# chapter 4

## Kinematic and Dynamic Theory

(Chapter 11, 13,18)

For interpretation of intensities in diffraction pattern, single scattering would be ideal
- i.e. "*kinematical*" scattering

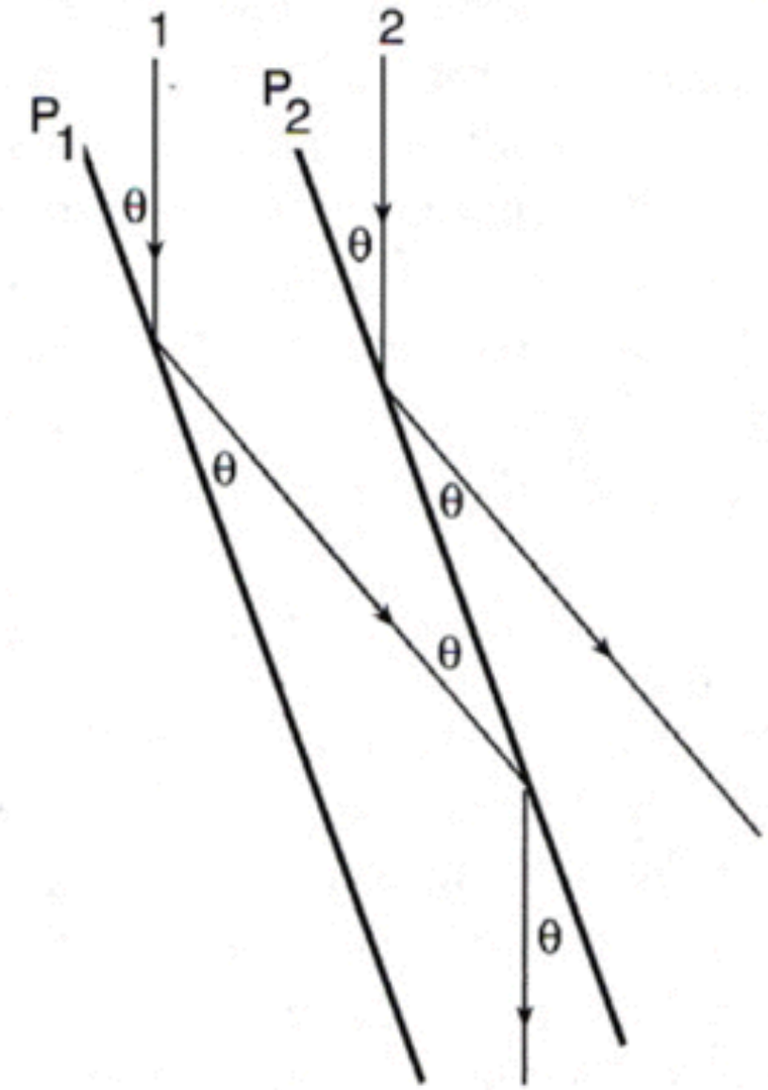
However, in electron diffraction there is often multiple elastic scattering:
i.e. "*dynamical*" behaviour

(Chapter 11, 13,18, 24)

This dynamical scattering has a high probability because a Bragg-scattered beam is at the perfect angle to be Bragg-scattered again (and again...)

As a result, scattering of different beams is not independent from each other

(Chapter 26)



- 運動學理論在以下兩個條件下可被接受
- 為第一近似

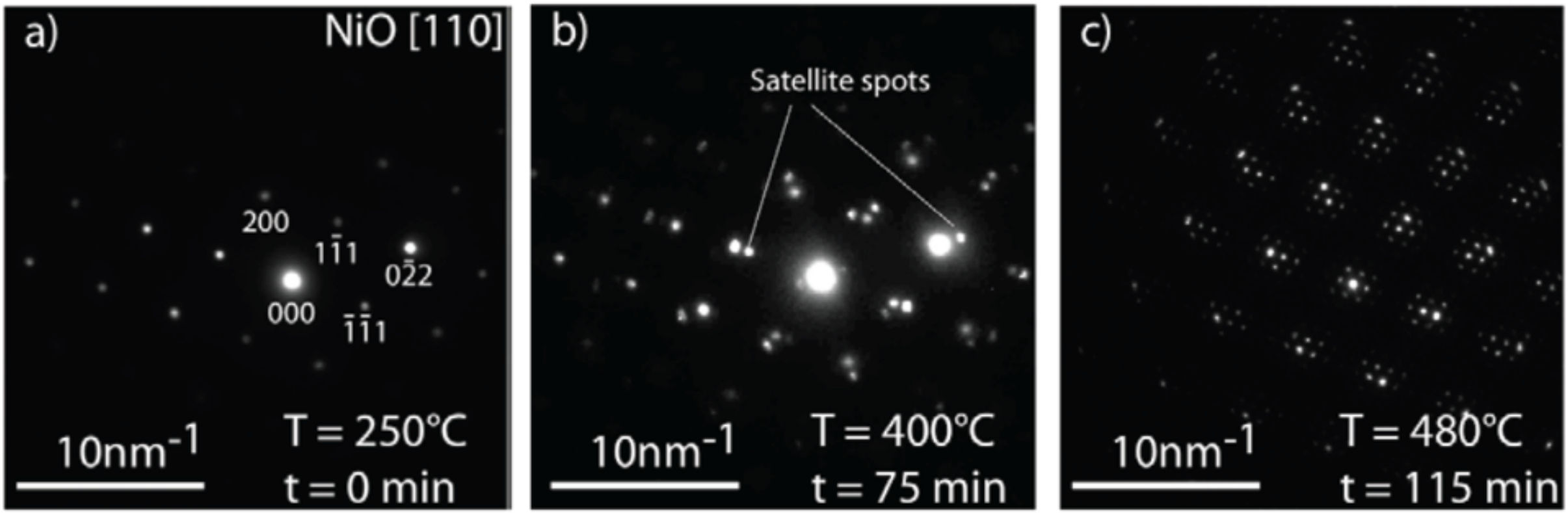
- （1）當樣品很薄時：沒有足夠的“繞射中心”去建
- 立足夠強的繞射光
- （2）當晶體遠離真正的繞射中心時：弱光

# Double diffraction (Chapter 18)

Special type of multiple elastic scattering: diffracted beam travelling through a crystal is rediffracted

Example 1: rediffraction in different crystal - NiO being reduced to Ni in-situ in TEM

Epitaxial relationship between the two FCC structures (NiO: $a$ = 0.42 nm Ni: $a$ = 0.37 nm)




Formation of satellite spots around Bragg reflections

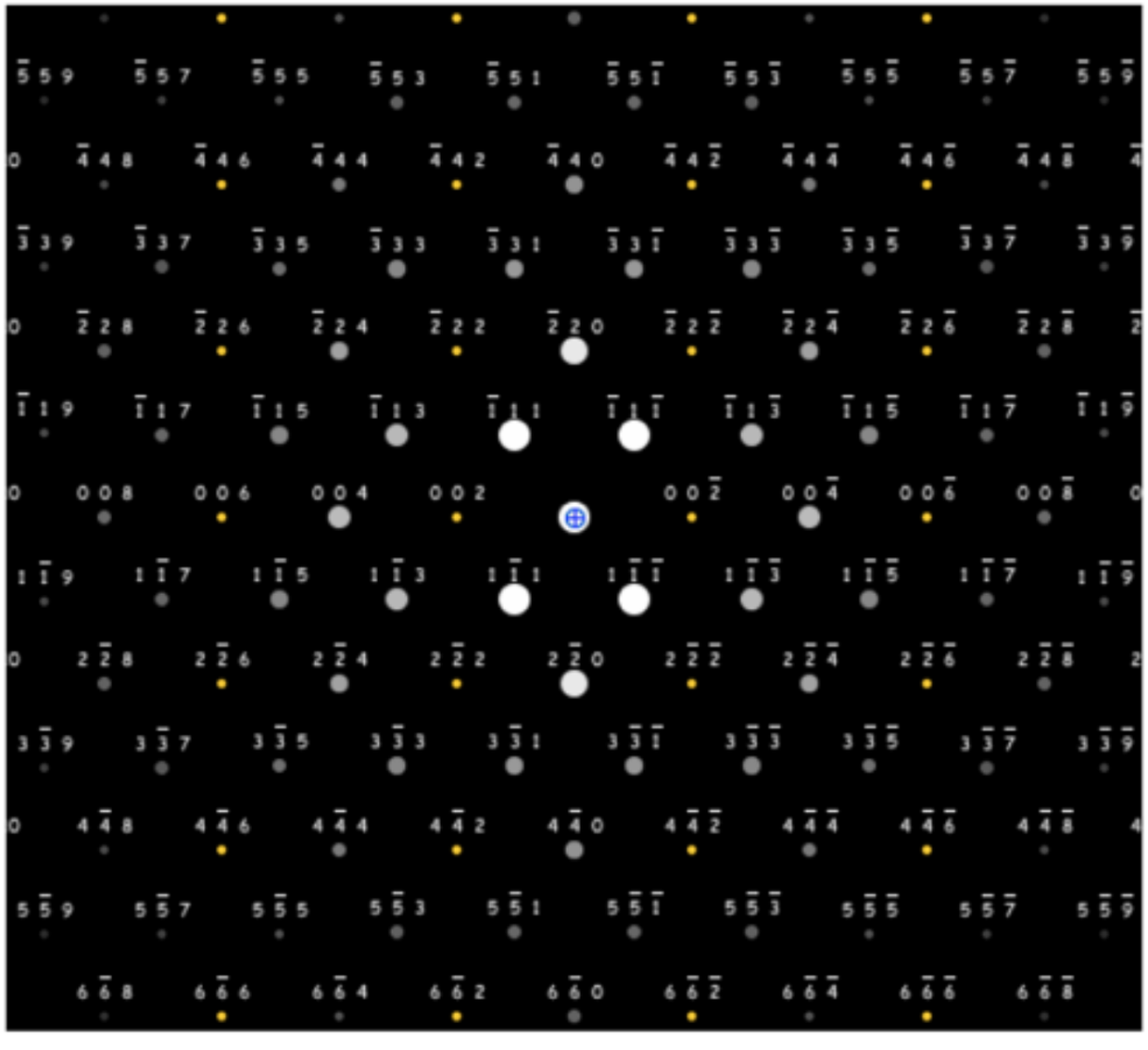
# Double diffraction (Chapter 18)

Example 11: rediffraction in the same crystal; appearance of forbidden reflections

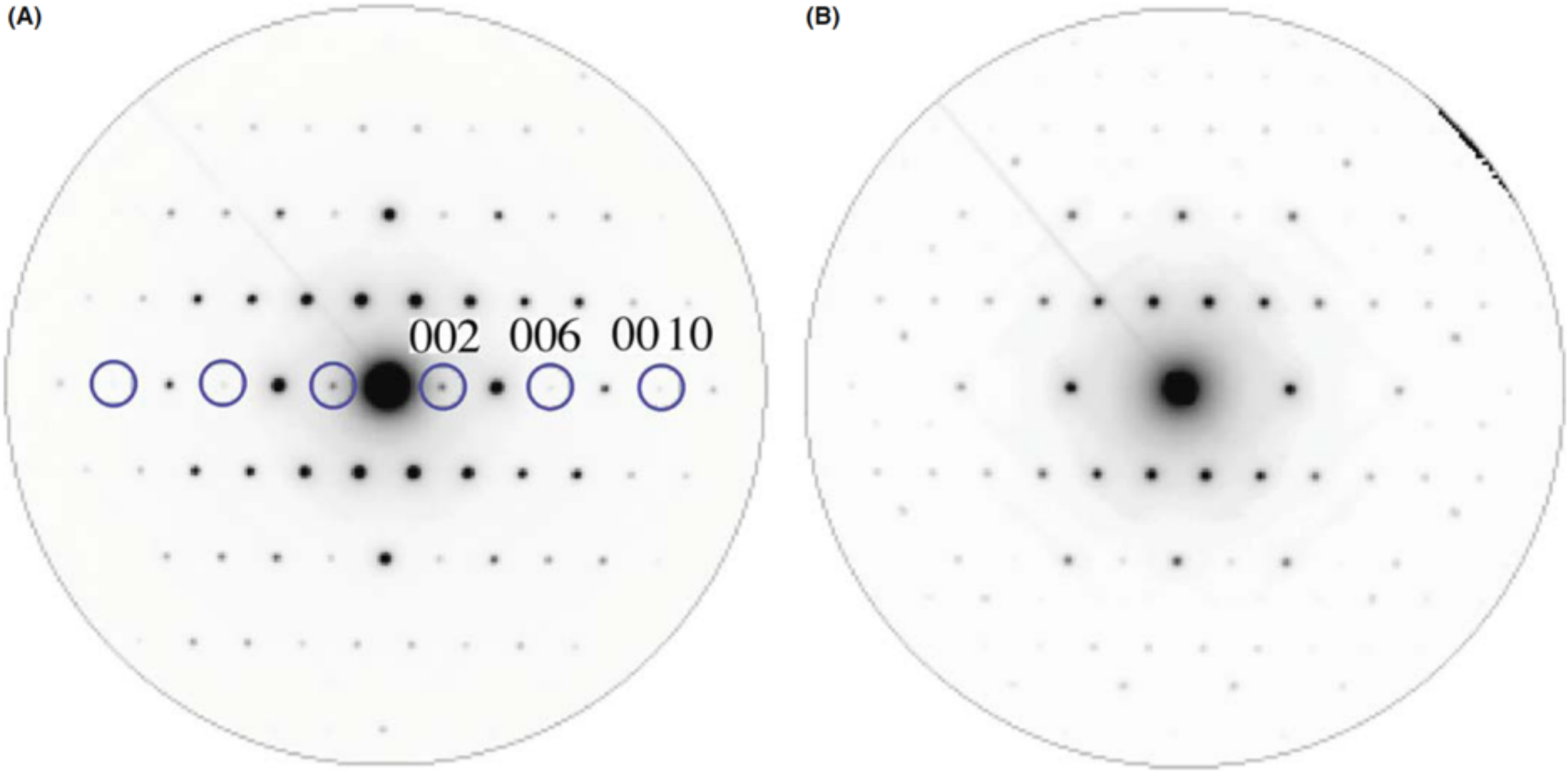
Example of silicon; from symmetry of the structure {2 0 0} reflections should be absent

