

Fifty Years of Defect Imaging – Focusing on Dislocation Core Structure

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Over fifty years have elapsed since the dynamical theory of electron diffraction was developed [1], [2], [3] to interpret the early TEM diffraction contrast images of crystal defects including dislocations. Subsequent progress in experimental technique, instrumentation and theoretical interpretation has resulted in dramatically improved resolution of the dislocation core region. Dislocation mobility and other significant properties are determined by the core structure. Although the resolution was initially limited by the diffraction contrast mechanism rather than by instrumental aberrations, for widely dissociated core structures a bridge could be built via stacking fault energy between metal plasticity and electronic properties. With the weak beam imaging method [4] and more accurate simulations [5], core structure resolution reached about 1.5nm and is still widely used although the results are not always unambiguous.

For dislocations precisely aligned with the microscope axis, the attractions of direct structure imaging are irresistible. With aberration-corrected HREM or HAADF STEM, atomic columns are now routinely imaged in 2-d projection showing details of the core region for different dislocation configurations in many materials. Although the core scattering contribution is maximized in this projection configuration, some issues in the interpretation of these results are as yet incompletely resolved.

Crucially important features of dislocation core structure such as jogs and kinks are likely to be inadequately registered or even to escape detection altogether in projection imaging. Matching of images with quantitative simulations might alert microscopists to such deviations from the assumed 2-d structure but are still very rarely attempted in structure imaging. Only recently have continuing difficulties over the quantitative simulation of image intensities even in perfect crystals (the Stobbs factor [6]) shown signs of being resolved. Fast electron scattering in the dislocation core region should also ideally be based on a scattering potential taking full account of electron density redistribution.

Using forbidden reflections, kinks have been successfully observed in high resolution, plan view images of dislocations [7]. In such images, minimization of background intensity from surface and other diffuse scattering mechanisms is important. With this in mind it could be useful to employ energy filtering to allow still higher resolution in weak beam imaging. Weak beam electron holography also offers the possibility of rejecting thermal diffuse scattering and of providing the phase information generally missing in diffraction contrast imaging.

[1] M. J. Whelan and P. B. Hirsch *Phil. Mag.* **1957**, *2*, 1121-1142; 1303-1324. [2] A. Howie and M. J. Whelan *Proc. Roy. Soc. A* **1961**, *263*, 217-237. [3] A. Howie and M. J. Whelan *Proc. Roy. Soc. A* **1962**, *267*, 206-230. [4] D. J. H. Cockayne, I. L. F. Ray and M. J. Whelan *Phil. Mag.* **1969**, *20*, 1265-1270. [5] A. Howie and Z. S. Basinski *Phil. Mag.* **1968**, *17*, 1039-1063. [6] M. J. Hytch and W. M. Stobbs *Ultramicroscopy* **1994**, *53*, 191-203. [7] H. Kolar, J. Spence and H. Alexander *Phys. Rev. Lett.* **1996**, *77*, 4031-4034.

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