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Bouncing Around Between Real and Reciprocal Space with Electrons and X-rays, an Adventure with John Spence.

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John liked to summarise things clearly and succinctly. If there is one question that motivated his extensive career in science it would be "Where are the Atoms?"

Our probes for determining structure are imperfect. Electrons can be focused to a limited extent and can provide real space images directly giving atomic positions in some cases. However they interact strongly with the atomic potential making quantitative analysis difficult, and in practice direct structural determination is limited to cases with a "perfect" projection (2D materials represent a special limiting case). If electron lenses are bad, X-ray optics is even worse, so for all practical purposes X-rays can't be focused. They don't interact as strongly so theories based on first order scattering are usually adequate. For both electrons and X-rays radiation damage sets the limit to the information that can be extracted in any experiment.

In practice both electron and X-ray scattering require combining information from both real and reciprocal (or scattering angle) space and this is an overarching theme of John's work. It was during his time in Oxford as a postdoc that he became interested in phase contrast electron imaging, and this led to his book "Experimental High Resolution Electron Microscopy" [1]. After moving to Arizona State to join John Cowley as the second physics faculty member in electron microscopy he became more interested in phase contrast in STEM. In collaboration with John Cowley he showed that lattice resolution in STEM was a consequence of interference and a coherent probe [2]. This became the starting point for my own work in this area [3]. John was always open to new ideas and he then became intrigued by the possibility of using channeling from dynamical diffraction (ALCHEMI) as a way of determining which atoms were at different crystallographic sites [4].

John always realized that new frontiers were opened up with instrumentation developments. It started with combining STM with TEM, and that led to point projection microscopy and eventually lens-less imaging techniques that were also relevant for X-ray imaging. In parallel he was pushing developments in detectors, improved TV cameras and the use of imaging plates. Improved recording of convergent beam patterns led to taking quantitative electron microscopy and diffraction to new limits, not just where are the atoms but where are the electrons [5]! The analogies between X-ray and electron coherent diffraction led to an interest in coherent X-ray imaging at synchrotrons and the development of algorithms for phasing X-ray scattering based on support constraints.
For many years John was fascinated by the possibility of innovations in recording diffraction patterns. John was the leader in developing techniques to use femtosecond X-ray pulses to outrun radiation damage and record diffraction patterns before a sensitive protein structures were destroyed. This spectacularly came to fruition with the demonstration of its use in solving the structure of PS2, and other proteins that were difficult to crystallize [6]. However John realized that for structural biology, cryo EM would prove to be more generally applicable and was took the lead in acquiring a Krios at ASU. He saw the future in terms of time resolution, and watching "chemistry" take place in real time.

He hadn't forgotten about electrons. For more than half a century those of us who have a passion for scattering theory had been trying to find a way to invert dynamical diffraction, to go back from diffracted intensities (or even an exit wave function) to the crystal potential and atomic positions. In collaboration with J. Donatelli in Berkeley he published a solution to this long-standing problem [7]. It was a crowning intellectual achievement, to a long and productive career in microscopy and diffraction.

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