However, normally see them because of double diffraction

Simulate diffraction pattern on [1 1 0] zone axis:



# Double Diffraction (Chapter 18)

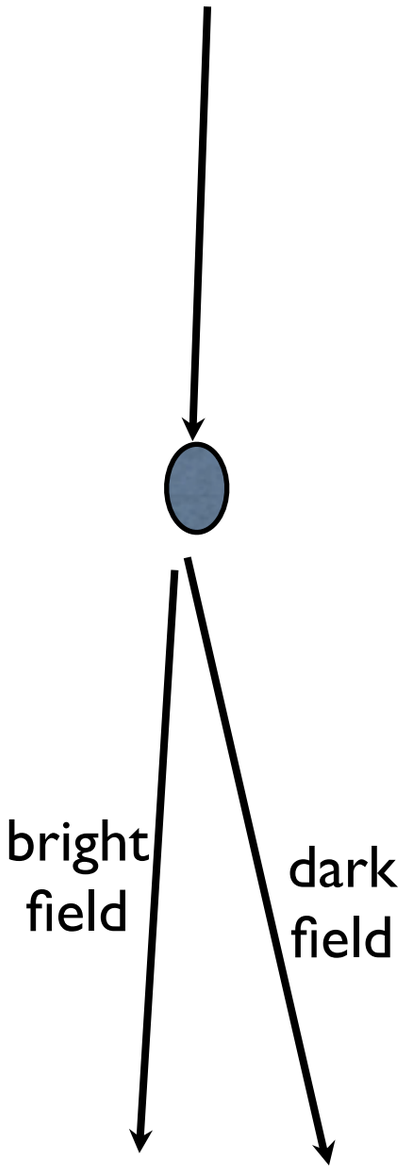



Si[130]

# 4.1 運動學強度(Kinematical Intensity)

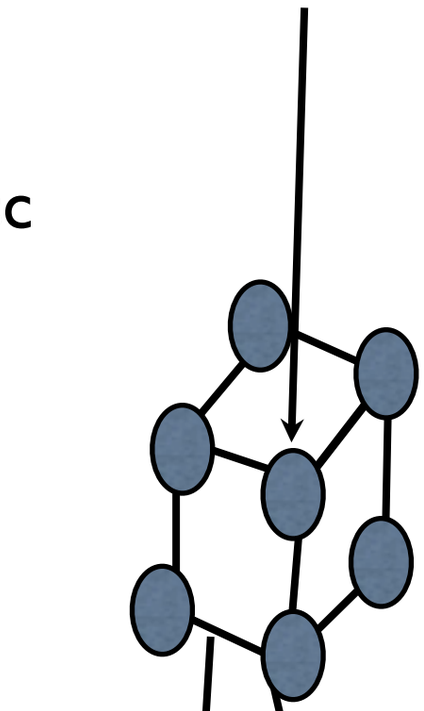
## single atom

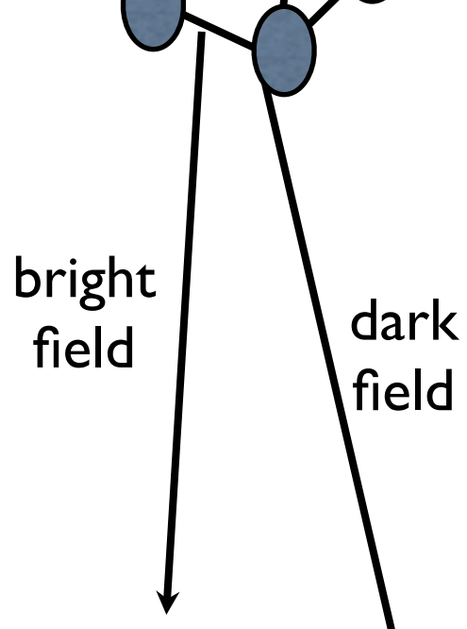
$I_o = I - I_{sc}$




$I_o$ $I_{sc} \propto |f(\theta)|^2$

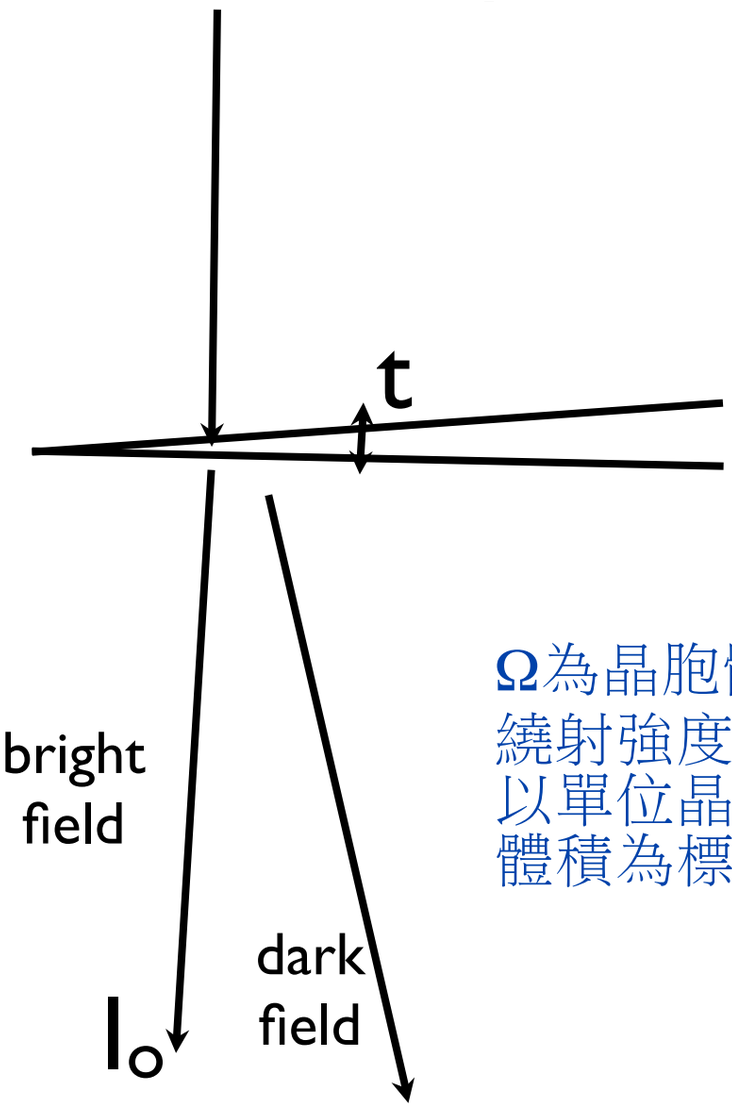
## Recall Unit cell






$I_o$ $I_{sc} \propto |F(\theta)|^2$

## Thin sample



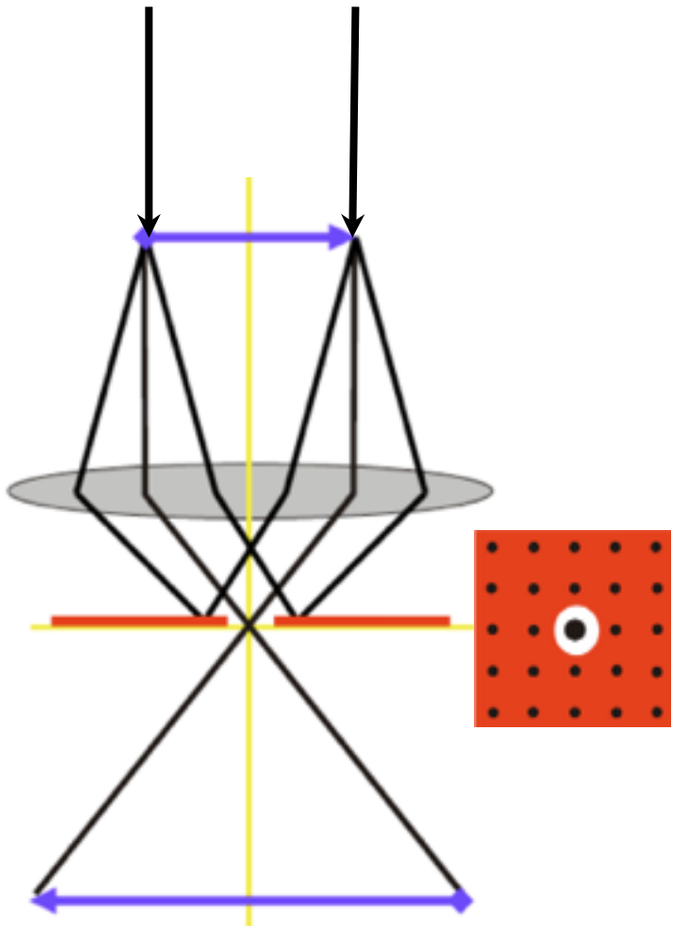

$I_o$ $I_{sc} \propto |F(\theta)|^2 \frac{\sin^2(\pi ts)}{(\pi s)^2}$

Ω為晶胞體積
繞射強度
以單位晶胞
體積為標準

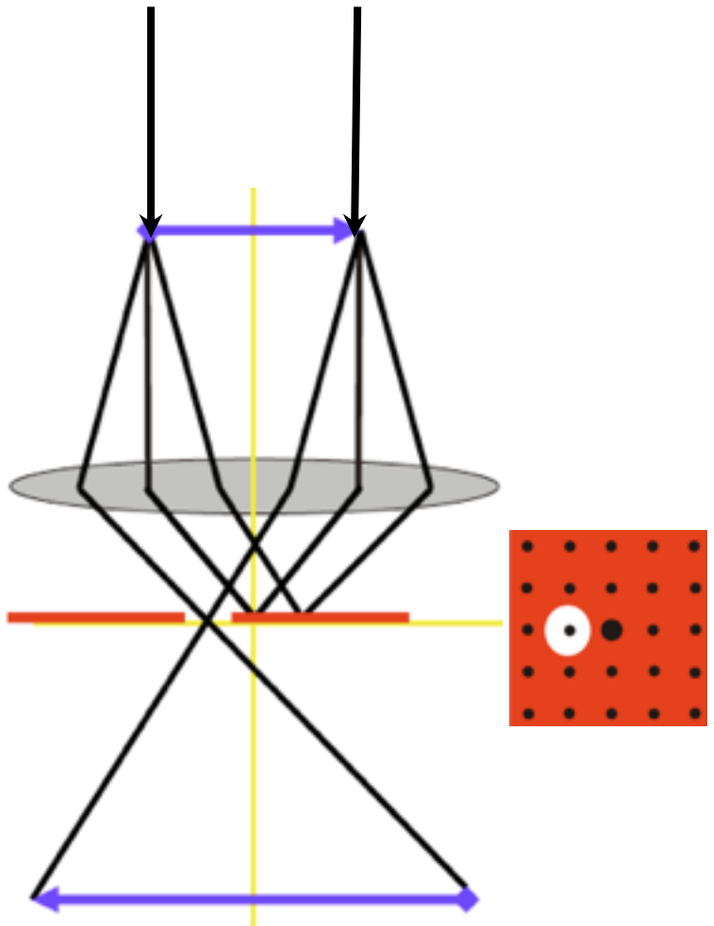
$$I_{sc} = \frac{\lambda^2 F^2(H)}{\Omega^2} \frac{\sin^2(\pi ts)}{(\pi s)^2}$$

