Automated processing for X-ray Pair Distribution Function data

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The XPDF project at Diamond Light Source aims to provide high quality X-ray Pair Distribution Function data to members of the materials science community who are not expert synchrotron users. To this end, the project aims to combine a sophisticated LIMS with automatic processing of the data. The data management is provided by SynchWeb[1], working as the GUI in front of the ISPyB database[2]. Users upload the details of their sample and experimental conditions using this LIMS. Once the X-ray diffraction data have been obtained on the I15-1 beamline at DLS, the collected metadata is used to drive automatic processing using the Dawn data analysis system[3]. Two approaches will be described and compared: a process based on first-principles ray-tracing and one based on scattering data generated by the XRMC simulation software[4]. The data management pipeline will also be described and the challenges of providing automatic data processing for non-expert users discussed.

References

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