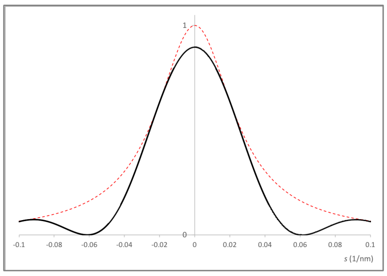
Assignment Week 5 – Answers

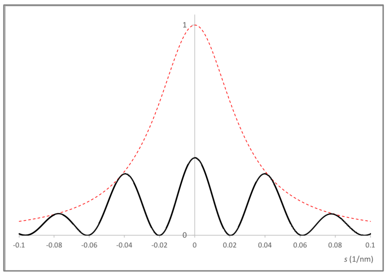
Assignment 5.1

a) Below are shown the four different rocking curves for the diffracted beam intensity (in solid black lines) and their envelope functions (in dashed red lines).

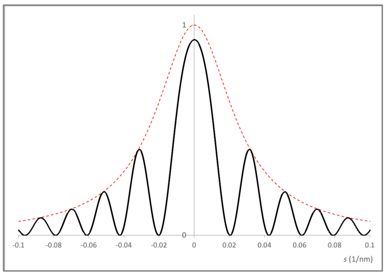
t = 15 nm:



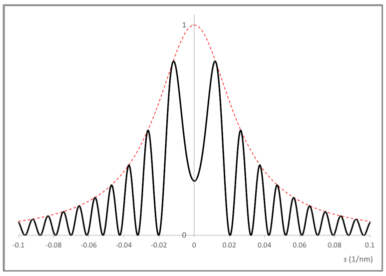
t = 30 nm:



t = 60 nm:



t = 120 nm:



Do the plots match well those shown in these corrections?

b) For the plots made in part a):

i. As the thickness t increases, the frequency of sinusoidal modulations in excitation error s also increases.

ii. The envelope function does not change with specimen thickness. This is because the envelope function is given by the expression:

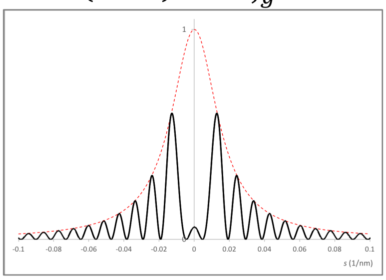
$$\frac{1}{1+\xi_g^2 s^2}$$

iii. The increased frequency of sinusoidal oscillations with thickness in part i) is an effect similar to what was seen using the kinematical approximation, as derived from the approximation that the intensity distribution along the length of the reciprocal lattice rod is the Fourier transform of the sample thickness.

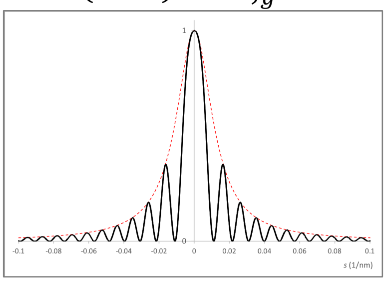
iv. Only the 15 nm and 60 nm specimen thicknesses would be suitable for dark-field imaging at the exact Bragg condition, because they are the only two images which would give a strong intensity in the diffracted beam (i.e. intensity close to 1), and hence a strong image intensity.

c) The envelope function can be modified by choosing a plane from another family of planes to excite in the 2-beam condition, such that it has a different extinction distance ξ_g. For a correct answer this should be done for two different types of planes.
As an example, curves are shown here for:

Plane $(2\ 2\ 0)$ with $\xi_g = 62.43$ nm:

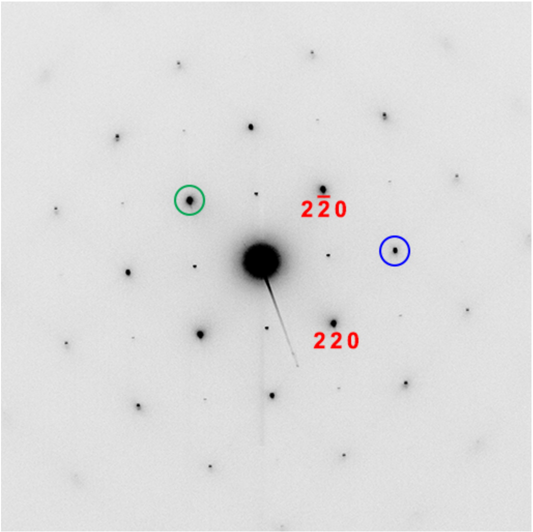


Plane $(2\ 2\ 2)$ with $\xi_g = 80.23$ nm:



