Diffraction Contrast Imaging

Lecture 10
Categories of imaging

Mass-thickness contrast
- Contrast appears in the image due to differences in the inherent scattering from the sample
- Z-contrast imaging (a high-resolution version of same)

Diffraction contrast
- In crystalline materials, diffraction occurs.
- Utilizing the objective aperture, either the direct (‘un-diffracted’) beam or one of the diffract beams is selected to form the image
  - Results in crystallographic information being conveyed in the image

Phase contrast (‘high-resolution’ imaging)
- Direct and diffracted beams undergo phase shifts in the material
- An image if formed by recombining all beams and observing the resulting interference pattern
Bright Field / Dark Field Imaging

BF image formed from the direct beam

Displaced aperture DF image formed with off-axis scattered beam

CTF image where the incident beam is tilted so that the scattered beam remain on axis

Optic axis
Reflecting plane
Incident beam
θ specimen
2Θ
Objective lens
Direct beam
Diffracted beam
Objective aperture

Optic axis
Reflecting plane
Incident beam
θ specimen
2Θ
Objective lens
Direct beam
Diffracted beam
Objective aperture

Optic axis
Direction of tilt of incident beam
2Θ = angle of tilt of incident beam
θ
Objective lens
Diffracted beam
Objective aperture
Direct beam
Diffracted beam
Optic axis
 Objective aperture
Diffracted beam
Direct beam
Two beam imaging

Primary imaging mode is the “two-beam” condition
Allows readily interpretable images
Two-beam conditions

Examples of two-beam conditions near the 011 Zone Axis
**Assumptions**

- Only two diffracted beams considered, direct and one diffracted.
- Intensity of diffracted beam is small.
- Single scattering event.
- No ‘absorption’ i.e.: $I_{\text{diffracted}} \ll I_{\text{transmitted}}$.

\[
I_{\text{Diff}} = \frac{\sin^2(\pi z s)}{\zeta_s s^2}
\]

\[
I_{\text{Trans}} = 1 - I_{\text{Diff}}
\]
Kinematic vs. Dynamical

Can be used to explain (to first approximation) the origin much of much what we see in the microscope

However, cannot be used to accurately calculate intensity relationships

Use dynamical theory:
- Considers multiple beams
- Intensity in one or more diffracted beams can be large in comparison with transmitted beam
- Multiple scattering allowed
- “Absorption” (loss of electrons) allowed
- Can explain intensity accurately
- Very complicated to utilize practically
Kinematic diffraction in perfect crystals

**Thickness contours:**

- At exact Bragg condition ($s = 0$), the intensity of the direct and diffracted beam oscillate in a complementary way.

- For a wedge specimen, the separation of the fringes in the image is determined by the angle of the wedge and the extinction distance, $\xi_g$.

- Thus, the image may appear to be black or white depending on the thickness of the specimen where you are observing it.
Kinematic diffraction in perfect crystals

Representative bright field (a), and dark field (b) micrograph showing thickness fringes

Courtesy V.R. Radmilovic
Translation / rotation between two crystals yields fringes in images

- Stacking faults
- Grain boundaries
- Translation boundaries
- Phase boundaries
- Surfaces (if stepped)

Electron wave has a different amplitude & phase in each crystal

- Results in a fringe pattern
Kinematic diffraction in imperfect crystals

Strain field of dislocation causes local diffraction differences

Seen as line of contrast in the image (if oriented correctly ...)

\[ \mathbf{g} \cdot \mathbf{R} \text{ causes the contrast and for dislocations, } \mathbf{R} \text{ changes with } z. \]

\[ \mathbf{g} \cdot \mathbf{b} = n; \text{ if we know } \mathbf{g} \text{ and we determine } n, \text{ then we know } \mathbf{b}. \]
If $g \cdot b = 0$, then you won’t see any contrast because the diffracting planes are then parallel to $R$. This is termed the invisibility criterion.
Dislocations in Si. Left: BF image in two-beam condition with strong (220) diffraction. Right: $g-3g$ WBDF image with weak (220) diffraction. Compare the intensities of the active diffractions (circled in inserts).
Dark field images of new Al-2at.%Cu-1at.%Si-1 at.%Ge alloy aged 1h and 3hrs (right) at 190°C; imaged using 112θ reflection.

Courtesy V.R. Radmilovic
Weak-beam dark-field imaging

Diffraction condition

\[ |\phi_g|^2 = \left( \frac{\pi t}{\zeta_g} \right)^2 \cdot \frac{\sin^2(\pi t s_{eff})}{\left(\pi t s_{eff}\right)^2} \]

\[ s_{eff} = \sqrt{s^2 + \frac{1}{\zeta_g^2}} \]

\[ \zeta_{eff} = \frac{\zeta_g}{\sqrt{w^2 + 1}} \]

The Ewald sphere construction showing the diffraction conditions used to obtain weak-beam images. The sphere cuts the row of systematic reflections at “ng” where \( n \) is not necessarily an integer.
Kinematic diffraction in imperfect crystals

Bright field image
Dark field image
‘Weak beam’ dark field image

Al$_2$O$_3$
GaN
The origin of bend contours shown for a foil symmetrically bent on either side of the Bragg conditions. When the \( hkl \) planes are in the Bragg condition, the reflection \( G \) is excited.
Kinematic diffraction in perfect crystals

Bend Contours

Each diffracted plane produces two bend contours

[100] crystal orientation

[103] crystal orientation
g•b Contrast Analysis of Overlapping Stacking Faults and Superpartial Dislocations

- **Type A**: Leading dislocations of the SF’s $\Rightarrow 1/x$ [112]
- **Type B**: Trailing dislocations of the SF’s $\Rightarrow 1/x$ [112]
- **Type C**: Superpartials bounding the APB’s $\Rightarrow 1/2$ [101]
- Stacking Fault Displacement $R \Rightarrow 1/3$ [111]

$x=3$ or 6

Courtesy V.R. Radmilovic
Kinematic diffraction in imperfect crystals

**Off-axis Dark Field**

**On-axis Dark Field**
Weak-beam dark-field imaging

A DP obtained when the specimen is tilted to a suitable orientation for WB microscopy. Here \( g \) is a 220 reflection and \( 3g \) is

![Diagram showing the relationship between optic axis and Ewald sphere for BF and DF imaging.](image)

Relationship between the orientation of the Ewald sphere and the position of the Kikuchi lines for the \( 0g \) (upper) and \( 3g \) (lower) diffraction conditions. The two pairs of diagrams are related by tilting the beam; the specimen has not tilted so the position of the Kikuchi lines is unchanged.