Type of presentation: Oral

# IT-9-O-2387 Retrieving nanoscale third-dimension information directly from TEM data using stacked-Bloch-wave simulations and artificial neural network tools

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Transmission electron microscope (TEM) specimens are three-dimensional, but TEM images and diffraction patterns are two-dimensional. To retrieve the "third-dimensional" information, we have developed a direct-retrieval algorithm including dynamical diffraction that can use TEM data (such as a single convergent-beam electron diffraction [CBED] pattern) and retrieve variations of a range of nanoscale specimen parameters, including strain, crystal tilt, and chemical composition. The retrieval algorithm itself is detailed elsewhere [1], and uses the stacked-Bloch-wave algorithm [2-3] and artificial neural network optimization tools [4]. In this work, we show the effectiveness of our algorithm and discuss considerations for applying this algorithm to realistic experimental data.

A demonstration of this algorithm’s third-dimension (depth-dependent) retrieval ability is seen in Figures 1 & 2. Figures 1 and 2 show CBED patterns of a 100-nm-thick Si specimen at 80 kV at the [110] zone axis, simulated using the stacked-Bloch-wave [2-3] forward-simulation algorithm and 197 zero-order-Laue-zone reflections. Figure 1 has "asymmetric" diffraction features due to the third-dimension variation of crystal tilt. Figure 2 is a CBED pattern like that in Figure 1 but without third-dimension variation, and fails to reproduce the correct diffraction features. Figures 3 and 4 demonstrate our algorithm’s effective and accurate retrieval of third-dimension variation in crystal tilt ($\Delta\alpha$, mean over all layers) from the specimen shown in Figure 1a, and decreasing mismatch between simulated and experimental CBED intensity (given by $\Delta E$, mean over all reciprocal-space points). Figure 4 shows how well the unknown $\alpha$ is determined for a known E mismatch.

This algorithm can retrieve third-dimension material properties from a single CBED pattern; however, other techniques like dark-field image series or large-angle rocking-beam electron diffraction (LARBED) series can also be used. Each technique has its own advantages and challenges, especially for analysis of strain or compositional variations. Large lattice-parameter variations can also require a modification to the algorithm in [1].

In this work, we present practical considerations for using our third-dimension information-retrieval algorithm [1]. We demonstrate its effectiveness, discuss different acquisition techniques and consider how different parameters affect our algorithm.

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[2]: R. S. Pennington, F. Wang, C. T. Koch. Ultramicroscopy, 2014. http://dx.doi.org/10.1016/j.ultramic.2014.03.003
[3]: D. J. Eaglesham, C. J. Kiely, D. Cherns, and M. Missous. Phil. Mag. A 60, 161 (1989).
[4]: R. Rojas. Neural Networks: A Systematic Introduction (Springer Verlag, Berlin, 1993).

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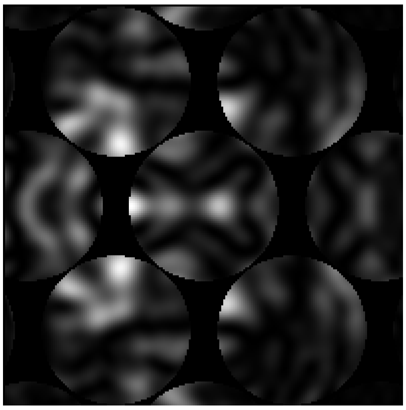

Fig. 1: Simulated zero-loss-filtered convergent-beam electron diffraction (CBED) pattern, generated from a specimen with third-dimension crystal tilt variation. The specimen has ten 10 nm layers, tilted along the [001] direction {0.00, -0.04, -0.10, -0.20, -0.30, -0.30, -0.20, -0.14, -0.06, 0.00} degrees, respectively.

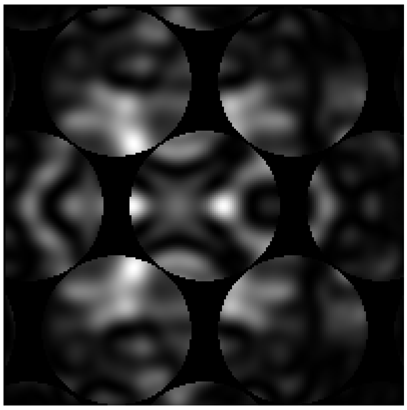

Fig. 2: A CBED pattern like Figure 1, but generated from a specimen with no layer-by-layer crystal tilt variation but with the same mean crystal tilt, which fails to reproduce the "asymmetric" diffraction features seen.

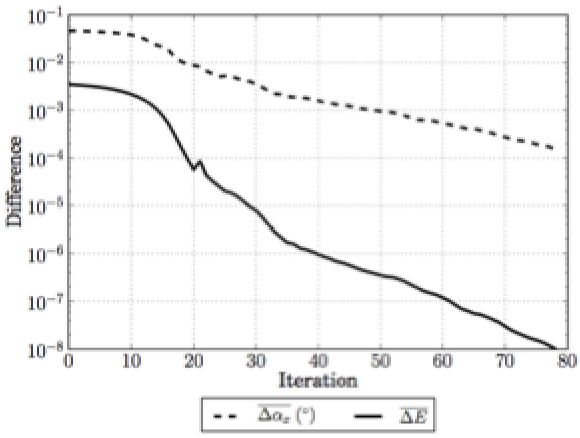


Fig. 3: Our algorithm [1] retrieves third-dimensional variation in crystal tilt (see text) using a (13x13) point reciprocal-space grid, each point 0.05 degrees apart, starting at the 000 point and moving in the [001] and [-110] directions. (This area does not correspond to the discs in Figure 1, but is from the same specimen.)

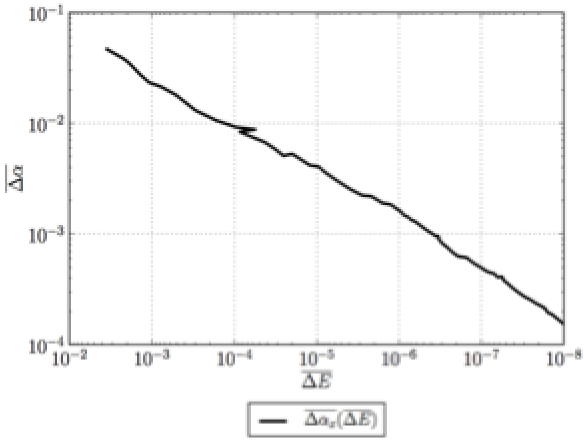


Fig. 4: The unknown third-dimension parameter mismatch (Δα, mean over all layers), plotted as a function of the known intensity mismatch (ΔE, mean over all points).