Assignment 5.2

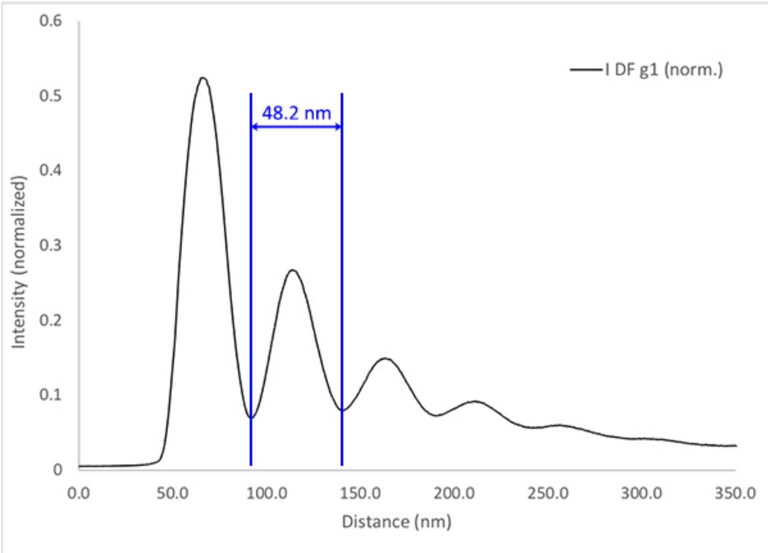
a) If we compare the SADPs under conditions $\boldsymbol{g}_1$ and $\boldsymbol{g}_2$ with the zone axis SADP, then we can see that $\boldsymbol{g}_1$ corresponds to the reflection circled in blue below, and $\boldsymbol{g}_2$ to the reflection circled in green:

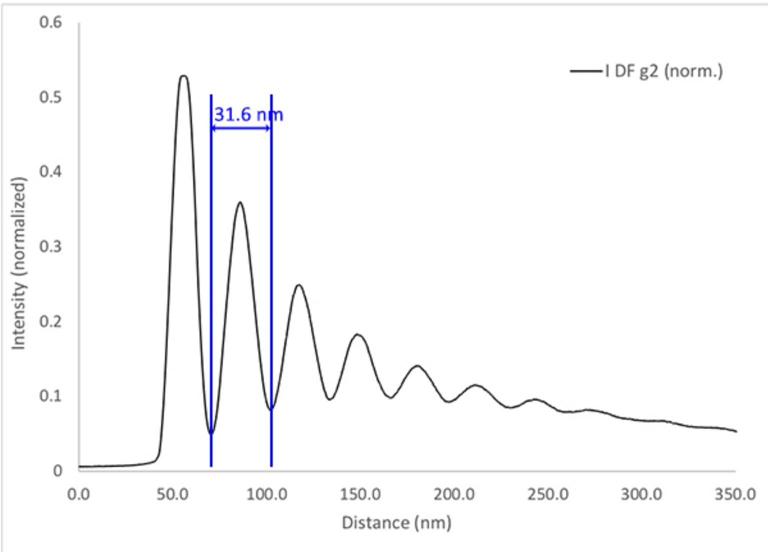


From the indices given in the zone axis SADP:
$\boldsymbol{g}_1$ corresponds to: $(2\ \bar{2}\ 0) + (2\ 2\ 0) = (4\ 0\ 0)$
$\boldsymbol{g}_2$ corresponds to: $-(2\ 2\ 0) = (\bar{2}\ \bar{2}\ 0)$

It can be commented that the thickness fringes are broader for the reflection $\boldsymbol{g}_1$, plane $(4\ 0\ 0)$, than for the reflection $\boldsymbol{g}_2$, plane $(\bar{2}\ \bar{2}\ 0)$.

b) The plotted curves are shown below. Here they are plotted on separate graphs, but they can be plotted on the same graph as well.





From the curves, the lateral distances for between peaks or valleys of intensity are:

$\boldsymbol{g}_1$: 48.2 nm

$\boldsymbol{g}_2$: 31.6 nm

Using the 2x relationship of extinction distance to lateral distance for the cleaved wedge geometry, this gives estimated extinction distances of:

$\xi_{g1} \approx$ 96.4 nm (more generally: $\xi_{g1}\left(or\ \xi_{g\,(4\,0\,0)}\right) =$ value in the range of 94 – 100 nm)

$\xi_{g2} \approx$ 63.2 nm (more generally: $\xi_{g2}\left(or\ \xi_{g\,(\bar{2}\,\bar{2}\,0)}\right) =$ value in the range of 58 – 64 nm)

Note that for measuring from the first to second peak gives a slightly different answer to measuring other peak-to-peak or valley-to-valley combinations. Perhaps this is because of rounding of the edge of the cleaved wedge from oxidation.

c) Clearly the two values of extinction distances are different. This is because each of them is for a plane from a different family. Because the scattering angle for the $(4\ 0\ 0)$ plane is larger than for the $(\bar{2}\ \bar{2}\ 0)$ plane, its atomic form factors are lower, thereby reducing the plane's structure factor compared to the $(\bar{2}\ \bar{2}\ 0)$ plane. This in turn gives it a greater extinction distance.

d) In the table, the modelled extinction distances for these two families of planes are:

$$\xi_{g\ (4\ 0\ 0)} = 103.76 \text{ nm}$$

$$\xi_{g\ (\bar{2}\ \bar{2}\ 0)} = \xi_{g\ (2\ 2\ 0)} = 70.3 \text{ nm}$$

Their ratio is therefore:

$$\frac{\xi_{g\ (4\ 0\ 0)}}{\xi_{g\ (2\ 2\ 0)}} = 1.5$$

The corresponding ratio for the experimental data is:

$$\frac{\xi_{g1}}{\xi_{g2}} = \frac{96.4}{63.2} = 1.5$$

We can see that the two ratios are in excellent agreement. Therefore, even if there is a discrepancy between the absolute values of modelled to experimental extinction distances (because of challenges in modelling the atomic form factors accurately), this discrepancy is rather uniform and extinction distance ratios match well.
(Note that for a correct answer the inverse ratio can instead by specified, value of 0.66–0.67).