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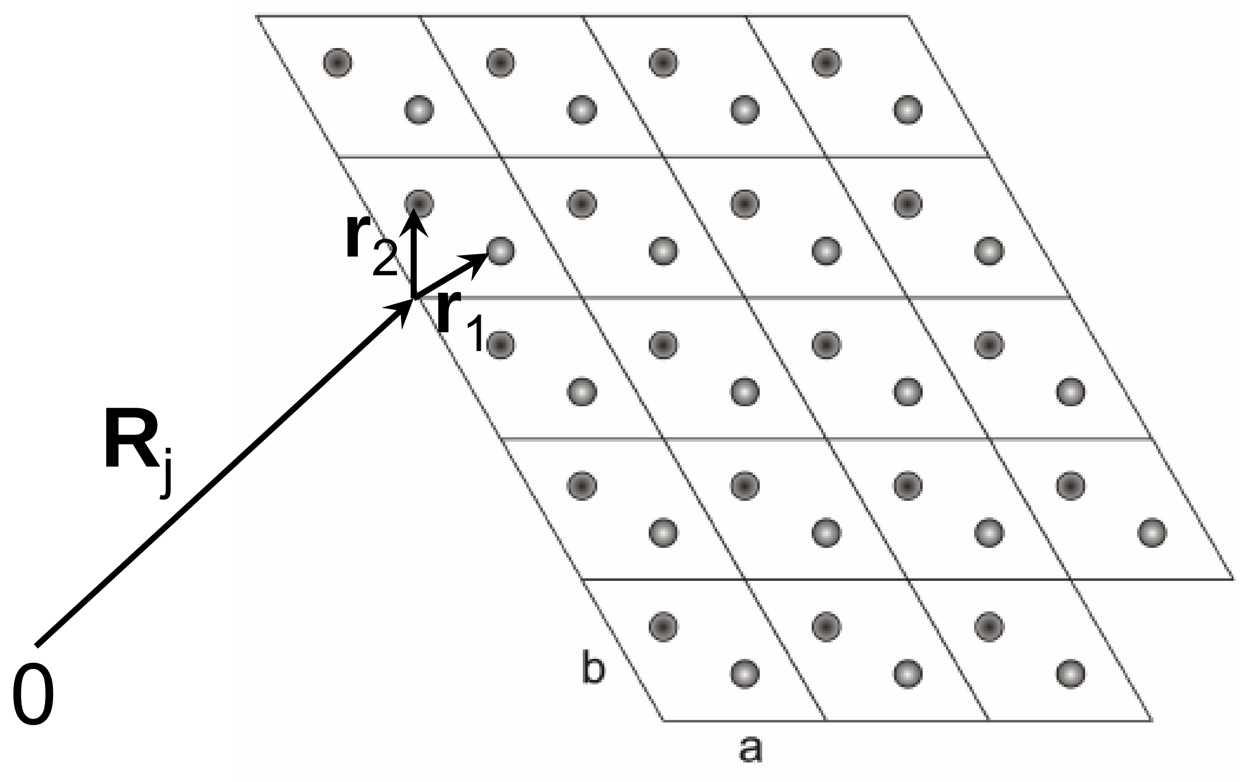
# *Лекция 4. Основы теории ядерного рассеяния нейтронов.*

- *Несколько атомов в элементарной ячейке*
- *Методы измерения брэгговского рассеяния*
- *Когерентное однофононное рассеяние*

# Случай нескольких атомов в элементарной ячейке

$$\mathbf{R}_j(t) \quad \rightarrow \quad \mathbf{R}_{j,d}(t) = \mathbf{R}_j^{(0)} + \mathbf{r}_d + \mathbf{u}_{j,d}(t)$$



# Случай нескольких атомов в элементарной ячейке

$$\left(\frac{d^2\sigma}{dE_f\, d\Omega_f}\right)_{\mathrm{coh}} =$$

$$\frac{k_f}{k_i}\frac{1}{2\pi\hbar}\sum_{j,d}\sum_{n,s}\bar{b}_d\,\bar{b}_s\, e^{i\mathbf{Q}\left(\mathbf{R}_n^{(0)}+\mathbf{r}_s-\mathbf{R}_j^{(0)}-\mathbf{r}_d\right)}\int_{-\infty}^{\infty}\left\langle e^{-i\mathbf{Q}\mathbf{u}_{j,d}(0)}e^{i\mathbf{Q}\mathbf{u}_{n,s}(t)}\right\rangle e^{-i\omega t}dt$$

$$\left(\frac{d\sigma}{d\Omega_f}\right)_{\mathrm{coh,el}} = N\sum_j e^{i\mathbf{Q}\mathbf{R}_j^{(0)}}\left|\sum_d \bar{b}_d e^{i\mathbf{Q}\mathbf{r}_d}e^{-W_d}\right|^2$$

