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Towards a Uniform Model for Lattice Defect Image Simulations

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For more than seven decades, diffraction contrast in the TEM has been used for the study of both linear and planar lattice defects, such as dislocations, stacking faults, anti-phase boundaries, and so on. In recent years, several alternative approaches for defect imaging have become available: using a standard annular dark field detector, the STEM diffraction contrast image (DCI) mode produces medium angle annular dark field (MAADF) images which display strong defect contrast, even for relatively thick foils [1], while suppressing contrast due to foil bending and such. Both systematic row and zone axis orientations can be used in the STEM-DCI technique, in contrast with conventional TEM bright field/dark field imaging, where the zone axis orientation is mostly avoided. The arsenal of scanning electron microscopy (SEM) modalities has been extended with the electron channeling contrast imaging (ECCI) approach, which allows for the imaging of low density surface penetrating lattice defects over large sample areas. It is to be noted that in all of these techniques, the diffraction contrast is caused by the same dynamical scattering mechanisms; the only differences are the instrument accelerating voltage, the illumination mode (parallel or conical, stationary or scanning), and the shape and position of the detector (CCD, annular detector). The common underlying physics principles suggest that a single computational approach to defect image simulations might be possible, covering all the above mentioned observations modes.

In this contribution, we will describe a unified numerical approach to defect contrast image simulations for conventional TEM, STEM-DCI, and ECCI modalities. We begin with the displacement field, $\mathbf{R}(\mathrm{r})$, which can be modelled analytically for certain defects (straight dislocations in an anisotropic medium, planar faults), but requires a numerical model for the more general case. Using a plane wave expansion for the sample exit wave function, one can show that the Darwin-Howie-Whelan (DHW) equations for the beam amplitudes $S_g(z)$ can be written as:

$$\frac{\mathrm{d}S_{\mathbf{g}}(z)}{\mathrm{d}z} = 2\pi \mathrm{i} s_{\mathbf{g}} S_{\mathbf{g}}(z) + \mathrm{i}\pi \sum_{\mathbf{g}'} \frac{\mathrm{e}^{-\mathrm{i}\alpha_{\mathbf{g}-\mathbf{g}'}(\mathbf{r})}}{q_{\mathbf{g}-\mathbf{g}'}} S_{\mathbf{g}'}(z),$$

where s_g is the excitation error, $1/q_g$ are proportional to the Fourier coefficients of the optical potential, and $\alpha_g(\mathbf{r}) = 2\pi g\ \mathbf{R}(\mathbf{r})$. In matrix form, we have:

$$\frac{\mathrm{d}\mathbf{S}(z)}{\mathrm{d}z} = \mathrm{i}\mathcal{A}(\mathbf{r})\mathbf{S}(z),$$

where $\mathcal{A}$ is the structure matrix, which has $2\pi s_{\mathbf{g}} + \pi/q_0$ along its diagonal, and $\pi \exp[-\mathrm{i}\alpha_{\mathbf{g}-\mathbf{g}'}(\mathbf{r})]/q_{\mathbf{g}-\mathbf{g}'}$ on the off-diagonal. Formally, the solution to this equation for a foil of thickness ε can be written as:

$$\mathbf{S}(\epsilon) = e^{\mathrm{i}\mathcal{A}\epsilon}\mathbf{S}(0) = \mathcal{S}(\epsilon)\mathbf{S}(0),$$

where $S(\varepsilon)$ is the scattering matrix. The matrix exponential can be computed efficiently using the Padde approximation. Defect image simulations then use the column approximation, with one column corresponding to each image pixel; each column is sub-divided into N_t slices of thickness ε, for a sample thickness (or integration depth, for the SEM modalities) of $t = N_t\varepsilon$. The most elementary computational

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step is the propagation of the wave function from slice i to slice $i + 1$. In the scattering matrix formalism, this is readily accomplished by a matrix-vector multiplication, once the scattering matrix is known. Since the defect phase factors are periodic functions, one can pre-compute an array of scattering matrices, and use complex bi-linear interpolation to select the relevant matrix for each slice. In zone axis orientation, one identifies two short reciprocal vectors g_a and g_b, and writes all reflections as linear combinations of these two vectors; the defect phase factor can then be decomposed as:

$$e^{-i\alpha_{\mathbf{g}-\mathbf{g}'}(\mathbf{r})} \rightarrow e^{-2\pi i(m-m')\mathbf{g}_a\cdot\mathbf{R}(\mathbf{r})} e^{-2\pi i(n-n')\mathbf{g}_b\cdot\mathbf{R}(\mathbf{r})};$$

in the exponents, only the values $(m - m')g_a \cdot \mathbf{R}(\mathbf{r})$ mod 1 and $(n - n')g_b \cdot \mathbf{R}(\mathbf{r})$ mod 1 are relevant, due to the periodicity of the complex exponential. For a given perfect crystal structure matrix A, one can then pre-compute a 2-D array of scattering matrices for which the exponents uniformly sample the interval [0 . . . 1]. The remainder of the dynamical scattering simulation then involves products of wave amplitudes by the appropriate scattering matrices as the waves propagate down the integration column.

Using this elementary computational step, we have implemented defect image simulations for the three modalities mentioned above: conventional TEM bright field/dark field imaging requires only a single integration for each image column, corresponding to the incident beam direction k. For the STEM-DCI approach, a range of incident beam directions is specified (corresponding to the illumination cone), and the integrations are carried out for each beam direction; the computed intensities are then stored as individual diffraction disks, similar to a CBED pattern, so that the annular detector geometry and microscope camera length can be imposed afterwards. For the ECCI imaging modality, one can show that the probability of back-scattered electron generation can be computed by means of the following relation:

$$\mathcal{P}(\mathbf{k}_0) = \sum_{\mathbf{g}}\sum_{\mathbf{h}} S_{\mathbf{gh}} L_{\mathbf{gh}},$$

where the matrices are defined as:

$$S_{\mathbf{gh}} \equiv \sum_{n}\sum_{i\in\mathcal{S}_n} Z_n^2\, e^{-M^{(n)}_{\mathbf{h}-\mathbf{g}}}\, e^{2\pi i(\mathbf{h}-\mathbf{g})\cdot\mathbf{r}_i} e^{i(\theta_{\mathbf{h}}-\theta_{\mathbf{g}})};$$

$$L_{\mathbf{gh}} \equiv \frac{1}{z_0}\int_0^{z_0} dz\, S^*_{\mathbf{g}}(z) S_{\mathbf{h}}(z) \approx \frac{1}{N}\sum_{i=1}^{N} S^*_{\mathbf{g}}(z_i) S_{\mathbf{h}}(z_i);$$

In the final equation, the scattered amplitudes are computed using the same algorithm as for the TEM and STEM-DCI approaches. In addition to the scattering matrix algorithm, our approach also requires a routine to automatically determine all the contributing reflections for a given crystal structure and incident wave vector, as well as an automated routine to apply the Bethe potential perturbation approach to reducing the size of the dynamical matrix. We will illustrate these approaches with a number of application examples, including ECCI images of stacking-fault pyramids in GaP and STEM-DCI images of dislocations in Ni-based super alloys. Extensions of the model to multi-phase compounds will also be discussed. All fortran 90 source code as well as several visualization interfaces written in the Interactive Data Language are made available in the public domain.

References

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