Diffraction contrast imaging

Lecture 11

Thickness fringes

Bend contours

Planar faults

What is 'contrast'

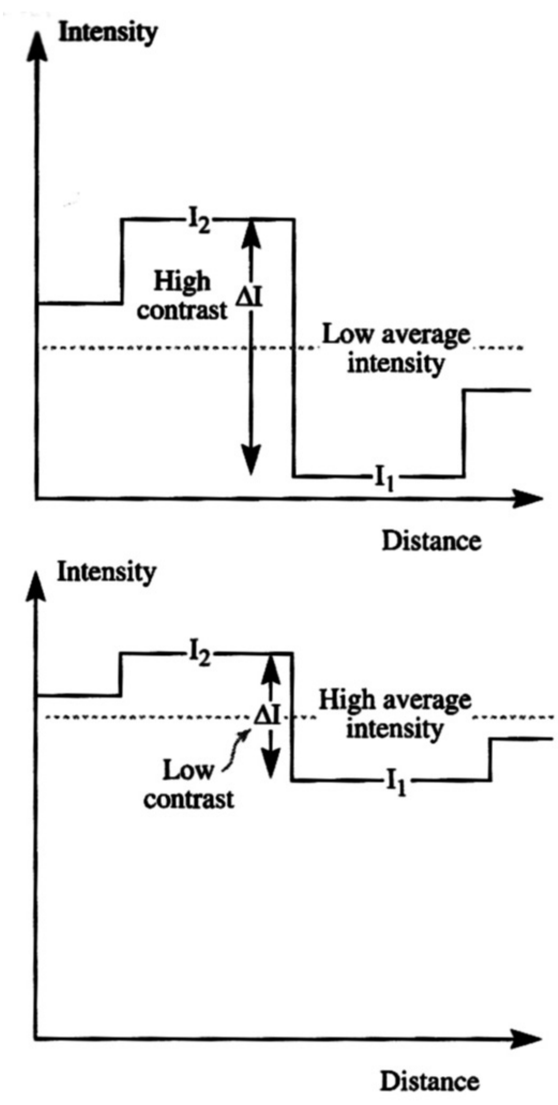
Contrast:

$$C = \frac{(I_1 - I_2)}{I_2} = \frac{\Delta I}{I_2}$$

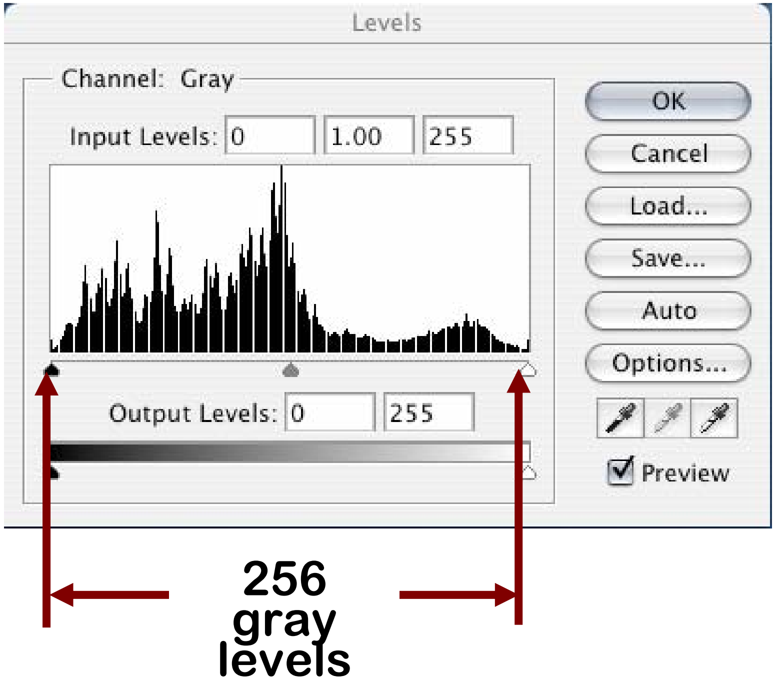
Generally, the goal with all imaging is to maximize contrast, not intensity

- i.e. want <u>differences</u> in intensity, not just more intensity

Also, generally lower average intensity allows more contrast



The perfect ‘image’ …

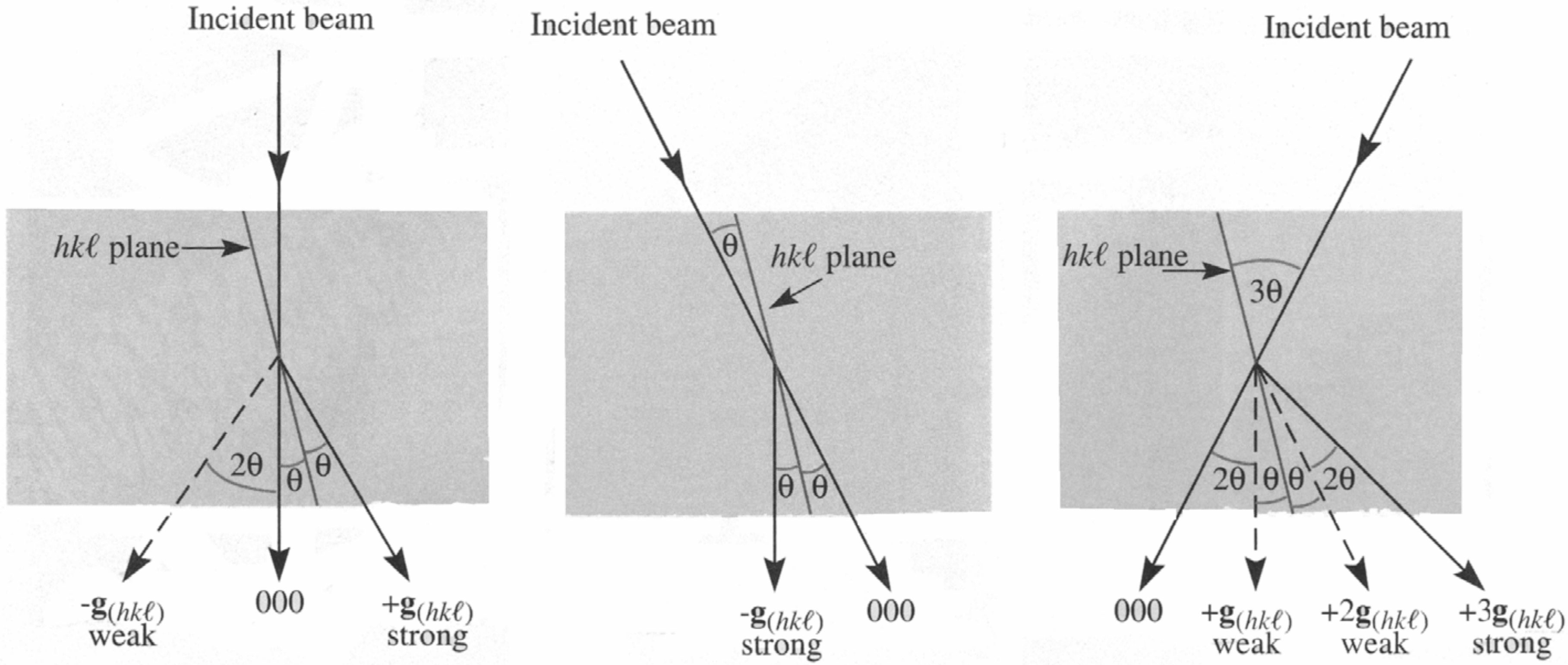


… is one that fills the available gray levels completely and as uniformly as possible

… has a low to medium level of average contrast

… has a very low intensities at 0 & 256 gray levels

Two beam imaging

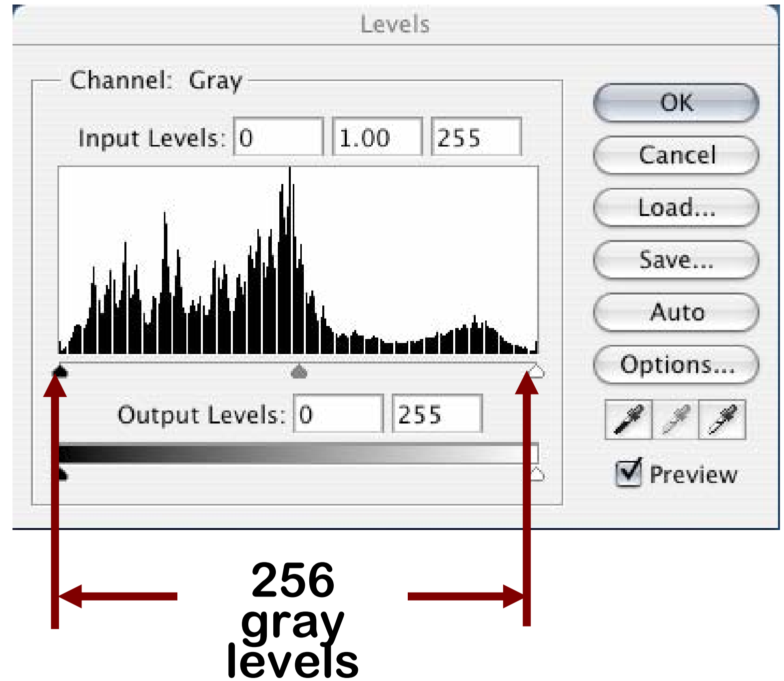


Bright Field Image **Dark Field Image** **Weak-Beam Dark Field Image**

Primary imaging mode is the "two-beam" condition

Objective aperture is used to select between beams

The perfect 'image' …



… is one that fills the available gray levels completely and as uniformly as possible

… has a low to medium level of average contrast

… has a very low intensities at 0 & 256 gray levels

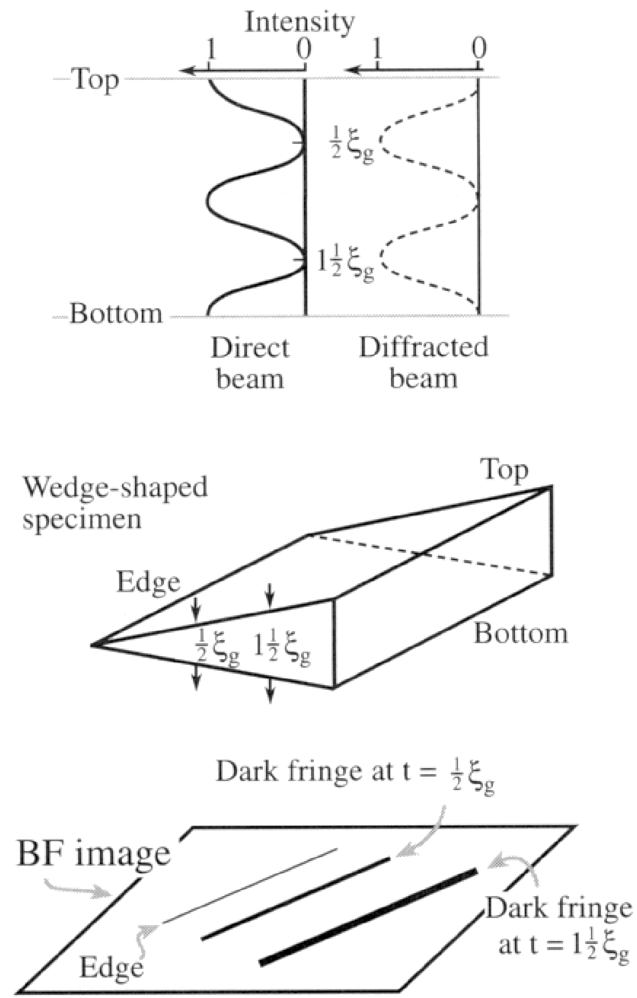
Thickness "fringes"

- This is now obvious to us after our discussion of both dynamical diffraction & Bloch waves
- But it does represent the first and most obvious example of diffraction contrast imaging

