Case for 1-2 permanent DMSC staff dedicated to computational powder diffraction science - development of the ESS Rietveld package.

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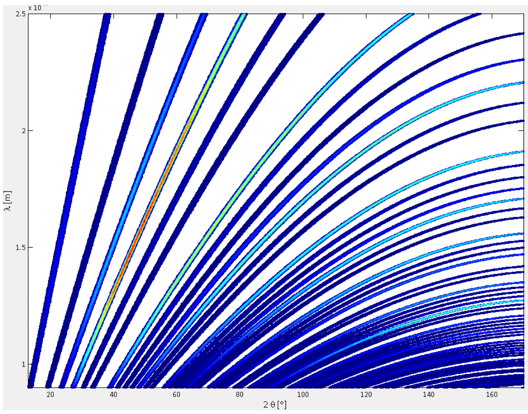
Powder diffraction is one of the more popular and productive neutron techniques. It is applied to a wide range of solids, including battery and fuel cell materials for clean energy applications, superconductors and magnets, minerals and ceramics, and molecular materials such as pharmaceuticals. Virtually all powder neutron diffraction analyses and subsequent publications use a computational profile fitting method first developed in the 1960's by H. Rietveld, then a researcher at the Dutch Petten reactor neutron facility. Although the central algorithm is quite simple, Rietveld programmes have grown into large and sophisticated packages where models may be fitted to multiple neutron and x-ray profiles, with details of crystal or magnetic ordered structures including incommensurate modes, and microstructural features such as sample texture being refined freely or under suitable constraints.

Neutron facilities have developed Rietveld packages for their users with varying degrees of success. The two most successful and widely-used packages are GSAS (developed by A.C. Larson and R.B. von Dreele at Los Alamos National Lab, and now supported by B. Toby at Argonne National Lab) and Fullprof (from J. Rodriguez at ILL, Grenoble). Their success has resulted from consistent support and development by the latter individuals over many years. Facilities or university groups that have tried to develop and maintain Rietveld codes through short term support have generally not been successful.

Several powder neutron diffractometers are currently under discussion for ESS, and it is likely that at least one will be included in the first phase of 7 instruments, with several more in the eventual suite of 22 public instruments. It is thus essential that ESS develops a coherent plan to ensure that suitable Rietveld software is available to users. Reliance on the use of GSAS, Fullprof or other software written elsewhere is a risky approach, and these may not handle the novel characteristics of ESS data (e.g. resulting from the long neutron pulse) well. Furthermore, much of the data emerging from ESS instruments will be intrinsically '2-dimensional' as illustrated by the Figure. Only cuts in the vertical (wavelength) or horizontal (2theta) directions can be analysed with existing Rietveld programs, so new software is needed to make use of the full information content of ESS powder diffraction data. Additional dimensions to the data will result from variable time, temperature, pressure etc. experiments facilitated by the very high flux of ESS instruments.



The DMSC proposal provides the ideal opportunity to ensure that Rietveld fitting of ESS powder neutron diffraction data is possible. At least one permanent staff member is required, and given the other computational needs of powder diffraction, for example in pre-processing and visualisation of data, and in pdf-type fitting of diffuse scattering, a more sensible approach would be to dedicate two permanent staff to computational powder diffraction science. They could build up a group of postdoctoral researchers and PhD students from the international ESS community. Developing an ESS Rietveld package (from scratch, or better, through collaboration with the existing teams) would be a principal activity. This large task should start soon, so that the package can be tested on data from a variety of sources while ESS is being constructed, and hence will be fully ready when initial powder neutron diffraction data emerge from the new source.