3D RECONSTRUCTION OF SUB-NM BEAM PROFILES IN STEM

G. Möbus, R.E. Dunin-Borkowski, C.J.D. Hetherington, J.L. Hutchison

Department of Materials, Oxford University, Oxford OX1 3PH, UK

Introduction: Atomically resolved chemical analysis using techniques such as electron energy loss spectroscopy and annular dark field imaging relies on the ability to form a well-characterised sub-nm electron beam in a FEGTEM/STEM [1-2]. To understand EELS+EDX-signal formation upon propagation of a sub-nm beam through materials we first have to assess precisely the beam intensity distribution in vacuum and find conditions for the best obtainable resolution.

Experimental Details: Modern TEM/STEM instruments combine features of both imaging and scanning technology. The beam forming capability approaches closely that for dedicated STEMs, while CCD recording devices allow us to measure the beam profile by direct imaging at magnifications up to 1.5 M. The recording of a "z-section" series through the 3D intensity distribution of the cross-over can therefore be realised by recording of a "condenser focal series". The microscope tested in this way is the Oxford JEM-3000F FEGTEM (300kV) with a guaranteed probe size in EDX-mode of <0.4nm [1, 2] and Cs = 0.6mm. The combination of the sections into a 3D reconstruction is a simple tomography/laminography problem for which various commercial software exists such as IDL (RSI inc., Boulder, USA).

Results: Experimental data from two focal series are shows in Figs 1-3. From various focal series it is found that the probe size at the chosen demagnification is not limited by diffraction. Instead the smallest aperture yields the smallest probe. Fig 1 shows a z-series of central line profiles of a cross-over which shows good azimuthal symmetry with a 0.4nm width (FWHM) at ~2-3 pA beam current. Another cross-over with distinct asymmetry due to 3-fold astigmatism has been with a minimum probe size approaching down to 0.2nm at only <1pA emission current. Several members of this focal series are printed with central line profiles in Fig. 3, one of them, strongly underfocused, is picked for matching in Fig 2 (left), and a 3D rendering of the intensity I(x,y,z) is printed for two semitransparent iso-intensity surfaces in Fig 2 (right).

Comparison with calculations: By means of the reciprocity theorem [3], STEM beam profiles can be modelled with aberration-simulation software identical to that used for HREM. Here an EMS [4] implementation is used [5]. A two step filtering process is applied to the input signal, which is an ideal delta-function in "source space". The first filter (complex valued) applies all lens aberrations (Cs, defocus, and astigmatism) and calculates the Fresnel-zone plate, which focuses the beam into a spot on the specimen with a selected convergence angle. The second filter applies an envelope to account for beam broadening due to: (i) a finite width of the source (here modelled by a Gaussian) which is assumed to consist of a lateral distribution of self-luminous points, (ii) the MTF of the CCD camera, (iii) an exit/entrance- pupil ratio < 1, which reduces beam resolution without affecting the convergence angle, and (iv) possible defocusing/widening due to the beam imaging process. The match of calculated to experimental profiles (Fig 1+2) is found to be good. However, particular details for large apertures have not been matched perfectly yet.

Outlook: The importance of 3D beam modelling and experimental reconstruction lies in the extension towards beams propagating through specimens, which affects STEM imaging resolution, the interpretation of annular dark field images (Z-contrast), and EELS or EDX experiments, especially of the ALCHEMI [6] type. A 3D intensity distribution inside a 45nm Al_2O_3 grain boundary specimen (see also [7]) is shown as iso-surface of constant electron density in Fig 4. [8]

References:

1. J.L. Hutchison et al, JEOL News, 34E, No. (1999), 10-15.
2. J.L Hutchison et al., J. Electr. Microsc., in preparation.
3. E.J. Kirkland, Advanced Computing in Electron Microscopy, Plenum, N.Y., USA (1998).
4. P. Stadelmann, Ultramicroscopy, 21 (1987), 131.
5. G. Möbus, Proceed. EUREM 12, L. Frank, F. Ciampor eds, Brno, Vol I, 385 (2000).
6. J.C.H. Spence and J. Tafto, J. Microscopy, 130, (1983). 147.
7. G. Möbus and S. Nufer, this volume.

8. Funding by EPSRC for the FEGTEM (GR/L22324) and an Advanced Fellowship (G.M.) is gratefully acknowledged. We thank H.Banzhof & M. Lehmann for providing their LI2 subroutine for EMS.

