This module will cover the basics of undertaking Rietveld and Le Bail analysis using GSAS. It is designed for users who collect XRD data and compare to databases but wish to learn more about their materials. In other words, users who want to refine the structural model with the collected data. The course will be interactive and you will require a working copy of the GSAS suite on your own laptop.

GSAS is available at no cost for MacOSX, Linux and Windows at: https://subversion.xor.aps.anl.gov/trac/EXPGUI (you will require both GSAS and the EXPGUI graphical user interface for GSAS)

Please note, there are a number of refinement programs available including HighScore, Jana2006, Topas, Rietica, Rietan, FullProf, etc…, however the details and methods learnt in this course are easily applicable to these other software suites – they use the same analytical approach but the interface is different.

The tutorial will work through converting data to acceptable formats, loading XRD data and crystallographic models, and the process of refining models. This last step will be the focus of the majority of the tutorial detailing why certain parameters are refined and in what order. To finish off the tutorial, a sequential refinement will be undertaken - this is where 100s of XRD data can be refined simultaneously and is often undertaken as a function of temperature or electrochemical charge/discharge or applied electric or magnetic field, etc…

The course will be interactive and further topics can be covered, please contact Neeraj (neeraj.sharma@unsw.edu.au) for a discussion of these options. Additionally, if researchers are interested in an advanced or troubleshooting course please contact Neeraj or Chris as we are thinking of running one later in the year.

External applicants from other universities, institutes, or industry are more than welcome, please contact c.marjo@unsw.edu.au for pre-payment details. For UNSW researchers, please register by emailing c.marjo@unsw.edu.au with the module name, your name, the school, and UNSW account code.

Cost is $30 ex-GST and the course is limited to 20 people