Diffraction contrast imaging

Lecture 13

Weak beam dark field imaging
Simulation of diffraction contrast
Weak beam dark field imaging
Weak beam dark field images

Goal: ‘high resolution’ diffraction contrast image of defects

Method: establish a kinematical condition (large $s$)

This gives a small $\xi_{\text{eff}}$

Result is a narrow dislocation image (since this is proportional to $\xi_{\text{eff}}$)
Weak beam dark field images

Why high-resolution images?

Often want to look at:
- Jogs & kinks
- Separation between partial dislocations
- Interaction between dislocations
- Interaction with other defects & precipitates

Again, these images can help correlate specifics of dislocation motion with overall plastic deformation response
Weak beam dark field imaging

By setting \( s \) ‘large’ most of the sample is not oriented in a strong Bragg condition.

However, defect locally bends planes back to Bragg angle.

The region over which this occurs is very small, as the strain needed must be large.

Thus the defect image is quite narrow.

The image ‘peak’ is thus close to the dislocation core.

- Will switch with sign of \( g \)
Weak beam dark field imaging

Steps:

1. Establish two beam condition with $s$ slightly greater than zero

2. Tilt the strong $g$ to the optic axis using dark field tilts
   - You will note that it becomes quite dim
   - You will also see $3g$ become strong
     - This is purely a geometric effect

3. Insert objective aperture & check centering

4. Now both BF & WBDF are well established
Weak beam dark field imaging

Nothing ‘magical’ about the g-3g condition
  – It’s just one that ‘often’ works

Any two-beam condition where corresponding DF has $s >> 0$ will work, and some may work better

For calculation purposes, may need to know $s$ precisely
  – Measurement method described in W&C text

Resulting WBDF image will have ‘weak’ intensity
  – May require very long exposures
  – Resolution limit may be stage drift
Weak beam dark field imaging

A bit of theory

\[ I_g = |\phi_g|^2 = \left( \frac{\pi t}{\xi g} \right)^2 \frac{\sin^2(\pi s_{\text{eff}} t)}{(\pi s_{\text{eff}})^2} \]

\[ s_{\text{eff}} = \sqrt{s^2 + \frac{1}{\xi g^2}} \]

If \( s \gg 0 \), then \( s_{\text{eff}} \approx s \)

Resulting image largely insensitive to \( \xi_{\text{eff}} \)

Image is ‘kinematical’

\[ I \propto \frac{\sin^2(\pi s_z t)}{(\pi s_z)^2} \]
Weak beam dark field imaging

So - in most of the image - we have kinematical contrast
- $\mathbf{0}$ and $\mathbf{g}$ are not strongly coupled

However - local to the defect - the two beams are strongly coupled
- The defect is the connecting link
- Strong dynamical contrast only local to the defect

Bloch wave explanation:
- Defect causes local change in scattering from Bloch Wave #1 to Bloch Wave #2
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Weak beam dark field imaging

Can more readily see dissociation & interaction effects
Weak beam dark field imaging

Inside-outside contrast also sensitive to small changes in $s$ during WBDF imaging
Weak beam dark field imaging

Many more fringes seen in SF images

Spacing very sensitive to $s$
Weak beam dark field imaging

Strong effect on thickness fringe spacing as well

Large $s$ reduces effective extinction distance $\xi_{\text{eff}}$

Cross section $t$

$\xi_{\text{eff}} = \frac{1}{s_{\text{eff}}}$

slope $t$, fringe separation $t$, fringe width $t$
Simulation of diffraction contrast
Computational solutions to HW Eqns

Use:
\[
\frac{d\phi_g}{dz} = \frac{\pi i}{\xi_g} \phi_o \exp \left[ -2\pi i (sz + g \cdot R) \right] + \frac{\pi i}{\xi_o} \phi_g
\]

and
\[
\frac{d\phi_o}{dz} = \frac{\pi i}{\xi_g} \phi_o + \frac{\pi i}{\xi_o} \phi_g \exp \left[ 2\pi i (sz + g \cdot R) \right]
\]

or:
\[
\frac{d\phi_o}{dz} = \frac{\pi i}{\xi_o} \phi_g
\]

and
\[
\frac{d\phi_g}{dz} = \frac{\pi i}{\xi_g} \phi_o + \left[ 2\pi i \left( sz + g \cdot \frac{dR}{dz} \right) \right] \phi_g
\]
Computational solutions to HW Eqns

Figure 8.4. Theoretical profiles of thickness fringes. (a) No absorption. (b) $\xi_g/\xi_s = 0.05$. (c) $\xi_g/\xi_s = 0.10$. Note the reduced visibility of the fringes in the thick regions of (c). Continuous and broken lines refer to bright-field and dark-field images respectively.

