

Chemical Crystallography with neutrons at OPAL - KOALA fulfils a promise

Monday, 2 December 2019 14:15 (15 minutes)

A strong case for the inclusion of a single-crystal diffractometer was made in the scoping of the initial suite of instruments to be built at the OPAL Reactor facility. The choice of a Laue instrument appeared to offer significant opportunities for a broad community of potential users. In particular the potential to undertake single-crystal chemical crystallography experiments on crystals of sizes less than a cubic millimetre was a particular attraction of using Laue diffraction. The instrument procured was largely based on the VIVALDI instrument which was being implemented at the Institut Laue Langevin in Grenoble, France.

By the time our instrument, KOALA was available for users, the world-wide output of single-crystal chemical crystallography studies (as included in the Cambridge Data Base) from the various neutron sources had, for a range of reasons, slowed to a trickle. This was despite the availability of several instruments which had promised a significant increase in the availability of such studies for application in areas of chemistry where definitive characterization of materials could only properly be achieved by this means.

The implementation of KOALA at ANSTO is compatible with applications to many fields of science, those in the physics applications had been strongly developed at the various neutron facilities across decades, whilst the applications in chemistry still had considerable scope to develop. Two critical developments at ANSTO have been the implementation of Oxford Cryosystems COBRA™ cryostream technology (developed for X-ray Crystallography). This has facilitated the examination of crystals under conditions compatible with their chemical and physical properties.

The most important development has been the creation of the LAUEG suite by Dr Ross Piltz which facilitates straightforward extraction of a data file in a format which chemical crystallographers are accustomed to use for routine crystals, and a suite of tools to manage the processing in non-routine cases.

In the first ten years of operation, it has been possible to build a strong chemical crystallography single-crystal neutron diffraction activity with KOALA. From the outset publications results from KOALA have appeared in the primary reports of the chemistry in high impact journals. More recently, as the capabilities of the instrument have become more widely known, access to KOALA has been sought to undertake key studies which underpin publication in journals of the highest standing.

Many of our users have little prior experience of neutron scattering, and at times, their exposure to crystallography has also been of limited extent. Four student theses have relied heavily on data collected at KOALA and all these students have proceeded to careers in which their well developed critical and analytical skills are required

This talk will highlight the important papers and findings which have reached the literature to date from KOALA with emphasis on what the single-crystal neutron diffraction experiment added to the chemistry under study.

Level of Expertise

Expert

Do you wish to take part in the poster slam

No

Travel Funding

Speakers Gender

Female

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Session Classification: Session 6

Track Classification: Chemistry and crystallography