# Day 1 Materials

CHRNS Neutron School

## Goals

* Reduce a data set
* Calculate expected SLDs using the NIST neutron activation calculator
* Generate a model of a thin film sample
* Fit a data set using Refl1D

## Data sets

### Sample

A TiO2 film was deposited on a silicon wafer by sputter deposition. Nominal thickness is 140 Å. The sample was mounted in the NCNR flow cell; the liquid reservoir was then filled with fully deuterated (d9-2-propanol, or dIPA) or fully hydrogenated 2-propanol (hIPA)

(Note: this was done in preparation for solvent exchange. We were interested not just in the structure of bilayers formed by slow solvent exchange, but also in the mechanism of bilayer formation. So, after characterizing the thin film by itself, we added lipids dissolved in deuterated IPA and hydrogenated IPA to get a sense for surface adsorption. Then we did the slow solvent exchange to form the bilayer, which we will analyze from a different experiment during Day 2.)

### Data path

ncnrdata/cgd/202003/23396/data/

Intensity scans (high Q): ch090, scans 26129 and 26130

dIPA data set: ch127 (specular, backgrounds, low Q intensity scan)

hIPA data set: ch128 (specular, backgrounds, low Q intensity scan)

To think about:

Calculate the expected SLD of TiO2 (what information do you need to do this?). How does this value compare to the fit result?

## Links

Reductus: <https://reductus.nist.gov>

Refl1D: [Reflectometry Software Installation | NIST](https://www.nist.gov/ncnr/chrns/education-and-outreach/chrns-summer-school-neutron-scattering/course-materials-0)

Neutron activation (and SLD) calculator: <https://www.ncnr.nist.gov/resources/activation/>

or <https://bmaranville.github.io/activation/activation/index_pyodide.html>