

X-RAY IMAGING

Achieving the third dimension using coherence

X-ray imaging in three dimensions is now possible from a set of 2D coherent Bragg diffraction patterns. This approach overcomes the necessity of having to rotate the sample for a 3D reconstruction.

Ian Robinson and Xiaojing Huang

X-ray imaging is extensively used in medical and materials science. Traditionally, the depth dimension is obtained by turning the sample to gain different views. The famous penetrating properties of X-rays mean that projection views of the subject sample can be readily obtained in the linear absorption regime. 180 degrees of projections can then be combined using computed tomography (CT) methods to obtain a full 3D image, a technique extensively used in medical imaging. In the work now presented in *Nature Materials*, Stephan Hruszkewycz and colleagues have demonstrated genuine 3D imaging by a new method called 3D Bragg projection ptychography¹. This approach combines the 'side view' capability of using Bragg diffraction from a crystalline sample with the coherence capabilities of ptychography. It therefore results in a 3D image from a 2D raster scan of a coherent beam across a sample that does not have to be rotated.

In recent years there have been a number of attempts to gain 3D information without the inconvenience of collecting a wide range of views by rotating the sample or camera. Bragg coherent diffractive imaging (BCDI) makes use of the fact that the Bragg diffracted beam emerges at a large angle to the incident beam, and therefore already provides a different view of the sample². Small rotations of the sample — less than one degree — can traverse the rocking curve and provide a full 3D image. The advantage here comes from the large offset of the origin in reciprocal space caused by the large momentum transfer of the selected Bragg peak.

X-ray ptychography uses coherent interference effects by combining overlapping regions of the sample to obtain images, again in projection. Tomographic ptychography can take this to three dimensions in the same way as CT, which has been used very effectively

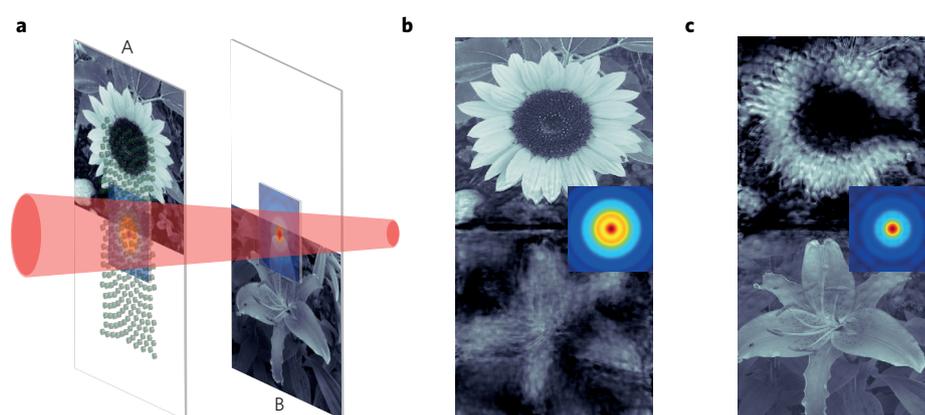


Figure 1 | Illustration of the depth resolution of ptychography. **a**, Simulated ptychographic dataset from an object made up of two photographs in different planes illuminated by a convergent X-ray beam.

b, Reconstruction of the data using the complex wavefront at the position of the left-hand plane as the probe. **c**, The same as **b**, but using the right-hand plane as the probe. The shapes and phase structure (colour) of the two probes are shown inset in **b** and **c**.

for submicrometre 3D imaging of the internal structure of a mouse femur³. From an optical perspective, there are more interesting methods based on wave propagation between planes within the sample to sections along the beam [Au: ok?]; this has been demonstrated for *Spirogyra*, a spiral-shaped algae 15 micrometres in diameter, using visible light ptychography⁴. Clear, well-separated images of the top and bottom sides of the algae were seen, but the depth resolution was a bit limited.

Hruszkewycz and colleagues have combined the capabilities of Bragg diffraction imaging and ptychography; they image a lithographically structured semiconductor thin film that shows a distinct pattern of strain adjacent to the edges of the patterned block of GeSi crystalline material, in agreement with finite-element modelling of the device. The strain sensitivity arises in exactly the same way as in conventional BCDI, where rigid displacements of the crystal lattice, a fraction of a lattice spacing in

magnitude, result in phase shifts in the 3D image of that block of material². Because it incorporates wave interference, X-ray ptychography obtains phase contrast images and, as with BCDI, the phase information is often found to be more reliable than the image amplitude. Phase contrast is an inherent strength of the ptychographic method.

Another, less well-documented strength of the ptychography approach is its ability to constrain the absolute location of the object plane with respect to the probe. Since the diffraction pattern at each location of the scan is given by the Fourier transform of the product of the object and a fixed 'probe', and the two functions are uniquely factorized by the overlap of the scan positions, the plane is fixed by the choice of the probe. Whenever a focused beam (or otherwise structured wavefront) is used as a probe, as by Hruszkewycz *et al.*, the probe structure evolves strongly with propagation and fixes the plane of the image. This is in stark contrast to BCDI, where the true 3D image

is indistinguishable from a Fresnel wave-propagated sister copy of itself⁵, as both copies have the same magnitude of their Fourier transforms (the Fresnel propagation step is a convolution, so the Fourier transform of the sister copy is the product of that of the original image and the Fourier transform of the Fresnel propagator, which has unit magnitude).

This ability of ptychography is illustrated in Fig. 1. A two-plane object, made of images A and B placed side-by-side but offset along the beam direction, is used to simulate a ptychography data set, including the propagation of the illuminating probe between the two planes. When the image

is reconstructed using the correct probe defined at plane A, image A appears in focus and image B appears out-of-focus. The reverse happens when the reconstruction probe is chosen to be that defined at plane B.

In the work reported by Hruszkewycz and colleagues, any propagation of the image is restricted further by the use of a 'support' which constrains it within a volume of space a little thicker than the semiconductor thin film. The consistency of the diffraction pattern of the image with the data then assures us that it is correct in all three directions of space. Such an approach successfully overcomes the need to rotate the sample and achieves genuine 3D X-ray

imaging, which constitutes an important tool for Bragg ptychography experiments. □

Ian Robinson and Xiaojing Huang are at the Brookhaven National Laboratory, Upton, New York 11973, USA. I.R. is also at the London Centre for Nanotechnology, London WC1 6BT, UK. e-mail: i.robinson@ucl.ac.uk

References

1. Hruszkewycz, S. O. *et al. Nat. Mater.* XXX (2016).
2. Robinson, I. & Harder, R. *Nat. Mater.* **8**, 291–298 (2009).
3. Dierolf, M. *et al. Nature* **467**, 436–439 (2010).
4. Godden, T. M., Suman, R., Humphry, M. J., Rodenburg, J. M., & Maiden, A. M. *Opt. Express* **22**, 12513–12523 (2014).
5. Huang, X., Harder, R., Xiong, G., Shi, X. & Robinson, I. *Phys. Rev. B* **83**, 224109 (2011).