

## A24. Liquid and Amorphous Materials

Adrian Barnes

H.H.Wills Physics Laboratory, University of Bristol, Royal Fort  
Tyndall Avenue, Bristol, BS8 1TL, United Kingdom

Liquid and amorphous materials are ubiquitous in the world around us and play an important role in both life and technology; examples include, the subtle biological interactions in the body, the chemical processing of materials and the use of glasses for optics and in lasers, to name but a few. To understand their properties and function we need to understand the detailed inter-atomic arrangements and interactions in the materials. However, in the absence of long range ordering, that gives rise to Bragg scattering, diffraction patterns show only a smooth oscillatory behaviour that reflects the underlying local *short* (bonding) and *intermediate* range order. In these lectures I will present the underlying theory necessary to understand X-ray and neutron diffraction patterns from disordered systems and show how they can be used to obtain the real space inter-atomic pair distribution functions,  $g_{\alpha\beta}(r)$ . Attention will be paid to multi-component systems where the overlap of these correlations in real space means it is not possible to obtain the individual  $g_{\alpha\beta}(r)$  from a single diffraction experiment. In particular, I will describe and show how the multi-pattern techniques of *neutron diffraction and isotopic substitution* (NDIS), *anomalous X-ray diffraction* (AXD) and *combined X-ray and neutron diffraction* can, in some cases, be used to determine the individual  $g_{\alpha\beta}(r)$  of the system under study. Throughout the lecture I will give examples of current work, especially with regards to instrumentation at current European neutron and X-ray sources, with emphasis on the stringent experimental techniques that are needed to obtain reliable data. Finally I will introduce the ideas behind current structural refinement techniques such as Reverse Monte Carlo (RMC) and Empirical Potential Structure Refinement (EPSR) and show how they may be used to obtain structural models of the systems under study.