# 4.2 Kinematic Contrast

- mass/ thickness contrast
- Bragg (orientation) contrast



Bright Field



Dark Field

Mass contrast, thickness fringe and orientation contrast

$$I_{SC} = \frac{\lambda^2 F^2(H)}{\Omega^2} \frac{\sin^2(\pi t s)}{(\pi s)^2}$$

$$\xi_g^e \equiv \left\{ \frac{\lambda F(g)}{\pi \Omega} \right\}^{-1}$$

$$I_{sc} = \frac{\sin^2(\pi t s)}{(s\xi_g)^2}$$

# 定義：

$$\xi_g^e \equiv \{\frac{\lambda F(g)}{\pi\Omega}\}^{-1} \cong \{\frac{4\times10^{-12}m\times10^{-9}m}{3\times12.5\times10^{-30}m^3}\}$$

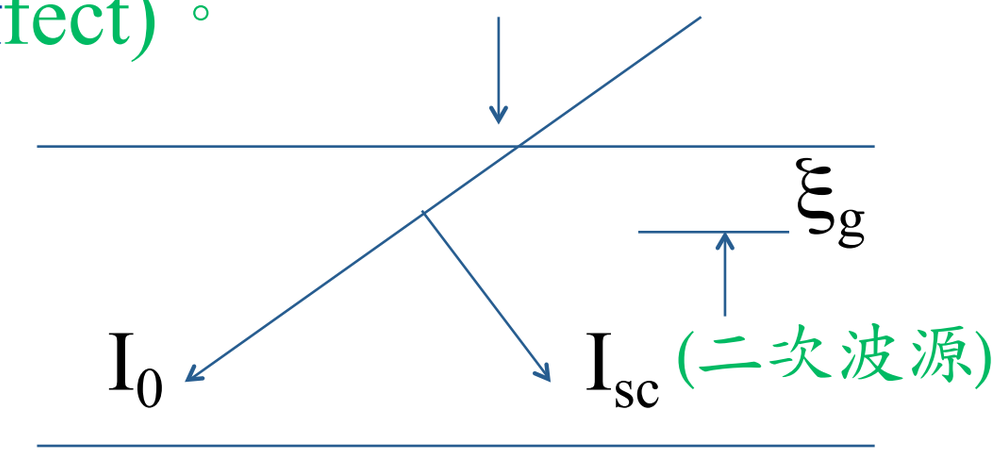
$$= 10^{-7}m = 1000\,\text{Å}$$

$$I_{sc} = \frac{\sin^2(\pi ts)}{(s\xi_g)^2}$$

運動學強度
- 光只被散射一次
- $I_{SC} << I_0 = 1$

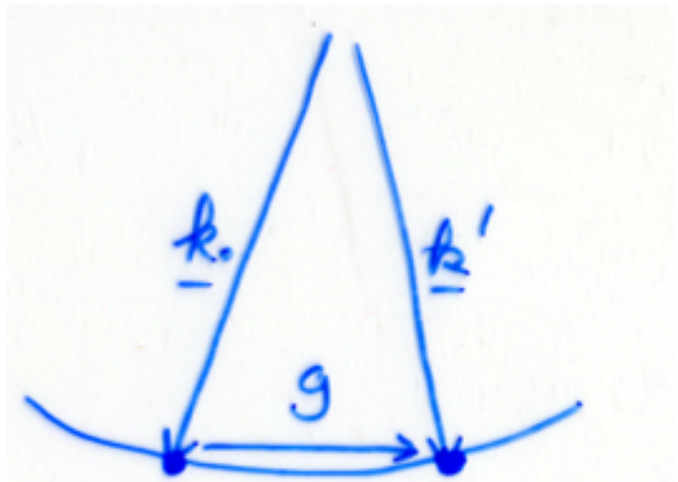
(遠離Bragg's條件)

- $\xi^x_g = \sim\mu m$
- $\xi_g$我們稱之為消光距離（extinction distance)
- 消光距離的物理意義就是當試片的厚度大於$\xi_g$時，散射光g的強度大於入射光強度（入射光的能量完全轉移至散射光方向）
- 我們因此必須考慮到由散射光束所引起之第二次散射。我們稱之為動力學效應(dynamical effect)。

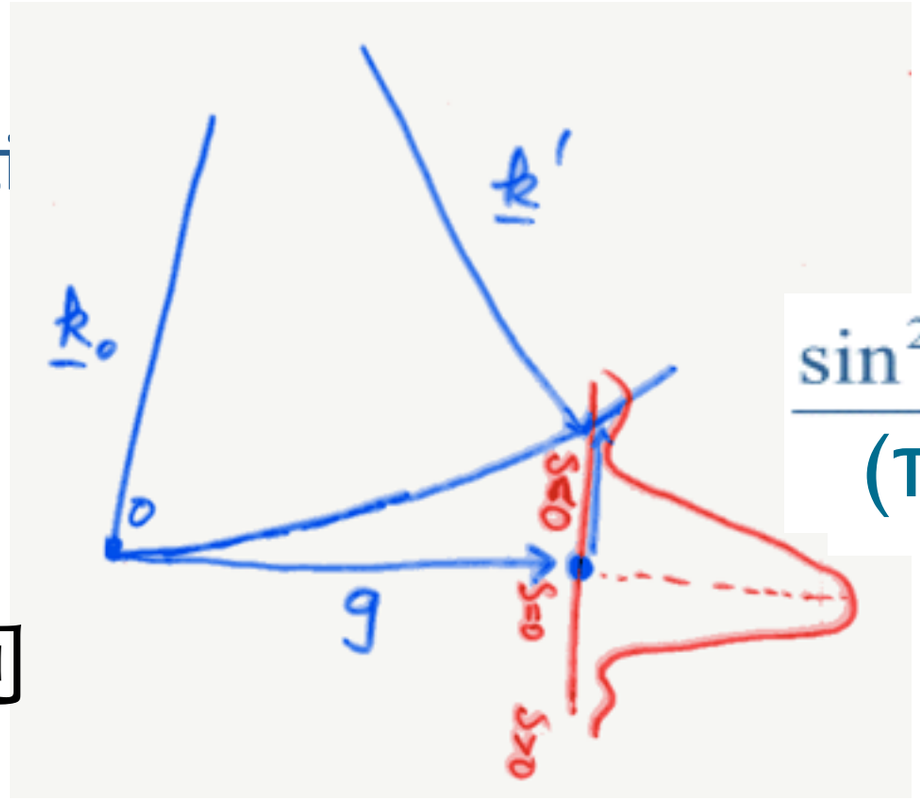


# 4.1 運動學強度(Kinematical Intensity)

- 回顧：薄膜的電子繞射並不一定要100%滿足Bragg's繞射條件
- Bragg's繞射條件 $2d\sin\theta = \lambda$
- $k'-k_0 = g$




- 繞射光的強度(結構因子的振幅)
- 與倒晶格點到Ewald球的距離
- 有關(s)
- 另s為激發誤差(deviation or excitati
- error)
- $\vec{H} = \vec{k}' - \vec{k}_0 = \vec{g} + \vec{s}$
- (relaxed Bragg's condition)

