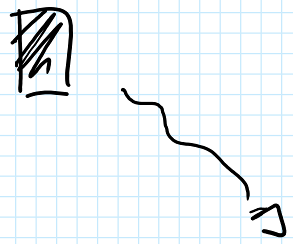
1 Röntgenbeugung (XRD)

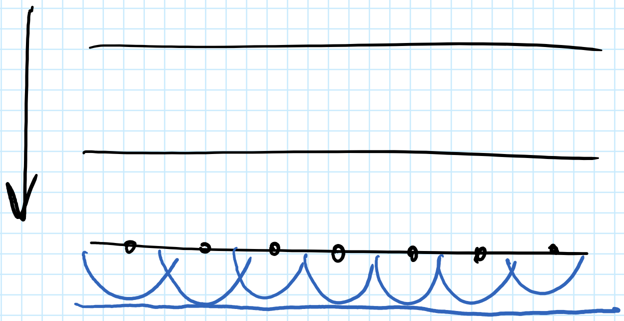
periodische Strukturen

X-ray

Wellen

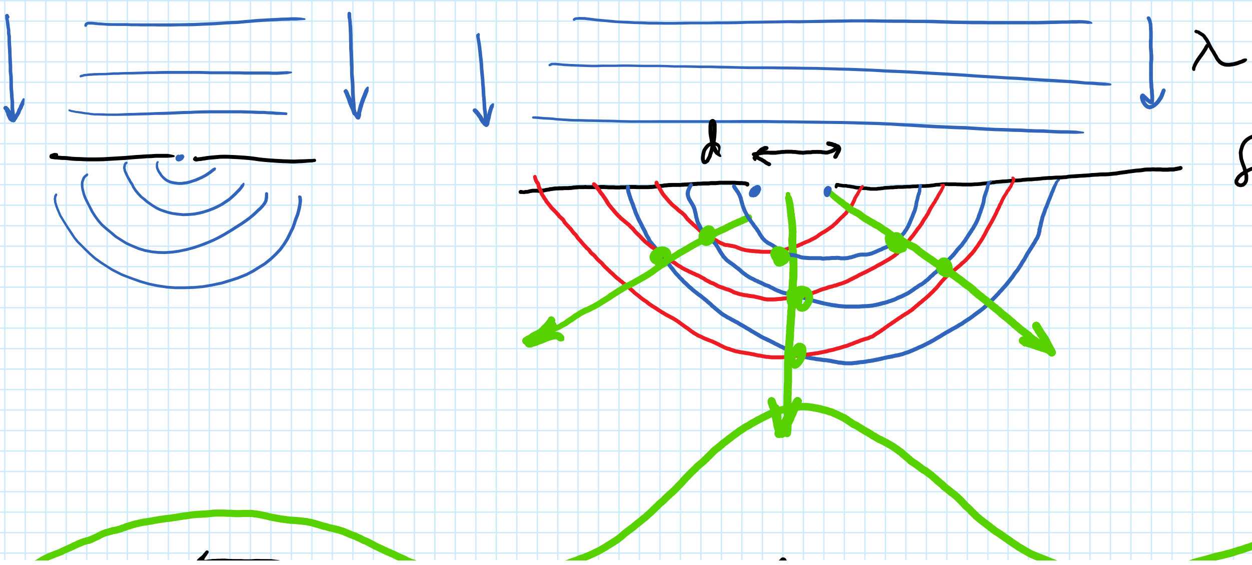


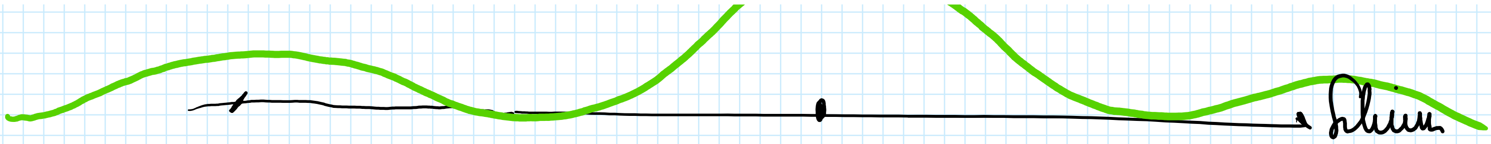
Huygen'sches Prinzip



Wellenfront

neue Wellenfront





$$\lambda \approx d$$

Röntgenstrahlung : $\lambda \approx$ Å (1895)

