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An Optical Sectioning Method for 3D Reconstruction Using 4D-STEM

Hamish Brown[1], Phillipp Pelz[1], Shang-Lin Hsu[2], Ramamoorthy Ramesh[2], Mary Scott[1], Scott Findlay[3], Leslie Allen[4], Colin Ophus[1] and Jim Ciston[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, California, United States, [2]University of California, Berkeley, Berkeley, California, United States, [3]Monash University, Clayton, Victoria, Australia, [4]The University of Melbourne, Parkville, Victoria, Australia

Investigating novel and interesting phenomena in materials such as ferroelectric polarization vortices, octahedral rotations and magnetic skyrmion materials requires techniques that characterise complex materials whose structure varies in three dimensions. For compact samples, such as nanoparticles, three-dimensional atomic resolution information can be accessed in scanning transmission electron microscopy (STEM) by tomographic reconstruction from a tilt series [1]. Many samples, such as thin films, have a geometry that means that tilting the specimen to all required orientations is unfeasible. In this talk we discuss an alternative novel approach to 3D reconstruction in TEM using an optical sectioning approach with 4D-STEM data, where a diffraction pattern of the STEM probe is read out at a speed approaching typical STEM probe dwell times [2], as the input. This approach is complimentary to conventional annular dark-field (ADF) STEM depth-sectioning, which is sensitive to the 3D positions of heavy atoms in the sample [3], in that our method can reveal the positions of both light and heavy atoms.

Recently it has been shown how this 4D-STEM experimental data can be used to reconstruct the scattering matrix [4,5]: a mathematical object that encapsulates how the specimen scatters electrons from the different orientations that make up a converged STEM probe. In that work the projected electrostatic potential for a thick, strongly scattering crystalline sample was reconstructed [5]. In our optical sectioning approach we use the information contained within the scattering matrix to synthesise imaging modes that would not be possible with direct, live imaging within the electron microscope [6]. Figure 1 illustrates our approach for a hypothetical collection of O atoms shown in Fig. 1(a). The phases of a few of the components of a scattering matrix (which map plane-wave components of the probe to the exit-surface wave) for a 300 keV probe are shown in Fig. 1(b), along with a sketch indicating the corresponding plane-wave component of the STEM probe. The different z-coordinates of the each of the atoms are apparent in these components from differing amounts of propagation for each atom and also by a geometric “shift” away from the in-plane position of the atoms (indicated by colored dots) proportional to the depth of the atom and the scattering matrix component’s transverse wave vector [indicated by an arrow in the upper part of Fig. 1(a)]. An optical-sectioning reconstruction involves taking the sum of all available scattering matrix components with inverse propagation and shift operations. This reconstruction for the heights of each of the atoms is shown in (c) including scattering matrix components out to 30 mrad.

Figure 2 shows a possible application of the technique, a 4D-STEM datasets were simulated for a heterostructure, shown in Fig. 2(a), comprising a 100 Å layer of PbTiO3, with polarization in the plane of the layer, capped top and bottom with 50 Å layers of SrTiO3. Optical sections of Fig. 2(b) the top SrTiO3 layer, Fig. 2(c) the middle PbTiO3 layer and Fig. 2(d) the bottom SrTiO3 layer are shown and polarization is clearly visible in the $PbTiO_3$ layer due to the relative shift of the O atoms relative to the Pb and Ti atoms in the unit cell [7].

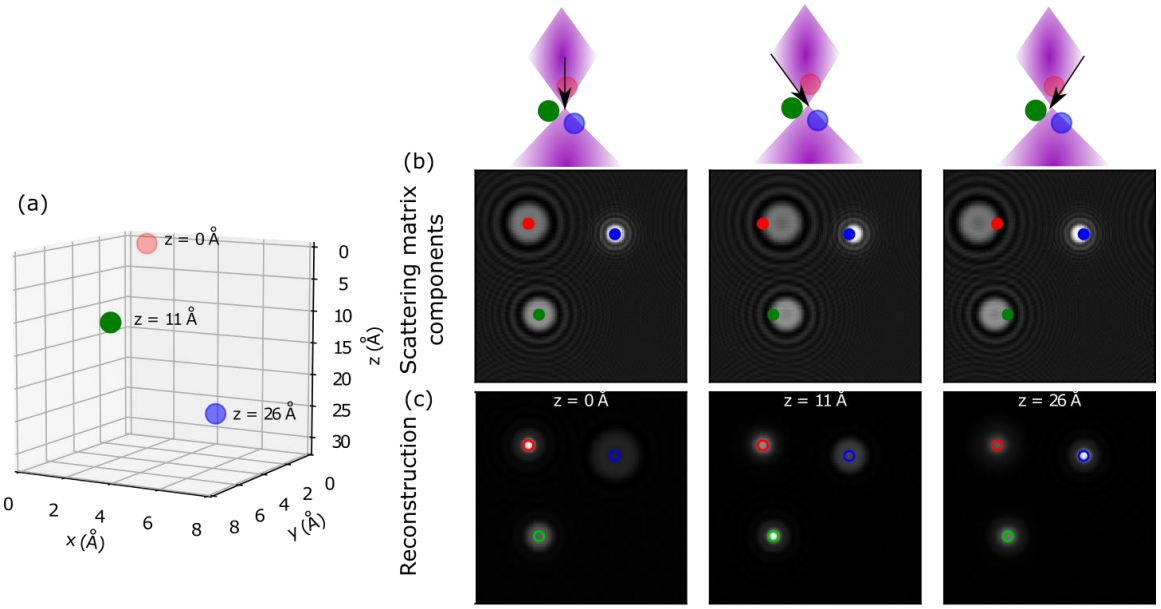

Figure 1. (a) Hypothetical collection of atoms (b) select components of the Scattering matrix for this system (c) An optical-sectioning reconstruction from the full scattering matrix

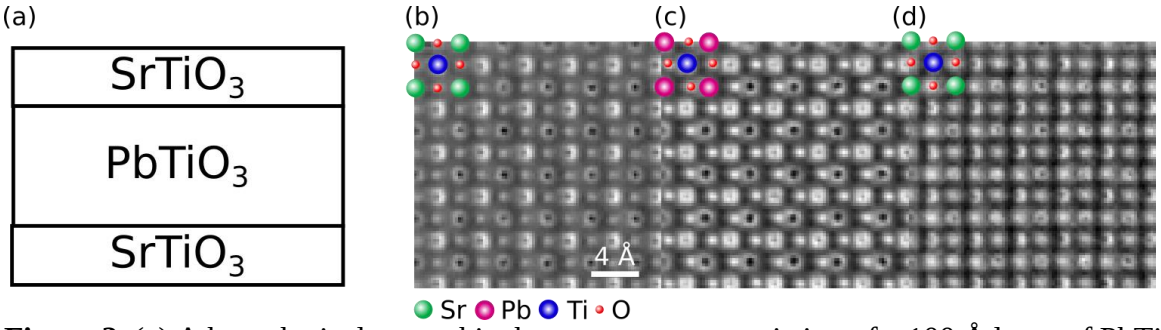

Figure 2. (a) A hypothetical perovskite heterostructure consisting of a 100 Å layer of PbTiO3 capped top and bottom with 50 Å layers of SrTiO3. Shown are scattering matrix optical sectioning reconstructions of the (b) top SrTiO3 layer, (c) middle PbTiO3 layer and (d) bottom SrTiO3 layer.

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