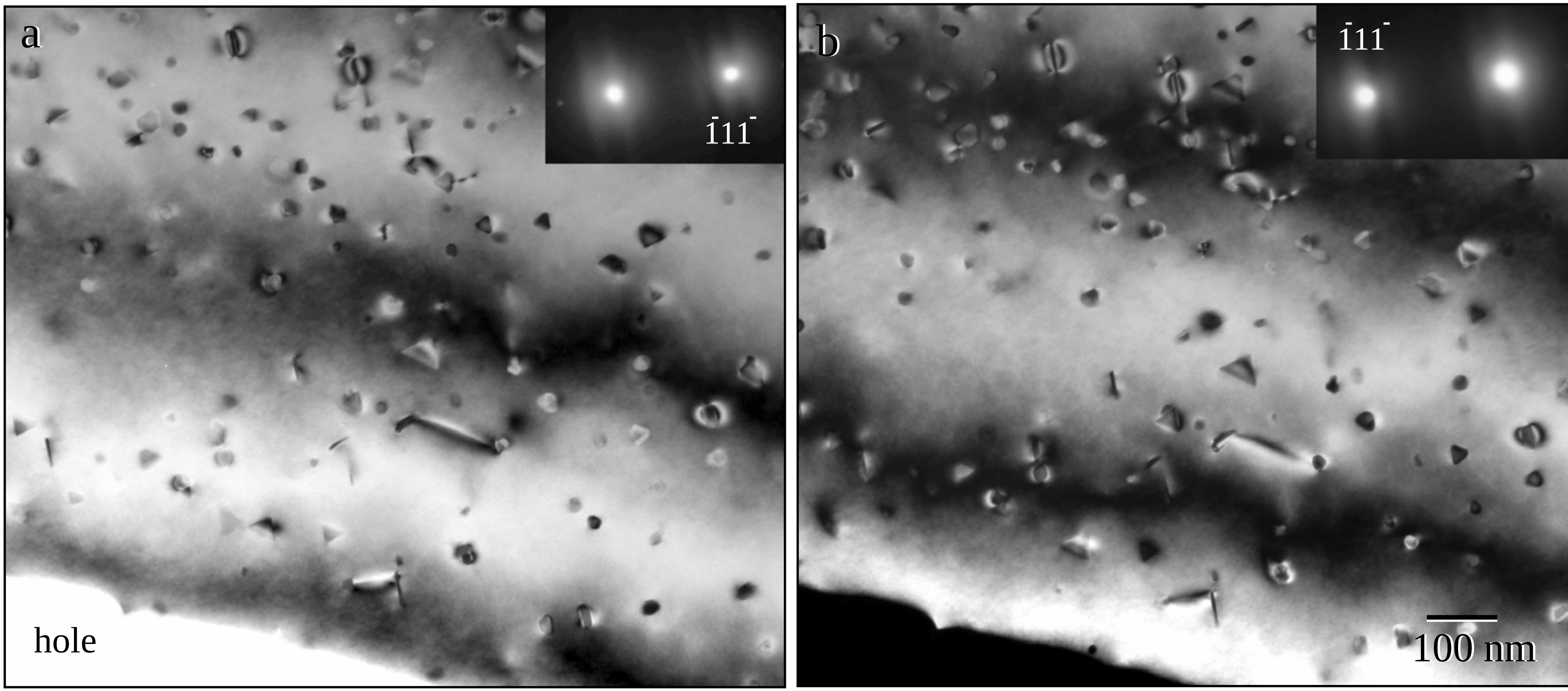
$$I_o = 1 - I_g$$

$$I_g = |\phi_g|^2 = \left(\frac{\pi t}{\xi_g}\right)^2 \frac{\sin^2(\pi s_{eff} t)}{(\pi s_{eff})^2}$$

$$\text{with: } s_{eff} = \sqrt{s^2 + \frac{1}{\xi_g}^2}$$



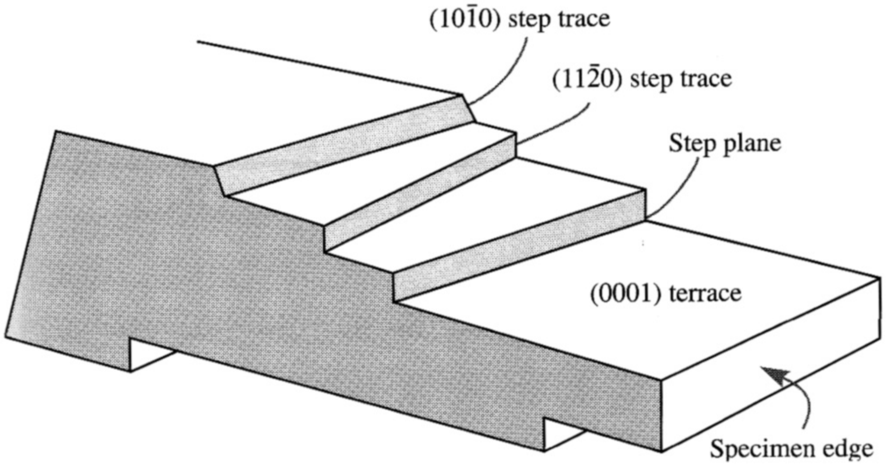
Thickness "fringes"

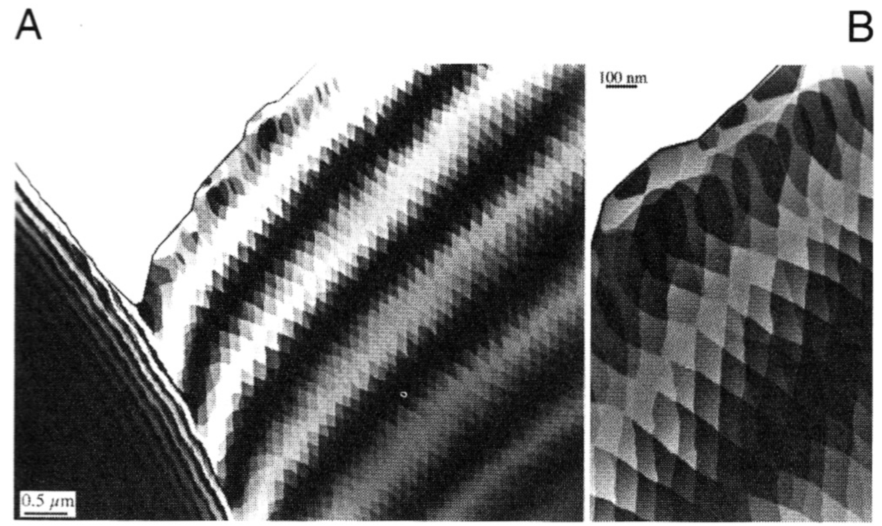


Representative (a) bright field, and (b) dark field micrographs showing thickness fringes

Thickness "fringes"

Nice example showing 'quantization' of thickness fringes due to the presence of steps in a sample





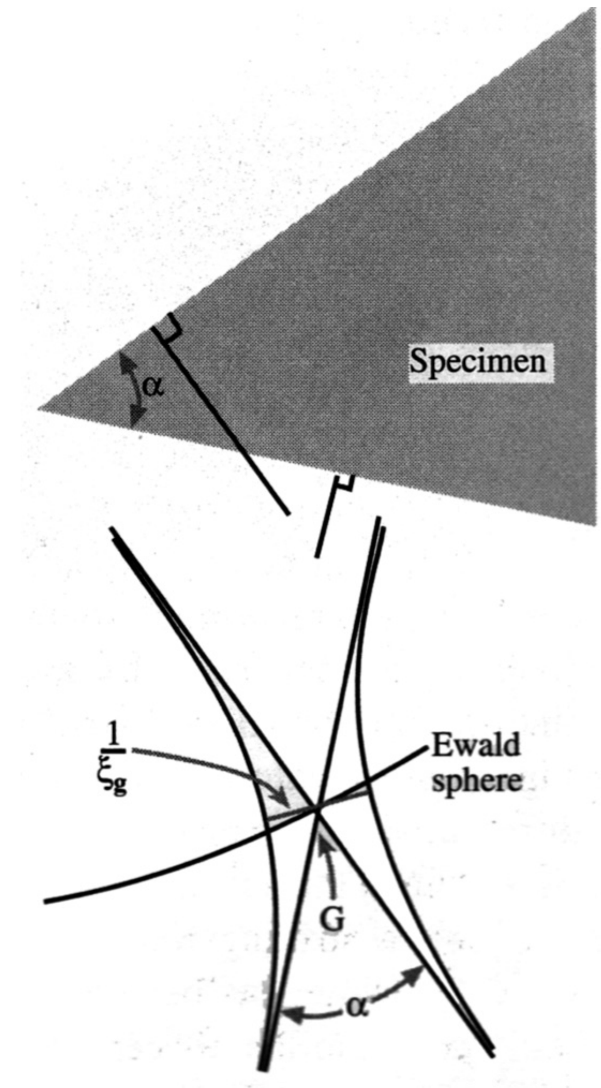
Effects in diffraction patterns

When you have a wedge, there are two rel-rods in the diffraction pattern

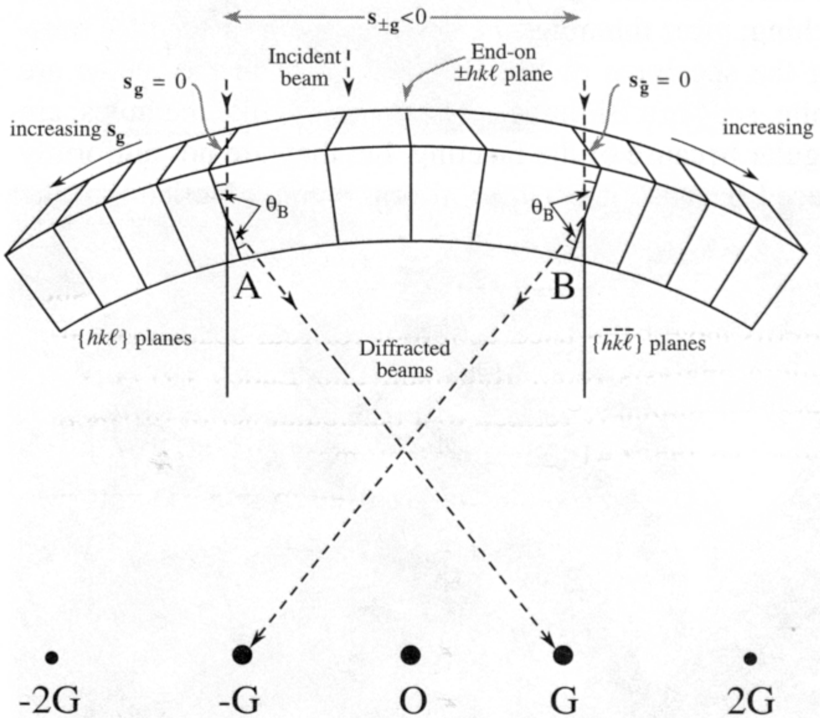
The rel-rods become curved, instead of straight

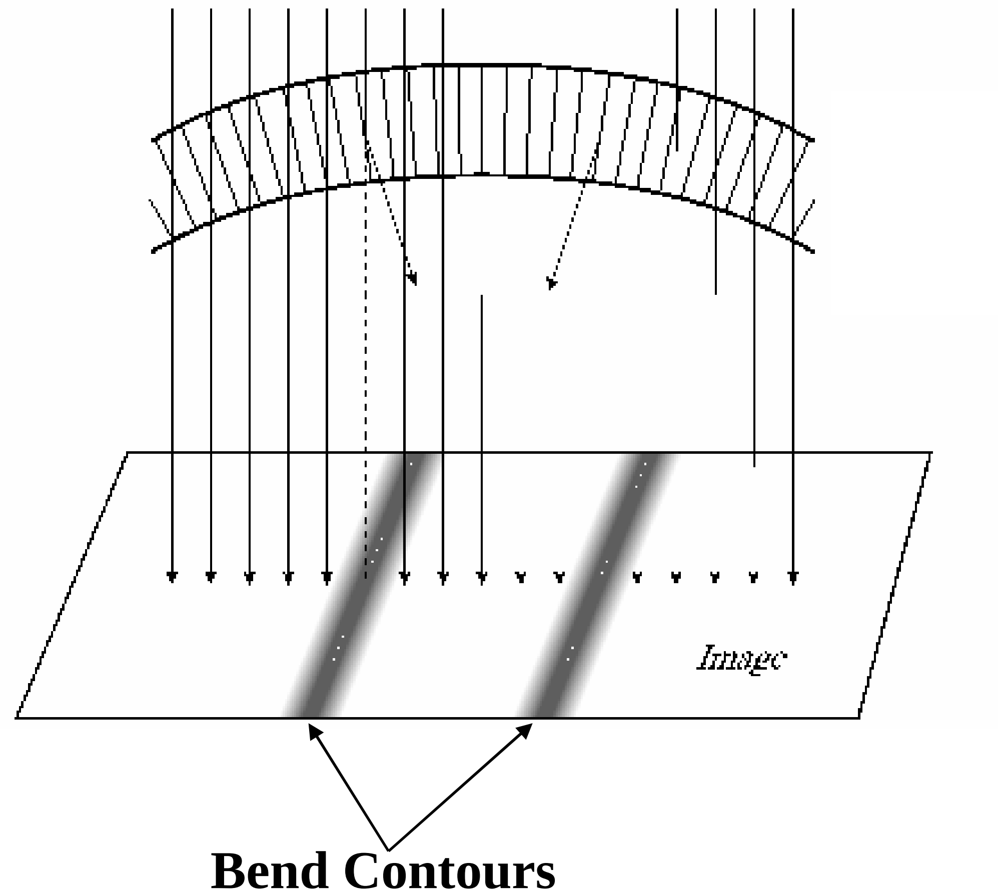
Reason is again related to strong dynamical coupling of the two beams

