Off-specular scattering with focus on time-of-flight

Philipp Gutfreund

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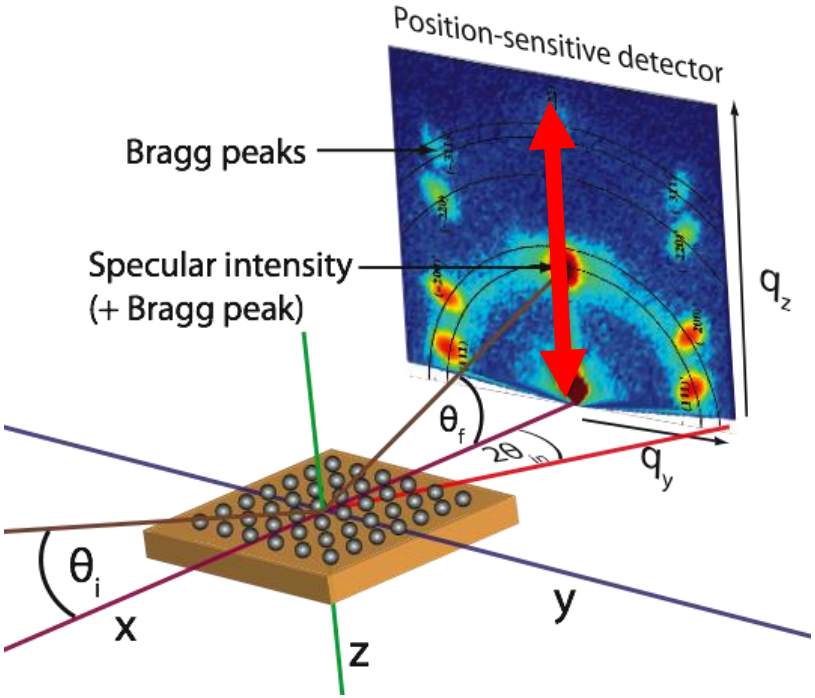
Reflectometry, OSS and GISANS



$$q_x = \frac{2\pi}{\lambda}(\cos\theta_f \cos 2\theta_{in} - \cos\theta_i)$$

$$q_y = \frac{2\pi}{\lambda}(\cos\theta_f \sin 2\theta_{in})$$

$$q_z = \frac{2\pi}{\lambda}(\sin\theta_i + \sin\theta_f)$$

Accessible q-range:

$$10^{-5}\,\text{Å}^{-1} \leq q_x \leq 10^{-3}\,\text{Å}^{-1} \equiv 1 - 100\,\mu m$$

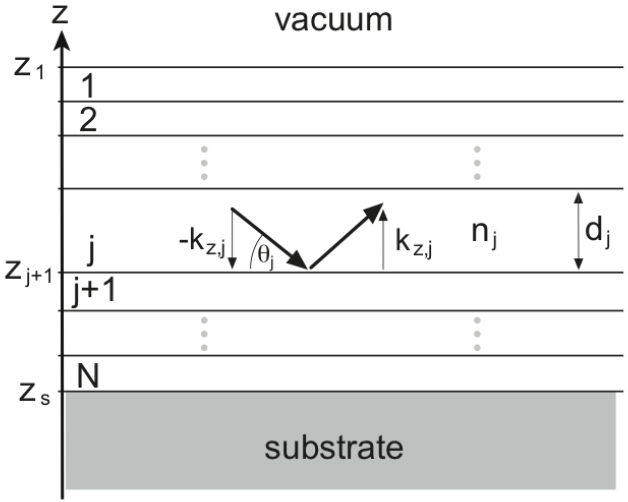
$$10^{-3}\,\text{Å}^{-1} \leq q_y \leq 10\,\text{Å}^{-1} \equiv 1 - 10000\,\text{Å}$$

$$10^{-3}\,\text{Å}^{-1} \leq q_z \leq 1\,\text{Å}^{-1} \equiv 10 - 10000\,\text{Å}$$

Distorted-wave Born Approximation(DWBA)

$$V(\vec{r}) = \bar{V}(z) + \delta V(\vec{r})$$

Separation of real system into z-projection and the rest



$$\phi_i = a_i \mathrm{e}^{i\vec{k}\vec{r}}$$

$$< 2|V(\vec{r})|\phi_i > \approx < \psi_2|\bar{V}(z)|\phi_i > + < \psi_2|\delta V(\vec{r})|\psi_1 >$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{spec} + \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{OS}$$

