916 CD
DOI: 10.1017/S1431927606066645

Microsc Microanal 12(Supp 2), 2006

# Diffuse Scattering of Electrons by Individual nm-sized Defects Reveals New Structural Details.

M. A. Kirk[1], R. S. Davidson[1], Z. Zhou[2], S. L Dudarev[3], M. L. Jenkins[2] and A. P. Sutton[4]

[1]Materials Science Division, Argonne National Laboratory, Argonne IL 60439
[2]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, UK
[3]EURATOM/UKAEA Fusion Association, Culham Science Centre, OX14 3DB, UK
[4]Department of Physics, Imperial College, London SW7 2AZ, UK

Elastic diffuse scattering of electrons by individual nm-sized dislocation loops and stacking fault tetrahedra has been studied recently both experimentally [1] and theoretically [2]. In this paper we present the possibilities for further analysis of similar data which suggest more complete structural characterizations of these defects, along with evidence for diffuse intensity which may be attributed to local modes of thermal vibration associated with the defect.

The diffuse intensity from a single defect is measured using a small parallel beam and energy filtered diffraction. Intensity from and around a weakly excited Bragg reflection with the beam placed near the defect is subtracted from the same reflection with the beam placed on the defect [1]. Intensity differences are mainly positive (except at the Bragg peak) and represent a direct measure of diffuse scattering by the defect and associated strain field. Some limited areas of "negative" intensity difference have now been found and may be associated with a difference in thermal diffuse scattering from the local defect modes.

Some features of defect structure are illustrated in Figure 1. (This and Figure 2 are best viewed in color on the CD-ROM.) By comparison with simulations of diffuse intensity from various dislocation loop geometries [2], it is possible to identify this defect as an edge-on Frank loop. Diffuse streaks in [-111] on both sides of the Bragg position (black center) identify this defect as vacancy based due to the stacking fault. Nodal surfaces of zero intensity (white dashed lines), also in [-111], indicate a defect size of 3.2 nm diameter. Other diffuse streaks may come from some dissociation onto the other edge-on (111) plane. Further defect modeling and scattering simulations are needed to verify this suggestion.

Diffuse scattering from what appears in an image (not shown) as a complete 5 nm tetrahedron is illustrated in Figure 2. Interpretation is speculative at this point, but some three-fold symmetry is suggested in patches of intensity, two of which correspond to the normals to the edge-on stack faults. The majority of positive diffuse intensity (red and orange on [-200] side) may be associated with the end-on stairrod dislocation in this orientation, and in addition indicates a vacancy based defect. The shades of blue darker than the main background reveal a negative intensity difference which may result from local modes of thermal diffuse scattering due to the defect. Note two patches of this intensity are symmetric about [200]. Obviously, much further experimental and simulation work is needed to confirm these suggestions.

[1] Kirk, M. A., Davidson, R. S., Jenkins, M. L., and Twesten, R. D., Phil. Mag. **85** (2005) 497.
[2] Zhou, Z., Sutton, A. P., Dudarev, S. L., Jenkins, M. L., and Kirk, M. A., Proc. Roy. Soc. A, doi:10.1098/rspa.2005.1542.