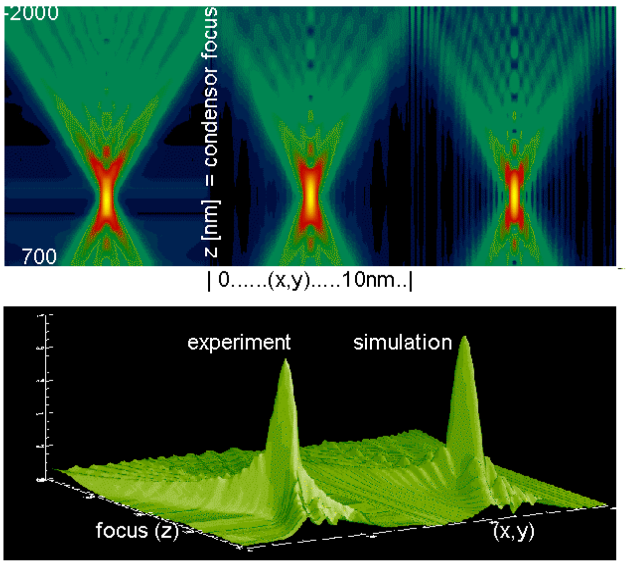


Fig 1: Circular symmetric cross-over   (left: experiment (middle: best match simulation, right: ideal probe) bottom: 3d plot of top-left and top-middle images

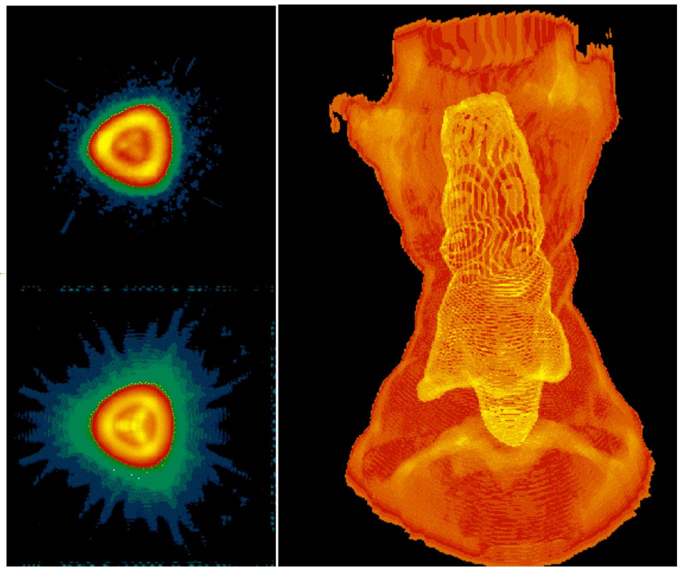
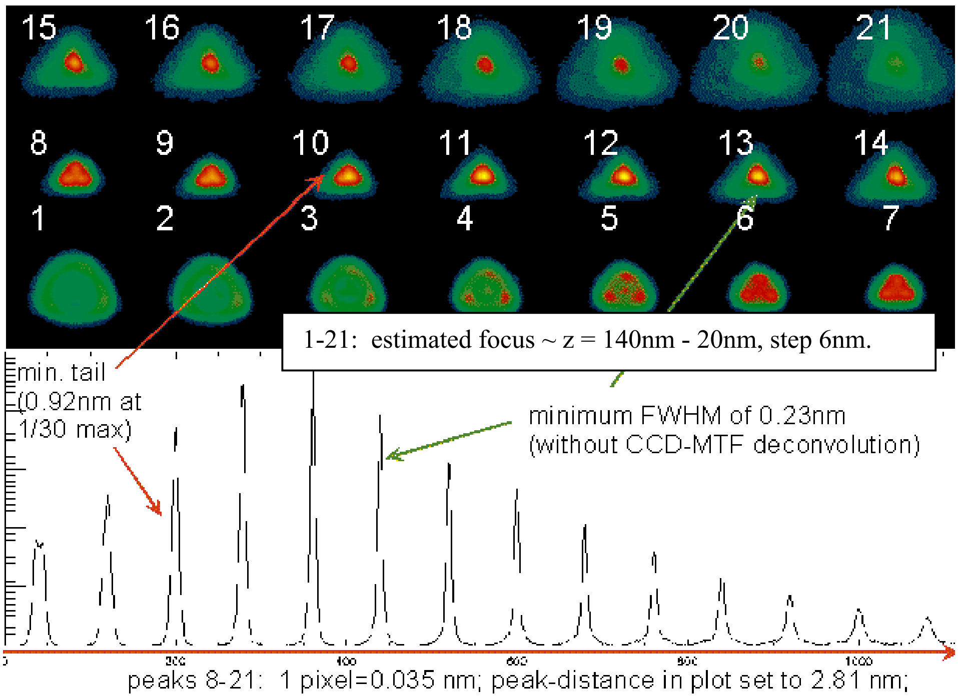


Fig 2: Experiment (up. left) and simulation (bot. left) (image widths = 5nm) plus tomographic reconstruction (right) for a cross-over (Fig 3) with visible 3-f. astigmatism (A3=500nm).



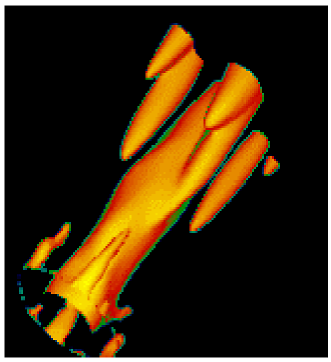


Fig 4: Calculation of beam propagation in a light atomic weight material (Al2O3) with the nominal beam focus located in the interior of the specimen. Chanelling along atomic columns and Fresnel propagation are superimposed.

Fig 3 Experimental focal series (as Fig 2) to show focus dependency of beam half/tail width.