$$W_d = \frac{1}{2}\left\langle\left(\mathbf{Q}\mathbf{u}_{j,d}\right)^2\right\rangle$$

$$\mathbf{u}_{j,d} = \sqrt{\frac{\hbar}{2M_d N}} \sum_{s=1}^{3\nu} \sum_{\mathbf{q}} \frac{1}{\sqrt{\omega_s(\mathbf{q})}} \left( a_{\mathbf{q},s} \mathbf{e}_{s,d}(\mathbf{q}) e^{i\mathbf{q}\mathbf{R}_j^{(0)}} + a_{\mathbf{q},s}^{+} \mathbf{e}_{s,d}(\mathbf{q})^{*} e^{-i\mathbf{q}\mathbf{R}_j^{(0)}} \right)$$

$$2W_d = \frac{\hbar}{2M_d N} \sum_{s=1}^{3\nu} \sum_{\mathbf{q}} \frac{\left|\mathbf{Q}\mathbf{e}_{s,d}(\mathbf{q})\right|^2}{\omega_s(\mathbf{q})} \left\langle 2n_{\mathbf{q},s} + 1 \right\rangle$$

$$= \frac{\hbar}{2M_d N} \sum_{s=1}^{3\nu} \sum_{\mathbf{q}} \frac{\left|\mathbf{Q}\mathbf{e}_{s,d}(\mathbf{q})\right|^2}{\omega_s(\mathbf{q})} \coth\left( \frac{\hbar\omega_s(\mathbf{q})}{2k_B T} \right)$$

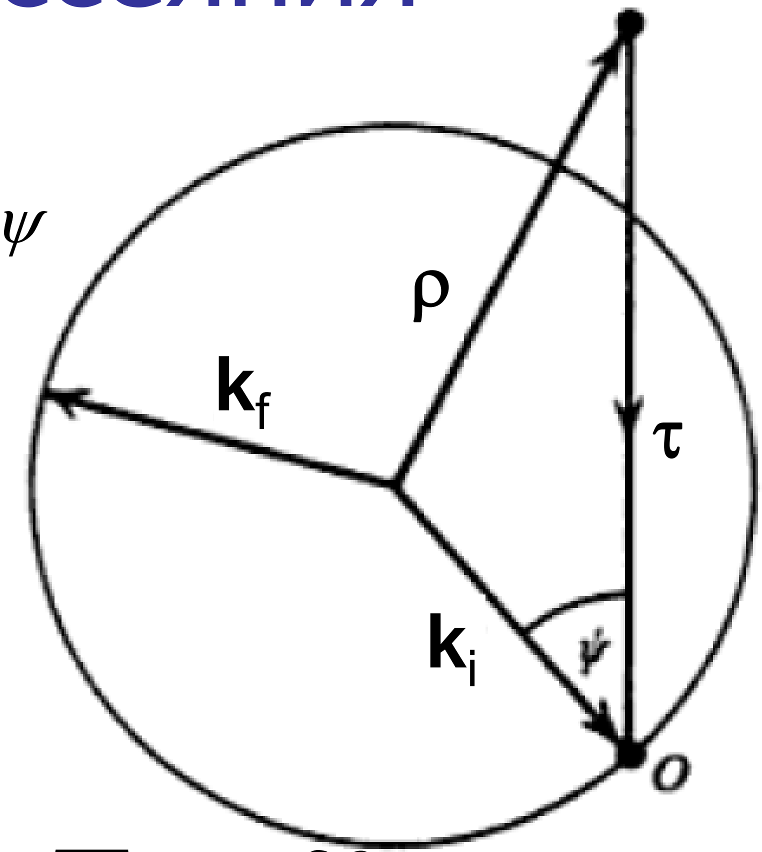
$$\left( \frac{d\sigma}{d\Omega_f} \right)_{\mathrm{coh,el}} = N \frac{(2\pi)^3}{\mathrm{v}_0} \sum_{\boldsymbol{\tau}} \delta(\mathbf{Q} - \boldsymbol{\tau}) \left| F_N(\mathbf{Q}) \right|^2$$

$$F_N(\mathbf{Q}) = \sum_d \bar{b}_d e^{i\mathbf{Q}\mathbf{d}} e^{-W_d}$$

Ядерный форм-фактор

# Методы измерения брэгговского рассеяния

$$\boldsymbol{\rho} = \mathbf{k}_i - \boldsymbol{\tau} \qquad \rho^2 = k^2 + \tau^2 - 2k\tau\cos\psi$$