Can see that as *s* changes, the distance between the spots will change



Bend contours

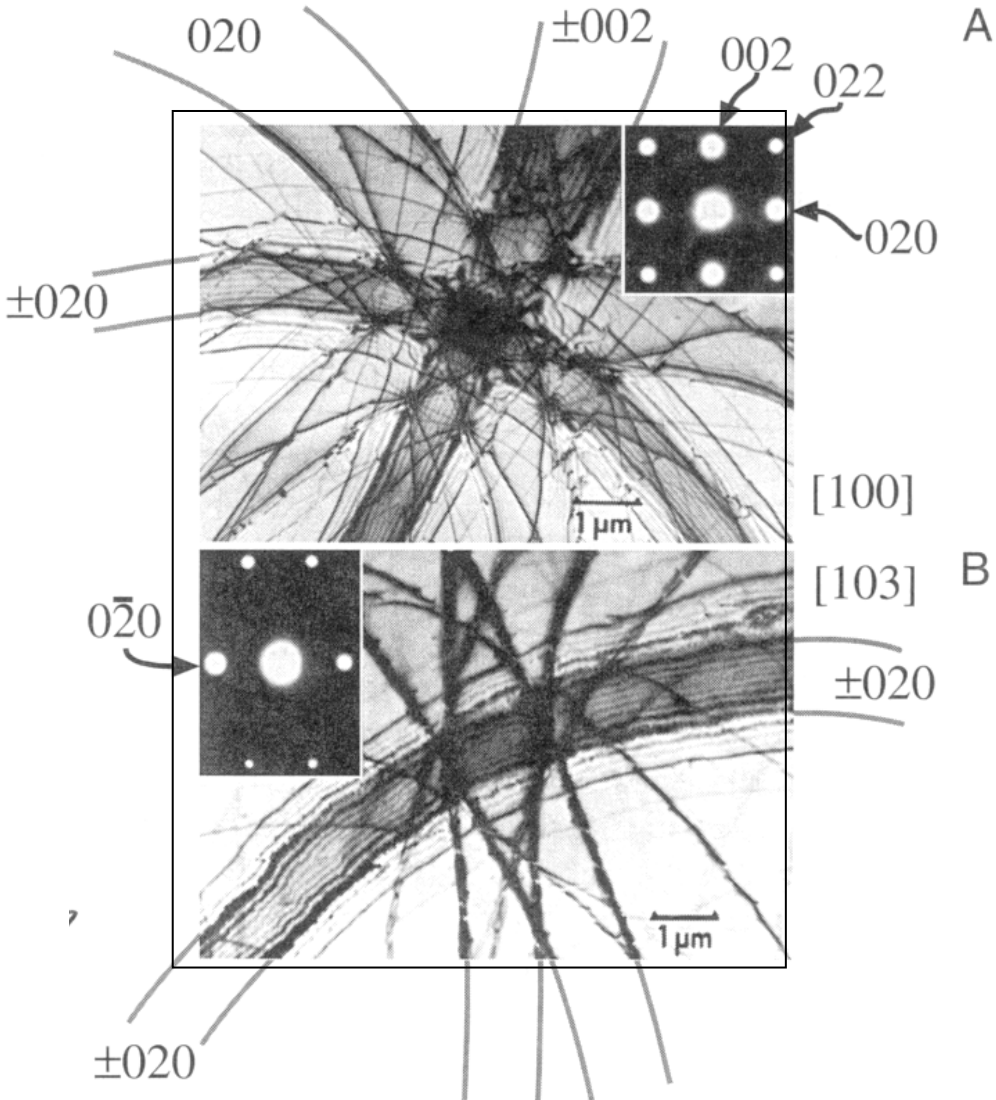




The origin of bend contours shown for a foil symmetrically bent on either side of the Bragg conditions. When the *hkl* planes are in the Bragg condition, the reflection G is excited.

Bend contours

Each diffracted plane produces two bend contours

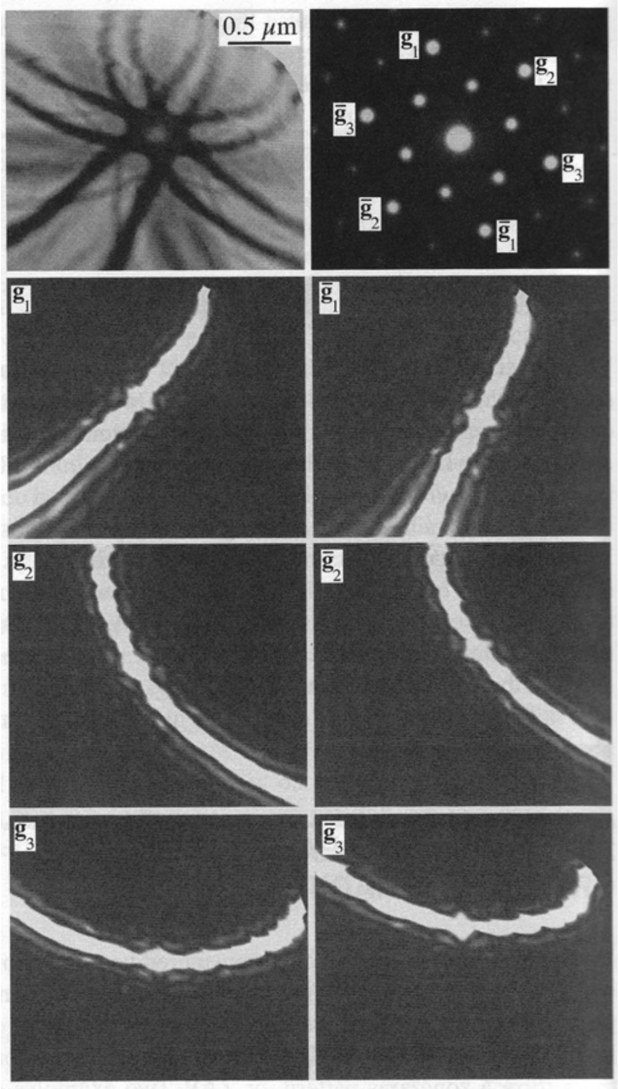


[100] crystal orientation

[103] crystal orientation

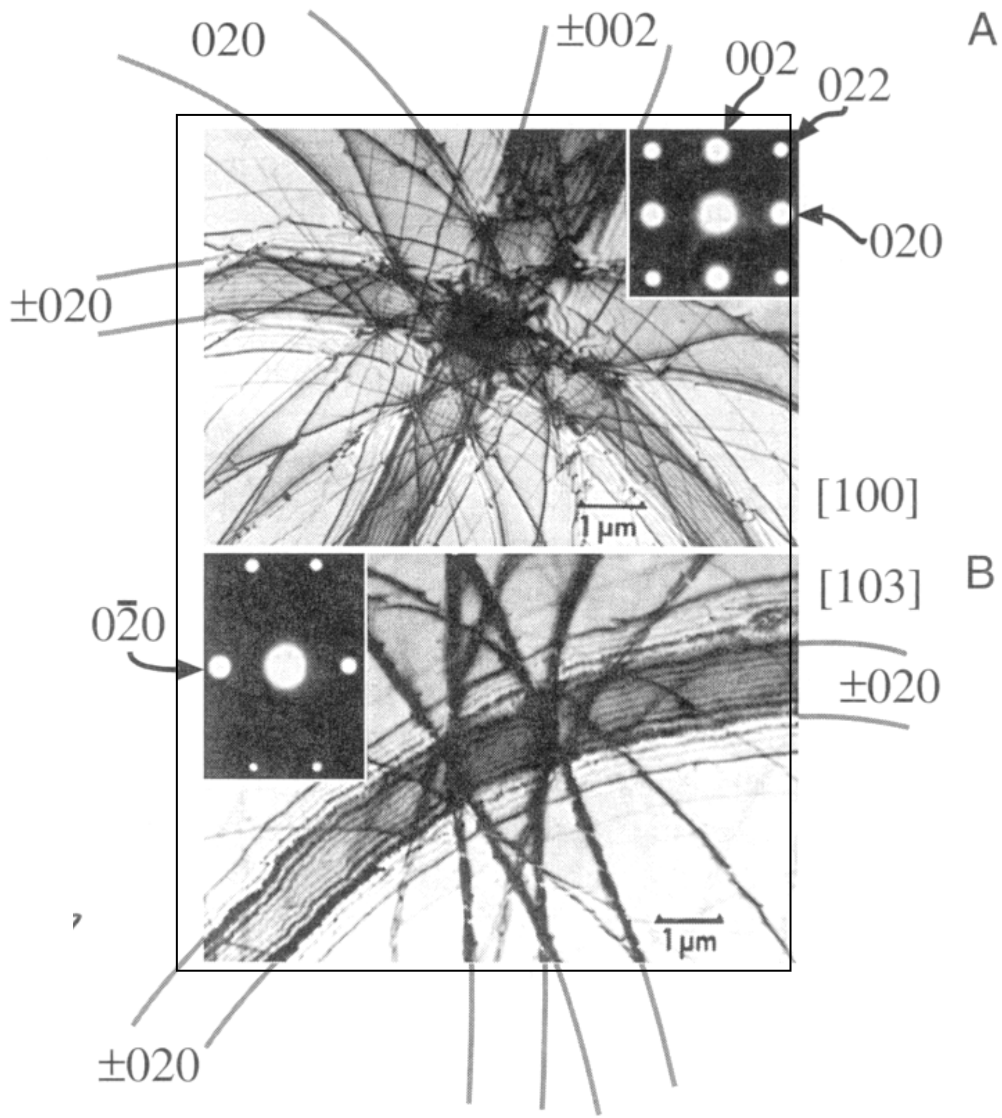
Bend contour

- There is a direct correlation between the bend contour lines in the image and the diffraction pattern
- If you select one of the diffracted spots with the objective aperture, one bend contour line will be visible
  - It will run 'approximately' perpendicular to the diffraction spot



Bend contours

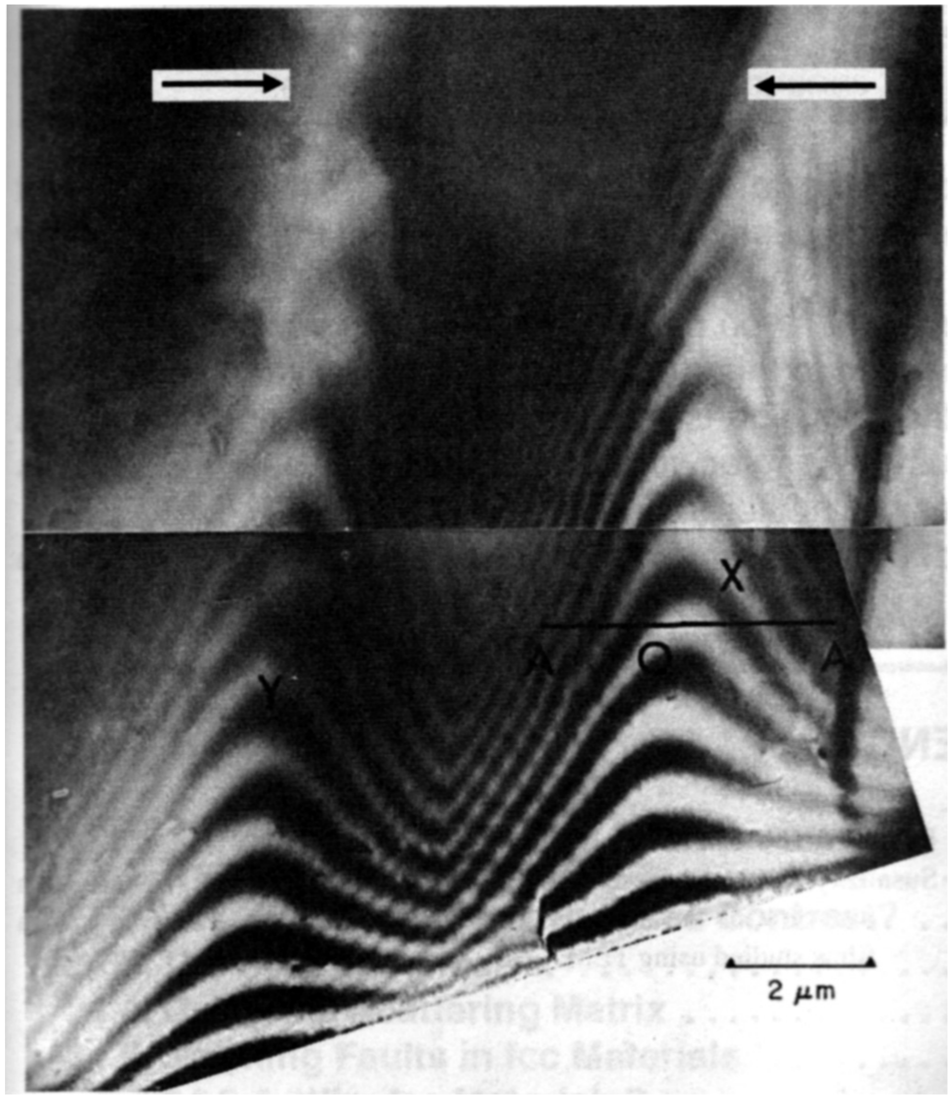
Each diffracted plane produces two bend contours



