# Documentation for SWXF demo file

December 13, 2021

## 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

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

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 $\sigma_a$ we would like to calculate the total scattering cross section $\sigma_T$. 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 $\Phi$ 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 $\rho_N$ each with cross section $\sigma$. Then the total cross section of scatterers in the beam is $\sigma_T = \rho_N \sigma_a A_0 \Lambda$. Here $\Lambda$ 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, $\sigma_N$. 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 $\alpha$ 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:

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