$$\int \delta(\mathbf{Q}-\boldsymbol{\tau})d\Omega = \int \delta(\mathbf{k}_i - \mathbf{k}_f - \boldsymbol{\tau})d\Omega$$

$$= \int \delta(\boldsymbol{\rho} - \mathbf{k}_f)d\Omega = c\delta(\rho^2 - k_f^2)$$

$$\int \delta(\boldsymbol{\rho} - \mathbf{k}_f)d\mathbf{k}_f = 1$$

$$\int \delta(\boldsymbol{\rho} - \mathbf{k}_f)d\mathbf{k}_f = \int \delta(\boldsymbol{\rho} - \mathbf{k}_f)k_f^2 dk_f d\Omega$$

$$= \frac{1}{2}\int \delta(\boldsymbol{\rho} - \mathbf{k}_f)k_f dk_f^2 d\Omega = \frac{c}{2}\int \delta(\rho^2 - k_f^2)\sqrt{k_f^2}dk_f^2 = \frac{c\rho}{2}$$

$$\int \delta(\mathbf{Q}-\boldsymbol{\tau})d\Omega = \int \delta(\boldsymbol{\rho} - \mathbf{k}_f)d\Omega = \frac{2}{\rho}\delta\left(\rho^2 - k_f^2\right) = \frac{2}{\rho}\delta\left(\tau^2 - 2k\tau\cos\psi\right)$$

# Интенсивность брэгговского пика. Общее выражение.

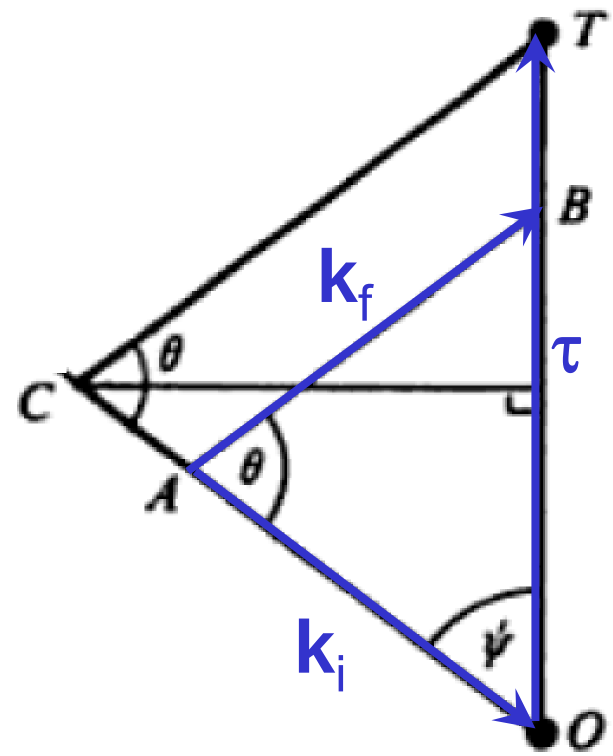
$$\left(\frac{d\sigma}{d\Omega_f}\right)_{\text{coh,el}} = N\frac{(2\pi)^3}{\mathrm{v}_0}\sum_{\boldsymbol{\tau}}\delta(\mathbf{Q}-\boldsymbol{\tau})\left|F_N(\mathbf{Q})\right|^2$$

$$F_N(\mathbf{Q}) = \sum_d \bar{b}_d e^{i\mathbf{Qd}} e^{-W_d}$$

$$\sigma_{tot\ \boldsymbol{\tau}} = \int\left(\frac{d\sigma}{d\Omega_f}\right)_{\text{coh,el}} d\Omega_f = N\frac{(2\pi)^3}{\mathrm{v}_0}\left|F_N(\boldsymbol{\tau})\right|^2\frac{2}{\rho}\delta\left(\tau^2 - 2k\tau\cos\psi\right)$$

# Метод Лауэ

$$k = \frac{\tau}{2\cos\psi} = \frac{\tau}{2\sin\frac{\theta}{2}}$$




$$I = \int_0^\infty \phi(\lambda)\sigma_{tot\,\boldsymbol{\tau}} d\lambda$$

$$= N\frac{(2\pi)^3}{v_0}\left|F_N(\boldsymbol{\tau})\right|^2 \int_0^\infty \frac{2}{\rho}\delta\left(\tau^2 - 2k\tau\cos\psi\right)\phi(\lambda)d\lambda$$

$$k = \frac{2\pi}{\lambda} \qquad \rho = k$$

$$I = N\frac{(2\pi)^3}{v_0}\left|F_N(\boldsymbol{\tau})\right|^2 \int_0^\infty \frac{2}{k}\delta\left(\tau^2 - 2\frac{2\pi}{\lambda}\tau\cos\psi\right)\phi(\lambda)d\lambda$$

