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STEM Dislocation Analysis and Image Simulations

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Conventional transmission electron microscopy (CTEM) continues to take on a prominent role in crystalline defect analysis. CTEM imaging modes such as bright field (BF), dark field (DF), and weak-beam dark field (WBDF) are well documented, and simulation programs are available for each. However, it has been demonstrated that scanning transmission electron microscopy (STEM) can be applied to defect analysis in a similar fashion, yet holds many advantages over CTEM [1-3]. For example, auxiliary contrast effects (bend contours, etc) are suppressed, and thicker specimens can be analyzed while retaining diffraction contrast; additionally, many diffraction contrast rules in CTEM remain valid in STEM, such as g · b, g · R, and invisibility conditions [4]. Although the principle of reciprocity has shown the imaging processes of STEM and CTEM to be equivalent [5], it is the case that the angular requirements for STEM are rather stringent and thus need to be relaxed in order to achieve optimal imaging conditions and many of the aforementioned benefits. Consequently, a computational basis is necessary to validate the application of STEM to diffraction contrast work. A previous publication by the authors addresses many of these issues, including reciprocity, while systematically exploring the contrast of a stacking fault under various STEM imaging conditions [4]. The present contribution will extend this developed methodology of STEM diffraction contrast analysis to dislocations.

Experimental STEM images were acquired on an FEI Tecnai F20 field emission 200 kV S/TEM with a probe convergence angle of 5.9 mrad. Two sets of oppositely-signed near-screw dislocations, ±b = $\frac{1}{3}$[1120], present in a Ti6Al foil were imaged in either a systematic row (two-beam or 3g) or zone axis configuration. The 3g imaging mode yields contrast similar to that observed in CTEM WBDF, however, in the STEM case, the crystal is tilted to s3g =0, such that the Bragg condition is satisfied at the center of the 3g diffraction disk. Computational STEM images were calculated by solving the Darwin-Howie-Whelan dynamical multi-beam equations for the systematic row and zone axis orientations over the range of incident beam directions given by the converged probe. The algorithm is described in detail in [4].

Fig. 1 displays a subset of all experimental and computational results. Although not shown below, systematic variations were made to the acceptance angles of the bright field and annular dark field (ADF) detectors for each imaging mode, which can be adjusted via the microscope camera length (CL). For each row in Fig. 1, the first two and last two columns represent BF and ADF images, respectively, with the leftmost in each case being the simulated image. Fig. 1a was obtained in a [1210] zone axis configuration at a CL of 163 mm. The two-beam condition used for row b (diffraction vector $g_{20\bar{2}1}$) results in |g · b| =2, hence the double-peaked dislocation contrast. Fig. 1c highlights the 3g imaging mode (diffraction vector $3g_{10\bar{1}1}$), which indeed provides dislocations of high contrast and narrow widths. In all cases, the experimental and computed images are in good agreement. It should be noted that there exist two additional dislocations amidst the lower set of three dislocations, with Burgers vectors parallel to the approximate beam direction of [1210]; hence, no contrast is observed. These dislocations are not accounted for in the computations, and may be the cause of some auxiliary contrast in the experimental results. The aforementioned imaging modes will be discussed in further detail, with respect to the detector acceptance angles and other geometrical parameters. Given the inherent benefits of STEM, the ability to obtain and interpret diffraction contrast images with high fidelity will no doubt be a boon to the field of crystalline defect characterization.

References
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Figure 1: Simulated and experimental BF and ADF images acquired in STEM under various diffraction conditions; a) [1210] zone axis, CL = 163 mm; b) two-beam obtained with $g_{20\bar{2}1}$ at a CL of 327 mm; c) $3g_{10\bar{1}1}$, CL = 163 mm. See text for details.