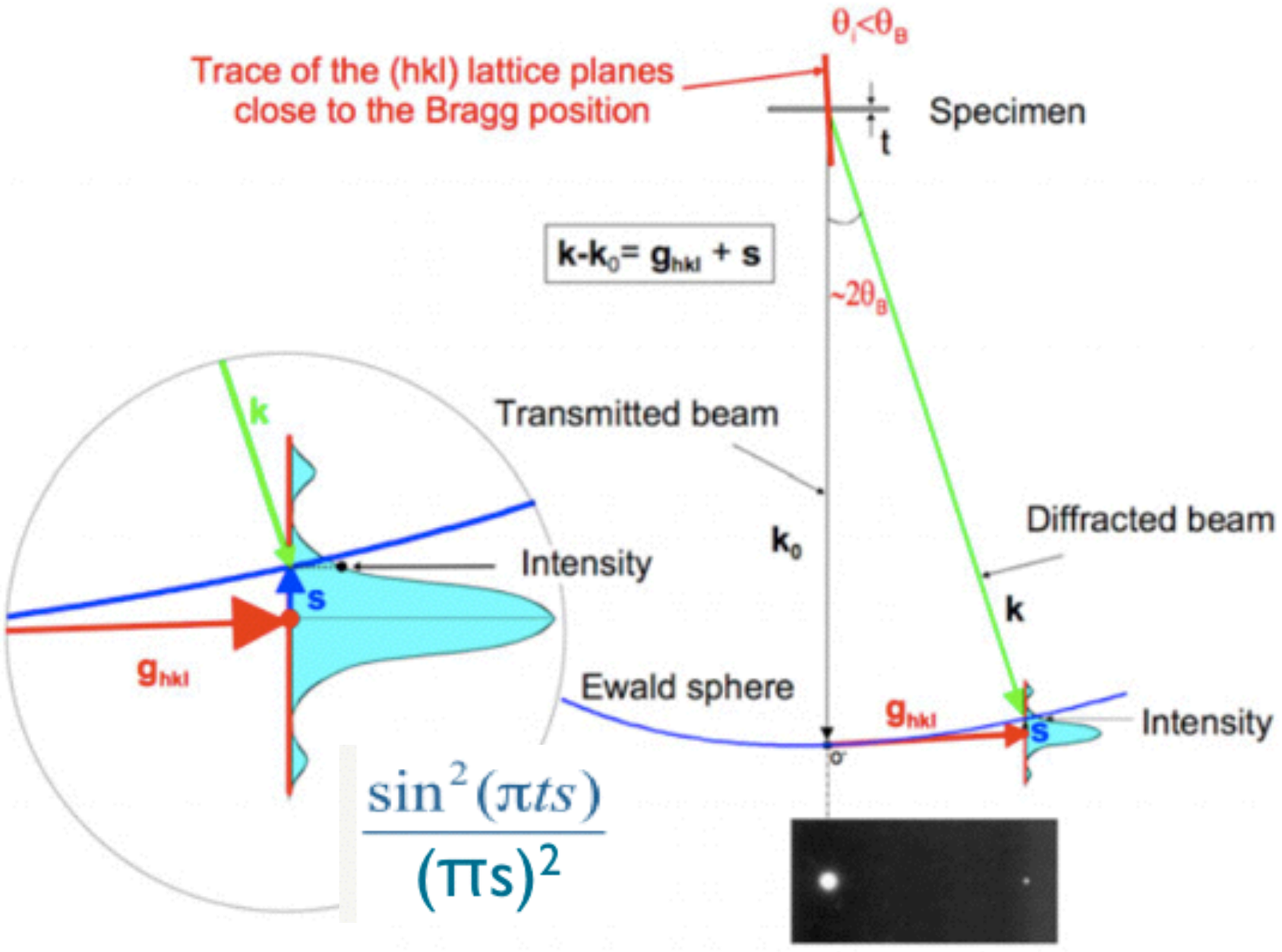



$$\frac{\sin^2(\pi ts)}{(\pi s)^2}$$

s: electron/ crystal 之相對方向

t: thickness

# Excitation error

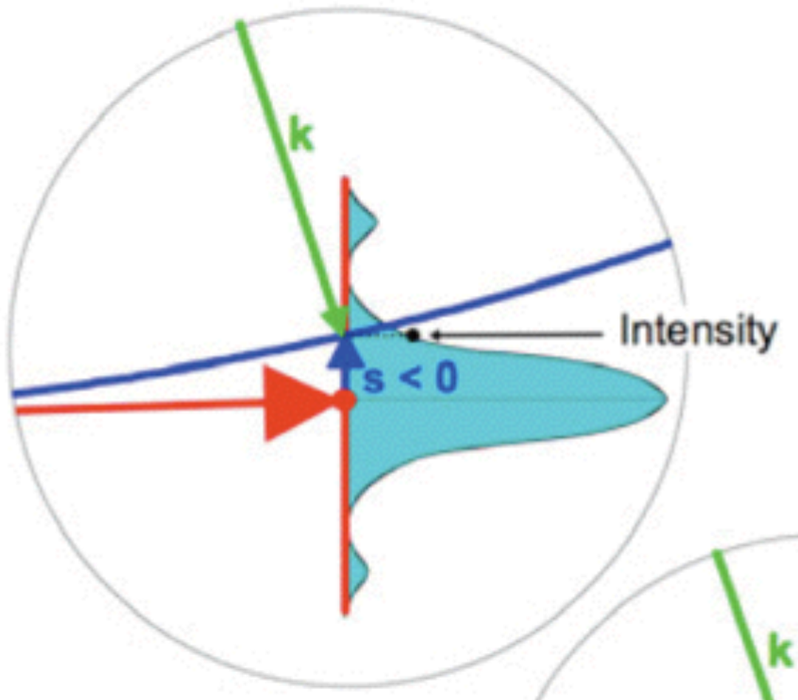


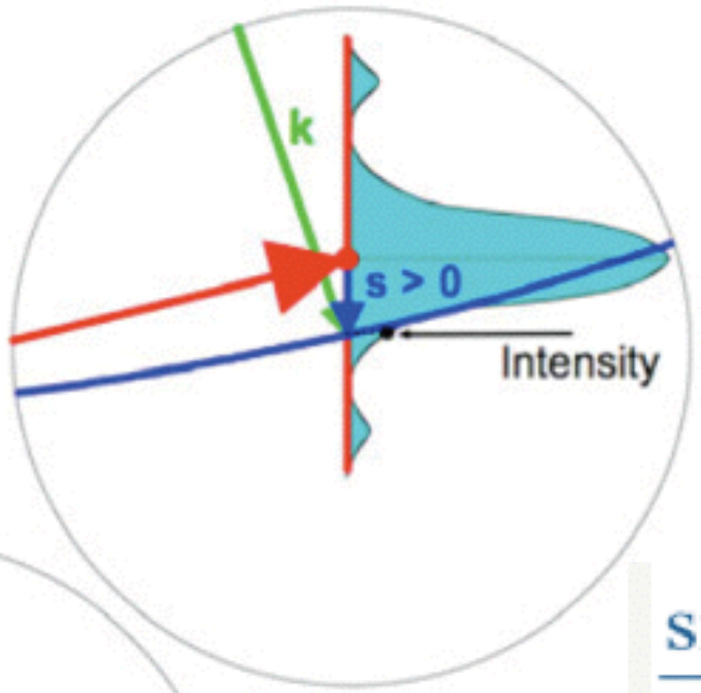

Tilted slightly off Bragg condition, intensity of diffraction spot much lower

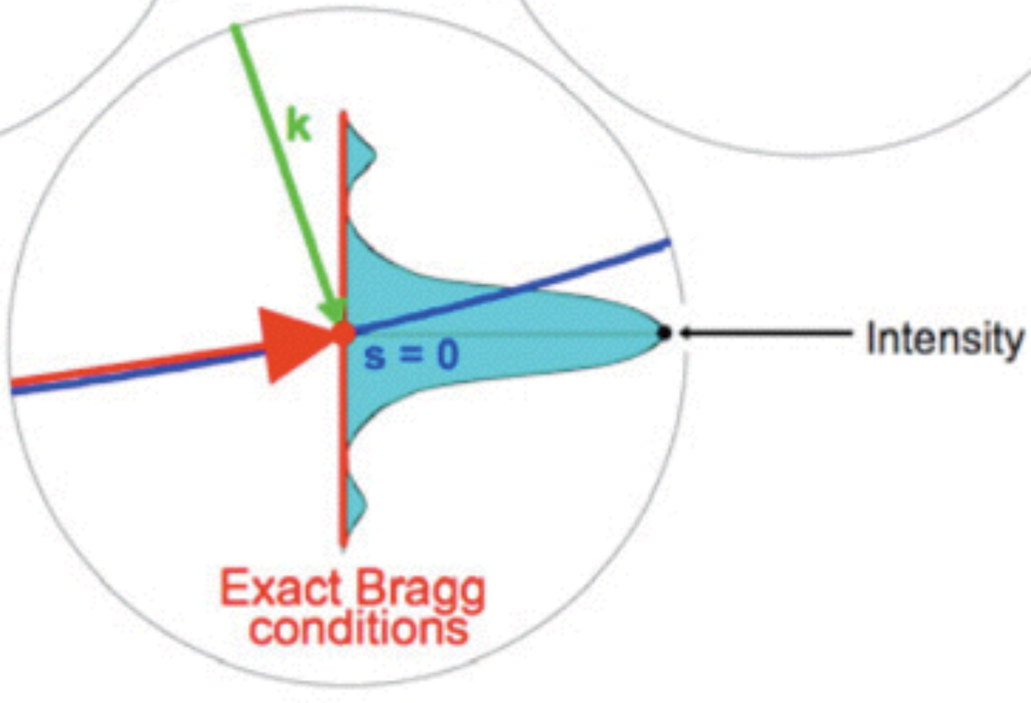
Introduce new vector **s** - "*the excitation error*" that measures deviation from exact Bragg condition