# Метод Лауэ

$$I = N\frac{(2\pi)^3}{\mathrm{v}_0}\left|F_N(\boldsymbol{\tau})\right|^2 \int_0^\infty \frac{\lambda}{\pi}\delta\left(\frac{\tau^2}{\lambda}\left(\lambda - \frac{4\pi}{\tau}\cos\psi\right)\right)\phi(\lambda)d\lambda$$

$$= N\frac{(2\pi)^3}{\mathrm{v}_0}\left|F_N(\boldsymbol{\tau})\right|^2 \int_0^\infty \frac{\lambda^2}{\pi\tau^2}\delta\left(\lambda - \frac{4\pi}{\tau}\cos\psi\right)\phi(\lambda)d\lambda$$

$$= N\frac{(2\pi)^3}{\mathrm{v}_0}\left|F_N(\boldsymbol{\tau})\right|^2 \int_0^\infty \frac{\lambda^4}{\pi\left(4\pi\cos\psi\right)^2}\delta\left(\lambda - \frac{4\pi}{\tau}\cos\psi\right)\phi(\lambda)d\lambda$$

$$I = \frac{N}{\mathrm{v}_0}\phi(\lambda)\frac{\lambda^4}{2\sin^2\left(\frac{\theta}{2}\right)}\left|F_N(\boldsymbol{\tau})\right|^2 \qquad \psi = \frac{\pi - \theta}{2}$$

# Метод вращения кристалла

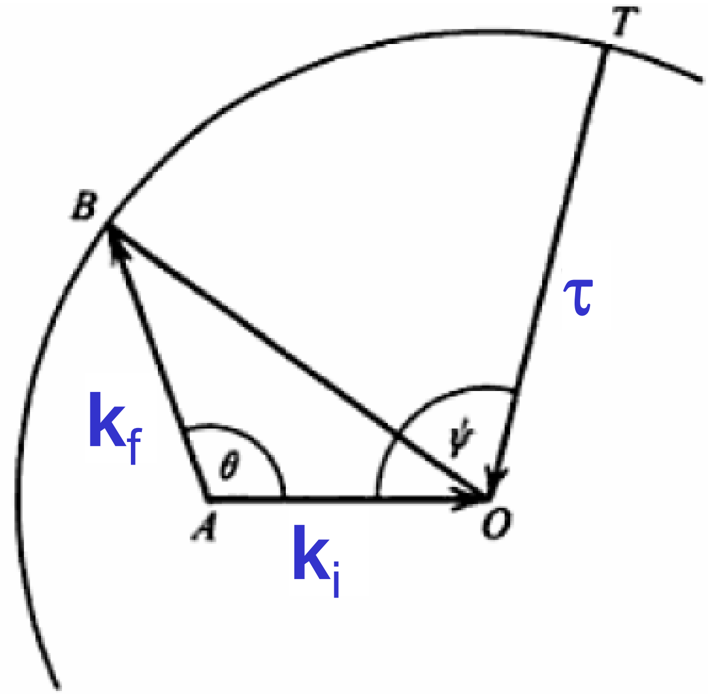
$$I = \Phi \int_0^{\pi} \sigma_{tot\ \boldsymbol{\tau}} d\psi = \Phi N \frac{(2\pi)^3}{v_0} \left| F_N(\boldsymbol{\tau}) \right|^2 \int_0^{\pi} \frac{2}{\rho} \delta\left(\tau^2 - 2k\tau\cos\psi\right) d\psi$$

$$x = 2k\tau\cos\psi$$

$$dx = -2k\tau\sin\psi\, d\psi$$

$$dx = -2k\tau\sqrt{1 - \frac{x^2}{(2k\tau)^2}}\, d\psi$$

$$dx = -\sqrt{(2k\tau)^2 - x^2}\, d\psi$$




$$I = \Phi N \frac{(2\pi)^3}{v_0} \left| F_N(\boldsymbol{\tau}) \right|^2 \int_{-2k\tau}^{2k\tau} \frac{2}{\rho} \delta\left(\tau^2 - x\right) \frac{dx}{\sqrt{(2k\tau)^2 - x^2}}$$

# Метод вращения кристалла

$$I = \Phi N \frac{(2\pi)^3}{\mathrm{v}_0} \left|F_N(\boldsymbol{\tau})\right|^2 \int_{-2k\tau}^{2k\tau} \frac{2}{\rho} \delta\left(\tau^2 - x\right) \frac{dx}{\sqrt{\left(2k\tau\right)^2 - x^2}}$$

$$= \Phi N \frac{(2\pi)^3}{\mathrm{v}_0} \left|F_N(\boldsymbol{\tau})\right|^2 \frac{2}{k} \frac{1}{\sqrt{\left(2k\tau\right)^2 - \tau^4}} = \Phi N \frac{(2\pi)^3}{\mathrm{v}_0} \left|F_N(\boldsymbol{\tau})\right|^2 \frac{2}{k\tau} \frac{1}{\sqrt{4k^2 - \tau^2}}$$