The OSS has to be <<1

Perturbed step potential

$$V(\vec{r}) = \bar{V}(\vec{r}) + \delta V(\vec{r})$$

Splitting into z and in-plane dependence:

$$\psi_1(\mathbf{r}) = \begin{cases} \mathrm{e}^{\mathrm{i}\mathbf{k}^{\parallel}\mathbf{r}_{\parallel}}(a_i(z)\mathrm{e}^{\mathrm{i}k_z^i z} + a_f(z)\mathrm{e}^{-\mathrm{i}k_z^f z}) & \text{for } z < 0 \\ \mathrm{e}^{\mathrm{i}\mathbf{k}^{\parallel}\mathbf{r}_{\parallel}} a'(z)\mathrm{e}^{ik'_z z} & \text{for } z > 0, \end{cases}$$

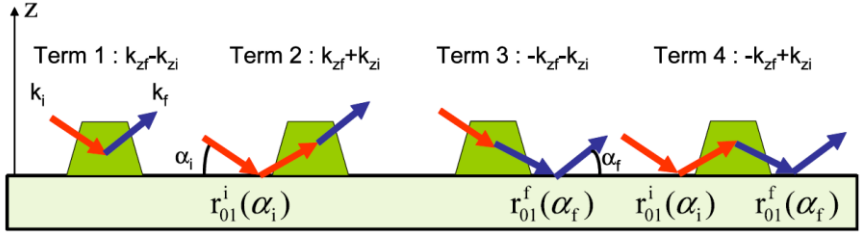
$$\psi_2(\mathbf{r}) = \begin{cases} \mathrm{e}^{\mathrm{i}\mathbf{k}^{\parallel}\mathbf{r}_{\parallel}}(a_i(z)\mathrm{e}^{-\mathrm{i}k_z^i z} + a_f(z)\mathrm{e}^{\mathrm{i}k_z^f z}) & \text{for } z < 0 \\ \mathrm{e}^{\mathrm{i}\mathbf{k}^{\parallel}\mathbf{r}_{\parallel}} a'(z)\mathrm{e}^{-ik'_z z} & \text{for } z > 0, \end{cases}$$

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_{\mathrm{OS}} = \left| \int \mathrm{d}\mathbf{r}\Psi_1(\mathbf{r})\Delta\rho(\mathbf{r})\Psi_2(\mathbf{r}) \right|^2 \quad \rightarrow \quad \text{16 terms}$$

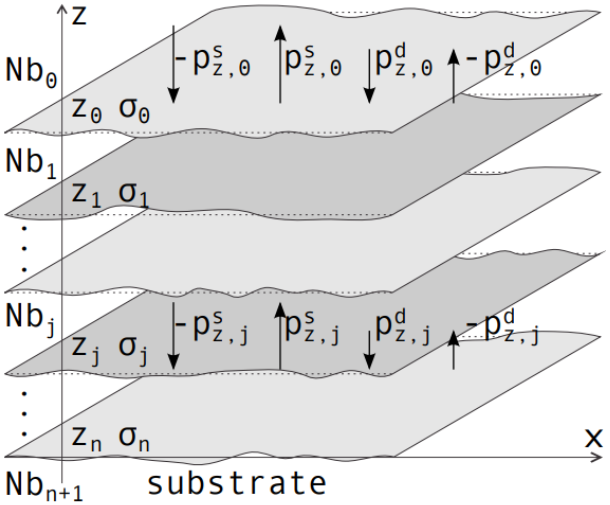
Perturbed step potential

5 distinct momentum transfers:

$$\mathbf{q_1} = \mathbf{q}_{\parallel}$$
$$\mathbf{q_2} = \mathbf{k_i} - \mathbf{k_f}$$
$$\mathbf{q_3} = \mathbf{k_i} + \mathbf{k_f}$$
$$\mathbf{q_4} = 2\mathbf{k_i}$$
$$\mathbf{q_5} = 2\mathbf{k_f}$$



R. Lazzari *et al.*, *Surf. Sci. Rep.* **64**, 255-380 (2009).



Upward and downward travelling refracted and reflected wave in each layer

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Calculated through Parratt formalism