**X-Ray Reflectivity—Substrate**

*General Notes*

- This experiment was performed to get a general sense of the thicknesses and surface roughnesses of each layer in the substrate.
- Sample was composed of the substrate only with no additional Nafion on top. Layers:
  - Silicon
  - Silicon oxide
  - Permalloy
  - Platinum
  - Air

*Active/Best Fit*

- LOCATION: `~\Active\X-Ray\`
- STATUS: Fit completed.
- FIT: DREAM, burn-in 100,000, population 20, initializer LHS, steps 2,000.
  - This fit is the UpdatedSLD fit from below, but I allowed it to run for the full number of burn-in and steps and added the background as a fit parameter.
  - This fit is good in the sense that it has converged, the variances appear to be normally distributed, and the correlations between parameters is small.
    - There is one exception: the intensity and rho of platinum are strongly correlated.
  - The model uncertainty is minimal, with some traces differing at the oxide layer.
  - The fitted XrSLD of the silicon oxide layer ($30.37 \times 10^{-6}$ Å$^{-2}$) is much higher than the nominal value ($18.83 \times 10^{-6}$ Å$^{-2}$), this indicates that the permalloy and silicon formed an alloy between them.
  - The thickness of the oxide layer is also greater (30 Å) than I would normally expect, ~ 10 Å, but this thickness is similar to what we see in the neutron data.
  - The thicknesses and surface roughnesses of the permalloy and platinum layers are very similar to the fitted values from the neutron data.

*Other Fits*

- LOCATION: `~\Active\X-Ray\~`
- STATUS: Fits completed
- FIT: DREAM, burn-in 100,000, population 20, initializer LHS, steps 2,000.
- Interfacial fits
  - I also ran four additional fits where I added an interfacial layer between each pair of layers in the substrate to test if there was an additional layer not accounted for in the base fit. There were four fits:
  - Silicon/Oxide
    - The first fit has an additional interfacial layer between the silicon and oxide layer.
    - This fit is slightly better than the base fit ($\chi^2 = 15.667$, BIC = 5659).
    - The fit parameters for the various layers are equal to the values in the base fit, with the exception of the oxide layer, which has an essentially zero thickness ($t = 3.4 \times 10^{-6}$ Å).
    - The interfacial layer replaces the oxide layer in the base fit and has the same parameters.
    - Despite being an improvement over the base fit, the vanishingly small oxide layer indicates that there is no additional layer between the silicon and oxide and this fit cannot be used.
    - I had attempted the fit by setting the lower bound of the oxide thickness to various non-zero values (5 Å, 10 Å, 20 Å) but every single one of these fits was lower limited, and the fit with a zero thickness was the only model that would fit the data.
  - Oxide/Permalloy
    - This fit is very similar to the above fit with the interfacial layer in between the silicon and oxide layers in that it offers a slight improvement in fit quality ($\chi 2 = 10.190$, BIC = 3720), but the interfacial layer replaces the permalloy layer, which in turn has an almost zero thickness ($t =$ 0.003 Å).

    - I also repeated this fit by forcing the thickness of this layer to be lower bound at 5 Å, 10 Å, and 15 Å, but they were consistently lower-bound limited and the near-zero thickness was the best model of the data.
    - Because this interfacial layer is essentially zero, we can assume that there is no interfacial layer between the oxide and permalloy layers.
- Permalloy/Platinum
    - This fit has a much thicker interfacial layer that takes up the majority of where the platinum layer was in the base fit, and the platinum layer corresponds to the surface of the sample in the base fit.
    - This fit is the best fit ($\chi^2 = 5.100$, BIC = 1917), however the difference between the SLD of the interfacial ($128.2 \times 10^{-6}$ Å$^{-2}$) and platinum ($122.6 \times 10^{-6}$ Å$^{-2}$) is minimal.
    - At the same time, the sum of the thicknesses of these two layers equals the fitted thickness of the platinum layer in the base fit. (40.57 Å + 9.30 Å = 49.87 Å, compared to 49.54 Å in the base).
    - The interface thickness and platinum interfaces correlates with many other parameters.
    - There are many different correlations between the parameters, which can be very large (platinum thickness and platinum irho) or less so, while still being significant (platinum interface and permalloy thickness).
    - I think that this fit is overfitting the data by splitting the platinum layer into two layers that do not exist and that we do not learn anything new from this fit.
    - The surface roughness of the platinum layer ($\sigma = 3.537$) is the similar to the base fit ($\sigma = 3.711$).
- Platinum/Air
    - Like the fit with an interfacial layer between the permalloy and platinum layers, this fit is significantly better than the base fit ($\chi 2 = 6.767$, BIC = 2508) but has many of the same issues as the other interfacial fit.
    - The platinum layer is split into two layers: platinum composes the majority of the layer while the interfacial layer represents the surface roughness of the total sample.
    - The sum of the thicknesses of these two layers is approximately the same as in the base fit (39.07 Å + 10.83 Å = 50.90, compared to 49.54 Å).
    - The various fit parameters exhibit correlations across many different parameters.
    - The surface roughness of the interfacial layer ($\sigma = 3.537$) is the similar to the base fit ($\sigma = 3.711$).
    - Comparing the interfacial layer in the previous fit to the platinum layer in this fit, and the platinum layer in the previous fit to the interfacial layer in this fit shows that the best fit parameters are similar. I interpret this to mean that the interfacial and platinum layers correspond to the same two layers in each fit.

*Take Aways*:
- The best-fit model of the data confirms that the sample is composed of four layers: silicon, oxide, permalloy, platinum.
- Additional models were tested by adding interfacial layers between each pair of layers above, but there is no evidence that there is any additional layers.
- In two of the fits, which had additional layers at the silicon/oxide and oxide/permalloy interfaces, the thickness of the interfacial layer was so small ($t \leq 0.01$ Å) that it can be assumed that the layer does not exist.
- In the other two fits, which had additional layers at the permalloy/platinum and platinum/air interfaces, the combination of the interfacial and platinum layers corresponds to the platinum layer in the base fit.
- The thicknesses of the permalloy, $t = 108$ Å, and platinum, $t = 49.54$ Å, layers are approximately the same as we requested from NanoFab.
- The SLDs of every layer is close to the theoretical values calculated for the Cu Kα X-ray wavelength[1], with the exception of the XrSLD of the oxide layer.
- The fitted XrSLD of the silicon oxide layer ($30.37 \times 10^{-6}$ Å$^{-2}$) is much higher than the nominal value ($18.83 \times 10^{-6}$ Å$^{-2}$), this indicates that the permalloy and silicon formed an alloy between them.

[1] $E = 8.04$ keV, $\lambda = 1.5406$ Å

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