Disorder and Diffuse Scattering

Experimental/Computational

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Introduction

To understand a material's properties, we need to understand how the atoms within it are arranged. Diffuse scattering is one of the most powerful tools available to explore ordering in materials. We use diffuse scattering data collected at ANU and around Australia and the world to revel important details about the ordering of atoms in materials. This information can then be used to make better materials with improved technological properties.

Description

The behaviour of a material (its electrical resistance, softness, hardness, magnetic behaviour, everything) depends on what atoms are in it and how they are arranged. This structure is usually discovered for crystalline materials (for example steel, ceramics, protein crystals, pharmaceuticals and even wood) using X-ray and sometimes neutron diffraction. Usually, we measure the strong, sharp Bragg peak reflections, which reveal the average long-range ordered structure. Often, the valuable properties of the material relate to the *disorder* (and short-range order) in the structure. This is revealed through diffuse scattering – broad, weak bands of scattering rather than sharp Bragg peaks (fig. 1).

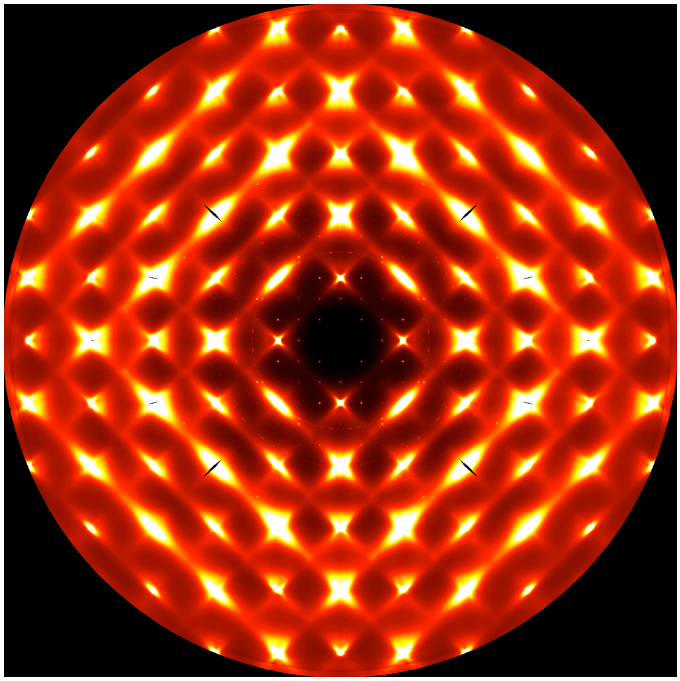

Figure 1: Diffuse X-ray scattering, measured at the Advanced Photon Source Synchrotron in Chicago. The material is PZN ($PbZn_{1/3}Nb_{2/3}O_3$), a material with electrical properties that make it useful in fields like energy conversion and micro-actuators.

Many systems can be examined using diffuse scattering, from molecular crystals such as pharmaceuticals to metals, ceramics (see figure 1) and even proteins.. Such a project may require sample preparation, data collecting (sometimes at a national or international facility) and data analysis using Monte Carlo modeling and other numerical techniques. ANU is a world leader in this growing field and can offer excellent links to national and international facilities and scientists.

The balance between experimental and computational in this project is very flexible and projects can be offered which are almost entirely computational or which contain a much larger experimental aspect. Projects can be offered at all levels from third year undergraduate to Ph.D.