Structural Science Technique Development

Computational

Darren Goossens, RSPE/RSC

goossens@rsc.anu.edu.au, 02 6125 3536

rsc.anu.edu.au/~goossens

Introduction

Analysis of diffuse scattering is hard! Even getting high quality data is hard. We are now working with large (>100GB) data sets of three-dimensional diffuse scattering data. The opportunity exists for an interested student with good computing skills, including programming, to contribute to the development of this cutting-edge field.

Description

We are tackling issues in data visualization, correction and reduction, and in how we can model the behaviour of disordered systems and calculate their diffraction patterns. Topics of interest include parallel processing (on GPUs for example), Monte Carlo and other forms of numerical modeling, model selection using genetic algorithms and other novel approaches, and model optimization.

This work could be conducted as a separate project at third or fourth year level, or as part of a wider diffuse scattering study of interesting materials as a Ph.D. project.

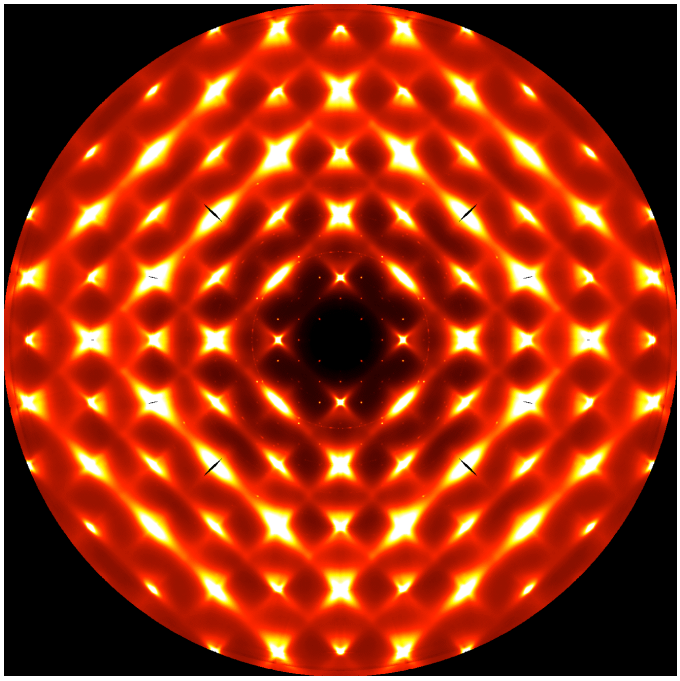

Figure 1: Diffuse X-ray scattering, measured at the Advanced Photon Source Synchrotron in Chicago. The material is PZN ($PbZn_{1/3}Nb_{2/3}O_3$), a material with electrical properties that make it useful in fields like energy conversion and micro-actuators. This is one 2-d cut through a 3-d data set.