Documentation for SWXF demo file

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1 Introduction

The file `SWXF_example_nov_2021.py` is an example file modeling the approach for calculating the expected signal from an x-ray standing wave fluorescence experiment. Sections in the code are marked off by `"#%%"`. Below we go through the sections one at a time

2 Section 1

In this section physical and mathematical constants are imported from scipy.constants. To the extent possible MKS units are assumed through the code. However, this is not always possible, as, for example, some of the functions in the x-ray database require energies in eV units. I will try to make the conversions obvious when they occur. Otherwise assume MKS. Metric prefixes are then used to convert from MKS. For example, 44*centi will be used to represent centimeters, where the unit of "meters" will have to be inferred from context. It is possible to attach units to quantities in python using the pint package, but this leads to complications when you use arrays, so I am skipping it.

3 Section 2

Here we define the fluorescent tag as a 5 nm diameter gold nanoparticle. I'm not sure if that will be the actual size of the nanoparticle used for fluorescent tags, this is something we need to consult on with Dr. Gaillard and the literature. But given the nanoparticle diameter, and assuming it is spherical, we can then calculate the number of atoms which we will need to get the fluorescent cross section.

4 Section 3

In section 3 we define the surface coverage in terms of the distance between gold nanoparticles on the surface. If we put one gold label per protein then this is the distance between proteins on the surface. We need to consult the literature to see what is a reasonable packing density of proteins in a supported lipid film. I guessed a spacing of every 100 nm. Perhaps this is conservative, we can probably pack them denser, but at some point they begin to interact with each other. However the denser the protein packing the stronger the signal.

5 Section 4

In section 4, we calculate the atomic absorption cross section. The atomic absorption cross section is given by the imaginary part of the atomic scattering factor f_2 via

$$\sigma = 2 f_2 r_0 \lambda. \tag{1}$$

We then correct this by the fluorescent yield in order to only calculate the fraction of absorbed x-rays that result in fluorescence.

Given a cross section per atom σ_a we would like to calculate the total scattering cross section σ_T. This will depend on the number of atoms intercepted by the beam. The total number of fluorescent photons produced is given by

$$N = \Phi \sigma_T \tag{2}$$

Here Φ is the incident beam flux (photons/m^2). However, typically we specify the beam in terms of the beam intensity I_0 and the area of the beam A_0. In this case $\Phi = I_0/A_0$. Assume that we have a density of atomic scatters ρ_N each with cross section σ. Then the total cross section of scatterers in the beam is $\sigma_T = \rho_N \sigma_a A_0 \Lambda$. Here Λ is the thickness of the sample. Thus we can rewrite eq. 2 as:

$$N = \frac{I_0}{A_0} \rho_N \sigma_a V = \frac{I_0}{A_0} \rho_N \sigma_a A_0 \Lambda = I_0 \rho_N \sigma_a \Lambda \tag{3}$$

We actually have a surface density of scatterers S_N not a volume density, σ_N. To convert between surface density and volume density we can use $\rho_N = S_N/h$ where h is the height of the beam.

We can now calculate the total fluorescence yield given the beam intensity, I_0. Let h be the beam height and α the incident angle. Since the beam comes in at grazing incidence, the thickness of sample intercepted by the beam is $\Lambda = h/\alpha$. Putting this into eq. 3 gives:

$$N = I_0 \frac{S_N}{h} \sigma_a \Lambda = I_0 \frac{S_N}{h} \sigma_a \frac{h}{\alpha} = I_0 S_N \sigma_a / \alpha \tag{4}$$

6 Refectivity functions

Here we discuss the functions `n_elem(elem,E)`, `n_water(E)`, `swave(alpha,z,E)` used to calculate the standing wave. The function `n_elem(elem,E)` takes an element and finds the x-ray index of refraction at the energy E given in eV. The function `n_water(E)` calculates the index of refraction for water. Since we are assuming scattering from a phospholipid bilayer submerged in water, these two materials form the interface if we ignore the bilayer.

