

**Simultaneous Local and Long Range Structure Determination:
Application to *in-situ* Studies**

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The ability to accurately determine structural disorder, both static and dynamic, requires the application of techniques that directly probe local atomic structure. Recently, the combined application of high energy X-rays, >70 keV, and area detectors have enabled the efficient collection of data suitable for PDF analysis in the time range from seconds to minutes - a three orders of magnitude reduction in measurement time from experiments using point detectors.[1] This has opened up the possibility of *in-situ*, time resolved experiments as complete data sets can be collected rapidly.

The potential of *in-situ* studies that probe both local and long-range structure has recently been demonstrated in a study of the phase transition of aluminum trifluoride, which used the combined approach of PDF analysis, Rietveld refinement, and molecular dynamics simulations.[2] The study, which used a sample environment with accurate temperature control and low background, showed clear deviations between the instantaneous local atomic structure and the long-range time averaged structure, as probed by the PDF method and Rietveld refinement, respectively.

[1] Chupas P.J., Qiu X, Lee P.L., Hanson J.C., Grey C.P., Billinge S.J.L., *J. Applied Cryst.*, 2003, **36**, 1342. [2] Chupas P.J., Chaudhuri S., et al., *J. Am. Chem. Soc.*, 2004, **126**, 4757.

Keywords: pair distribution function, powder diffraction under nonambient conditions, high energy x-rays