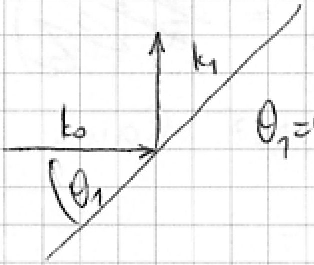
primitiver Gittervektor → $\cancel{k_{0,min} = \frac{b}{2}}$

$$b = \sqrt{2}\,|\vec{b}_1| = \frac{4\pi}{a}$$

$$k_{0,min} = \frac{b}{2} = \frac{2\pi}{a}$$

c)





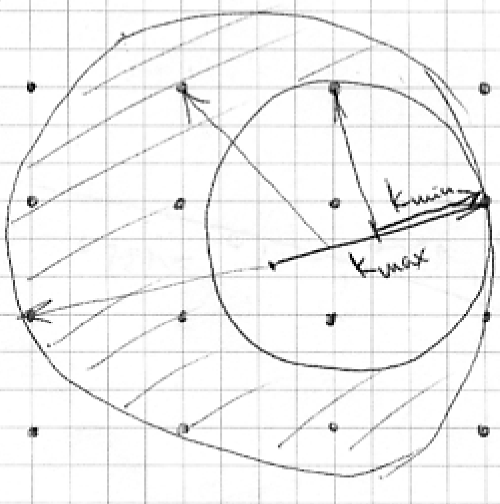
$\theta_1 = 45° \rightarrow (1\bar{1}0)$

$\theta_2 = 90°$, $\theta_3 = -45°$

$\downarrow$ (100) $\quad$ $\downarrow$ (110)

d)

<u>Laue:</u>

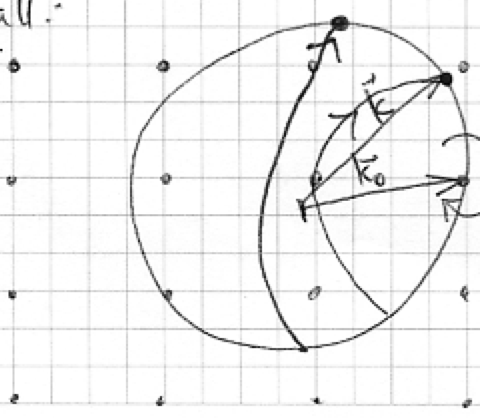


kontinuierliches Spektrum

→ $k_{min} \leq k \leq k_{max}$

⇒ alle • im //-Bereich können zu Reflexen beitragen

<u>Drehkristall:</u>



monochromatisch

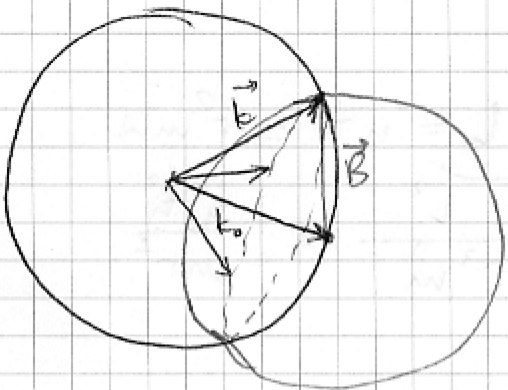
Drehung des Kristalls/Gitters

→ bei bestimmten Winkeln liegen Gitterpunkte auf Kreislinie

→ viele Reflexe

Debye-Scherrer

Pulverprobe, monochromatisch



$\vec{B}$ zufällig orientiert → zeigt auf die Oberfläche der O Kugel

→ Reflexe auf Kegeloberfläche

A2

a) $$\frac{N_L}{N}\Big|_{0{,}9T_M} = e^{S_L/k_B}\, e^{-\frac{E_L}{k_B T}} = 61{,}0 \cdot 10^{-6}$$

$$\frac{N_L}{N}\Big|_{20°C} = 2{,}32 \cdot 10^{-20}$$

b) $$\left.\begin{aligned} \Delta V &= V_{Ez} \cdot N_L \\ V &= V_{Ez} \cdot (N + N_L) \end{aligned}\right\} \quad \frac{\Delta V}{V} = \frac{N_L}{N + N_L} \approx \frac{N_L}{N}$$

