

Recent Developments in Total Scattering Data Collection and Interpretation

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The total structure factor and its Fourier transform, the total radial distribution function, provide key information for understanding the structure of liquid and amorphous materials. The experimental challenge is to obtain these structural functions as accurately and routinely as possible. The methodology is well established using neutron diffraction and recent advances in high-energy synchrotron x-ray diffraction mean that x-ray structure factors are now of comparable quality to their neutron counterpart. This talk will discuss developments using both neutron and x-ray diffraction, highlighting improved instrumentation and, in particular, developments in total scattering under non-ambient conditions.

In addition, the interpretation of total scattering data is becoming increasingly sophisticated with the application of, amongst others, computer modelling methods. Reverse Monte Carlo (RMC) modelling is extensively used to interpret scattering data from disordered materials (liquids, amorphous and crystalline materials), producing three-dimensional models of the structure consistent with the experimental data. The RMC method will be described, concentrating on recent developments for use with time-of-flight neutron scattering data, the incorporation of chemically appropriate local constraints and the importance of good quality initial structural models.

Examples from recent results will be given throughout the talk.