[100] crystal orientation

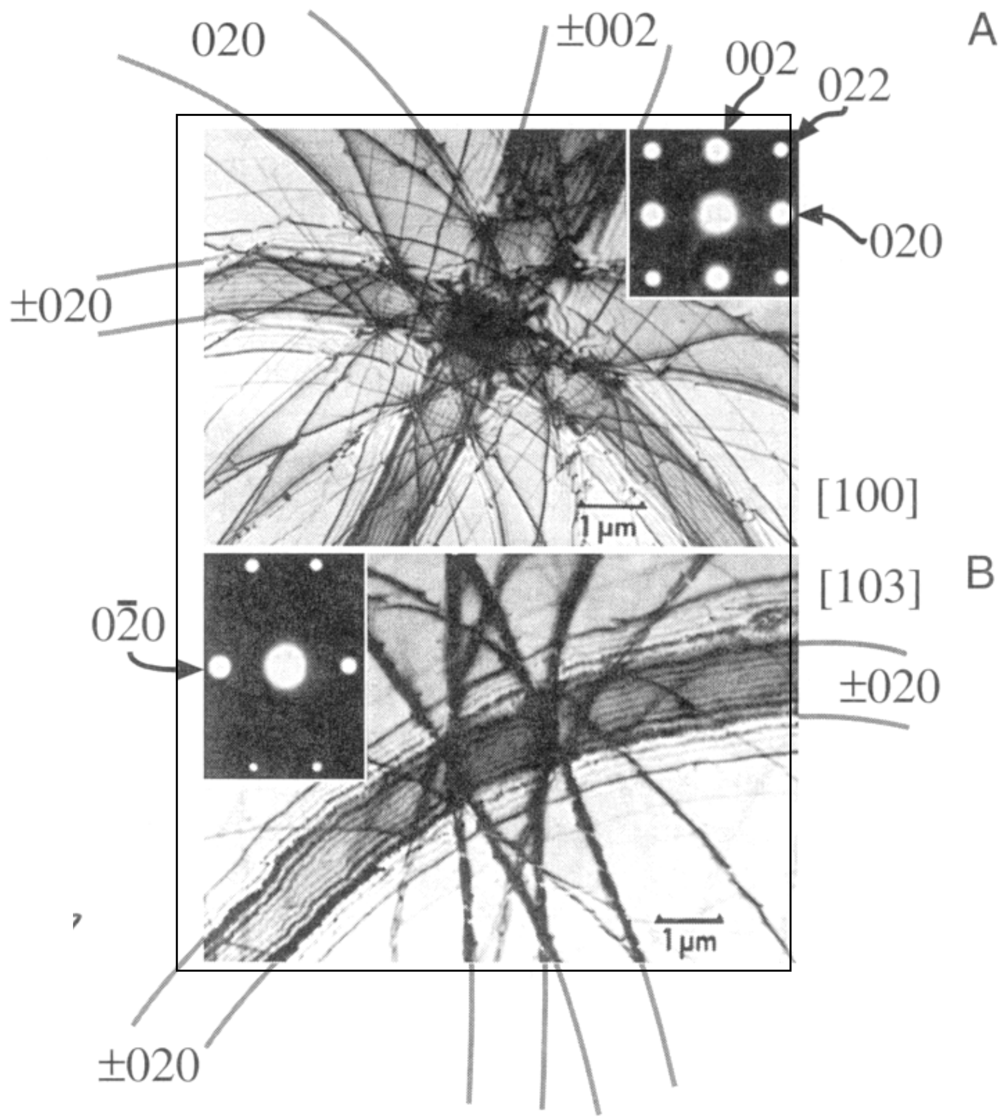
[103] crystal orientation

Thickness fringes & bend contours



Bend contours

Each diffracted plane produces two bend contours



[100] crystal orientation

[103] crystal orientation

Planar faults

Picture to right depicts a general planar interface

Translation boundary

- Any translation is allowed
- No rotation ($\theta = 0$)
- A stacking fault is a special case

Grain boundary

- Same chemistry & structure
- Any value of $R(\vec{r})$, $\vec{n}$ or θ allowed

Phase boundary

- Different chemistry or structure across boundary

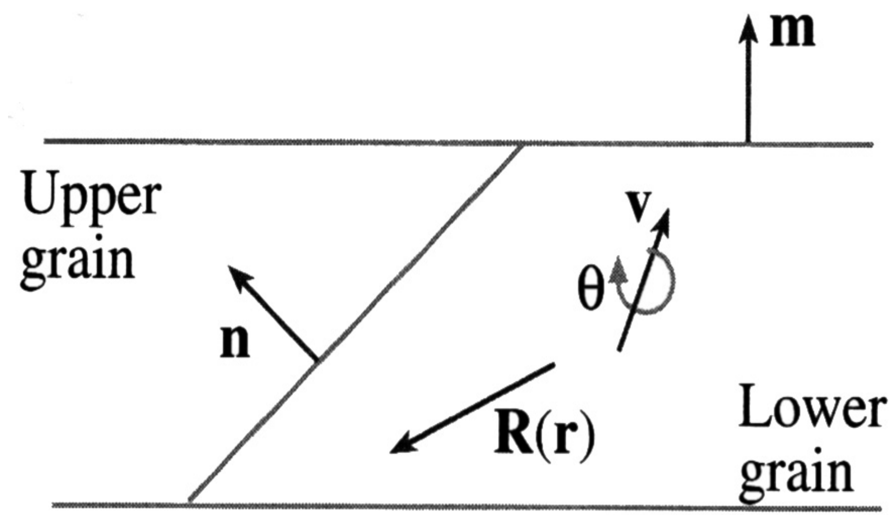
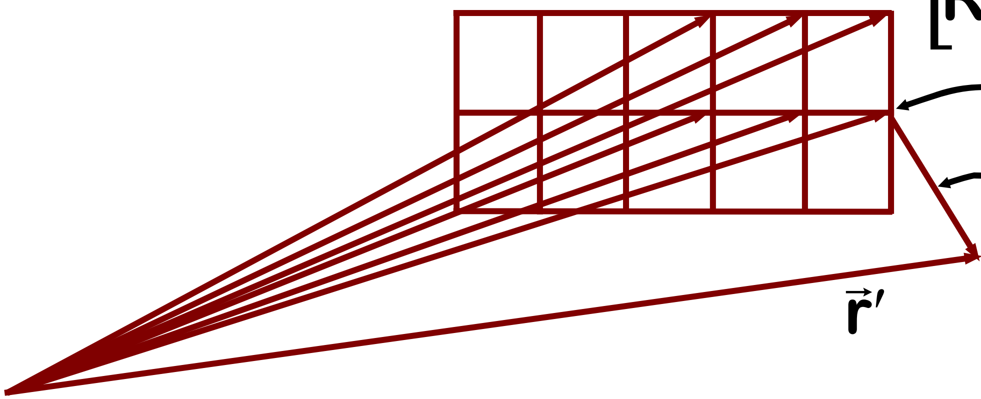


Table 24.1. Examples of Internal Planar Defects

Group	Structure	Example	Example
SF	Diamond-cubic, fcc, zinc blende	Cu, Ag, Si, GaAs	**R** = ⅓ [111] or **R** = ⅙ [11$\bar{2}$]
APB/IDB	Zinc blende, wurtzite	GaAs, AlN	inversion
APB	CsCl	NiAl	**R** = ½ [111]
APB/SF	Spinel	$MgAl_2O_4$	**R** = ¼ [110]
GB	All materials	Often denoted by Σ where Σ^{-1} is the fraction of coincident lattice sites	rotation plus **R**
PB	Any two different materials	Sometimes denoted by Σ_1,Σ_2, which are not equal	rotation plus **R** plus misfit

Scattering from a lattice



So scattered wave from an array of N atoms:

$$\Psi_{scatt}(\vec{K}) = \sum_{j}^{N} f_{el}(\vec{R}_j)\exp\left[-2\pi i(\vec{K}\cdot\vec{R}_j)\right]$$

Remember our earlier description of a crystal:

Crystal = lattice + basis + defect displacements

$$\vec{R}_j = \vec{r}_{lattice} + \vec{r}_{basis} + \vec{r}_{defects} = \vec{r}_l + \vec{r}_b + \vec{r}_d$$

What is the effect of displacements on images?

If you have a strained or displaced unit cell, it can be described by:

$$\mathbf{r}_n' = \mathbf{r}_n + \mathbf{R}_n$$

Location of defective unit cell → $\mathbf{r}_n'$

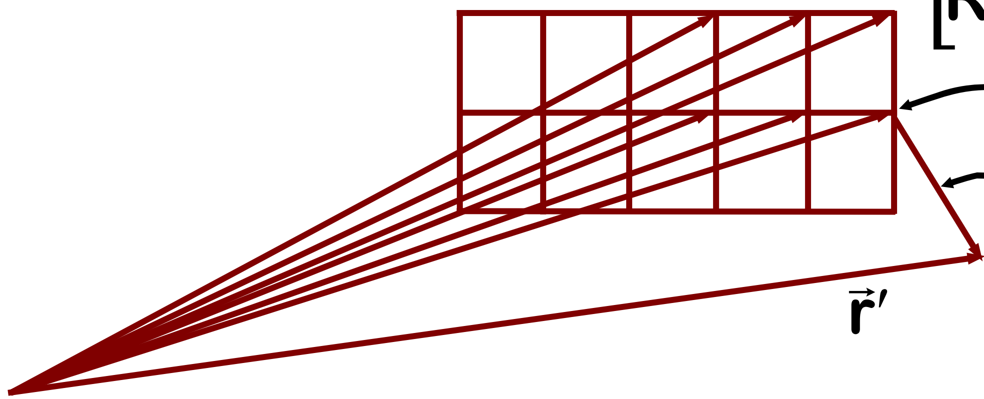
Regular lattice positions → $\mathbf{r}_n$

Displacement function → $\mathbf{R}_n$

Must substitute this into the phase term of our scattered wave

$$\Psi_{scatt}\left(\vec{K}\right) = \sum_{j}^{N} f_{el}\left(\vec{R}_j\right) \exp\left[-2\pi i\left(\vec{K}\cdot\vec{R}_j\right)\right]$$

Scattering from a lattice



So scattered wave from an array of N atoms:

$$\Psi_{scatt}\left(\vec{K}\right) = \sum_{j}^{N} f_{el}\left(\vec{R}_j\right) \exp\left[-2\pi i\left(\vec{K}\cdot\vec{R}_j\right)\right]$$

Remember our earlier description of a crystal:

Crystal = lattice + basis + defect displacements

$$\vec{R}_j = \vec{r}_{lattice} + \vec{r}_{basis} + \vec{r}_{defects} = \vec{r}_l + \vec{r}_b + \vec{r}_d$$

What is the effect of displacements on images?

