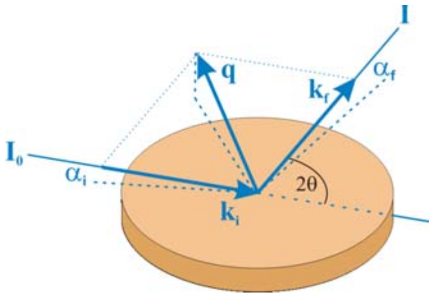
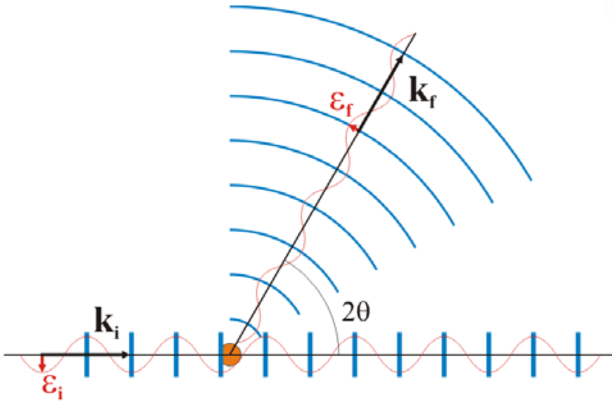
Streutheorie

$$q \equiv |\mathbf{q}| = 2k \cdot \sin(\theta) = \frac{4\pi}{\lambda} \cdot \sin(\theta)$$

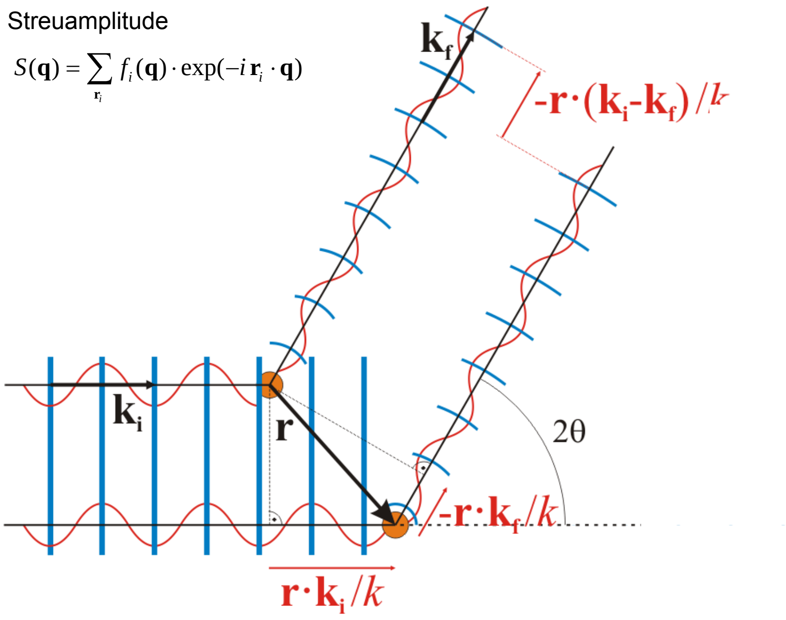




Streutheorie

Streuamplitude

$$S(\mathbf{q}) = \sum_{\mathbf{r}_i} f_i(\mathbf{q}) \cdot \exp(-i\,\mathbf{r}_i \cdot \mathbf{q})$$

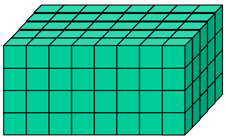


Streutheorie

Streuung an 3D Kristallgitter:

$$S(\mathbf{q}) = F(\mathbf{q}) \sum_{n_1}^{N_1-1} \sum_{n_2}^{N_2-1} \sum_{n_3}^{N_3-1} \exp\left[-i(n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}) \cdot \mathbf{q}\right]$$

$$= F(\mathbf{q}) \sum_{n_1}^{N_1-1} \exp(-i\, n_1\mathbf{a_1} \cdot \mathbf{q}) \sum_{n_2}^{N_2-1} \exp(-i\, n_2\mathbf{a_2} \cdot \mathbf{q}) \sum_{n_3}^{N_3-1} \exp(-i\, n_3\mathbf{a_3} \cdot \mathbf{q})$$



Interferenzfunktion für Beugung am N-fachen Mehrfachspalt:

$$S_N(x) = \sum_{n}^{N-1} \exp(-i\, n\, x) = \frac{1-\exp(-i\, N\, x)}{1-\exp(-i\, x)}$$

