Poster

Complementing XRD at the national level – 3DED and the UK National Electron Diffraction Facility (NEDF)

D.N. Rainer[1], J.P Tidey[2], R.D. Bannister[1], R. Beanland[2], M.E. Light[1], R.I. Walton[2], D. Walker[2], S.J. Coles[1]

[1]University of Southampton, United Kingdom, SO17 1BJ, [2]University of Warwick, United Kingdom, CV4 7AL

d.n.rainer@soton.ac.uk

The rapid development of 3DED techniques[1] has culminated in dedicated electron diffractometers now being commercially available. The recently established UK National Electron Diffraction Facility aims to harness the significant potential of employing electrons as a radiation source for diffraction experiments to expand the scope for structure determination to crystallites too small for single-crystal XRD (SCXRD) experiments. As a national facility, we provide the service to academic researchers across the UK, through panel-reviewed proposals akin to other large-scale facilities such as Diamond Light Source, as well as to users from industry on a contractual basis. The facility itself is a partnership between the University of Southampton, the University of Warwick, and Rigaku Oxford Diffraction, and has installed a Rigaku XtaLAB SynergyED instrument at both of the university sites. It acts as an additional pillar of the established National Crystallography Service (NCS, www.ncs.ac.uk), which has been providing researchers in the UK with X-ray derived crystal structures for almost half a century.

In this talk we share our insights and experiences of the foundational year for NEDF. We will touch on how the fundamental differences between SCXRD and 3DED require adaptations to sample submission, user-crystallographer interactions, data collections, structure determination, and finally reporting. Using examples generated by the facility, we will highlight how 3DED and obtained structures are complementary to XRD and demonstrate that 3DED is not trying to replace XRD, but rather stepping in where other crystal structure determination methods have reached their limitations. Finally, we give an outlook on how we are expanding on what we can offer users, ranging from elemental analysis using energy-dispersive X-ray spectroscopy, additional sample environments using dedicated holders, and keeping up to date with data processing and refinement software.

[1] Gemmi M., Mugnaioli E., Gorelik T.E., Kolb U., Palatinus L., Boullay P., Hovmöller S., & Abrahams J.P. (2019). *ACS Cent. Sci.* **5**, 1315–1329.