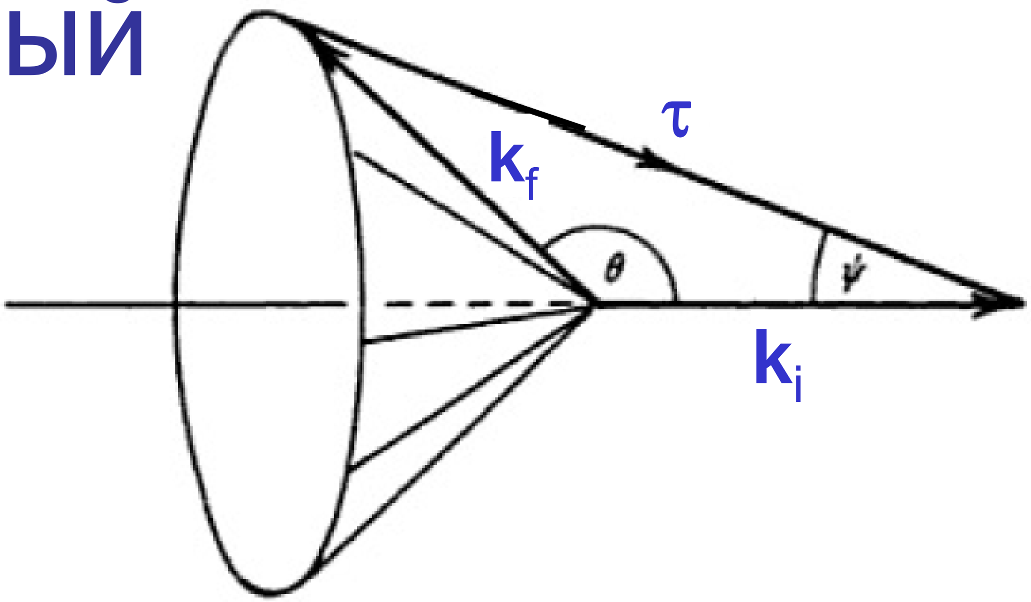
$$= \Phi N \frac{(2\pi)^3}{\mathrm{v}_0} \left|F_N(\boldsymbol{\tau})\right|^2 \frac{2}{k\sqrt{2k^2(1+\cos\theta)}} \frac{1}{\sqrt{2k^2 - 2k^2\cos\theta}}$$

$$\tau^2 = k^2 + k^2 + 2k^2\cos\theta \quad \Rightarrow \quad \tau = \sqrt{2k^2(1+\cos\theta)}$$

$$I = \Phi N \frac{(2\pi)^3}{\mathrm{v}_0} \left|F_N(\boldsymbol{\tau})\right|^2 \frac{1}{k^3 \sin\theta}$$

$$\frac{I_1}{I_2} = \frac{\left|F_N(\boldsymbol{\tau}_1)\right|^2}{\left|F_N(\boldsymbol{\tau}_2)\right|^2} \frac{\sin\theta_2}{\sin\theta_1}$$

# Порошковый метод




$$I = \Phi N \frac{(2\pi)^3}{v_0}\frac{2}{k}\sum_{\boldsymbol{\tau}}\left|F_N(\boldsymbol{\tau})\right|^2 \int_0^{\pi} \delta\left(\tau^2 - 2k\tau\cos\psi\right)\frac{2\pi\sin\psi\, d\psi}{4\pi}$$

$$x = \cos\psi \quad \Rightarrow \quad dx = -\sin\psi\, d\psi$$

$$I = \Phi N \frac{(2\pi)^3}{v_0}\frac{1}{k}\sum_{\boldsymbol{\tau}}\left|F_N(\boldsymbol{\tau})\right|^2 \int_{-1}^{1} \delta\left(\tau^2 - 2k\tau x\right) dx$$