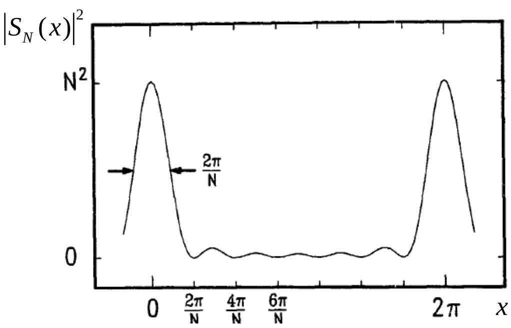
Streutheorie

Streuung an 3D Kristallgitter:

Intensität proportional zu:

$$\left|S_N(x)\right|^2 = \frac{\sin^2(N\, x/2)}{\sin^2(x/2)}$$

$$\left|S(\mathbf{q})\right|^2 = \left|F(\mathbf{q})\right|^2 \cdot \left|S_{N_1}(\mathbf{a_1} \cdot \mathbf{q})\right|^2 \cdot \left|S_{N_2}(\mathbf{a}_2 \cdot \mathbf{q})\right|^2 \cdot \left|S_{N_3}(\mathbf{a}_3 \cdot \mathbf{q})\right|^2$$



Streutheorie

Streuung an 3D Kristallgitter:

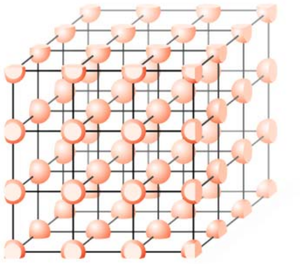
$$|S(\mathbf{q})|^2 = |F(\mathbf{q})|^2 \cdot |S_{N_1}(\mathbf{a}_1 \cdot \mathbf{q})|^2 \cdot |S_{N_2}(\mathbf{a}_2 \cdot \mathbf{q})|^2 \cdot |S_{N_3}(\mathbf{a}_3 \cdot \mathbf{q})|^2$$

→Laue Bedingungen:

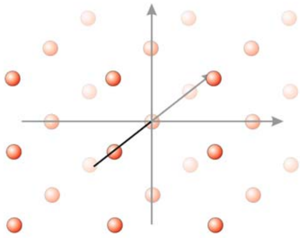
$$\mathbf{a}_1 \cdot \mathbf{q} = 2\pi h$$
$$\mathbf{a}_2 \cdot \mathbf{q} = 2\pi k$$
$$\mathbf{a}_3 \cdot \mathbf{q} = 2\pi l$$

→ Streuung lokalisiert an Punkten des reziproken Gitters

Realraum



Reziproker Raum



Streutheorie

Streuung an 2D Gitter:

$$|S(\mathbf{q})|^2 = |F(\mathbf{q})|^2 \cdot |S_{N_1}(\mathbf{a}_1 \cdot \mathbf{q})|^2 \cdot |S_{N_2}(\mathbf{a}_2 \cdot \mathbf{q})|^2$$

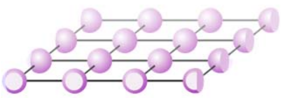
→Laue Bedingungen:

$$\mathbf{a}_1 \cdot \mathbf{q} = 2\pi h$$
$$\mathbf{a}_2 \cdot \mathbf{q} = 2\pi k$$

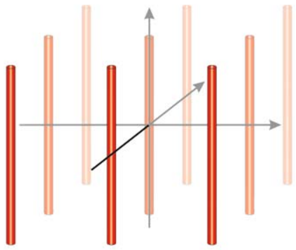
l beliebig!

→ Streuung lokalisiert an 2D periodischen Linien im reziproken Raum („Stäbe“)

Realraum



Reziproker Raum



Streutheorie

Streuung an halbunendlichem 3D Gitter (Kristalloberfläche):

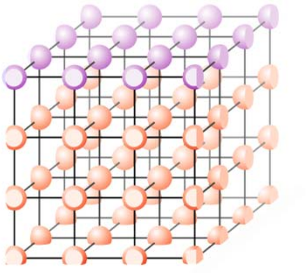
$$S(\mathbf{q}) = F(\mathbf{q})\sum_{n_1}\exp(-2\pi i\, n_1 h)\sum_{n_2}\exp(-2\pi i\, n_2 k)\sum_{n_3-\infty}^{0}\exp(-2\pi i\, n_3 l)\cdot\exp(-\beta\, n_3)$$

$$S_{CTR}(\mathbf{q}) = \sum_{n_3-\infty}^{0}\exp\left[(-2\pi i\, l-\beta)\cdot n_3\right] = \frac{1}{1-\exp(-2\pi i\, l-\beta)}$$

$$\left|S_{CTR}(\mathbf{q})\right|^2 \approx \frac{1}{4\sin^2(\pi l)}$$

→ Streuintensität entlang Stäben im reziproken Raum moduliert („Gitterstäbe“, CTRs)

Realraum



Reziproker Raum