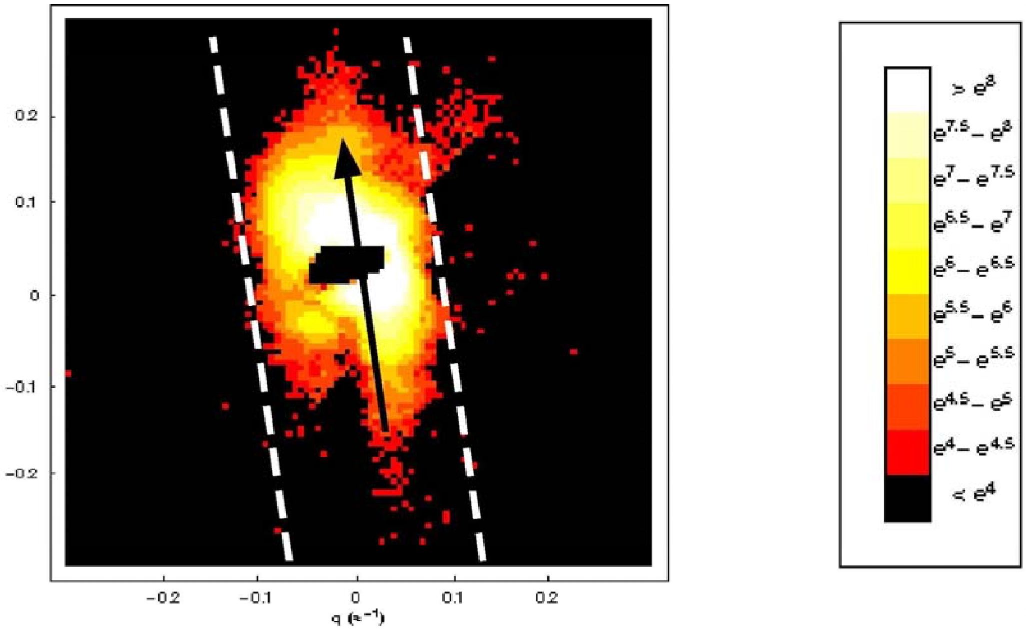

Figure 1. Absolute elastic diffuse intensity (electrons per pixel) from edge-on Frank loop around 222 Bragg peak with 444 excited near [0-11] pole. Arrow in [-111], loop normal.

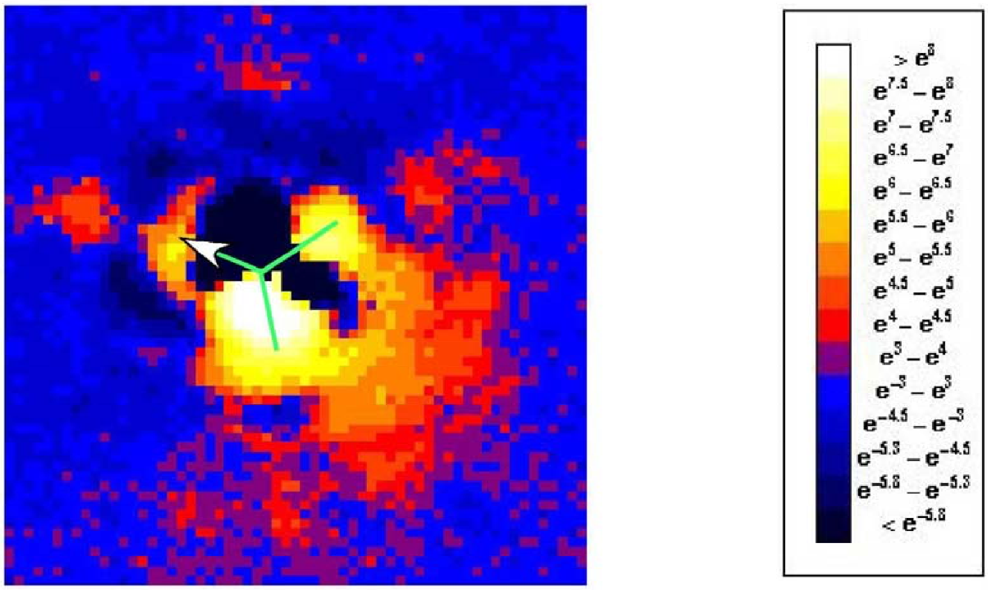

Figure 2. Elastic diffuse intensity from stacking fault tetrahedron around 400 Bragg peak with 800 excited near [0-11] pole. Arrow in [200] with legs in <111>. Scale about two times that of Figure 1. Blue shades(except the lightest) represent negative intensity differences.