Electron diffraction as part of a national diffraction service

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Electron Diffraction is about to revolutionise crystal structure determination in fields limited by crystallite size and quality. Across chemical and materials science, including supramolecular chemistry¹, catalysis² and pharmaceuticals, a new wealth and volume of accurate structural information will give a step-change in the science enabled. The UK National Crystallography Service (NCS), in partnership with the University of Warwick and Rigaku Oxford Diffraction, are setting up a UK national facility for electron diffraction. This complementary partnership will offer a combination of the right technology, the experience of delivering a successful national service and the knowledge and expertise required for technique development. This combination of skills and expertise, together, will continue to ensure the method of analysis is available nationally and continues to expand into new areas of chemistry.

The principal difference between electron diffraction and XRD is the strength of interaction. Electrons have an interaction roughly 10,000x stronger than X-rays³. This means that electron diffraction is suitable on crystallites below 1 µm in size. Data collections are extremely rapid and are experiments are performed by combining multiple datasets on a number of crystallites. This means a service would be extremely high throughput with a lot of staff time spent on data processing and solving. As such a slightly different model for a national service is required when compared to XRD.

Access to the service will be applied for through two separate routes. There will be a mixture of mail-in and ‘project’ access, where the latter is brief periods of in-person use. On top of providing a service, we also plan to offer dynamic training opportunities to our users, covering preparation and running of samples, and also how to process and analyse resulting data in order to enable the next generation of scientists to make the best possible use of this rapidly advancing technique for crystallographic structure determination. The service will strive to evolve as much of the project access as possible into a remote online steering of data collection so users can run their experiments from their home facility.

In order to fully explore the capabilities of the technique, the service will establish a development programme for in-situ controlled sample environment studies. This will be based on community demand, research backgrounds and the range of available technologies already developed for electron microscopy. The service will aim to be at the forefront of this research and will look to provide access for the whole scientific community.

This is an exciting time for a new and emerging technique and a national service has an imperative role of championing and driving forward developments. It is vital that it is able to maximise support to a range of users at all levels in a multitude of fields. Based on the experience of setting up such a facility, it’s operation mode, it’s capacity and demand, the NCS will be able to assess the national needs for electron diffraction, both scientifically and geographically.