Max von Laue

$$\lambda = \frac{h}{p} \quad \text{(de Broglie Beziehung)}$$

$p = m \cdot v$

Elektronen ($E \cong 100$ eV)

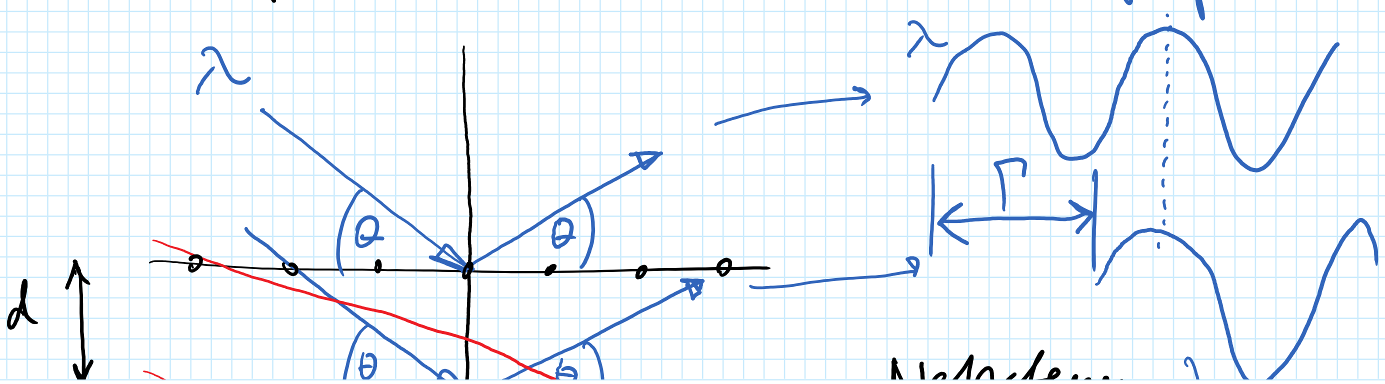
Protonen / Neutronen ($E \approx 10$ meV)

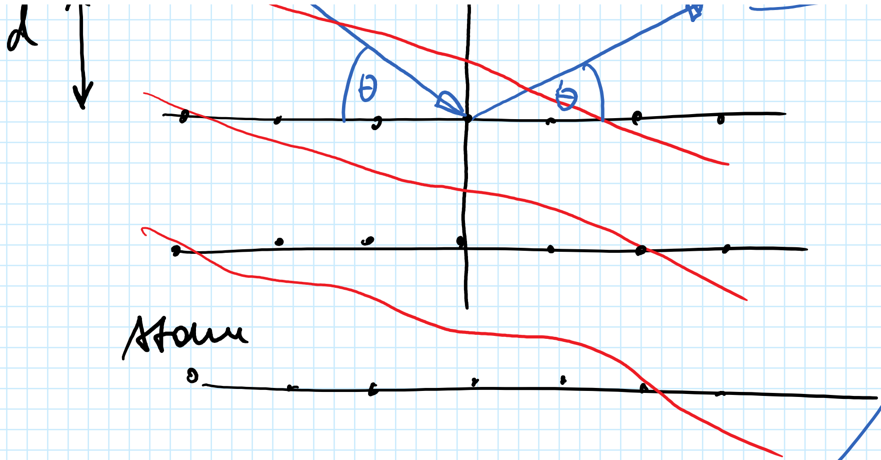
He Atome ($E \approx$ meV)

Polymere, C_{60}, ...