# Excitation error

Excitation vector **s**
Conventions

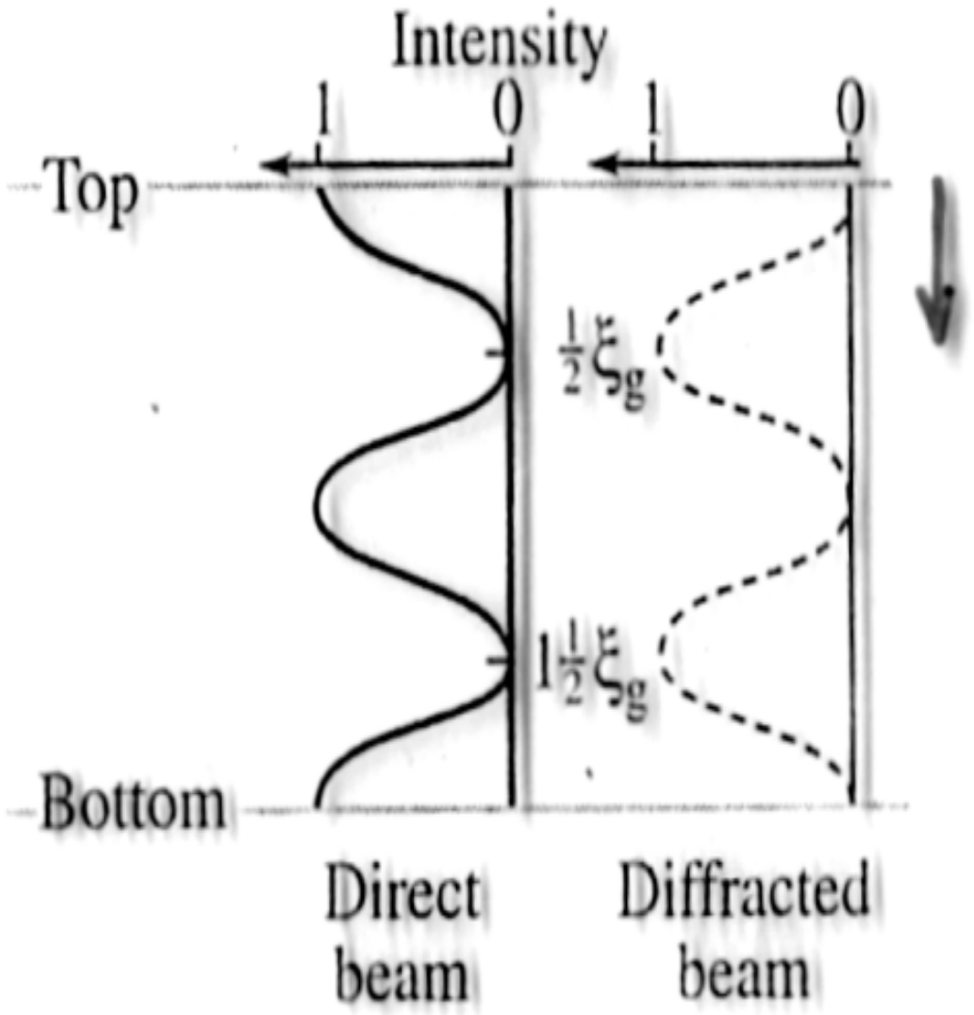


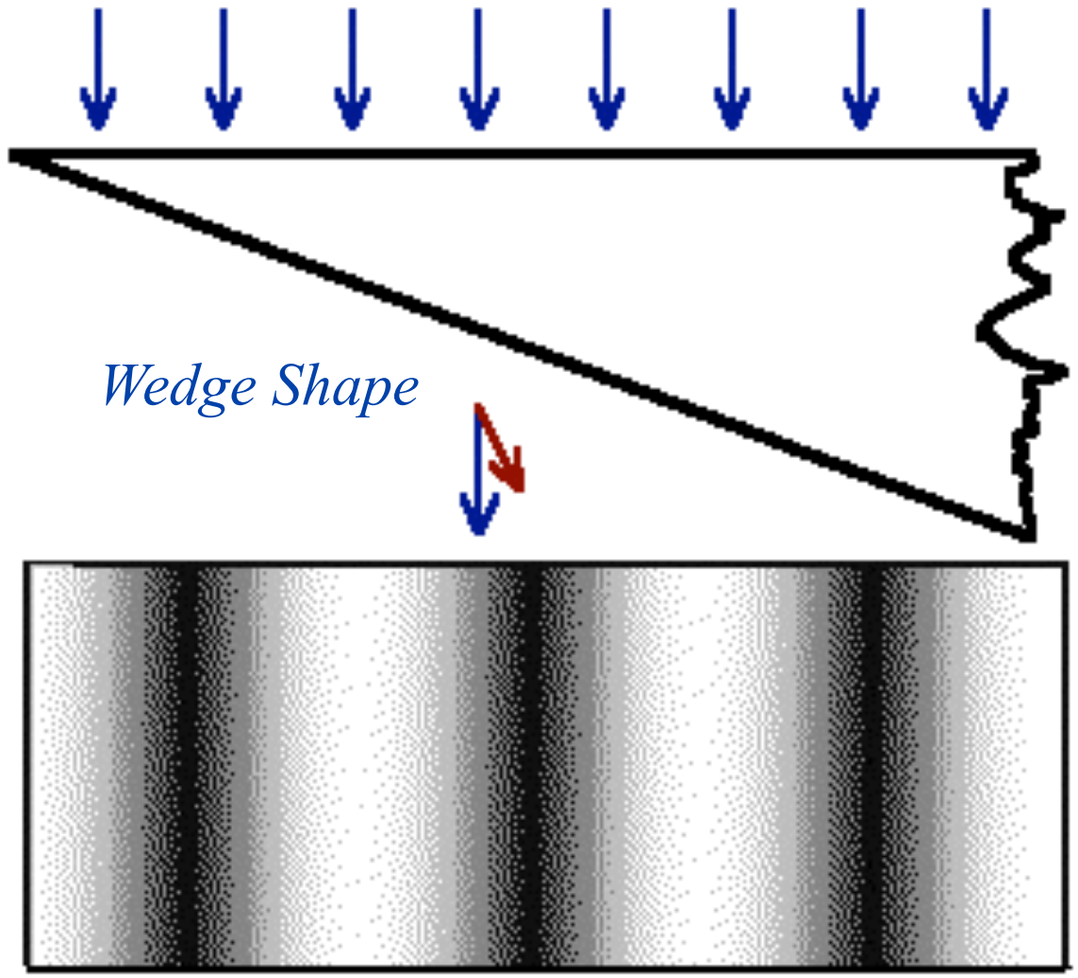



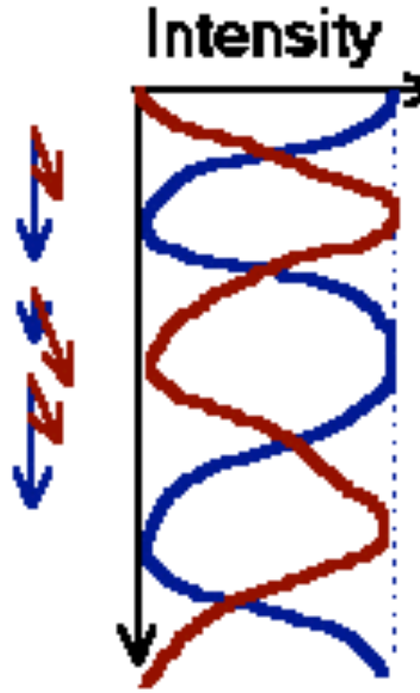




$$\frac{\sin^2(\pi t s)}{(\pi s)^2}$$

# 4.2.1 Thickness Fringe



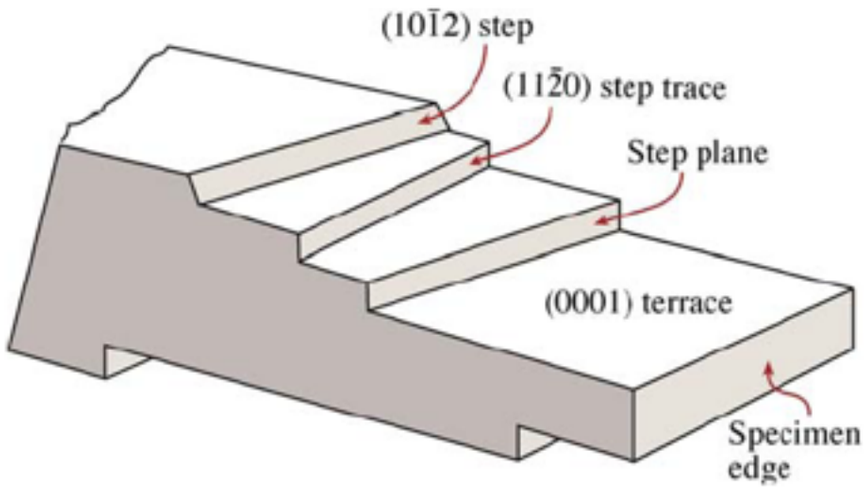

$I_o = 1 - I_{sc}$

Bright Field

$$I_{sc} = \frac{\lambda^2 F^2(H)}{\Omega^2} \frac{\sin^2(\pi t s)}{(\pi s)^2}$$

Dark Field

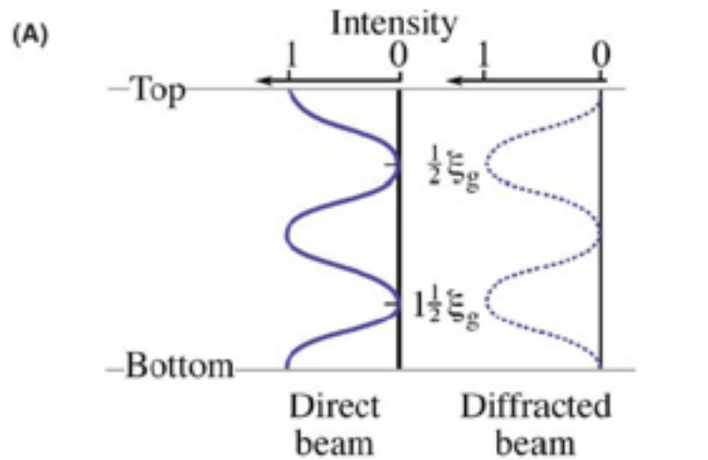
# (II) Thickness Fringes




*Wedge Shape*

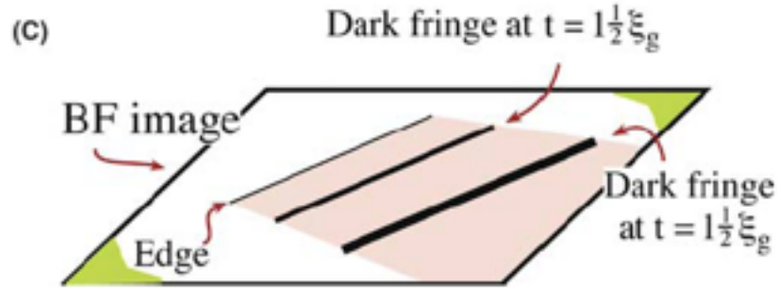
$$I_g = \frac{\pi^2}{\xi_g^{\,2}} \frac{\sin^2(\pi t s)}{(\pi s)^2}$$