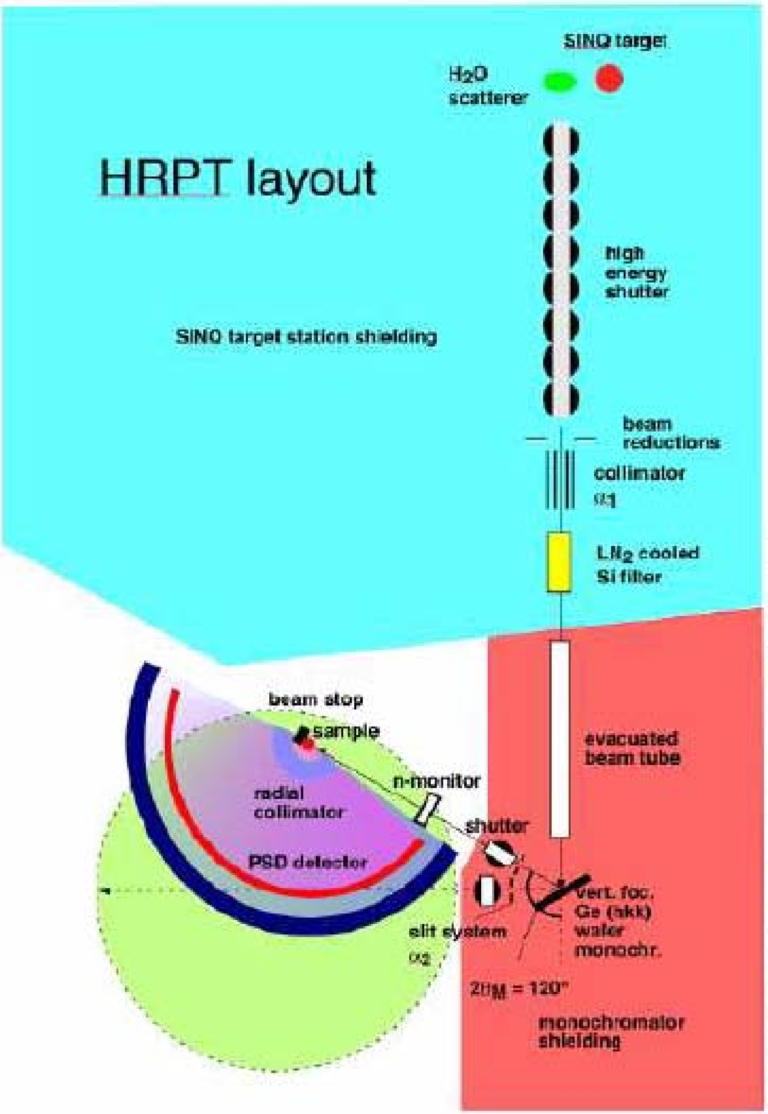
# Порошковый метод

$$I = \Phi N \frac{(2\pi)^3}{v_0} \frac{1}{k} \sum_{\boldsymbol{\tau}} \left| F_N(\boldsymbol{\tau}) \right|^2 \frac{1}{2k\tau} = \Phi N \frac{(2\pi)^3}{v_0} \frac{1}{4k^3 \sin\frac{\theta}{2}} \sum_{\boldsymbol{\tau}} \left| F_N(\boldsymbol{\tau}) \right|^2$$