(From Hashimoto, Howie and Whelan, 1962, by courtesy of The Royal Society)

"Rocking" Curve
Like a trace across a bend contour

$w = s\xi_g$

Figure 8.5. ‘Rocking Curves’ computed on the two-beam theory for a crystal of thickness $t = 4\xi_g$. Full curves are bright-field images; broken curves are dark-field images. The dark-field images are symmetrical about $w = s\xi_g = 0$. (a) No absorption, $\xi_g/\xi_s = 0$. (b) $\xi_g/\xi_s = 0.05$. (c) $\xi_g/\xi_s = 0.10$. The curves in (a) are complementary. Note the asymmetry of the bright-field images in (b) and (c) (corresponding to either edge of the dark band at D in Figure 8.3), and the reduced amplitude of the subsidiary oscillations in (c). In (b) and (c) $\xi_s = \xi_g$.

(From Hashimoto, Howie and Whelan, 1962, by courtesy of The Royal Society)
Computational solutions to HW Eqns

Obviously, can produce simulated images by calculating $\phi_o$ and $\phi_g$ along each column.

Figure 10.8. Computed stacking fault image profile for $\alpha = +2\pi/3$ with anomalous absorption effects included, $t|\xi_o' = 7.25$, $\xi_o' = \xi_g'$, $\xi_o' / \xi_g' = 0.075$, $w = -0.2$. Bright- and dark-field images are shown as continuous and broken lines respectively.

(From Hashimoto, Howie and Whelan, 1962, by courtesy of The Royal Society)

Figure 10.9. Computed stacking fault image profile for $\alpha = -2\pi/3$ with anomalous absorption effects included, $t|\xi_o' = 5$, $\xi_o' = \xi_g'$, $\xi_o' / \xi_g' = 0.07$, $w = 0$. Bright- and dark-field images are shown as continuous and broken lines respectively.

(From Hashimoto, Howie and Whelan, 1960, by courtesy of The Philosophical Magazine)
Computational solutions to HW Eqns

Dislocations show relatively sharp fall-offs in contrast

Due to the nature of \( \frac{dR}{dz} \)

\[ p = \frac{g \cdot b_e}{g \cdot b_s} \]

Figure 11.11. Computed bright-field images of mixed dislocations. The image width depends on the value of the parameter \( p \) shown for each curve. See text for discussion. (From Howie and Whelan, 1962, by courtesy of The Royal Society)

Figure 11.4. Computed bright-field (continuous line) and dark-field (broken line) images for a screw dislocation in the middle of a thick foil with \( t = 0.4 \), \( g \cdot b = 1 \), \( \xi_{e} / \xi_{s} = 0.1 \). In (a) \( \psi = 0 \); in (b) \( \psi = 0.3 \).

(From Howie and Whelan, 1962, by courtesy of The Royal Society)

Figure 11.5. Computed bright- and dark-field images for an edge dislocation in the middle of a thick foil with \( t = 0.4 \), \( g \cdot b = 1 \), \( \xi_{e} / \xi_{s} = 0.1 \), \( \psi = 0 \). Compare with Figure 11.4a.
Computational solutions to HW Eqns


CUFOUR:
Obviously, can produce simulated images by calculating $\phi_o$ and $\phi_g$ along each column.
Computational solutions to HW Eqns

“SIMCON”

A program that allows one to use the output form FEM modeling to generate simulated diffraction contrast


FIG. 3. (Color) ANSYS stress plot of γ-axis stresses (vertical in the plane of the gauge) surrounding the shallow isolation trench structures. Note: entire FE model not shown.

FIG. 1. (Color) Experimental (400) TEM image of shallow isolation trench structure and line scan (a). Simulated (400) TEM image of shallow isolation trench structure and line scan (b). Difference map created by subtracting a from b on a pixel by pixel basis (c). Boxes show the analyzed regions.