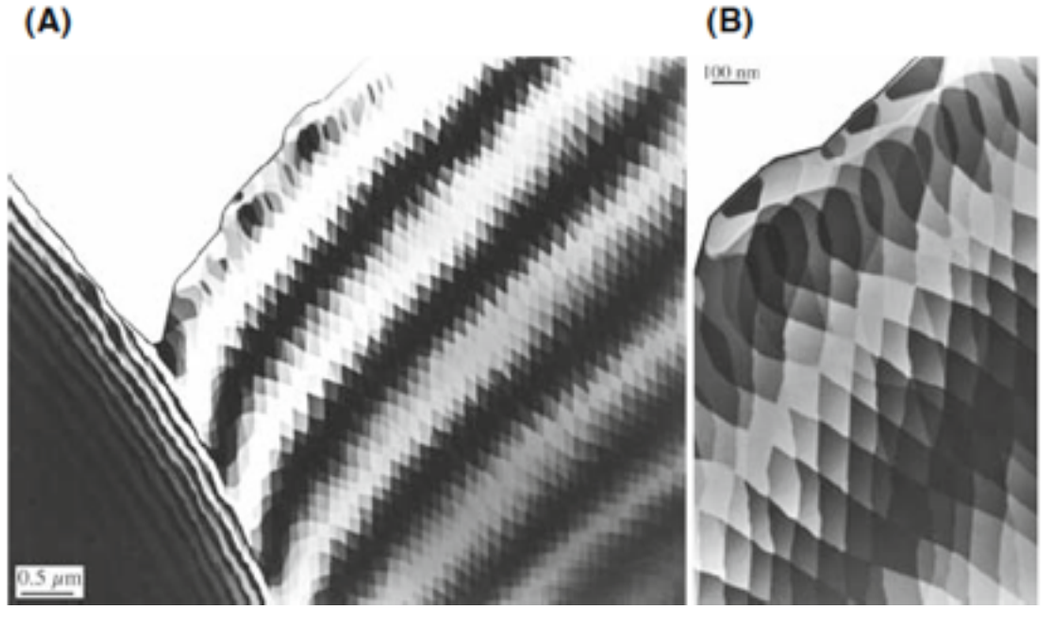
$$I_0 = 1 - I_g$$

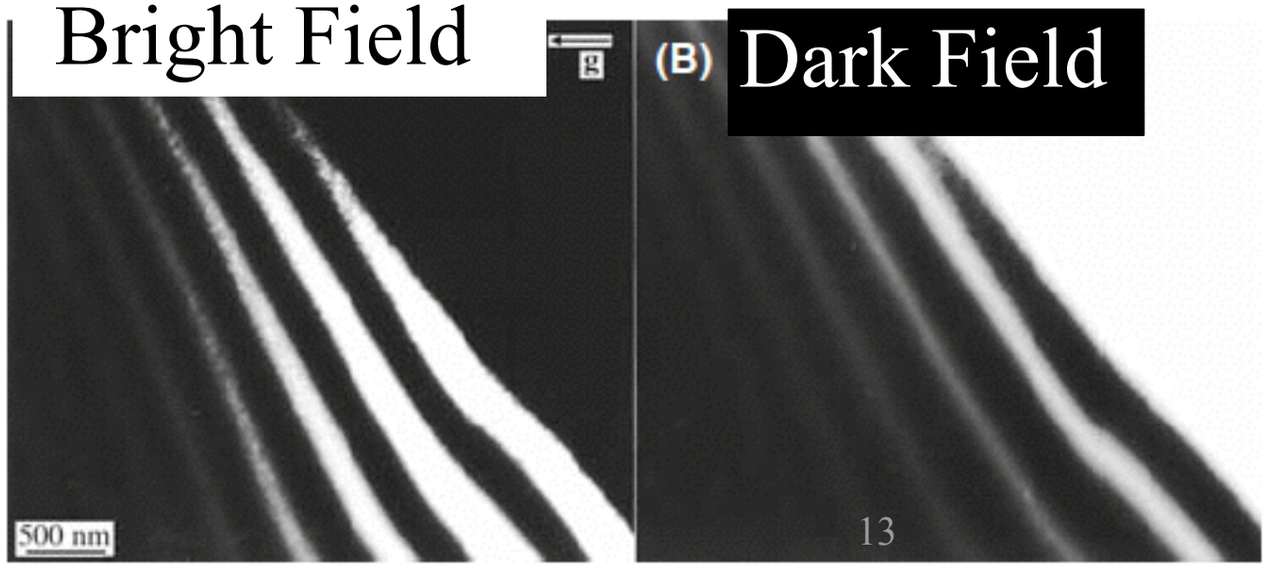



- 在運動學的範圍內有吸收的因素，明場與暗場之強度沒直接的關係

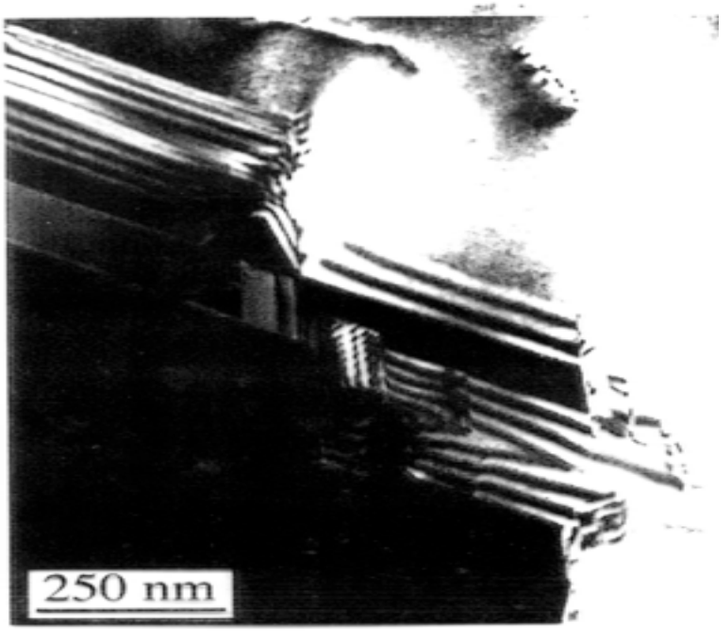
- 明場與暗場像是運動學的範圍才可能是互補

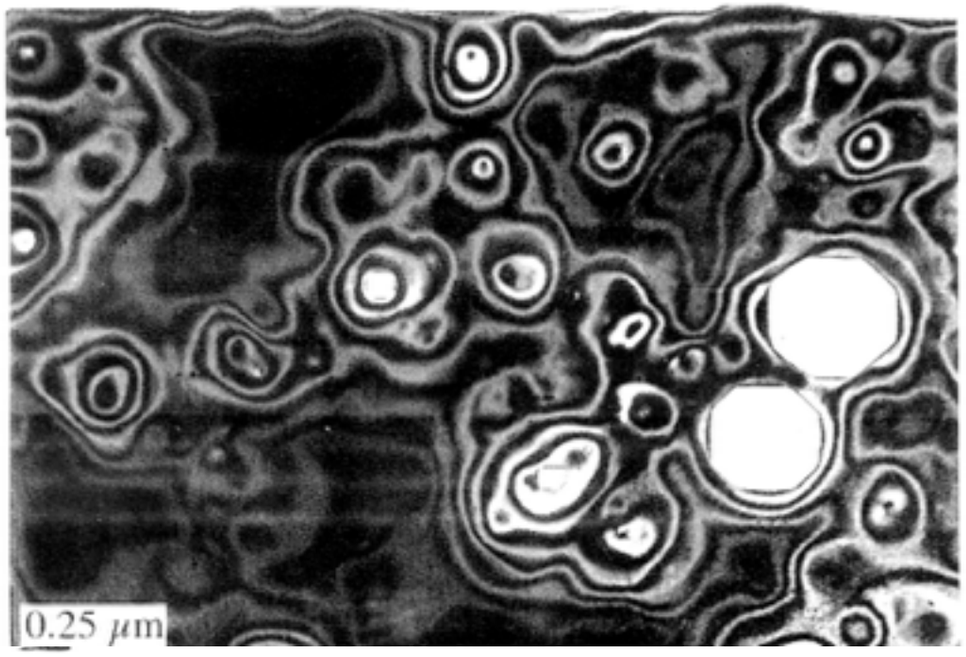


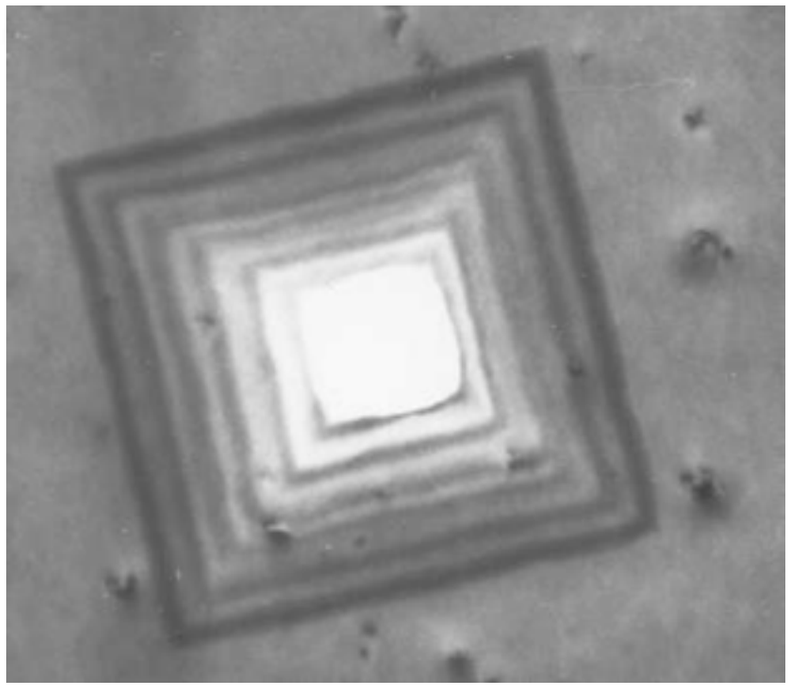



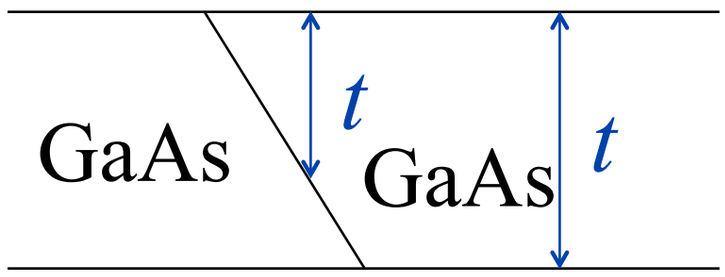



# (III) Thickness Fringes



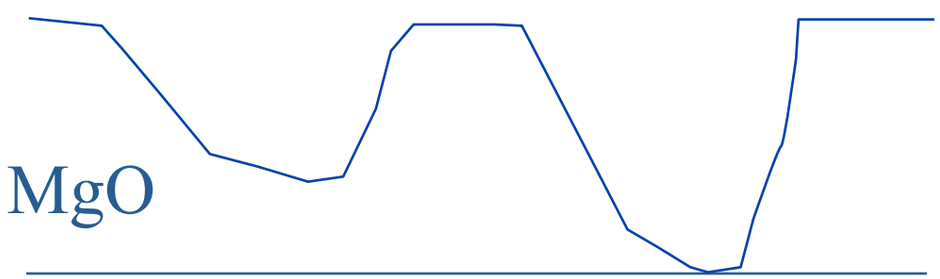



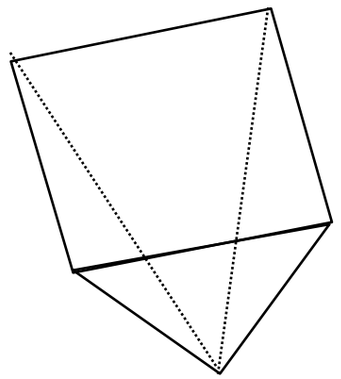



傾斜晶界

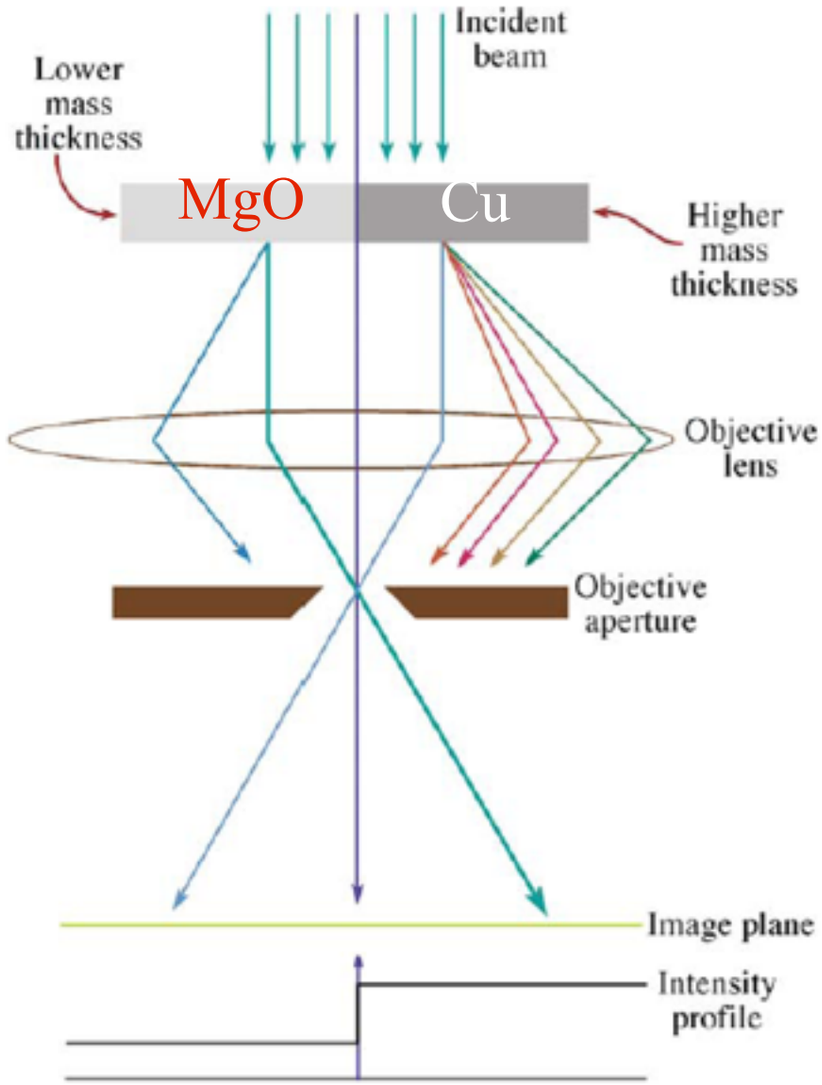
化學浸蝕破洞

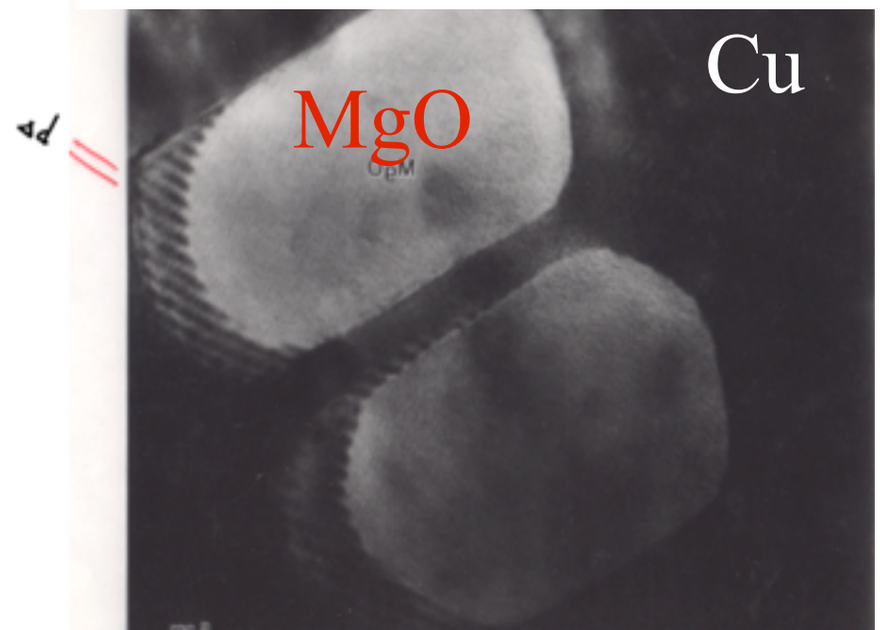



an etch pit in a **Ge** sample which is the usual inverted pyramid with **{111}** planes