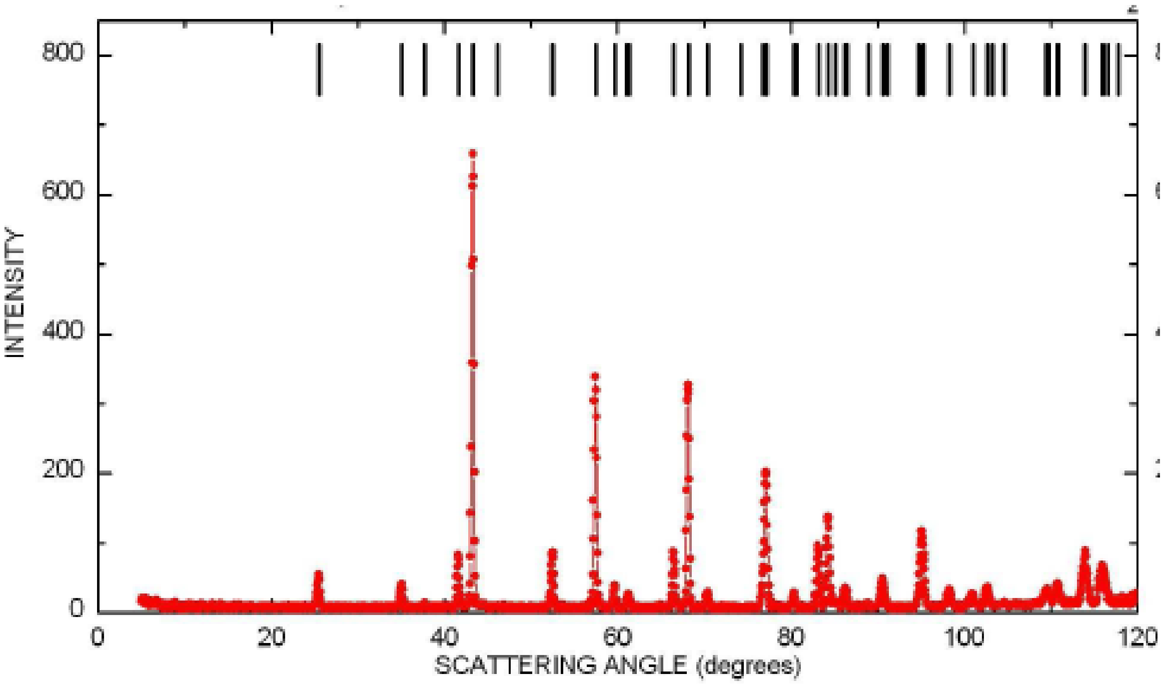
$$\tau = 2k \sin\frac{\theta}{2}$$

$$\boxed{I = \Phi \frac{N}{v_0} \frac{\lambda^3}{4 \sin\frac{\theta}{2}} \sum_{\boldsymbol{\tau}} \left| F_N(\boldsymbol{\tau}) \right|^2}$$

# Порошковый метод




# Порошковый метод. Эксперимент.



# Когерентное однофононное рассеяние

$$\left(\frac{d^2\sigma}{dE_f d\Omega_f}\right)_{\mathrm{coh}} = \frac{\sigma_{\mathrm{coh}}}{4\pi}\frac{k_f}{k_i}\frac{N}{2\pi\hbar} e^{\langle U^2\rangle}\sum_j e^{i\mathbf{QR}_j^{(0)}}\int_{-\infty}^{\infty} e^{\langle UV\rangle} e^{-i\omega t} dt$$

$$e^{\langle UV\rangle} = 1 + \langle UV\rangle + \frac{1}{2}\langle UV\rangle^2 + \ldots + \frac{1}{n!}\langle UV\rangle^n + \ldots$$

$$\langle\lambda|UV|\lambda\rangle$$

$$= \sum_{s=1}^{3}\sum_{\mathbf{q}}\sum_{s'=1}^{3}\sum_{\mathbf{q}'}\langle\lambda|\left(g_s(\mathbf{q})a_{\mathbf{q},s} + g_s^*(\mathbf{q})a_{\mathbf{q},s}^+\right)\left(h_{s'}(\mathbf{q}')a_{\mathbf{q}',s'} + h_{s'}^*(\mathbf{q}')a_{\mathbf{q}',s'}^+\right)|\lambda\rangle$$

$$= \sum_{s=1}^{3}\sum_{\mathbf{q}}\langle\lambda|g_s(\mathbf{q})h_s^*(\mathbf{q})a_{\mathbf{q},s}a_{\mathbf{q},s}^+ + g_s^*(\mathbf{q})h_{s'}(\mathbf{q})a_{\mathbf{q},s}^+a_{\mathbf{q},s}|\lambda\rangle$$

$$\langle\lambda|a_{\mathbf{q},s}a_{\mathbf{q},s}^+|\lambda\rangle = n_{\mathbf{q},s} + 1 \qquad \langle\lambda|a_{\mathbf{q},s}^+a_{\mathbf{q},s}|\lambda\rangle = n_{\mathbf{q},s}$$

# Сечение когерентного однофононного рассеяния

$$\langle UV \rangle = \sum_{s=1}^{3}\sum_{\mathbf{q}}\left( g_s(\mathbf{q}) h_s^*(\mathbf{q}) \langle n_{\mathbf{q},s}+1\rangle + g_s^*(\mathbf{q}) h_s(\mathbf{q}) \langle n_{\mathbf{q},s}\rangle \right)$$

$$= \frac{\hbar}{2MN}\sum_{s=1}^{3}\sum_{\mathbf{q}}\frac{\left|\mathbf{Qe}_s(\mathbf{q})\right|^2}{\omega_s(\mathbf{q})}\left( e^{-i(\mathbf{qR}_j^{(0)}-\omega_s(\mathbf{q})t)}\langle n_{\mathbf{q},s}+1\rangle + e^{i(\mathbf{qR}_j^{(0)}-\omega_s(\mathbf{q})t)}\langle n_{\mathbf{q},s}\rangle \right)$$

$$\left(\frac{d^2\sigma}{dE_f\, d\Omega_f}\right)_{\text{coh 1ph}} = \frac{\sigma_{\text{coh}}}{4\pi}\frac{k_f}{k_i}\frac{N}{2\pi\hbar}e^{-2W}\frac{\hbar}{2MN}\sum_{s=1}^{3}\sum_{\mathbf{q}}\frac{\left|\mathbf{Qe}_s(\mathbf{q})\right|^2}{\omega_s(\mathbf{q})}\sum_j e^{i\mathbf{QR}_j^{(0)}}$$

$$\times\int_{-\infty}^{\infty}\left( e^{-i(\mathbf{qR}_j^{(0)}-\omega_s(\mathbf{q})t)}\langle n_{\mathbf{q},s}+1\rangle + e^{i(\mathbf{qR}_j^{(0)}-\omega_s(\mathbf{q})t)}\langle n_{\mathbf{q},s}\rangle \right) e^{-i\omega t}\,dt$$

