Two beam toy model for dislocation contrast in ECCI

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Dislocation contrast in the SEM, as observed though electron channelling contrast imaging (ECCI), is commonly treated analogously to the contrast in the TEM. This perception is based on early studies done for dislocations parallel with the surface where the surface relaxation is negligible. However, for threading dislocations (TD) that interact with the surface (normal or inclined), as is the case for nitrides materials, $\mathbf{g} \cdot \mathbf{b}$ type invisibility criteria are no longer fully applicable to ECCI, especially in forward geometry [1].

Dislocations change locally the lattice curvature and Bragg diffraction conditions in the crystal, affecting the form and diffracting behaviour of the electron wavefunction in that region. More explicitly, Howie and Whelan [2] had shown that dislocation contrast is the result of interband transitions between Bloch waves states which, in turn, are caused by the change in the displacement field, $\mathbf{u}(\mathbf{r})$, around the dislocation or local "strain". Dynamical models have been used successfully to both predict and characterise dislocations in ECCI [3]. Nevertheless, the behaviour of dislocation contrast in ECCI in particular and diffraction contrast in the SEM in general remains somewhat opaque.

In the work we investigate the behaviour of contrast causing strain as a means of insight into this problem. We call the dislocation strain component to which ECCI is sensitive *ECCI-strain*, and we defined it, generalising Tunstall work [4], as being composed of the change in the $\mathbf{g}$ components of the displacement field in the direction of the incident beam $\mathbf{r}_{inc}$ (change in lattice curvature) plus a small part of its change in the direction of the diffraction condition $\mathbf{g}$:

$$\textit{ECCI-strain} = \frac{\partial u_g}{\partial r_{inc}} + \theta_B \frac{\partial u_g}{\partial r_g} \tag{1}$$

Negative (blue) and positive (red) isosurfaces of equal absolute value of the ECCI-strain are shown in Fig. 1 for both an edge (a) and a screw (b) normal threading dislocation in a wurtzite crystal for a 50° degree tilted sample. Notice that, not only can the surface relaxation be very large compared to the bulk effect for an edge dislocation, but the sign of the strain can flip.

We can also examine whether the dislocation character or the diffraction condition will have the greater qualitative effect on the strain profile and therefore contrast. Fig. 2 shows top sample view for an edge TD equidistant ECCI-strain isosurfaces. In the same diffraction condition, different edge dislocations (Fig. 2 a) and b)) will show ECCI-strain profiles rotated to each other, somewhat following the Burger vector. On the other hand, the same edge dislocation in different diffraction conditions will change less drastically its stain orientation but it will affect significantly its intensity. As expected, flipping the direction of the diffraction vector (c) and d)) or the that of the Burger's vector (b) and c)) flips the positive negative strain regions.

The dislocation contrast behaviour in ECCI will then follow closely the behaviour of the strain [5]. Note that numerical predictions of contrast involve adding backscattering probabilities along the incident beam direction.

References

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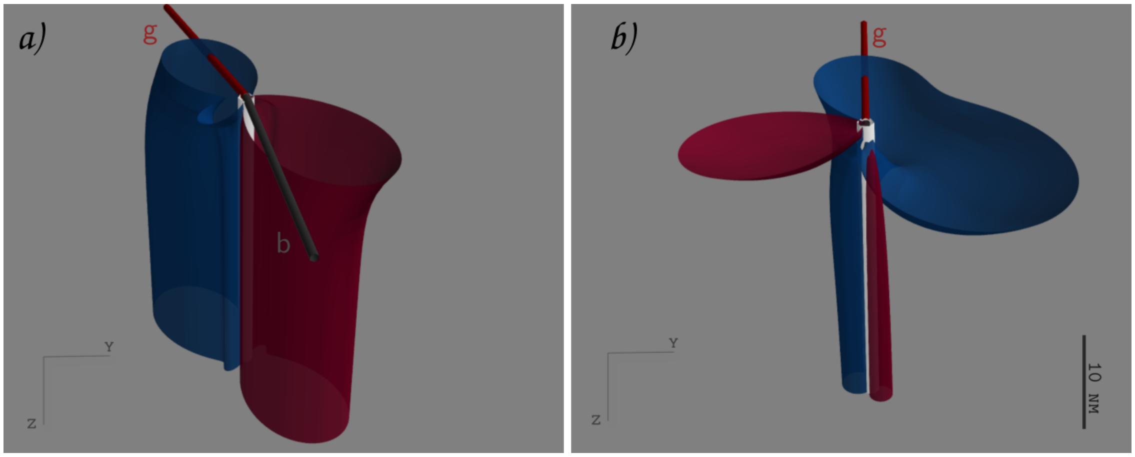