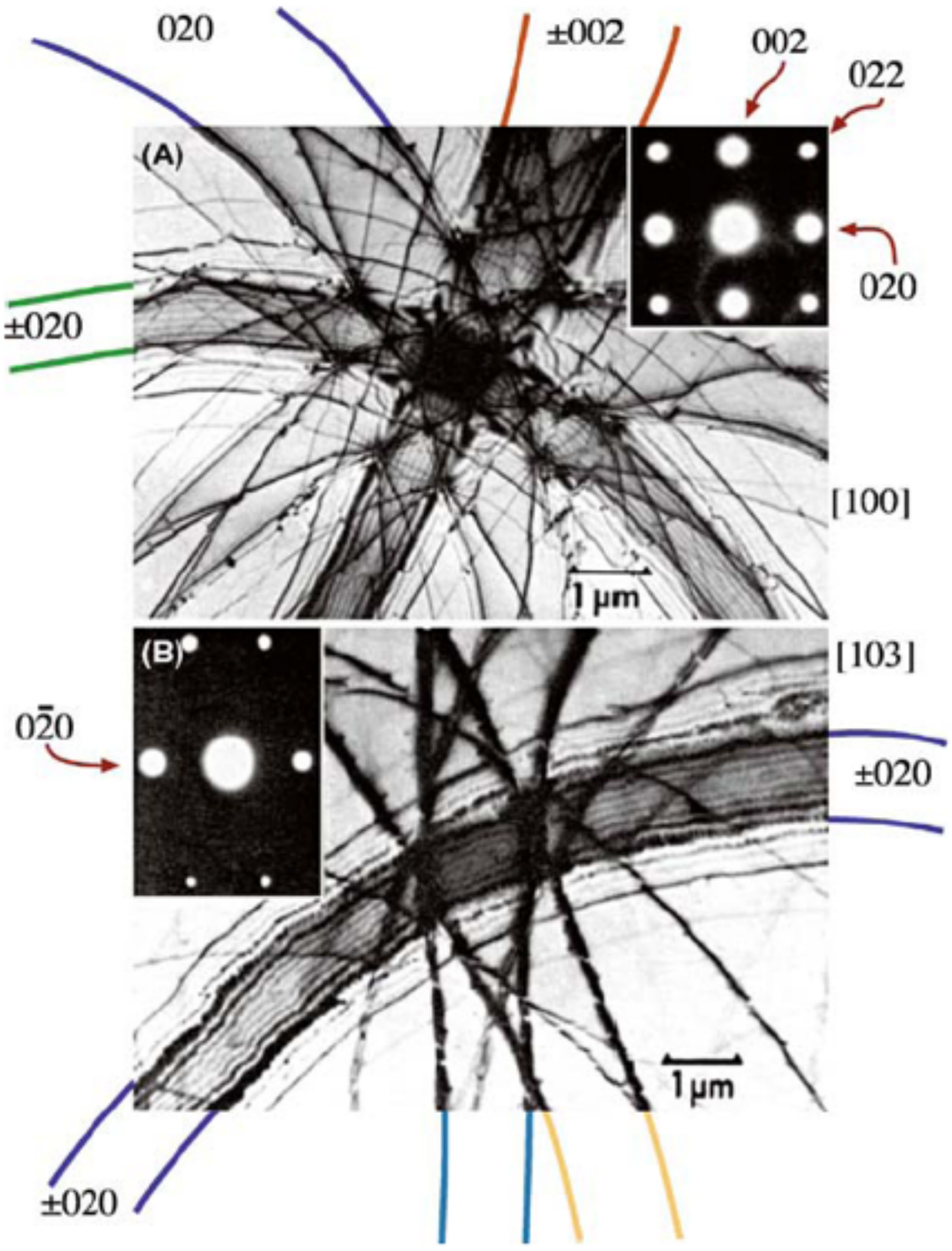


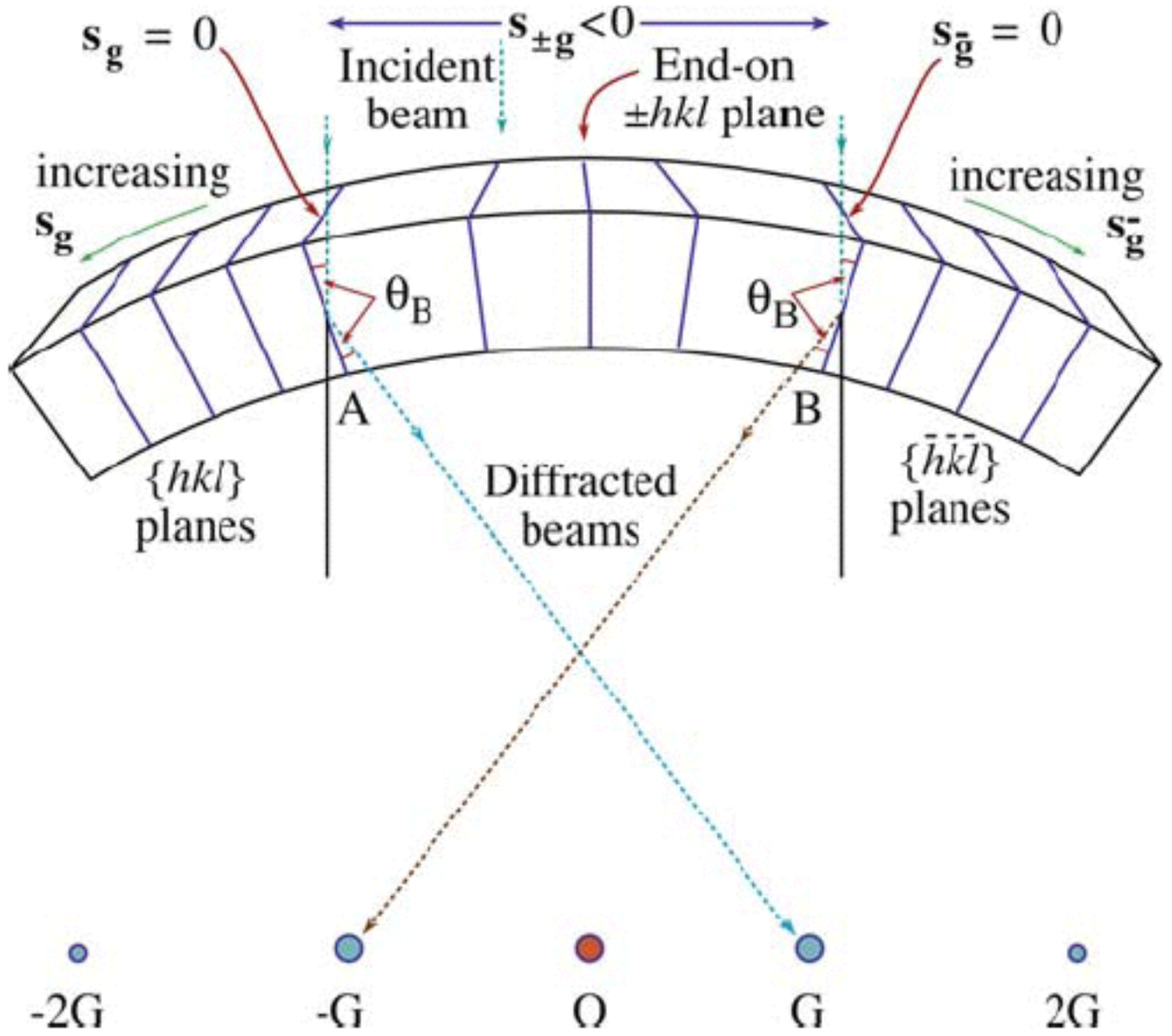
# 4.2.2 Mass Contrast

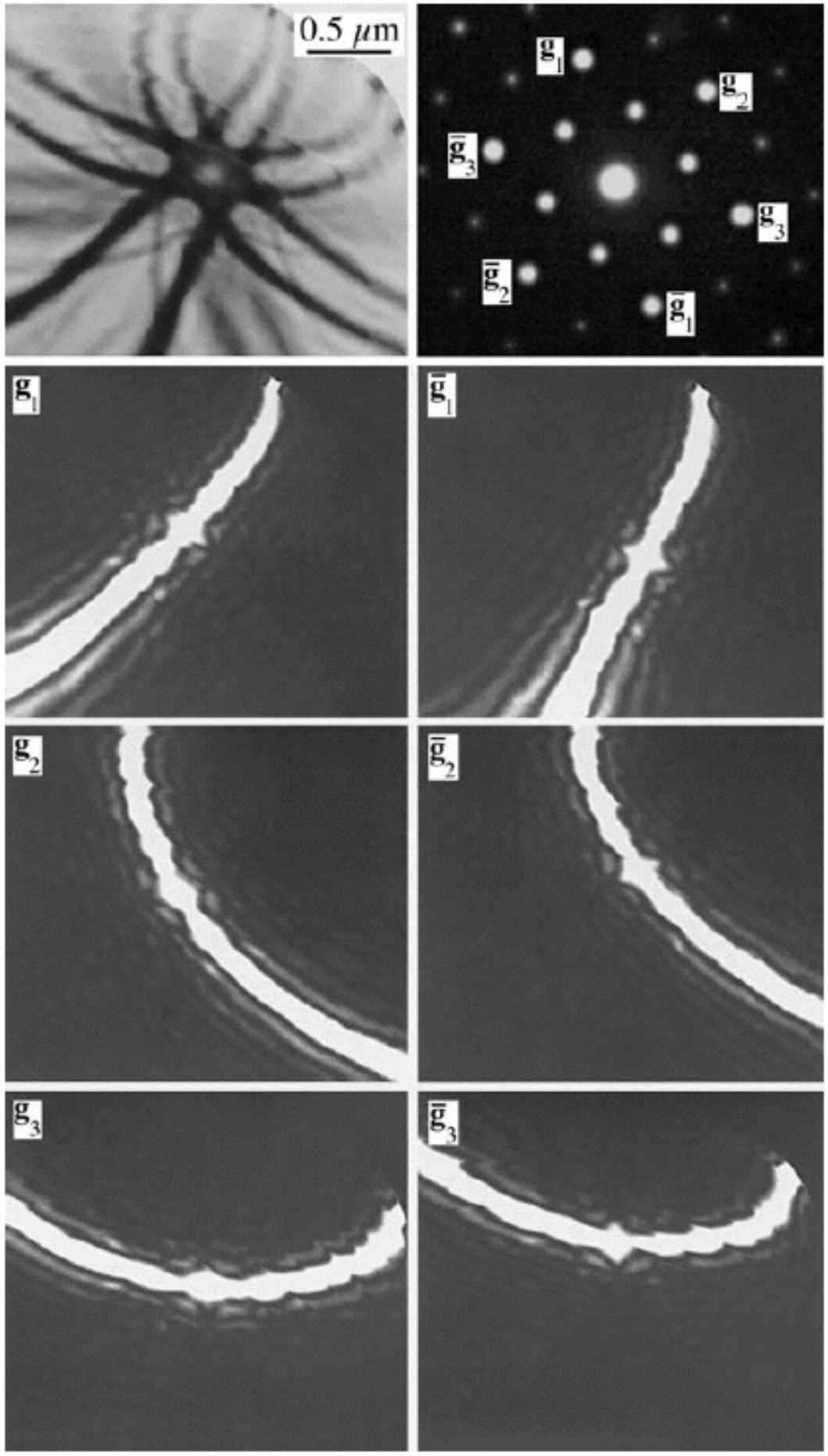


# 4.2.3 Bend Contours (Bragg contrast)
# (實空間結晶訊息)




0.5 μm
g1
g2
g3
g1
g2
g3
g1
g1
g2
g2
g3
g3

# • 4.3 電子繞射動力學

(Dynamic Diffraction Theory)

## (Chapter 13)

Strain Contrast

(defects: dislocation, interface, stacking fault)

•當 $t \approx \frac{\zeta_g}{\pi}$ $I_g = |\psi_g| \approx 1,\ I_0 = 1 - |\psi_g|^2 \approx 0$

$\Psi_g$可以當成二次波源，這時運動學不適用，必須考慮"動力學"

•對運動學而言，穿透光和繞射光不互相干擾

動力學而言，穿透光和繞射光互相修正（影響）

•考慮雙光束條件，只有一個g很強被激發，其他的繞射光
S>>0或S<<0

# 4.3.1 Howie- Whelan Equation

$$\frac{d\psi_0}{dz} = \frac{i\pi}{\xi_g}\psi_g(z)\exp(-2\pi isz) + \frac{i\pi}{\xi_0}\psi_0(z)$$

$$\frac{d\psi_g}{dz} = \frac{i\pi}{\xi_g}\psi_0(z)\exp(2\pi isz) + \frac{i\pi}{\xi_0}\psi_g(z)$$

其解，

$$w = s\xi_g$$

動力學強度

$$I_g = \frac{1}{1+w^2}\sin^2\left(\frac{\pi t}{\xi_g^{eff}}\right) = \left(\frac{\pi t}{\xi_g}\right)^2 \frac{\sin^2(\pi t S_{eff})}{(\pi t S_{eff})^2}$$

Bragg contrast

mass contrast

thickness contrast

$$\xi_g^{eff} = \frac{\xi_g}{(1+w^2)^{1/2}}$$

$S_{eff}=[(s^2+1)/\xi^2]^{1/2}$

有效的激發誤差 (描述電子與樣品作用之強弱) 則

運動學強度

$$I_0 = 1 - I_g, I_g = \frac{\sin^2(\pi ts)}{(\xi^2 s^2)}$$

$$\psi_g = i\lambda\frac{F_g}{\Omega}\frac{\sin(\pi ts)}{\pi s} = \frac{i}{\xi_g}\frac{\sin\pi ts}{s}$$

$$S_{eff}=[(s^2+1)/\xi^2]^{1/2}$$

有效的激發誤差 (描述電子與樣品作用之強弱) 則

- 當S=0時，$S_{eff}=\xi_g^{-1}$　　$I_0=1-I_g$

- 當|S|很大時，$S\sim S_{eff}$ (動力學退化與運動學相重合):弱光束

有晶格扭曲時（或位移），Howie-Whelan Eqn.之修正

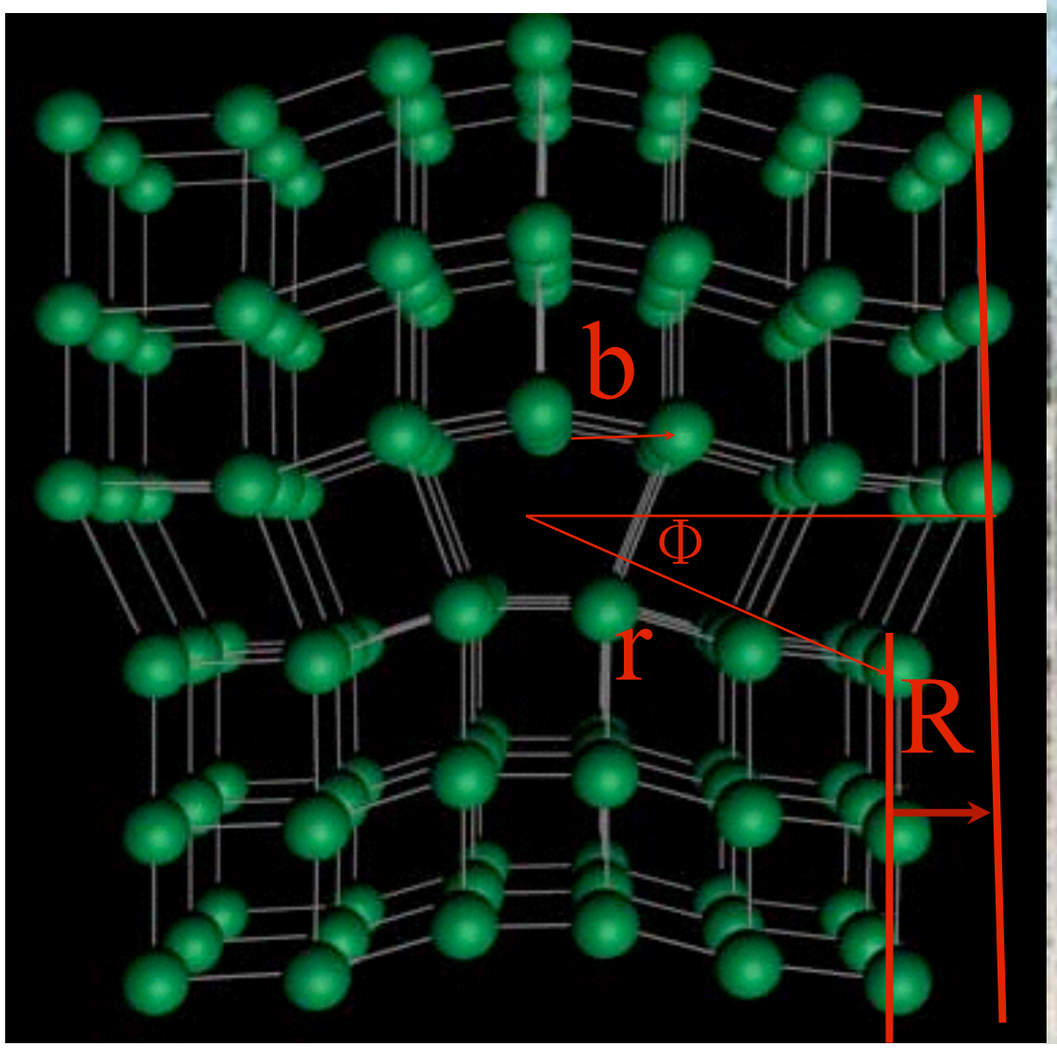
連續R　　固定R

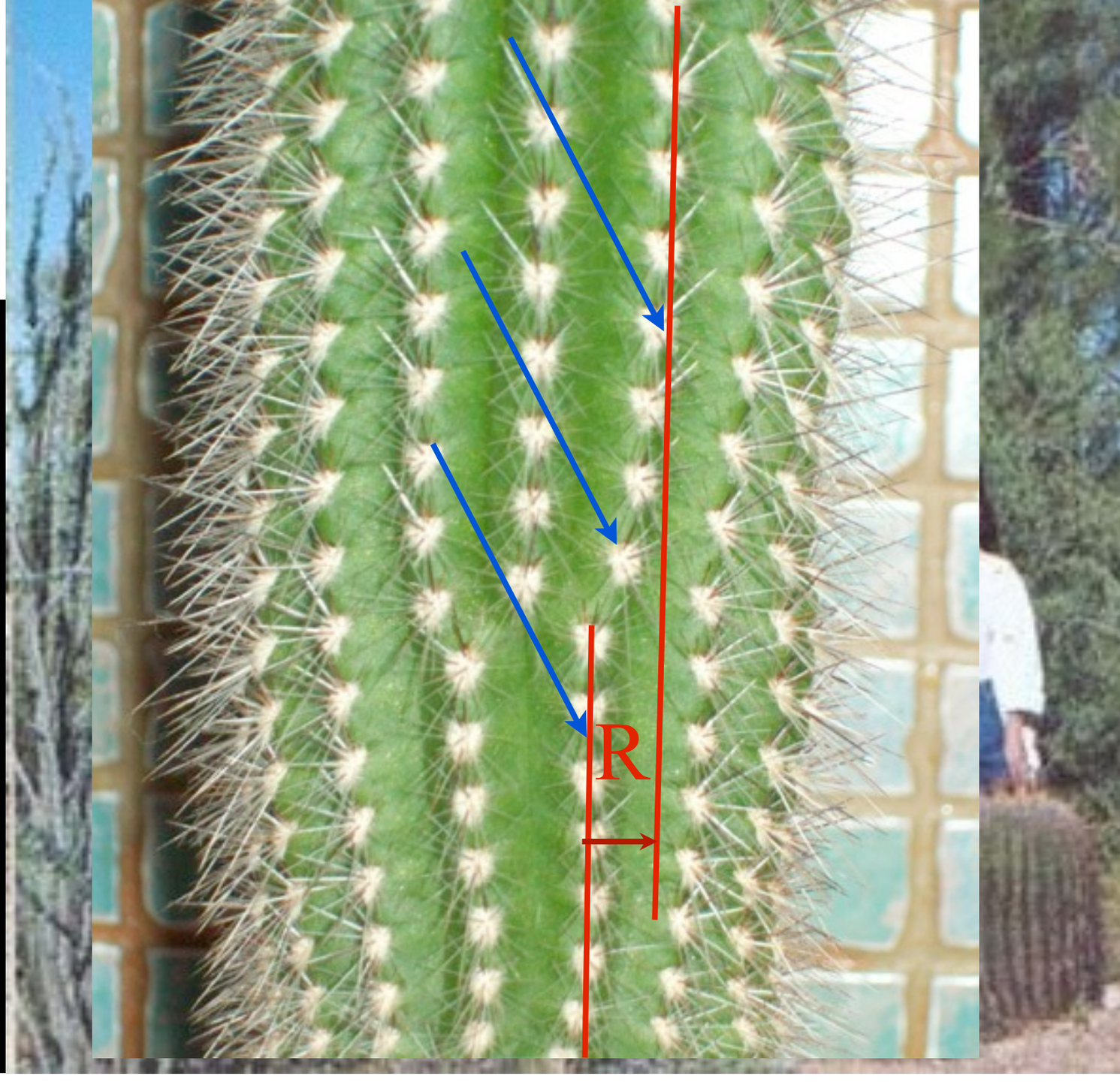
$$\frac{d\psi_g}{dz}=\frac{i\pi}{\xi_0}\psi_g(z)+\frac{\pi i}{\xi_g}\psi_0(z)\exp(2\pi i(sz+g\bullet R)$$

