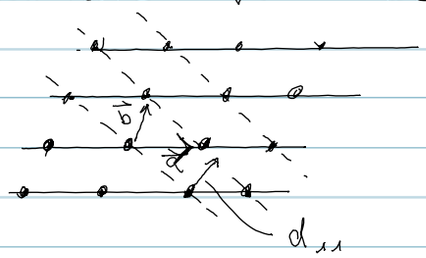
2.4. Netzebenen

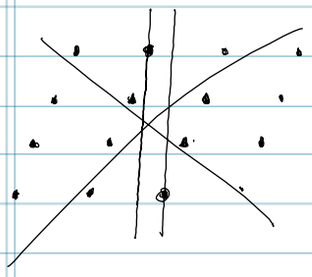
Scharen von Ebenen : ∥ äquidistante Ebenen



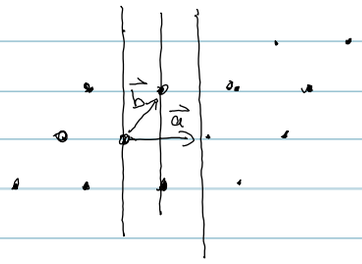
{0 1}
{1 1}

Miller-Indices hkl : Beziehung zw. Lage Netzebene u. EZ

h : Wie viele neue Ebenen entlang a-Achse?
k : b
l : c



{2 1}



alternativ

$h = \frac{a}{a'}$
$k = \frac{b}{b'}$
$l = \frac{c}{c'}$

a' = Abstand zw benachbarten Ebenen

Bsp: Netzebenen kub. Gitter

Zusammenhang zw. Netzebenenabstand u MI

orthorh. EZ $a \neq b \neq c$

$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

↳ Herleitung : 2. ÜB (2D)

z.B. Kub. EZ : $a = b = c$

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

$\{110\}$: $h, k = 1$; $l = 0$

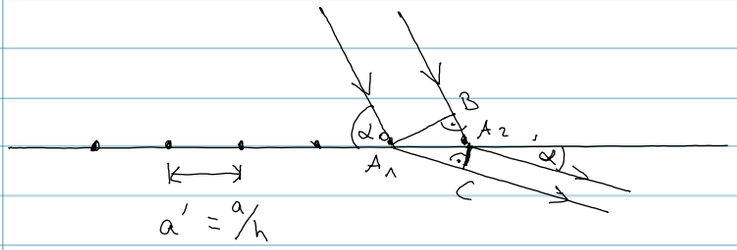
$$\frac{1}{d^2} = \frac{2}{a^2} \rightarrow d = \frac{a}{\sqrt{2}}$$

2.5 Röntgenbeugung

↳ Kristallstruktur

z.B. Einkristall → Beugungsmuster

Reflexe mit z.T. untersch. Intensität

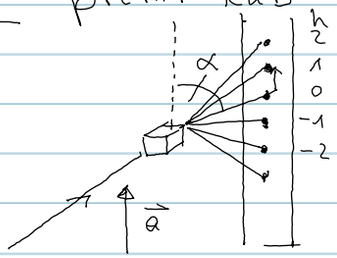


Weglängenunterschied $\Delta = \underbrace{\overline{A_1 C}}_{a' \cos\alpha} - \underbrace{\overline{B A_2}}_{a' \cos\alpha_0} = n\lambda$ ← Ordnung: 1, 2, 3, ...

$$\left.\begin{aligned} a'(\cos\alpha - \cos\alpha_0) &= n\lambda \\ a(\cos\alpha - \cos\alpha_0) &= nh\lambda \\ b(\cos\beta - \cos\beta_0) &= k\lambda \\ c(\cos\gamma - \cos\gamma_0) &= l\lambda \end{aligned}\right\} \text{ von Laue - Gleichungen}$$

$n = 1$

Bsp: prim. kub EZ ; $\{h00\}$



↳ $a \cos\alpha = h \cdot \lambda \qquad (n=1)$

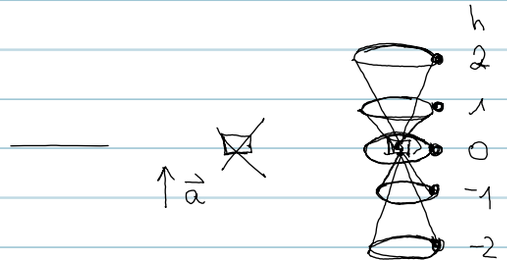
$h=0 \quad a\cos\alpha = 0$

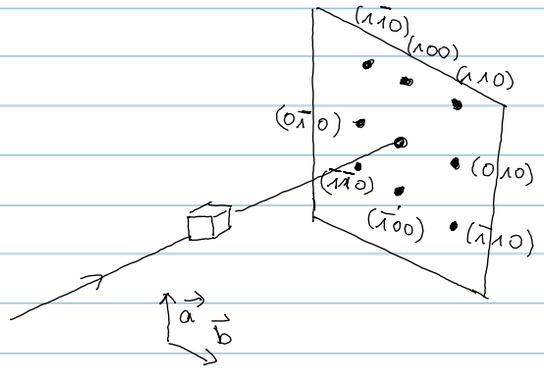
$h=1 \quad a\cos\alpha = \lambda \rightarrow \cos\alpha = \frac{\lambda}{a}$