1.2 Bragg'sches Gesetz

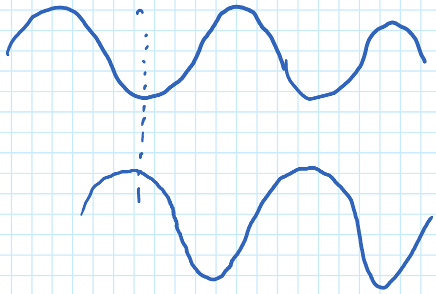
Γ = Gangunterschied





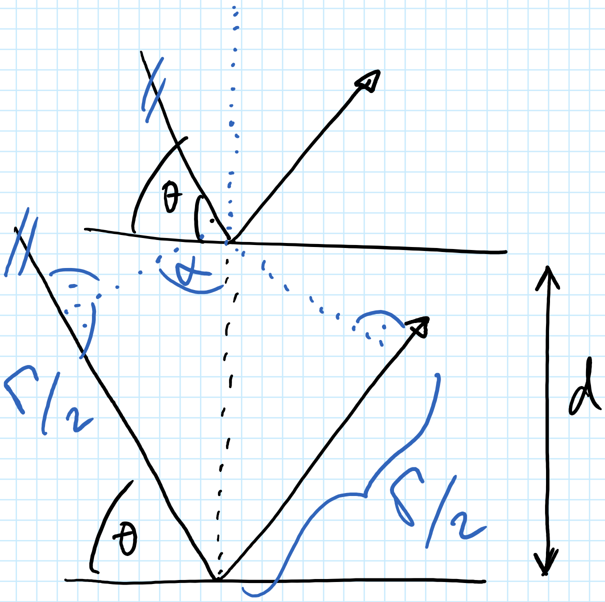
Netzebenen

kohär. Interferenz



$$\Gamma = n \cdot \lambda$$
$$(n = 0, 1, 2, 3, \ldots)$$

destruktive Interferenz



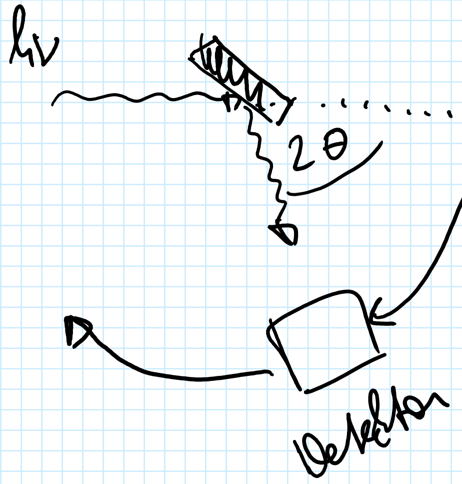
$$\sin \alpha = \frac{\Gamma/2}{d} = \frac{\Gamma}{2d}$$

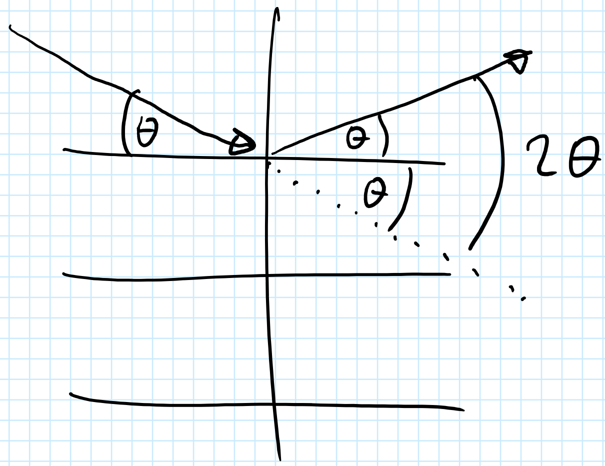
$$\theta + 90^\circ = \alpha + 90^\circ$$
$$\alpha = \theta$$