Figure 1: Side view of equidistant ECC-strain field isosurfaces for a) Edge with Burger vector direction b (grey rod) and b) Screw threading dislocation in a wurtzite crystal. The diffraction condition is indicated by g (red rod). (yz) indicate the sample coordinate frame.

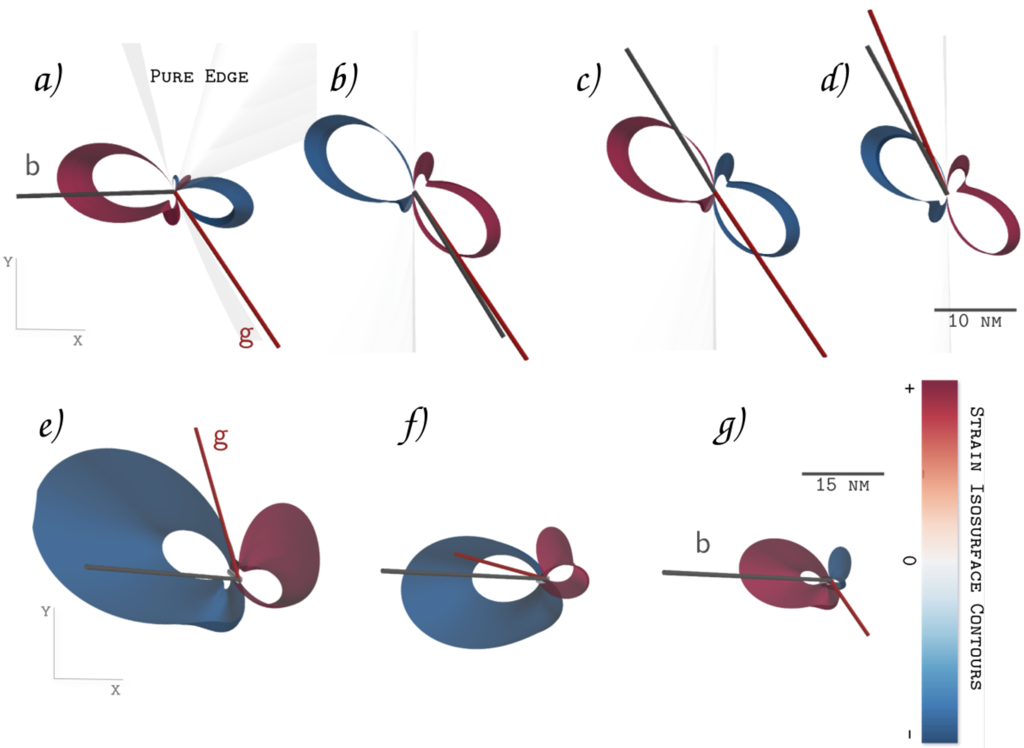

Figure 2: Top view of equidistant ECC-strain isosurfaces for a pure edge dislocation in a wurtzite crystal in different orientations indicated (see above caption). (xy) indicate the sample coordinate frame. The absolute values of red and blue isosurfaces is the same (equidistant). The white curves are the zero value isosurfaces. Note that top and bottom rows have slightly different scales.