Substituting

$$\vec{K}\cdot\vec{r} = (\vec{g}+\vec{s})\cdot(\vec{r}_n+\vec{R}_n)$$
$$= \vec{g}\cdot\vec{r}_n + \vec{g}\cdot\vec{R}_n + \vec{s}\cdot\vec{r}_n + \vec{s}\cdot\vec{R}_n$$

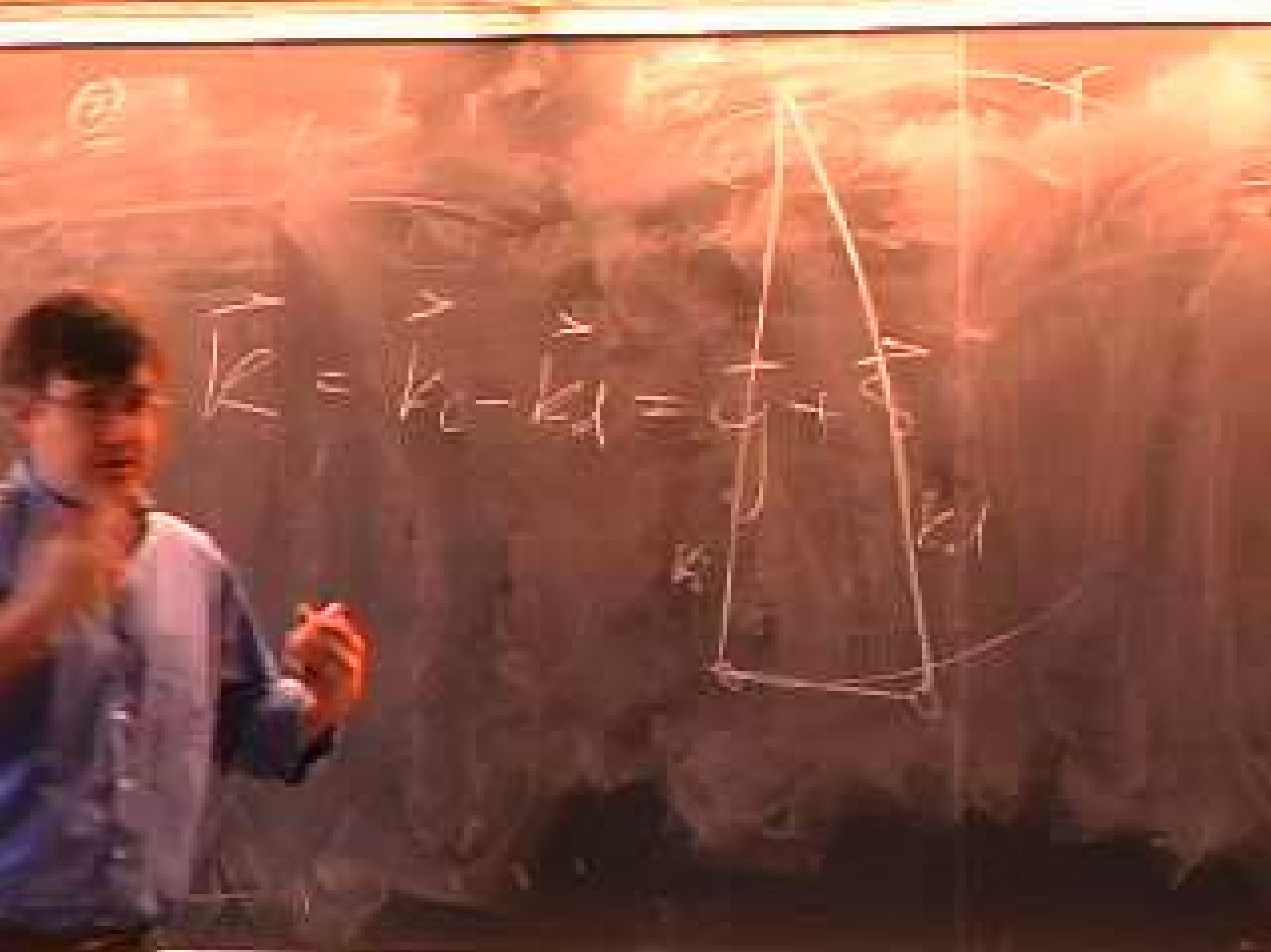
If s is small, this term is small …

integer

= sz

by high energy approximation

This is then the 'new' & important term


$\vec{k} = \vec{k}_i - \vec{k}_f$
k_i
k_f

What is the effect of displacements on images?

Substitute into Howie-Whelan Equations:

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

and

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

So, defect displacements (R) introduce a change in the phase term of the 0 and g beams (call this change α)

$$\alpha = 2\pi\vec{g}\cdot\vec{R}$$

Example: Stacking fault in FCC

Obviously, specifics of geometry are important

- i.e., vectorially, what is $\vec{g}$ & $\vec{R}$

In this example:

$$\vec{R} = \frac{1}{3}\left[11\bar{1}\right]$$

If $g = 2\bar{2}0$ then: $\vec{g}\cdot\vec{R} = 0$

- The SF is not visible

If $g = 02\bar{2}$ then:

$$\vec{g}\cdot\vec{R} = \pm\frac{4}{3} \quad \Rightarrow \quad \alpha = \pm\frac{8\pi}{3} = \pm\frac{2\pi}{3} = \pm 120^{\circ}$$

After passing through the SF, the electron wave undergoes a phase shift

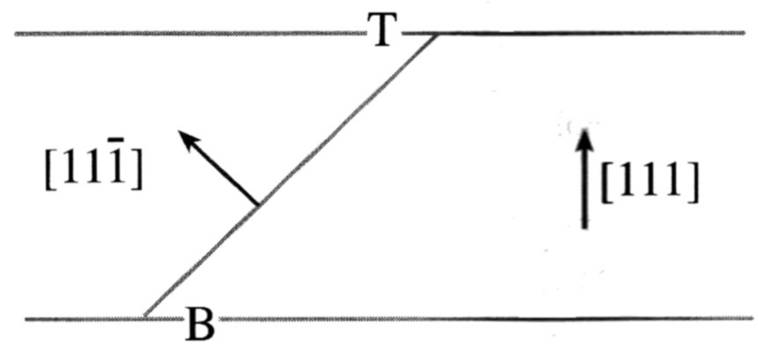
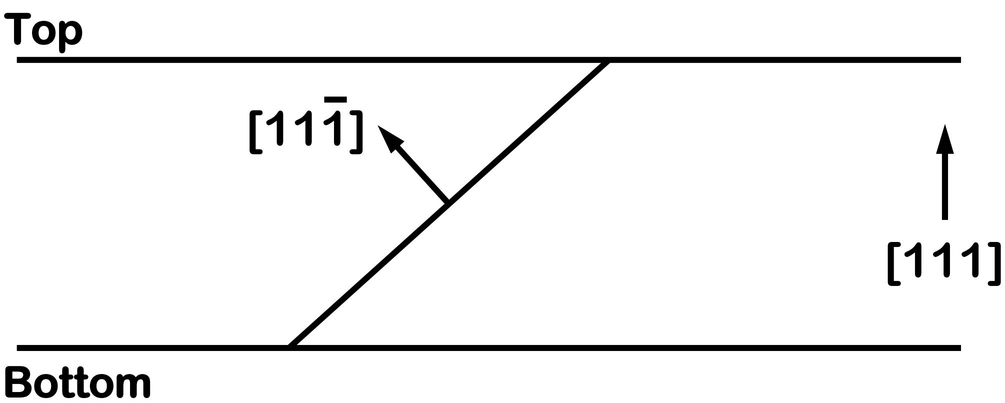
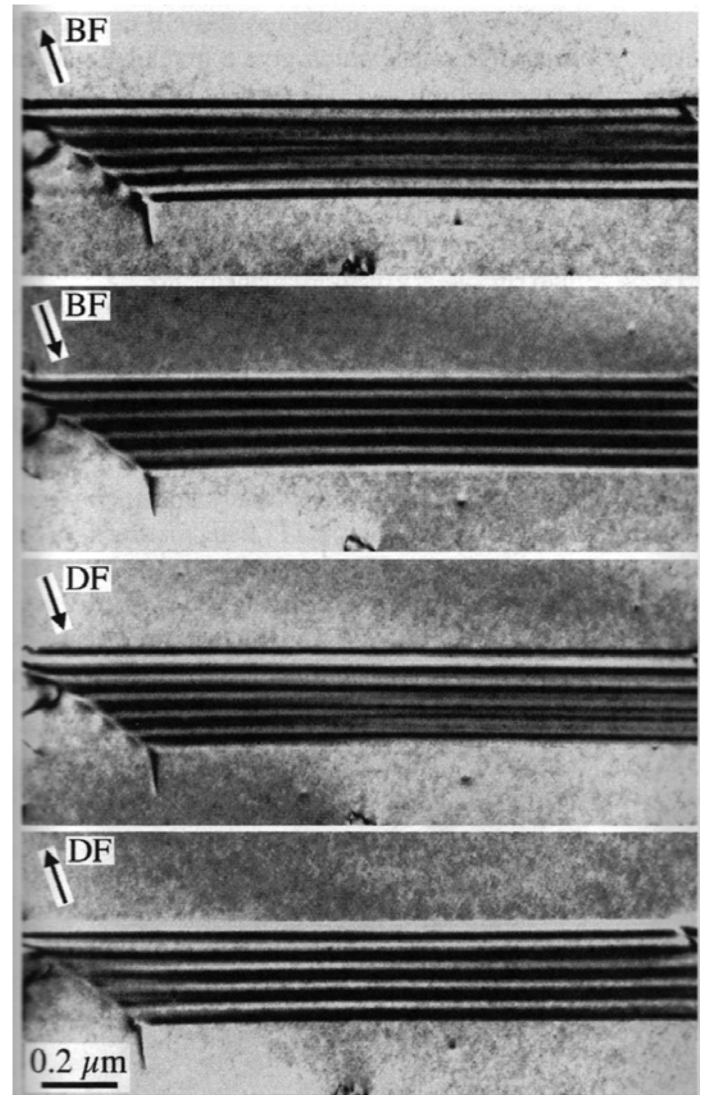


Figure 24.3. A stacking fault in a parallel-sided fcc specimen. The normal to the specimen is [111] and the normal to the SF is [11$\bar{1}$]. T and B indicate the top and bottom of the foil.

Example: Stacking fault in FCC





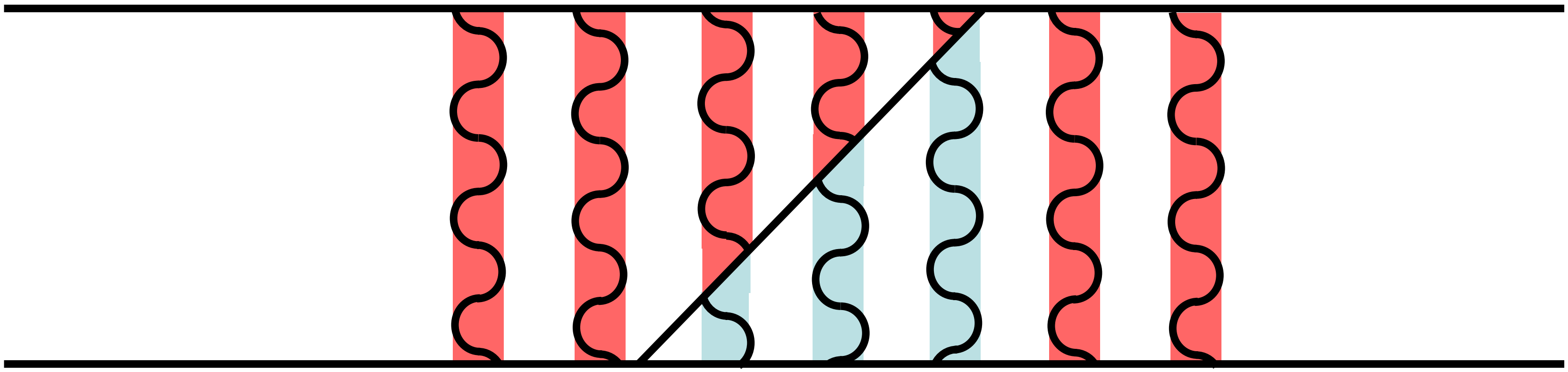
Fringe origin is difference in thickness over which this phase change occurs

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

and

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

Example: Stacking fault in FCC



Here's a visual representation of this phase shift using the 'column approximation' and considering just one of the two beams

Both the $\vec{0}$ and the $\vec{g}$ beams will undergo phase shifts of this type (of equal magnitude: $\alpha = 2\pi \vec{g} \cdot \vec{R}$)