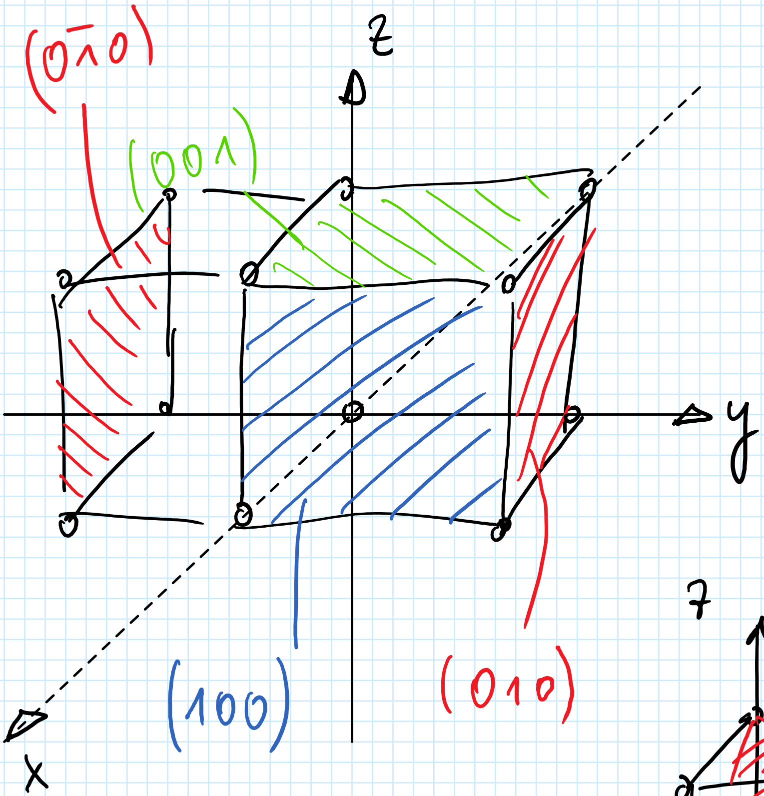
$$\sin \theta = \frac{\Gamma}{2d}$$

$$2d \cdot \sin \theta = \Gamma$$

Braggsches Gesetz: $\boxed{n\lambda = 2d \cdot \sin \theta}$





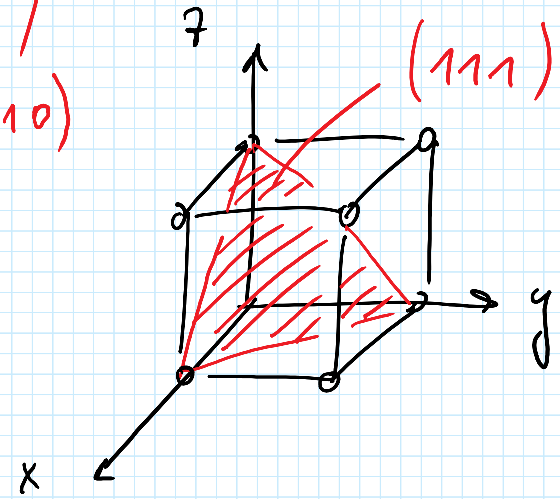


„kubisch primitiv"

Millersche Indices h, k, l

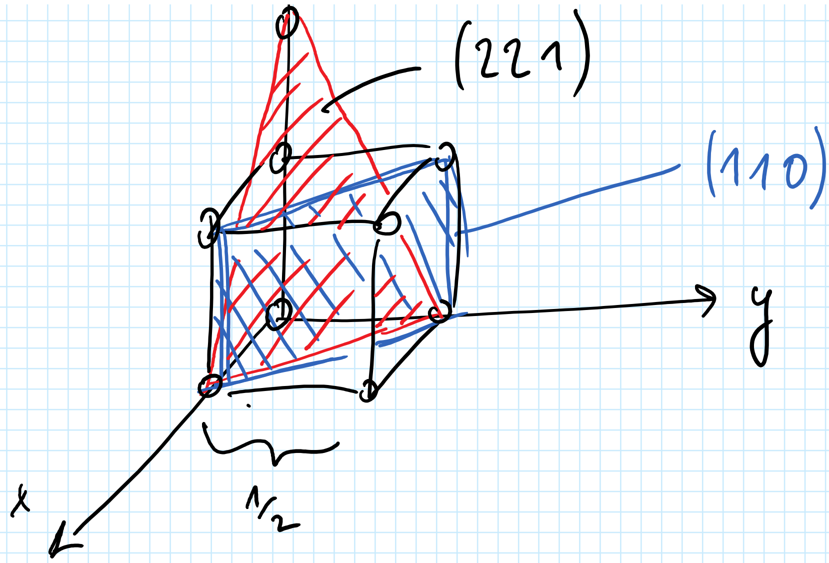
Netzebene (h, k, l)

(h k l)