The function `swave(alpha,z,E)` calculates the reflectivy of the interface from Fresnel's laws using the indices of refraction, then sums the incident and reflected waves and squares them to find the intensity of the standing wave at height z relative to the surface. We approximate Fresnel's laws in the limit of small angles. Here we can ignore polarization and we get

$$R(\alpha) = |r(\alpha)|^2 = \left|\frac{\alpha_{-}\alpha'}{\alpha + \alpha'}\right|^2 \tag{5}$$

Here α is the incident angle and $\alpha' = \sqrt{\alpha^2 - \theta_c^2}$ and θ_c is the critical angle for total external reflection.

The critical angle is given by Snell's law. This is typically written as

$$\frac{\sin(\phi_1)}{\sin(\phi_2)} = \frac{n_2}{n_1} \tag{6}$$

Where the angles ϕ_1 and ϕ_2 are defined with respect to the surface normal. Since in x-ray scattering the angles are typically defined with respect to the surface rather than the surface normal, we can write $\theta = 90 - \phi$ and thus $\sin(\phi) = \sin(90 - \theta) = \cos(\theta)$. Thus the condition for the critical angle is that $\cos(\theta_2) = 1$ since for smaller angles $\cos(\theta_2)$ would have to exceed 1, which implies an imaginary angle. Thus we can write the expression for the critical angle as:

$$\theta_c = \arccos\left(\frac{n_2}{n_1}\right) \tag{7}$$

We can also calculate the transmission of the interface

$$T(\alpha) = |t(\alpha)|^2 \left|\frac{2\alpha}{\alpha + \alpha'}\right|^2 \tag{8}$$

Given Snell's law and the reflection and transmission coefficients we can then calculate the x-ray field intensity above and below the interface. Below the interface the electric field is given by $E_T = tE_0 e^{i\vec{k}\cdot\vec{r}} = tE_0 e^{ik_0 z \sin(\alpha')}$. Here z is the height above (or below) the surface. This gives for the transimtted intensity, I_T:

$$I_T = I_0 T^{k_0 z\left(i\sin(\alpha') - i\sin(\alpha')^*\right)} \tag{9}$$

Normally, the exponential term cancels out, however, below the critical angle the refracted angle is purely imaginary so that this term leads to an exponential decay with z.

Above the surface we have the sum of two waves

$$E = E_0\left(e^{ik_0 z\sin(\alpha)} + re^{-ik_0 z\sin(\alpha)}\right) \tag{10}$$

giving the intensity $I = |E|^2$ which oscillates as a cosine

$$I/I_0 = 1 + r^2 + r\left(e^{2ik_0 z\sin(\alpha)} + e^{-2ik_0 z\sin(\alpha)}\right) = 1 + r^2 + 2r\cos(2k_0 z\sin(\alpha)) \tag{11}$$

Note that this results in a standing wave with an oscillation period of These relations are used in `swave(alpha,z,E)` to find the intensity of standing wave above and below the interface.

Note that we don't really need the intensity of the standing wave below the interface in order to calculate the fluorescence since the gold is above the interface, but we might need this later to estimate background scattering from the surface.

Also, note that this scheme is only an approximation. The reflection from the interface will be modified by the presence of the bilayer. However we will deal with that correction later.

For now there are two separate versions of the funciton `swave(alpha,z,E)`. `swave_z(alpha,z,E)` allows you to submit an array of incident z-values for a fixed angle and `swave_a(alpha,z,E)` allows you to submit an array of incident angles for a fixed height.

7 Section 6

In section 6, the functions are used to create plots. The first graph looks at the standing wave intensity vs. height for a fixed incident angle. This gives an indication of how sensitive the technique is to the position of the nanoparticle. The second graph plots the fluorescence yeild vs. angle for a nanoparticle at a fixed height.

8 Things to try next

1. Plot a graph of fluorescence yeild vs. particle size, or area coverage (trivial)
2. Superimpose plots of fluorescence yield vs. angle for different heights of nanoparticle
3. Calculate the fraction of fluorescence that would get into a detector for an acheivable experimental setup.
4. Modify the code to include the reflectivity from an interface with a bilayer.
5. Modify the code to include an estimate of Compton scattering background