A3

a) $F_C = -\frac{e^2}{4\pi\varepsilon_0\varepsilon_r r^2}$

$F_Z = m\omega^2 r$, $L = n\hbar = r^2 m\omega$

$\rightarrow -\frac{e^2}{4\pi\varepsilon_0\varepsilon_r r} = m\omega^2 r = \frac{L^2}{r^3 m} = \frac{n^2\hbar^2}{mr^3}$

$\Rightarrow r_n = \frac{4\pi\varepsilon_0\varepsilon_r n^2\hbar^2}{me^2}$

Energie $E_n = -\frac{1}{2}\frac{e^2}{4\pi\varepsilon_0\varepsilon_r r_n} = \int_r^\infty F_C\,dr$

$= -\frac{e^4 m}{8\pi\varepsilon_0\varepsilon_r 4\pi\varepsilon_0\varepsilon_r n^2\hbar^2} = -\frac{me^4}{32\pi^2\varepsilon_0^2\varepsilon_r^2 n^2\hbar^2}$

$= -\frac{me^4}{8\varepsilon_0^2\varepsilon_r^2 h^2 n^2}$

$\Delta E \overset{!}{=} E_2 - E_1 = -\frac{me^4}{8\varepsilon_0^2 n'^4 h^2}\left(\frac{1}{4}-1\right) = \frac{3me^4}{32\,\varepsilon_0^2 n'^4 h^2}$

b) Potentialtopf: $V(r) = \begin{cases} 0, & 0<r<R_0 \quad \mathrm{I} \\ \infty, & r \geq R_0 \quad \mathrm{II} \end{cases}$

I: SGL $-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(r) = E\psi(r)$

$\rightarrow \psi(r) = e^{\lambda r} \Rightarrow -\frac{\hbar^2}{2m}\lambda^2 = E$, $\lambda = \pm i\frac{\sqrt{2mE}}{\hbar}$

$\rightarrow \psi_{\mathrm{I}}(r) = c_1 e^{i\frac{\sqrt{2mE}}{\hbar}r} + c_2 e^{-i\frac{\sqrt{2mE}}{\hbar}r}$, $k := \frac{\sqrt{2mE}}{\hbar}$ Sur

Anschl. bed. (nach Versch. um R_0)

$$\psi(0) = 0 = \psi(2R_0)$$

$$\Rightarrow \quad c_1 + c_2 = 0$$

$$c_1 \left(e^{2i\varkappa R_0} - e^{-2i\varkappa R_0} \right) = 0$$

$$\rightarrow \quad e^{4i\varkappa R_0} = 1$$

$$\Rightarrow \quad 4\varkappa R_0 = n \cdot 2\pi \quad , n \in \mathbb{Z}$$

$$\rightarrow \quad 2\varkappa R_0 = n\pi$$

$$\Rightarrow \quad n\pi = 2R_0 \frac{\sqrt{2mE}}{\hbar}$$

$$\Rightarrow \quad E_n = \left(\frac{n\pi\hbar}{2R_0} \right)^2 \cdot \frac{1}{2m}$$

$$\Rightarrow \quad E_p = E_2 - E_1 = \frac{3\pi^2\hbar^2}{8R_0^2 m} = \frac{3h^2}{32 R_0^2 m}$$

$\parallel \frac{a}{2}$ ← Gitterkonst.

	$2R_0$/Å	n'	E_p/eV	E_w/eV
LiF	4,02	1,41	6,98	2,58
NaCl	5,64	1,56	3,55	1,72
RbI	7,34	1,65	2,09	1,38