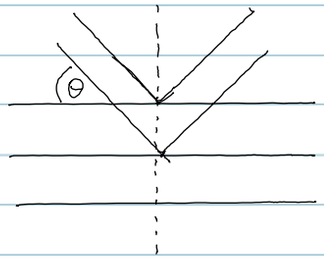
$h=2 \quad a\cos\alpha = 2\lambda \rightarrow \cos\alpha = \frac{2\lambda}{a}$

$k, l = 0 \; ; \; \beta = \beta_0 \; , \gamma = \gamma_0$

$\{hkl\}$







Bragg: $\boxed{2d \sin\Theta = n\lambda}$

Ordnung: 1, 2, 3

Beugung als Reflektion

Bragg und v. Laue sind äquivalent

z.B. kub. EZ

$$\frac{1}{d^2} = \frac{h^2+k^2+l^2}{a^2}$$

$$\sin^2\Theta = \frac{n^2\lambda^2}{4d^2} = \frac{n^2\lambda^2}{4a^2}\left(h^2+k^2+l^2\right)$$

Streuintensität

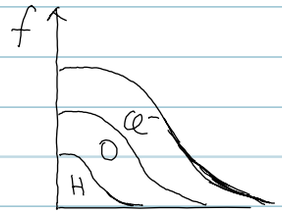
X-rays werden an e^- des Kristalls gestreut

Streufaktor $f = 4\pi \int_0^\infty \rho(r) \frac{\sin kr}{kr} r^2 dr$

$\rho(r)$: e^--Dichte

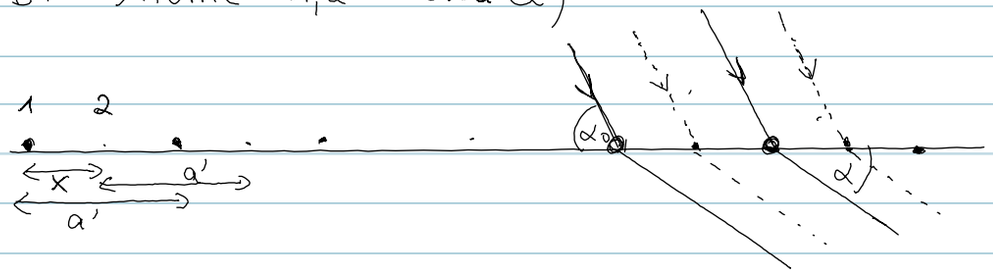
$\frac{\sin kr}{kr}$: beschreibt Interferenz gestreuter Strahlung

$k = 4\pi \frac{\sin\theta}{\lambda}$



$\rightarrow \frac{\sin\theta}{\lambda}$

z.B. Atome 1,2 (NaCl)



$\Delta_{11} = \Delta_{22} = \frac{a}{h}(\cos\alpha - \cos\alpha_0) = \lambda \quad (n=1)$

$\rightarrow (\cos\alpha - \cos\alpha_0) = \frac{h\lambda}{a}$

$\Delta_{12} = x(\cos\alpha - \cos\alpha_0) = x\frac{h\lambda}{a}$

Phasendiff.: $\phi = 2\pi \frac{\Delta_{12}}{\lambda} = 2\pi \cdot \frac{xh\lambda}{a\lambda} = 2\pi \frac{xh}{a}$

Amplitude: $A = f_1 e^{i\omega t} + f_2 e^{i(\omega t + \phi)}$

Intensität: $I \propto |A|^2 = \left[f_1 e^{i\omega t} + f_2 e^{i(\omega t+\phi)}\right]\left[f_1 e^{-i\omega t} + f_2 e^{-i(\omega t+\phi)}\right]$

$= f_1^2 + f_2^2 + f_1 f_2 e^{i\phi} + f_1 f_2 e^{-i\phi}$

$= f_1^2 + f_2^2 + 2 f_1 f_2 \cos\phi \neq f(\omega)$

Strukturfaktor: $F(h) = f_1 + f_2 e^{i\phi}$

Intensität: $I \propto |F(h)|^2$

allgemein: Atom j sei am Ort x_j, y_j, z_j

$$\hookrightarrow F(hkl) = \sum_j f_j e^{i2\pi\left(x_j\frac{h}{a} + y_j\frac{k}{b} + z_j\frac{l}{c}\right)}$$

$\hookrightarrow$ Int: $I \propto |F(hkl)|^2$

Bsp: Strukturfaktor von NaCl

Koordinaten Kation: $(0,0,0)$, $(1,0,0)$, $(0,1,0)$, $(0,0,1)$ ...
Koordinaten Anionen: $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $(\frac{1}{2},0,0)$, $(0,\frac{1}{2},0)$ ....

$$F(hkl) = \frac{1}{8}f_+\left[e^{2\pi i 0} + e^{2\pi i h} + \dots\right] + \frac{1}{2}f_+\left[e^{\pi i(h+k)} + \dots\right] + \frac{1}{4}f_-[\dots] + f_-\left[e^{\pi i(h+k+l)}\right]$$

$e^{2\pi i} = \cos 2\pi + i \sin 2\pi = 1$ $\quad$ $e^{\pi i} = \cos\pi + i\sin\pi = -1$

$\hookrightarrow e^{2\pi i h} = 1^h$ $\quad$ $\hookrightarrow e^{\pi i h} = (-1)^h$

$F(hkl) = 4(f_+ + f_-)$ wenn alle h,k,l gerade
$= 4(f_+ - f_-)$ " " ungerade

vgl. KCl $\quad$ K^+ u. Cl^- isoelektronisch
$\hookrightarrow f_+ \simeq f_-$
$\hookrightarrow F(hkl) \simeq 0$ für h,k,l ungerade