The fringes are a result of the difference in phase in this region of the electron wave at the exit of the sample

Example: Stacking fault in FCC

Have to look pretty carefully at images & calculations to get R(r) direction …

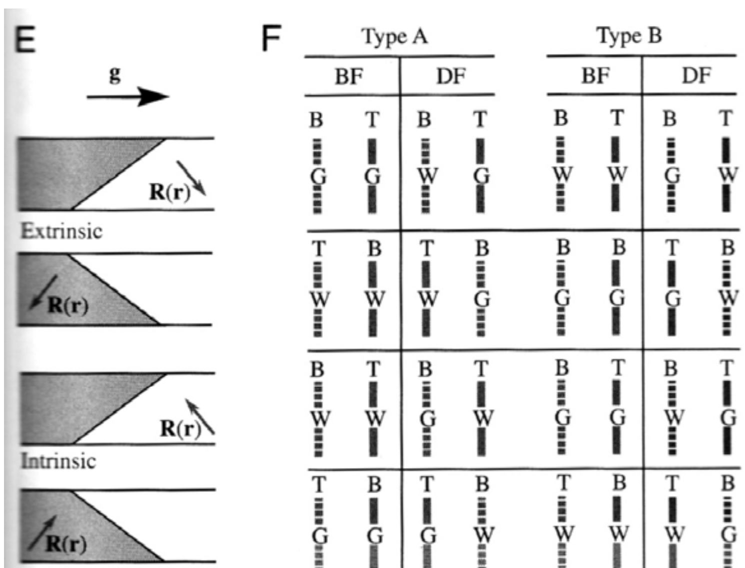
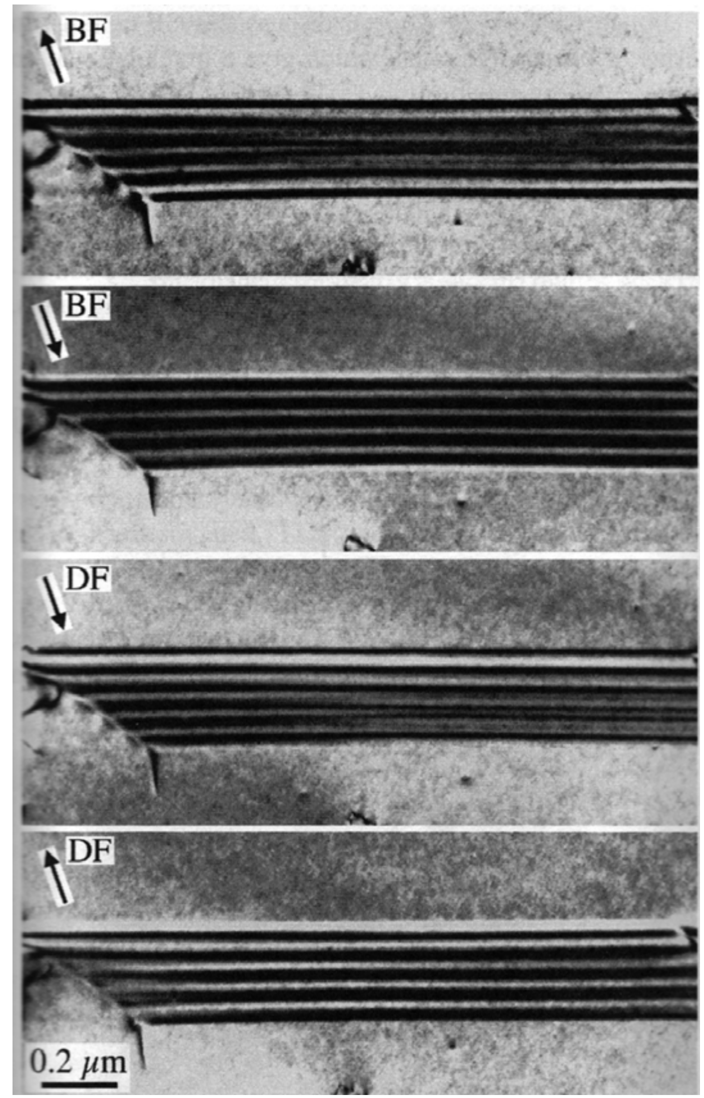
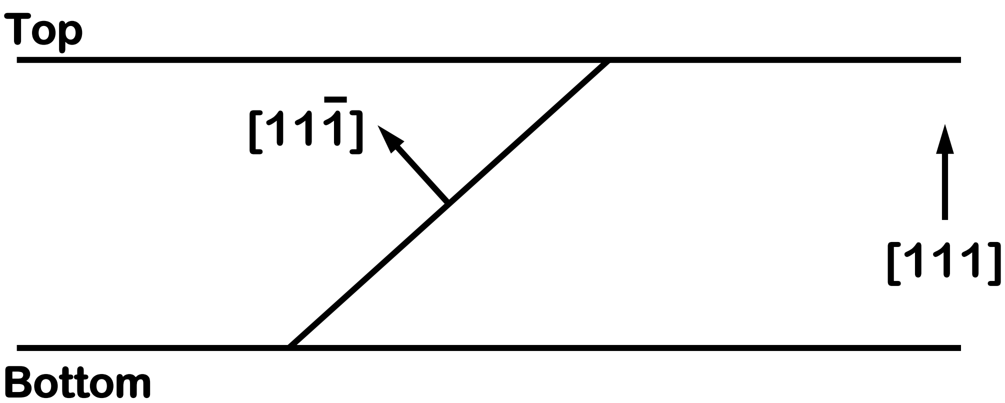
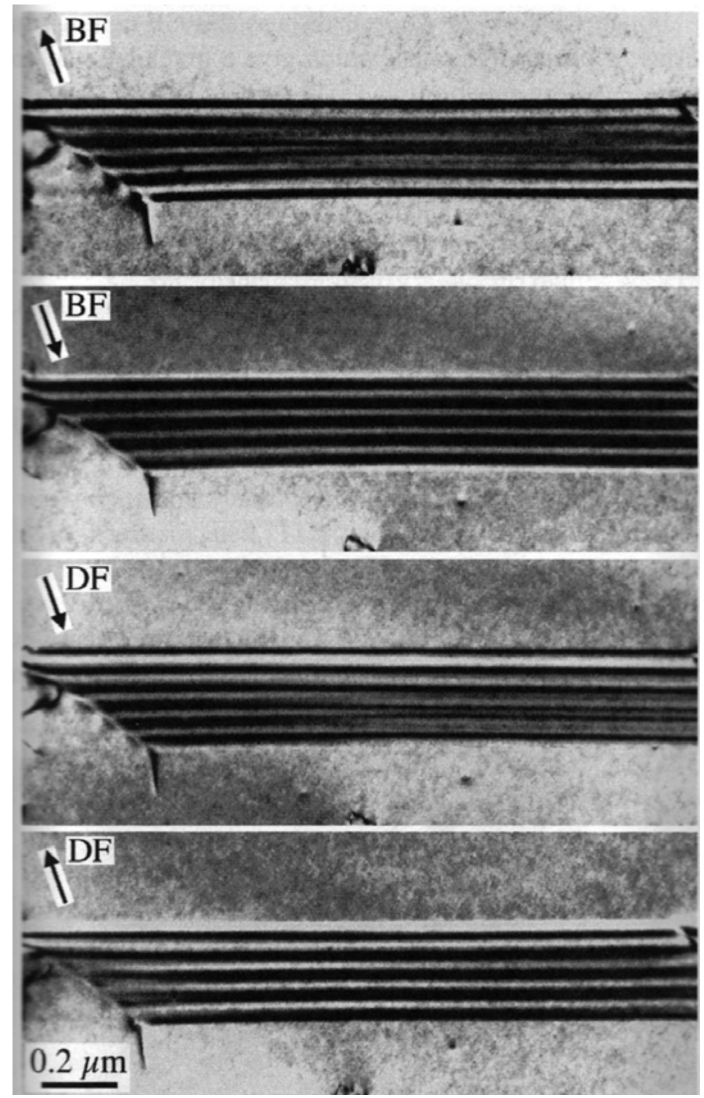


Figure 24.4. (A–D) Four strong-beam images of an SF recorded using ±**g** BF and ±**g** DF. The beam was nearly normal to the surfaces; the SF fringe intensity is similar at the top surface but complementary at the bottom surface. The rules are summarized in (E) and (F) where G and W indicate that the first fringe is gray or white, and (T,B) indicates top/bottom.



Example: Stacking fault in FCC





Fringe origin is difference in thickness over which this phase change occurs

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

and

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

Example: Stacking fault in FCC

Obviously, specifics of geometry are important

- i.e., vectorially, what is $\vec{g}$ & $\vec{R}$

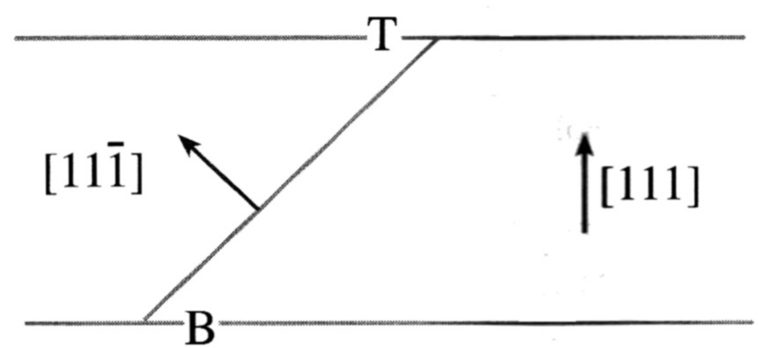


Figure 24.3. A stacking fault in a parallel-sided fcc specimen. The normal to the specimen is [111] and the normal to the SF is [11$\bar{1}$]. T and B indicate the top and bottom of the foil.

In this example:

$$\vec{R} = \frac{1}{3}\left[11\bar{1}\right]$$

If $g = 2\bar{2}0$ then: $\vec{g} \cdot \vec{R} = 0$

- The SF is not visible

If $g = 02\bar{2}$ then:

$$\vec{g} \cdot \vec{R} = \pm\frac{4}{3} \Rightarrow \alpha = \pm\frac{8\pi}{3} = \pm\frac{2\pi}{3} = \pm 120^{o}$$

After passing through the SF, the electron wave undergoes a phase shift

Example: Stacking fault in FCC

Have to look pretty carefully at images & calculations to get R(r) direction …

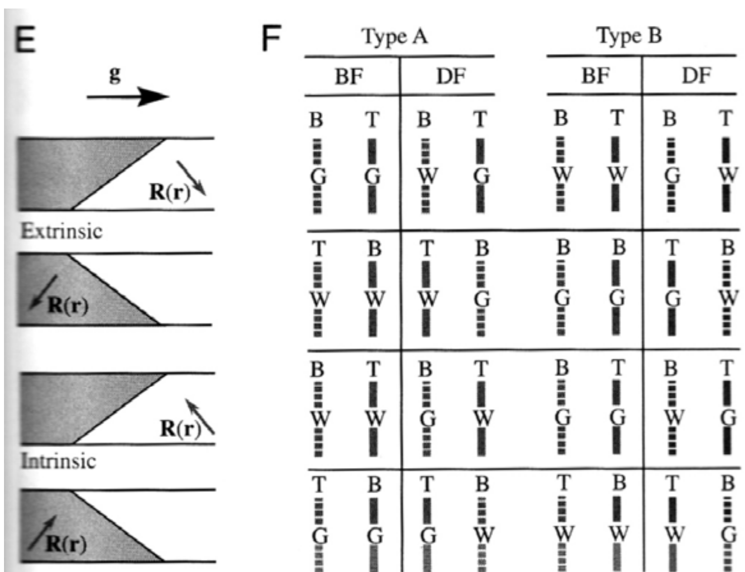
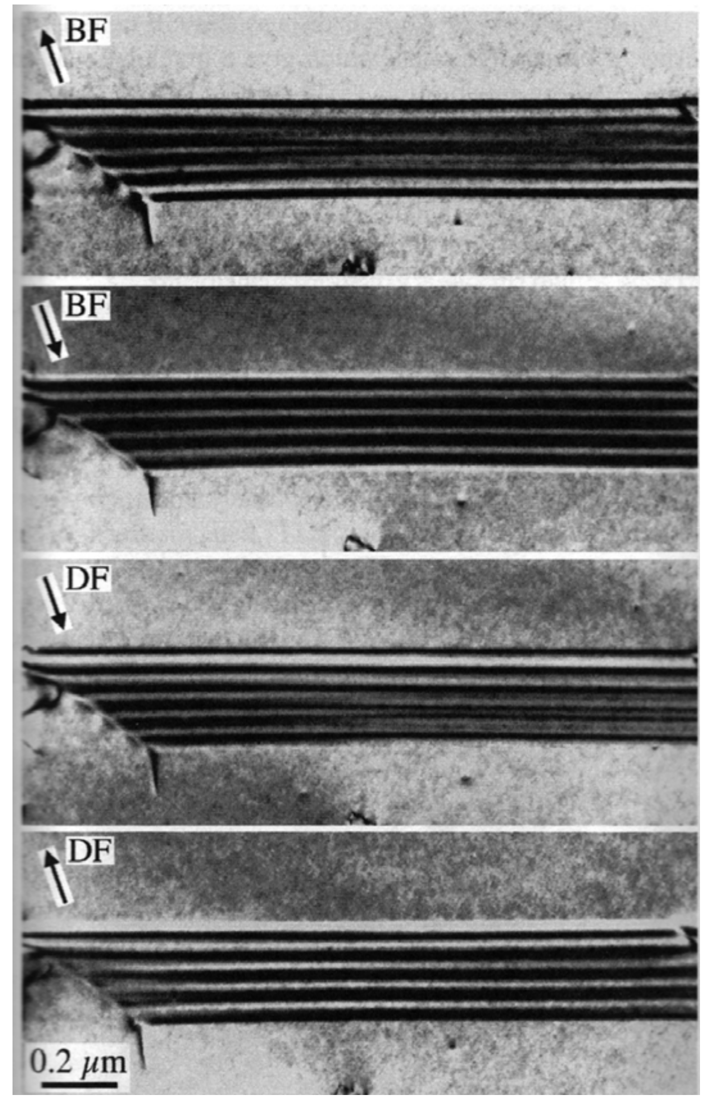


