Chapter 1

Resonant X-ray Electric Field Intensity

1.1 Experimental Setup

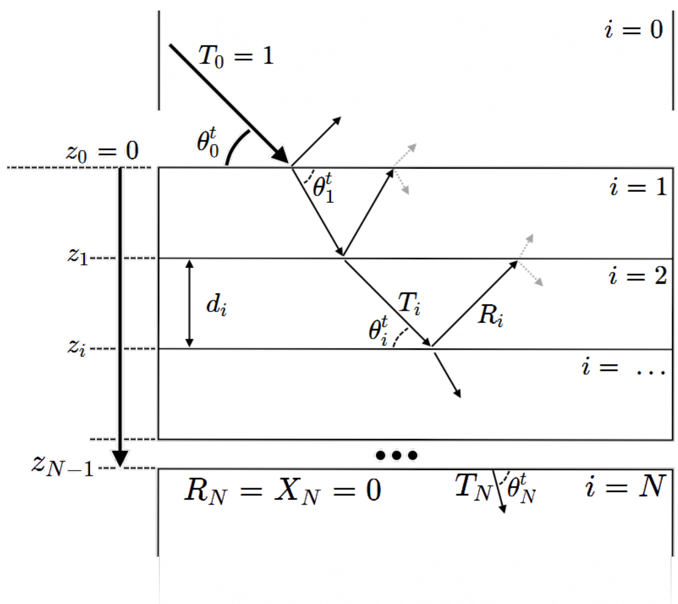

Figure 1.1: Experimental setup for measuring the X-ray electric field intensity. The X-ray beam is incident on a sample, and the reflected beam is analyzed to determine the electric field intensity.

1.1.1 Electric field

The total electric field of the X-ray beam in any given layer is given by the summation of two propogating waves.

$$\vec{E}_i(\vec{r}) = \vec{T}_i(\vec{r}) + \vec{R}_i(\vec{r}) \tag{1.1}$$

where

$$\vec{T}_i(\vec{r}) = T_i \cdot \exp\left(-\mathbf{i}\vec{k_i} \cdot \vec{r}\right) \tag{1.2}$$

$$\vec{R}_i(\vec{r}) = R_i \cdot \exp\left(+\mathbf{i}\vec{k_i} \cdot \vec{r}\right) \tag{1.3}$$

and $\vec{k_i}$ is the wavevector of the X-ray beam in layer i, at position $\vec{r}$.

Here the transmission and reflection components represent the sum of all multiple-scattering events in the layer. The complex constants T_i and R_i result of the requirement for continuity of the electric field vector at the boundary - more specifically, through a recursive solution using the Frensel coefficients for each interface.

Typically, especially for non-resonant X-ray scattering, the x-component wavevector k_x is ignored and the attenuation is treated as negligible.

1.1.2 Angle of incidence and wavevector

For any radiation of wavelength λ, and incident angle θ_0 coming from vacuum or a medium of complex refractive index N, the corresponding wavevector $\vec{k}$ is given by

$$\vec{k_0} = \frac{2\pi}{\lambda}\left(\cos(\theta_0)\hat{x} + \sin(\theta_0)\hat{z}\right) \tag{1.4}$$

As the X-ray propogates through the sample, the dielectric constant modifies the (now complex) angle of incidence and the complex wavevector, as per Snell's law (for grazing incidence).

$$\theta_i = \arccos\left(\frac{\cos(\theta_0) \times N_0}{N_i}\right) \tag{1.5}$$

$$\vec{k_i} = |\vec{k_0}|\left(\cos(\theta_i)\hat{x} + \sin(\theta_i)\hat{z}\right) \tag{1.6}$$

1.1.2.1 Critical angle

For any given refractive index $N_i < N_0$ [1], the critical angle occurs when $\cos(\theta_0) < \frac{N_i}{N_0}$. In the case where $N_0 \approxeq 1$ is air/vacuum, this critical angle corresponds to

$$\theta_0 = \sqrt{2\delta_i} \tag{1.7}$$

[1] This is usually the case for X-rays where $N_i = 1 - \delta_i + \mathbf{i}\beta_i$

1.2 Interface Calculation

To calculate the effect of refraction and reflection at each interface, a boundary condition is applied that the tangential component of the electric field must be continuous across the interface (both in $\hat{x}$ and $\hat{y}$ directions). This requires knowledge of the polarisation of the X-ray beam, as well as the refractive index of the medium.

1.2.1 Polarisation Dependence

An x-ray can be S-polarised (parallel to the planar surface, i.e. in the $\hat{y}$ or $\hat{x}$ direction) or P-polarised (parallel to the planar normal, i.e. in the $\hat{z}$ plane). These are also known as transverse electric (TE) and transverse magnetic (TM) polarisations, respectively.

Usually, the polarisation angle α can be defined as the angle between the electric field vector and the plane of incidence, with $\alpha = 0$ for S-polarised waves and $\alpha = \frac{\pi}{2}$ for P-polarised waves. Then the perpendicular and parallel components of the electric field vector can be defined as

$$E_{i,\perp} = E_i \cos(\alpha) \tag{1.8}$$
$$E_{i,\parallel} = E_i \sin(\alpha) \tag{1.9}$$

In the context of grazing incidence experiments, the X-ray beam is typically highly aligned and polarised. It will be routine to perform measurements with both S- and P-polarised X-rays.

1.2.2 Frensel Coefficients

Frensel coefficients describe the amplitude of reflected and transmitted waves at an interface between two media with different refractive indices. For S-polarised waves, the Frensel coefficients are given by

$$t_{s,i} = \frac{2k_{i,z}}{k_{i,z} + k_{t,z}} \tag{1.10}$$
$$r_{s,i} = \frac{k_{i,z} - k_{t,z}}{k_{i,z} + k_{t,z}} = t_{s,i} - 1 \tag{1.11}$$

For P-polarised waves, the Fresnel coefficients are given by

$$t_{p,i} = \frac{2k_{i,z}}{n^2 k_{i,z} + k_{t,z}} \tag{1.12}$$
$$r_{p,i} = \frac{n^2 k_{t,z} - k_{i,z}}{n^2 k_{t,z} + k_{i,z}} \tag{1.13}$$

At resonance, the refractive index n can be modified by a significant amount. Consider the imaginary component in Polystyrene (CH) at the carbon K edge changing magnitude from 1e-4 to 6e-3. For P3MEEET (C11H16O3S) at the resonant sulfur K edge, the magnitude changes from 9e-7 to 5.7e-6.

1.3 Taylor Series Derivation

Following the derivation of Borne & Wolf (1985) and Savakhin et al. (2020).

The total electric field is the sum of many reflections.

$$E = E_1 + E_2 + E_3 + ... + E_N \tag{1.14}$$

As we

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