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STEM Optical Sectioning for Imaging Screw Displacements in Dislocation Core Structures

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Aberration corrected (scanning) transmission electron microscopes (STEM) with sub-angstrom resolution have advanced our knowledge of the atomic structure of edge dislocations viewed end-on, with the tensile or compressive strain normal to the dislocation being clearly visible. Atomic displacements associated with screw dislocations however cannot be observed in end-on images because the helical screw displacements are parallel to the viewing direction. Such screw dislocations do however show small rotational displacements in thin foils due to surface stress relaxations known as the Eshelby twist. [1] We show that the helical displacements around a screw dislocation can be generally imaged with the dislocation lying transverse to the electron beam by "optical sectioning" in high-angle annular dark-field (HAADF) imaging in STEM. In optical sectioning, the few nanometre depth of focus of aberration corrected microscopes is utilized to extract information along the beam direction by focusing the electron probe at specific depths within the sample.

This novel technique is applied to the study of the screw component in the dissociation reaction of a mixed [**a**+**c**] dislocation in GaN. A focal series of experimental images were recorded using a Nion UltraSTEM100 aberration-corrected STEM operating at 100 kV. A 1μm thick sample of GaN, grown by metalorganic vapour phase epitaxy on a sapphire substrate, was thinned to be viewed along the a-axis. A dislocation was found lying in the plane of the sample, and characterized using weak-beam imaging to be of a mixed [**a**+**c**] type along [0001]. As the STEM electron beam is focused closer to the dislocation, the shearing of the (0002) planes becomes more localized in the image, and a more detailed observation of the screw displacements shows that the shearing occurs equally along two distinct lines along [0001] (see Figure 1). It is therefore apparent that the screw component of the dislocation has dissociated according to the reaction **c**=[½**c**+½**c**] confirming the assumption made in previous end-on observations. [2]

The dissociation of screw is also confirmed by comparing experiment with image simulations of both dissociated and undissociated structure models, and a good match is found between experiment and simulated images of the dissociated screw model. Quantitative analysis of the screw displacement field under a set of specimen thickness, defocus, and screw dissociation width conditions shows that the dissociation distance is around 1.65nm in this work, and this method provides sufficient sensitivity to detect a dissociated screw in GaN with a dissociation distance as small as 1.1nm (see Figure 2). [2] Details of the experiment results of STEM optical sectioning as well as image simulations will be presented. [3]

[1] Lozano, J.G. *et al*. Physical Review Letters 113, 135503. (2014)
[2] Yang, H. *et al*. Nature Communications (Under Review)
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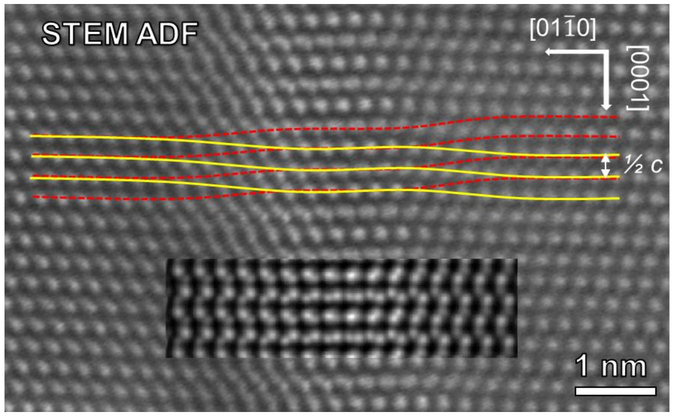

Figure 1. Experimental and simulated STEM-ADF image (inset) of the ½[a+c] + ½[a+c] dissociated dislocation lying perpendicular to the electron beam. The screw displacements associated with each of the partial dislocations can be observed, as indicated by the overlaid solid and dashed lines following the closer-to-focus stronger intensity peaks and further-from-focus weaker intensity peaks, respectively. A simulated image of an isotropic elastic model of a dissociated dislocation with a 1.65nm dissociation distance is overlaid. The simulation was done with the beam focused 5 nm below the top entrance surface of a 10-nm thick foil.

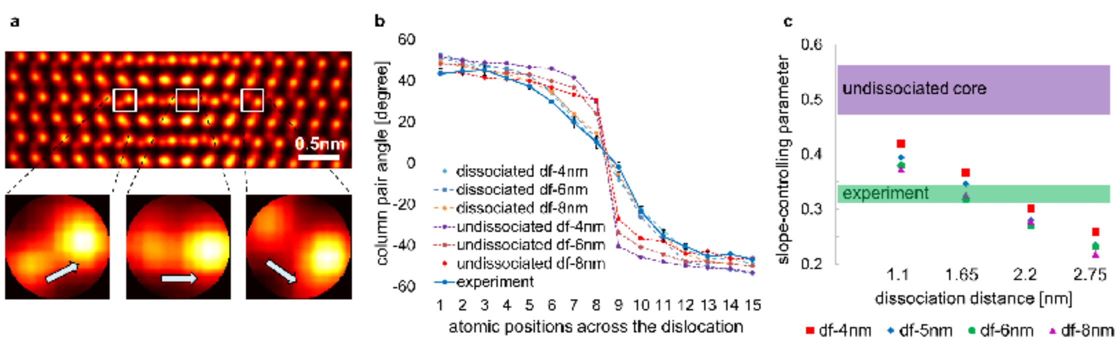

Figure 2. Determining screw dissociation through quantitative analysis of screw displacements near the dislocation. **(a)** The images in the fault region consist of pairs of closely-spaced peaks whose relative positions correlate with the amount of screw displacement. A Radon transform is used to measure changes in the column-pair angles across the dislocation. (**b**) The column pair angles have been measured for both the experimental and simulated images of dissociated screw (1.65nm dissociation distance) and undissociated screw dislocations, and a good match is found between experiment and the dissociated screw column angles, confirming the experimental observation of a dissociated screw. **(c)** The rate of angle change across the dislocation depends on the dissociation distance and probe defocus. By fitting sigmoid functions to the angle plots, and comparing the fitted slope-controlling parameter in the sigmoid functions of the experimental image with those of simulated images of different possible dissociation distance and defocus values, the dissociation distance of 1.65nm clearly gives the best agreement.

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