Figure 24.4. (A–D) Four strong-beam images of an SF recorded using ±**g** BF and ±**g** DF. The beam was nearly normal to the surfaces; the SF fringe intensity is similar at the top surface but complementary at the bottom surface. The rules are summarized in (E) and (F) where G and W indicate that the first fringe is gray or white, and (T,B) indicates top/bottom.



What is the effect of displacements on images?

Substitute into Howie-Whelan Equations:

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

and

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

So, defect displacements (R) introduce a change in the phase term of the 0 and g beams (call this change α)

$$\alpha = 2\pi\vec{g}\cdot\vec{R}$$

Example: Stacking fault in FCC

Obviously, specifics of geometry are important

- i.e., vectorially, what is $\vec{g}$ & $\vec{R}$

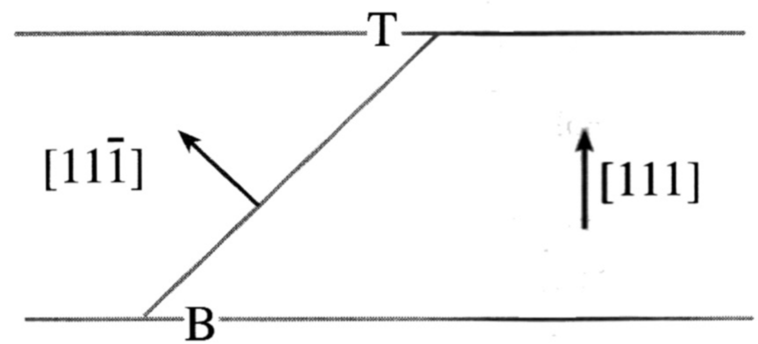


Figure 24.3. A stacking fault in a parallel-sided fcc specimen. The normal to the specimen is [111] and the normal to the SF is [11$\bar{1}$]. T and B indicate the top and bottom of the foil.

In this example:

$$\vec{R} = \frac{1}{3}\left[11\bar{1}\right]$$

If $g = 2\bar{2}0$ then: $\vec{g}\cdot\vec{R} = 0$

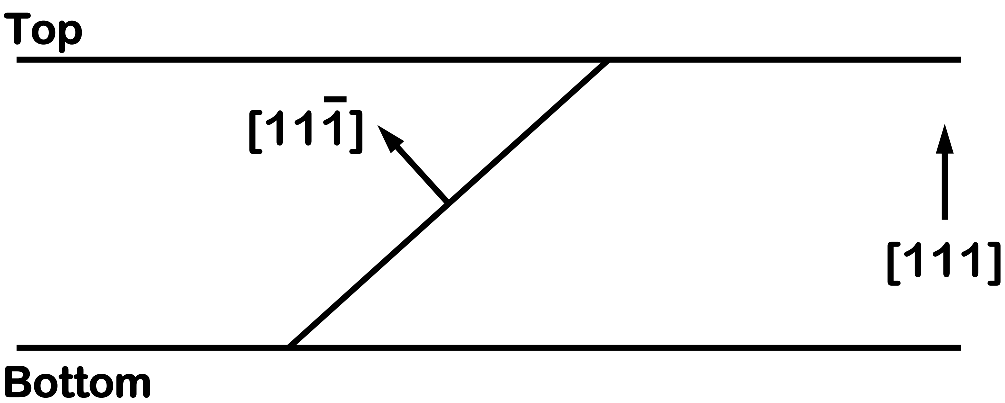
- The SF is not visible

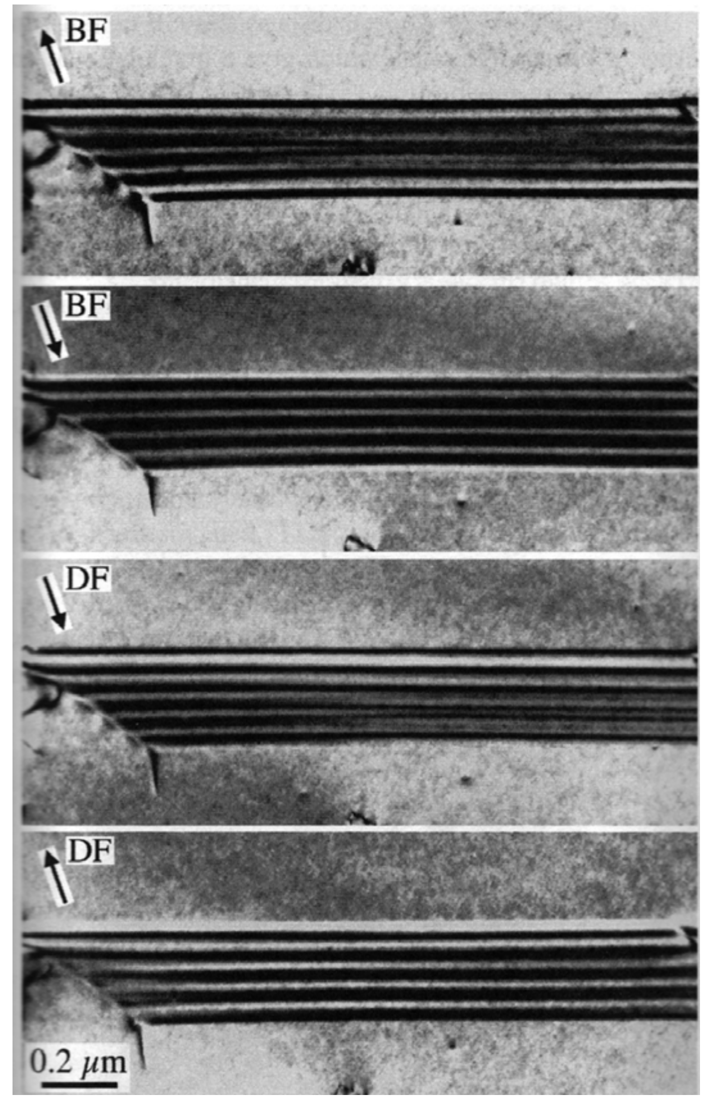
If $g = 02\bar{2}$ then:

$$\vec{g}\cdot\vec{R} = \pm\frac{4}{3} \Rightarrow \alpha = \pm\frac{8\pi}{3} = \pm\frac{2\pi}{3} = \pm 120^{o}$$

After passing through the SF, the electron wave undergoes a phase shift

Example: Stacking fault in FCC





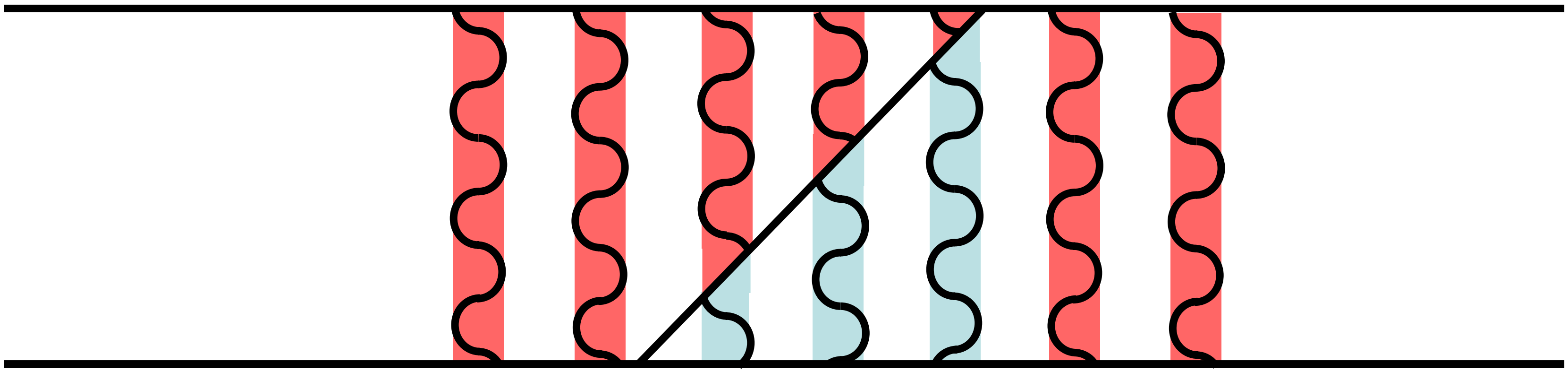
Fringe origin is difference in thickness over which this phase change occurs

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

and

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

Example: Stacking fault in FCC



Here's a visual representation of this phase shift using the 'column approximation' and considering just one of the two beams

Both the $\vec{0}$ and the $\vec{g}$ beams will undergo phase shifts of this type (of equal magnitude: $\alpha = 2\pi\vec{g}\cdot\vec{R}$)

The fringes are a result of the difference in phase in this region of the electron wave at the exit of the sample

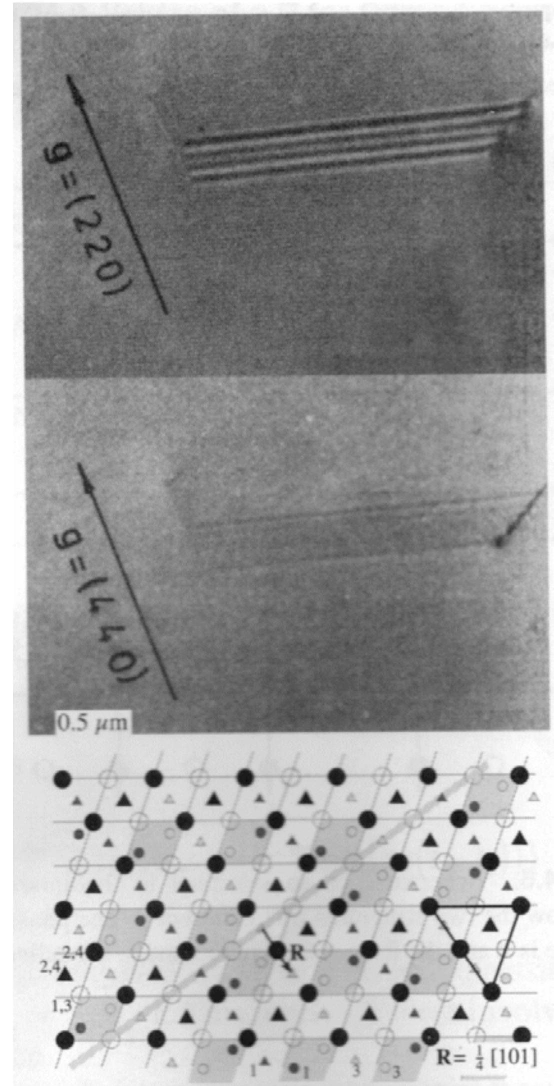
Anti-phase boundaries

In some conditions:

