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PhD project outline – modelling of electron diffraction for crystal structure solution and refinement

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Although electron diffraction (ED) took a leading role in establishing quantum mechanics in the 1920s, it never approached the utility and impact of X-ray diffraction, which has been the principal technique to determine the atomic structure of materials for over a century. The two main reasons for this failure were a) the lack of good data collection routines and quantitative electron detectors (e.g. film was only fully superseded by digital cameras in electron microscopes about 15 years ago) and b) multiple scattering, which changes diffracted intensities and requires more complicated modelling than XRD.

The first of these problems is now well and truly solved, with data collection methods developed by Hovmöller, Kolb and co-workers (recognised by the IUCr Gjønnes medal in 2020) [1]. Dedicated electron diffractometers – with direct detection cameras and optimised/automated operation – are now available. The University of Warwick was the first in the UK to have one of these machines, and forms part of the EPSRC National Electron Diffraction Facility (NEDF) [2]. The ability of electrons to study nanoscale crystals (much smaller than can be tackled by X-ray or neutron diffraction), to detect light elements like hydrogen and lithium, and to easily determine absolute structure and .crystal chirality, means that there is intense national and international interest in the new science enabled by these machines. However, there is still little work done on the second of the problems given above, which will be the focus of this PhD project.

Models of electron scattering from crystalline materials have principally been developed to support transmission electron microscopy and old ED methods. The calculation solves the time-independent Schrödinger equation for a fast electron in a crystalline material. This is currently done in two main ways, using wave propagation (multislice) or Bloch-wave methods. However both are relatively time consuming and there is currently only one implementation of Bloch-wave methods in crystallographic software, from the Palatinus group in Prague [3].

This project will develop the theory of electron scattering in ways that are optimised for the new methods of data collection and implement it in code that will support the international community in this rapidly growing field. The advances that it makes possible will be demonstrated using Warwick/NEDF experimental data.

[1] https://bit.ly/33SXI0K.
[2] https://www.ncs.ac.uk/nedf/.
[3] http://pets.fzu.cz/.

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