# Сечение когерентного однофононного рассеяния

$$\sum_j e^{i(\mathbf{Q}-\mathbf{q})\mathbf{R}_j^{(0)}} = \frac{(2\pi)^3}{\mathrm{v}_0}\sum_{\boldsymbol{\tau}}\delta(\mathbf{Q}-\mathbf{q}-\boldsymbol{\tau})$$

$$\int_{-\infty}^{\infty} e^{i(\omega_s(\mathbf{q})-\omega)t}dt = 2\pi\delta(\omega_s(\mathbf{q})-\omega)$$

$$\left(\frac{d^2\sigma}{dE_f d\Omega_f}\right)_{\text{coh 1ph}} = \frac{\sigma_{\text{coh}}}{4\pi}\frac{k_f}{k_i}\frac{1}{4\pi M}e^{-2W}\frac{(2\pi)^4}{\mathrm{v}_0}\sum_{s=1}^{3}\sum_{\mathbf{q}}\sum_{\boldsymbol{\tau}}\frac{\left|\mathbf{Q}\mathbf{e}_s(\mathbf{q})\right|^2}{\omega_s(\mathbf{q})}$$

$$\times\left(\delta(\omega_s(\mathbf{q})-\omega)\delta(\mathbf{Q}-\mathbf{q}-\boldsymbol{\tau})\left\langle n_{\mathbf{q},s}+1\right\rangle+\delta(\omega_s(\mathbf{q})+\omega)\delta(\mathbf{Q}+\mathbf{q}-\boldsymbol{\tau})\left\langle n_{\mathbf{q},s}\right\rangle\right)$$

# Сечение когерентного однофононного рассеяния

$$\left(\frac{d^2\sigma}{dE_f d\Omega_f}\right)_{\text{coh 1ph}} = \frac{\sigma_{\text{coh}}}{4\pi}\frac{k_f}{k_i}\frac{1}{2M}\frac{(2\pi)^3}{\text{v}_0}e^{-2W}\sum_{s=1}^{3}\sum_{\mathbf{q}}\sum_{\boldsymbol{\tau}}\frac{\left|\mathbf{Q}\mathbf{e}_s(\mathbf{q})\right|^2}{\omega_s(\mathbf{q})}$$

$$\times\Big(\delta(\omega_s(\mathbf{q})-\omega)\delta(\mathbf{Q}-\mathbf{q}-\boldsymbol{\tau})\left\langle n_{\mathbf{q},s}+1\right\rangle+\delta(\omega_s(\mathbf{q})+\omega)\delta(\mathbf{Q}+\mathbf{q}-\boldsymbol{\tau})\left\langle n_{\mathbf{q},s}\right\rangle\Big)$$

$$\hbar\omega = E_i - E_f \qquad E_i - E_f = \pm\hbar\omega_s(\mathbf{q}) \qquad \mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f = \pm\mathbf{q} - \boldsymbol{\tau}$$

$$T \to 0 \qquad \left\langle n_{\mathbf{q},s}+1\right\rangle \to 1, \quad \left\langle n_{\mathbf{q},s}\right\rangle \to 0$$

# Случай нескольких атомов в элементарной ячейке

$$\left(\frac{d^2\sigma}{dE_f\,d\Omega_f}\right)_{\text{coh 1ph}} = \frac{k_f}{k_i}\frac{(2\pi)^3}{2\mathrm{v}_0}\sum_{s=1}^{3\nu}\sum_{\mathbf{q}}\sum_{\boldsymbol{\tau}}\frac{1}{\omega_s(\mathbf{q})}\left|\sum_d \frac{\bar{b}_d}{\sqrt{M_d}} e^{i\mathbf{Qd}} e^{-W_d}\,\mathbf{Qe}_{s,d}(\mathbf{q})\right|^2$$

$$\times\Big(\delta(\omega_s(\mathbf{q})-\omega)\,\delta(\mathbf{Q}-\mathbf{q}-\boldsymbol{\tau})\langle n_s+1\rangle + \delta(\omega_s(\mathbf{q})+\omega)\,\delta(\mathbf{Q}+\mathbf{q}-\boldsymbol{\tau})\langle n_s\rangle\Big)$$