Data Collection and Batch Refinement

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This presentation will deal primarily with methods of collecting and refining large data sets, I shall refer to experimental methods that have been used with the Rapid2 detector which is located at station 6.2 of the SRS. Due to the high time resolution possible using this detector, it is possible to collect many 'frames' of data in a short time. This not only enables fast reactions to be monitored 'in-situ', but also presents the problem of dealing with large data sets which need to be refined. Due to this particular problem batch refinement is essential in order to handle these large data sets; it is from this point of view that I shall deliver the presentation.

However in our research group there are many areas in which large data sets are collected, so I would like to highlight the work being carried out at the moment to illustrate how it is possible to collect large amounts of data.

My presentation will be split equally into three parts with ten minutes being spent on each section, these sections will have the following titles;

1. Experimental methods and data collection.
2. Research in our group.
3. Batch refinement and associated pitfalls.

During the final section I shall talk about 'Le Bail' and 'Rietveld' refinement methods in the 'Fullprof' suite, This will include the importance of finding a good initial model before performing a refinement, and the fact that this model should be made as good as possible before carrying out a batch refinement. I will also highlight how data is converted from the raw format obtained at the synchrotron into a format which can be used by 'Fullprof'.