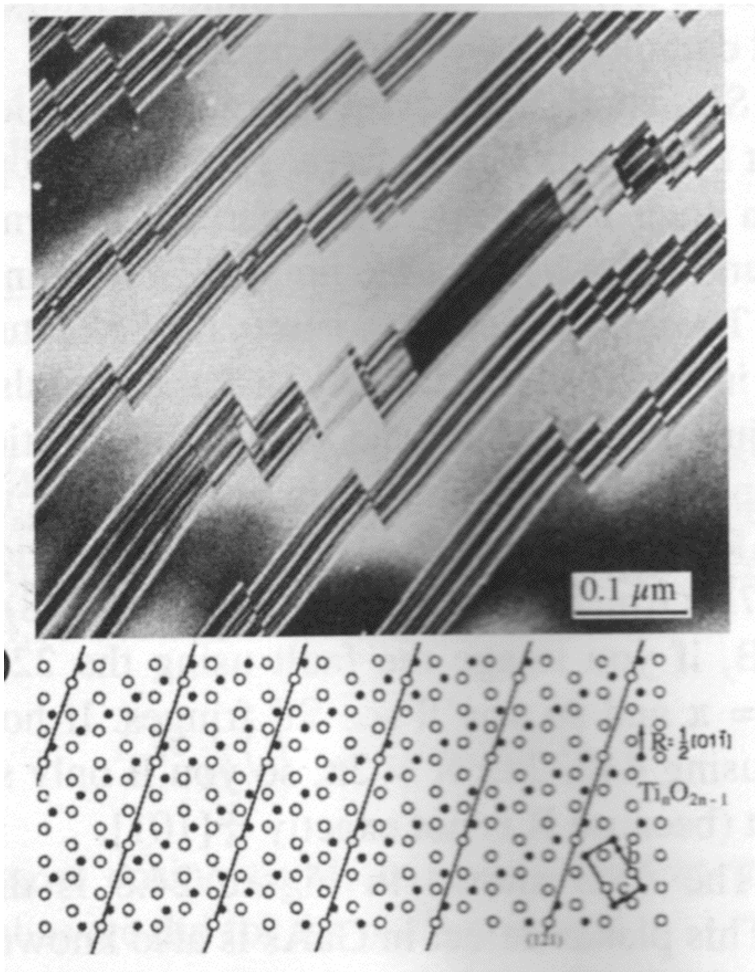
$$\vec{g}\cdot\vec{R} = \pm\frac{4}{3} \Rightarrow \alpha = \pi$$

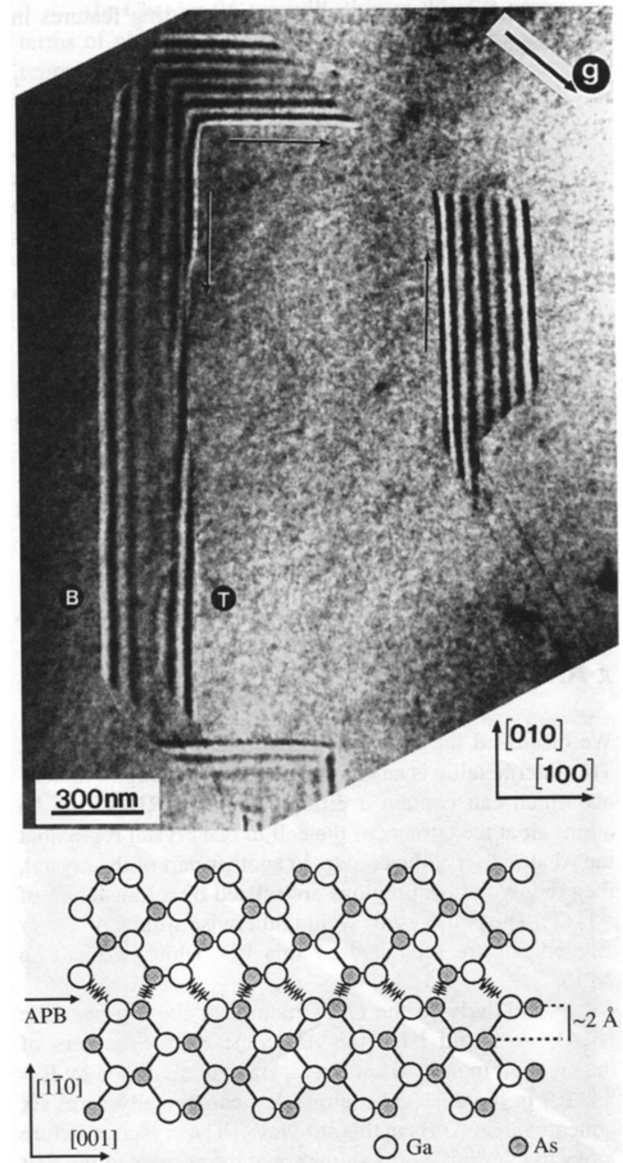
– "π fringes"

Other cases are more general examples of 'anti-phase boundaries"

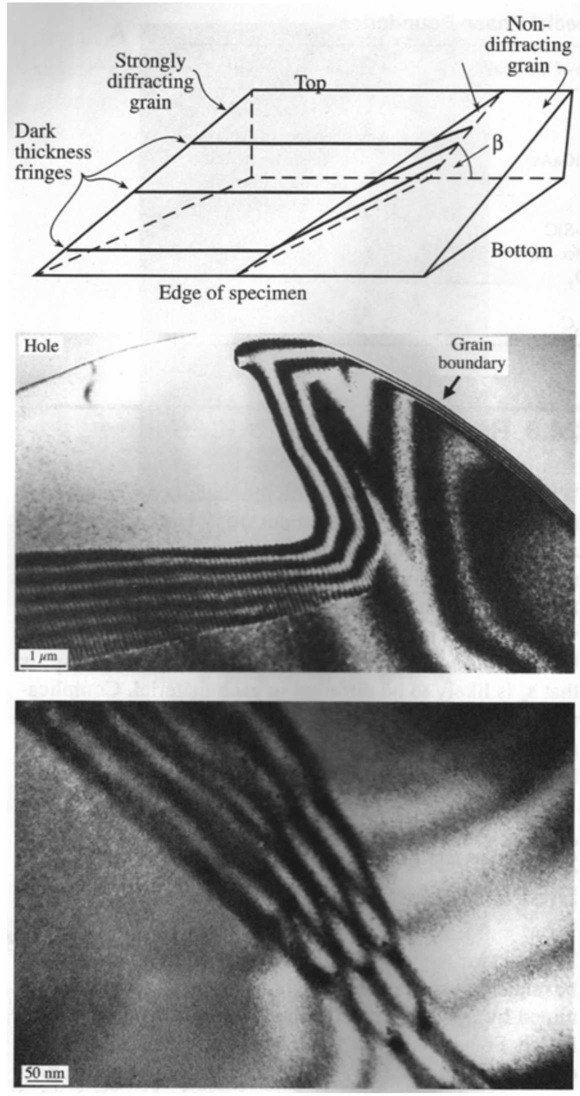


Anti-phase boundaries





Rotations

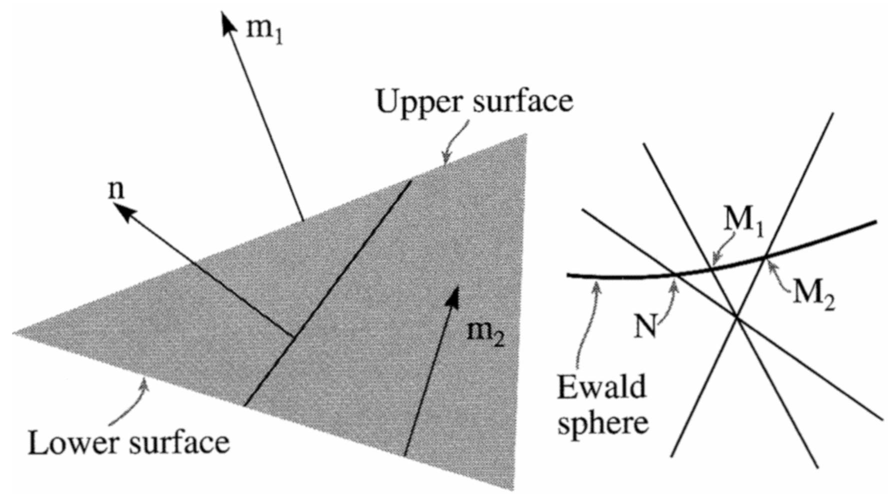


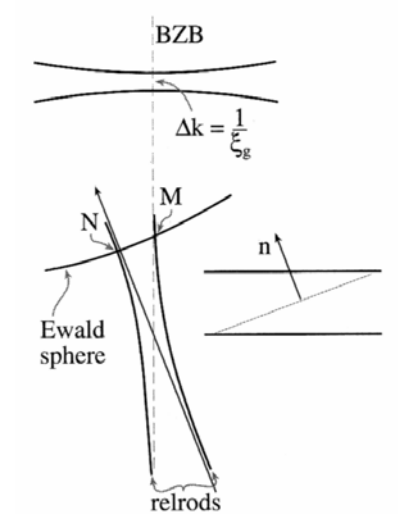
Strongly diffracting grain
Non-diffracting grain
Top
Dark thickness fringes
β
Bottom
Edge of specimen
Hole
Grain boundary
1 μm
50 nm

Effects in diffraction patterns

Same effects observed in diffraction pattern as we discussed in thickness fringes

Fundamentally* these are a result of the same strong coupling that gives rise to image fringes



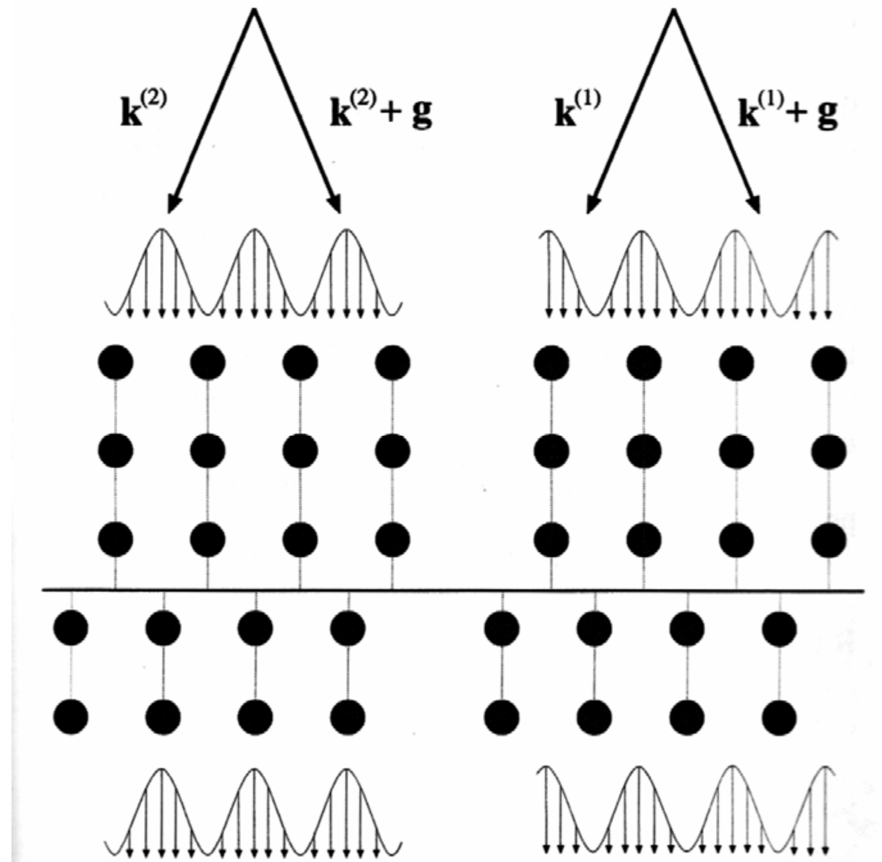


* i.e. can be shown from Bloch wave theory

Bloch waves

Remember, the real reason for everything we see has to do with Bloch waves

Planar defects cause phase shifts in the Bloch waves too



$$b^{(j)}(\vec{r}) = \sum_{g} C_{g}^{(j)} \exp\left[2\pi i \left(\vec{k}^{(j)} + \vec{g}\right) \cdot \left(\vec{r} \cdot \vec{R}\right)\right]$$