$h = 1$
$k = 1$
$l = 1$

x - Abschnitt : 1/2



x - Abschnitt : 1/2
y 1/2
z 1

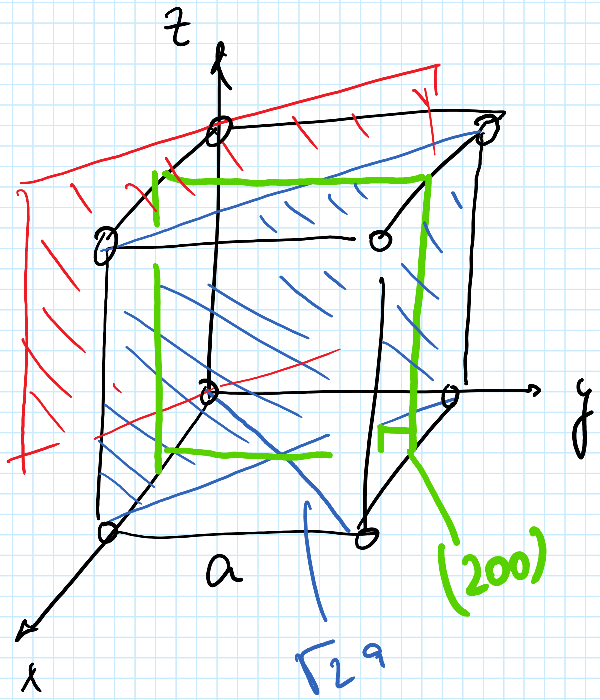
$\Rightarrow (221)$

Gruppen äquivalenter Ebenen : $\{h\,k\,l\}$

$\{100\}$: $(100),\ (010),\ (001)$

$(\bar{1}00),\ (0\bar{1}0),\ (00\bar{1})$

Netzebenenabstände ?

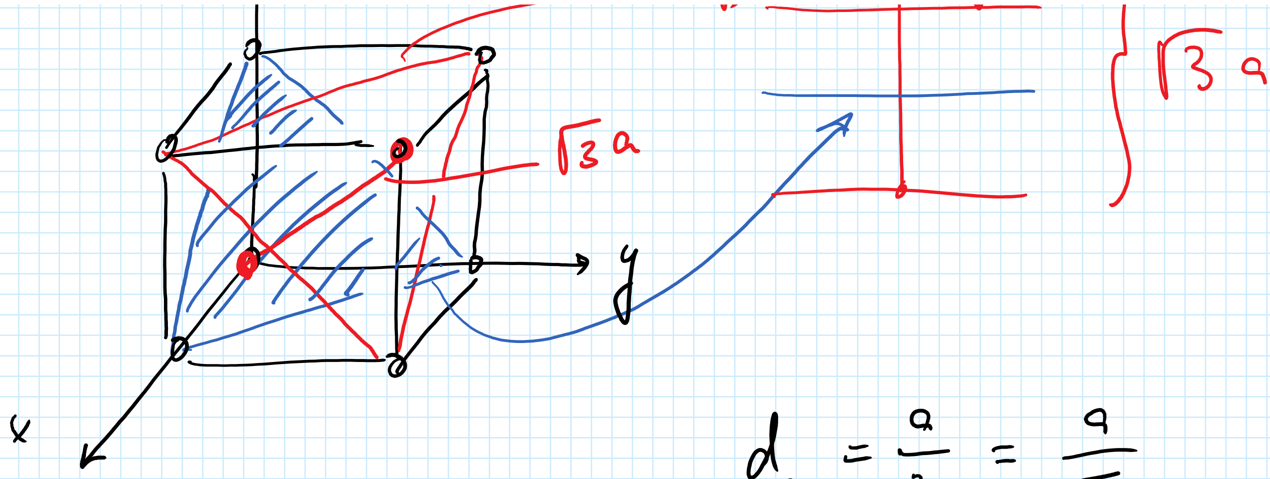


$$d_{100} = a$$

$$d_{110} = \frac{\sqrt{2}}{2}a = \frac{\sqrt{2}^{\,2}}{2\sqrt{2}}a$$

$$= \frac{2}{2\sqrt{2}}a = \frac{a}{\sqrt{2}}$$

$$d_{111} = \frac{\sqrt{3}}{3}a = \frac{a}{\sqrt{3}} \qquad \frac{\sqrt{3}}{3}a$$



