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Structure of Liquid and Amorphous Materials using Pair-Distribution Function Analysis

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The atomic-scale structure of liquids and glasses is a prerequisite for understanding their material properties. There is an absence, however, of translational periodicity that leads to the Bragg peaks observed in the diffraction pattern for a crystal. Instead, the diffraction pattern is diffuse, and it is a challenge to solve the structure.

In this talk I will outline the theory necessary for understanding the X-ray and neutron diffraction patterns that are measured for structurally disordered materials, and show how these patterns can be used to obtain real-space structural information in the form of partial pair-distribution functions $g_{\alpha\beta}(r)$ [1,2]. Attention will be paid to multi-component systems, where overlap of the pair-correlation functions means that it is not possible to obtain all of the individual $g_{\alpha\beta}(r)$ from a single diffraction experiment. In favourable cases, however, information can be gained by using multi-pattern techniques that include (i) neutron diffraction with isotope substitution (NDIS), (ii) anomalous X-ray diffraction (AXD), and (iii) a combination of X-ray and neutron diffraction. These methods will be illustrated by case studies taken from recent work at central neutron and X-ray facilities.

Finally, I will introduce the ideas behind structural refinement techniques such as reverse Monte Carlo (RMC) and empirical potential structure refinement (EPSR), where measured diffraction patterns are used to guide in the construction of atomistic models.

[1] H. E. Fischer, A. C. Barnes and P. S. Salmon, Rep. Prog. Phys. **69** (2006), 233.

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