Fast data processing for 4D-STEM

Aberration-corrected Annular Dark Field STEM (ac-ADF-STEM) has provided some beautiful images and valuable insights into materials such as 2D materials, functional oxides and semiconductors, with each atom clearly resolved. New developments in fast pixelated detectors now allow a four-dimensional (4D) dataset to be acquired, where for each position of the electron probe, scanned in a 2D raster over the sample, a 2D image of the diffraction plane is recorded. This huge jump in information content also comes with a big increase in data volumes that need to be interrogated and processed in order to extract the signals of interest.

Fig. 1 shows a set of simulated 4D-STEM data with a subatomic probe scanning across a single unit cell of [001] $SrTiO_3$. Each pattern corresponds to a change in position of the electron beam of a few picometres and would take a few microseconds to aquire. The patterns show a great deal of complexity due to multiple scattering effects. Nevertheless, a map of Center of Mass (CoM) displacement still points towards the heavier Ti and Sr atoms.

Methods are needed to distinguish changes in the patterns due to internal electric fields in the specimen and matching of 4D-STEM data to simulations. With modern computing methods and GPU acceleration, there is no reason why this analysis should not be performed in real time. The work envisaged requires a high level experimental techniques and data analysis, both with a significant computational element.

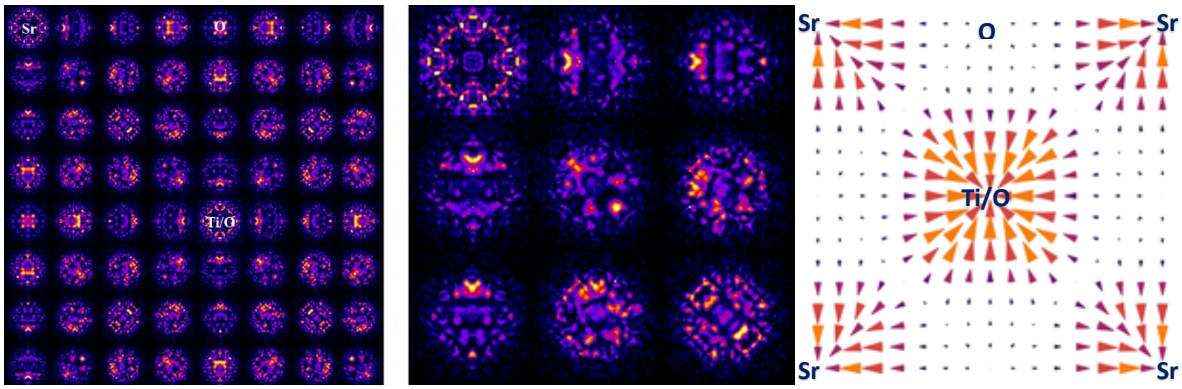

Fig. 1 (a) Scattering patterns [001] $SrTiO_3$ (b) Magnified image of 9 patterns from the top-left in (a). The complex intensity variations in the patterns are due to multiple scattering. (c) CoM shift extracted from (a).