$$d_{200} = \frac{a}{2} = \frac{a}{\sqrt{4}}$$

kubisch primitiv: $$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

$$n\lambda = 2d \sin\theta \longrightarrow \lambda = 2d \sin\theta$$

(2. Ordnung ≙ (200) Ebene) $\frac{d}{n}$

$$\sin\theta = \frac{\lambda}{2d} = \frac{\lambda}{2a}\sqrt{h^2+k^2+l^2}$$

$$\underline{a = \frac{\lambda}{2\sin\theta}\sqrt{h^2+k^2+l^2}}$$

Exp. : Poloniumkristall

$\lambda = 71\ \text{pm} = 71 \cdot 10^{-12}\ \text{m}$

2θ	θ	Ebenen	$\sqrt{h^2+k^2+l^2}$	a [pm]
12,1°	6,05°	(100)	$1 = \sqrt{1}$	337
17,1°	8,55°	(110)	$\sqrt{2}$	338
21,0°	10,5°	(111)	$\sqrt{3}$	337
24,3°	12,15°	(200)	$\sqrt{4}$	337
27,2°	13,6°	(210)	$\sqrt{5}$	338
29,9°	14,95°	(211)	$\sqrt{6}$	337
34,7°	17,35°	(220)	$\sqrt{8}$	337

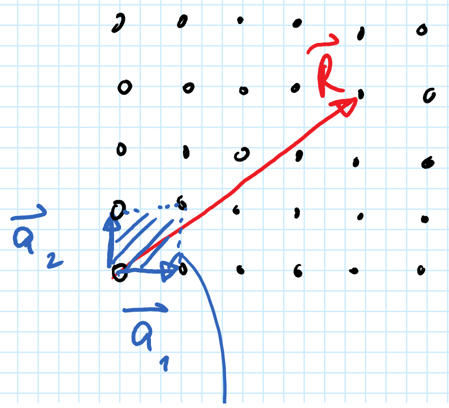
(Exp.)

kubisch primitiv

kubisch primitiv

$a = 3{,}37\ \text{Å}$

1.3 Laue Gleichungen



$$\vec{R} = 5\vec{a}_1 + 3\vec{a}_2$$

$$\vec{R} = m_1 \cdot \vec{a}_1 + m_2 \vec{a}_2 + m_3 \vec{a}_3$$

$$(m_{1,2,3} = 0, 1, 2, \ldots)$$

Einheitszelle

$(m_{1,2,3} = 0, 1, 2, \ldots)$

„Reziproker Raum"

$$\vec{G} = h_1 \vec{a}_1^{\,*} + h_2 \vec{a}_2^{\,*} + h_3 \vec{a}_3^{\,*}$$

$$(h_{1,2,3} = 0, 1, 2, \ldots)$$

$$\boxed{\vec{a}_i \cdot \vec{a}_j^{\,*} = 2\pi\, \delta_{ij}}$$

$i = 1,2,3$

$j = 1,2,3$

δ_{ij} = Kronecker Delta

$\delta_{ij} = 0 \quad (i \neq j)$

$\delta_{ij} = 1 \quad (i = j)$

$\vec{a}_1 \perp \vec{a}_2^{\,*}, \vec{a}_3^{\,*}$

$\vec{a}_2 \perp \vec{a}_1^{\,*}, \vec{a}_3^{\,*}$

$\vec{a}_3 \perp \vec{a}_1^{\,*}, \vec{a}_2^{\,*}$

$$\vec{R} \cdot \vec{G} = (m_1 \vec{a}_1 + m_2 \vec{a}_2 + m_3 \vec{a}_3)(h_1 \vec{a}_1^{\,*} + h_2 \vec{a}_2^{\,*} + h_3 \vec{a}_3^{\,*})$$

$$= m_1 h_1 \underbrace{\vec{a}_1 \vec{a}_1^{\,*}}_{2\pi} + m_2 h_2 \underbrace{\vec{a}_2 \vec{a}_2^{\,*}}_{2\pi} + m_3 h_3 \underbrace{\vec{a}_3 \vec{a}_3^{\,*}}_{2\pi}$$

$$= 2\pi (m_1 h_1 + m_2 h_2 + m_3 h_3)$$

$$\underbrace{\qquad\qquad\qquad}_{0,1,2,3,\dots}$$

$$\boxed{e^{i\vec{G}\cdot\vec{R}} = 1}$$

$$e^{ix} = \underbrace{\cos x}_{=1} + i \underbrace{\sin x}_{=0}$$

für $x = 0, 2\pi, 4\pi, 6\pi, \dots$