$$\frac{d\psi_0}{dz}=\frac{i\pi}{\xi_0}\psi_0(z)+\frac{\pi i}{\xi_{-g}}\psi_g(z)\exp(-2\pi i(sz+g\bullet R)$$

因為缺陷因素引起相位之變化

# 4.3.2 Line Defects




## Edge Dislocation
## (邊刃差排)

g-R 引起的方向變化

$$R = \frac{1}{2\pi}[b\frac{Sin2\Phi}{4(1-\nu)} + (b \wedge u)]\{\frac{1-2\nu}{2(1-\nu)}\ln r + \frac{Cos2\Phi}{4(1-\nu)}\}$$

有晶格扭曲時（或位移），Howie-Whelan Eqn.之修正

連續R　　固定R

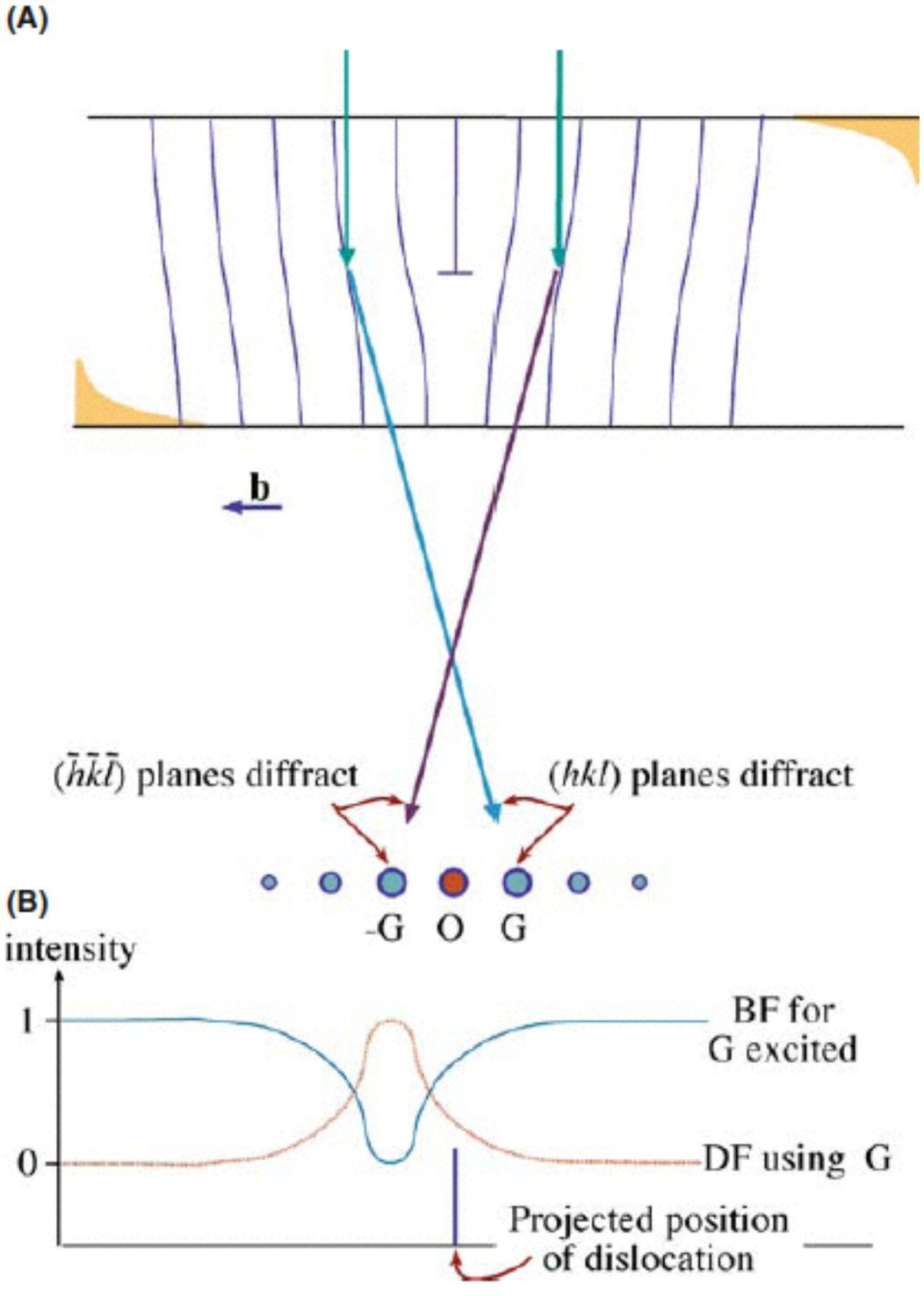
$$\frac{d\psi_g}{dz} = \frac{i\pi}{\xi_0}\psi_g(z) + \frac{\pi i}{\xi_g}\psi_0(z)\exp(2\pi i(sz + g\bullet R)$$

$$\frac{d\psi_0}{dz} = \frac{i\pi}{\xi_0}\psi_0(z) + \frac{\pi i}{\xi_{-g}}\psi_g(z)\exp(-2\pi i(sz + g\bullet R)$$

因為缺陷因素引起相位之變化

# (Chapter 26)

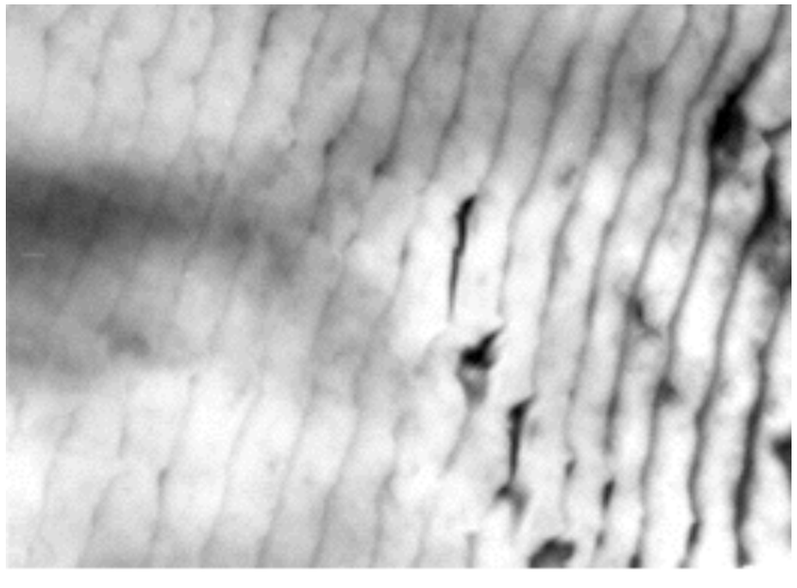
- 若g · R=0 則雖有缺陷，但不引起對比
- g · R是因為缺陷之應變場，使晶格扭曲，變形或位移，所以在TEM影像我們看到的是缺陷的應變場
- 若R(r)延續很遠（長程應變）則缺陷之影像是很寬的；相反的，若R (r) 是非常局部化則缺陷之對比亦侷限在很小區域

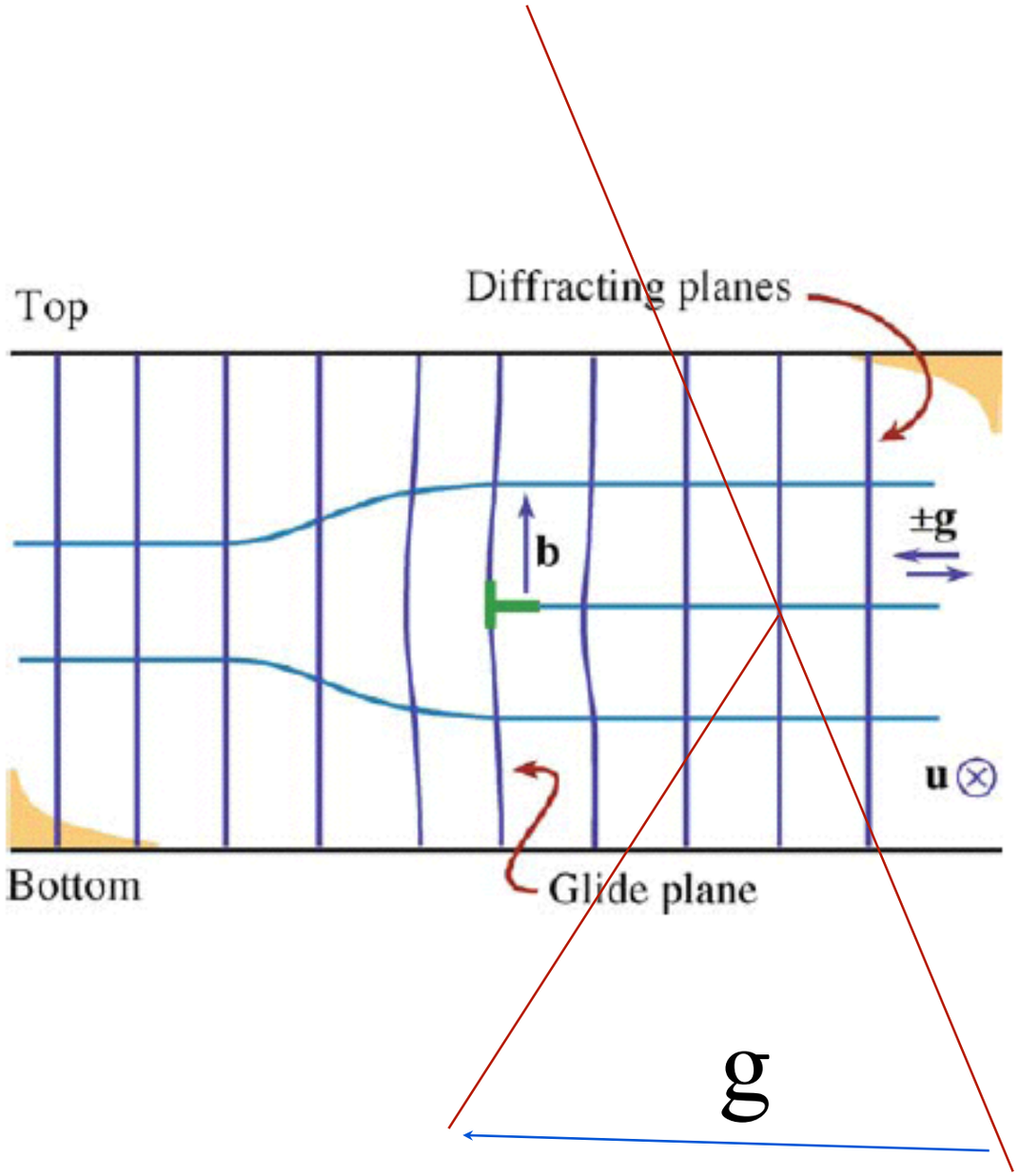



•因為局部應變場的變化，使得每一個column的繞射條件皆不同（$\vec{R}$不同）

•因而產生對比之分佈

•事實上，我們看到的是入射電子與應變場之作用結果（$\vec{g}\cdot\vec{R}$ 對比）

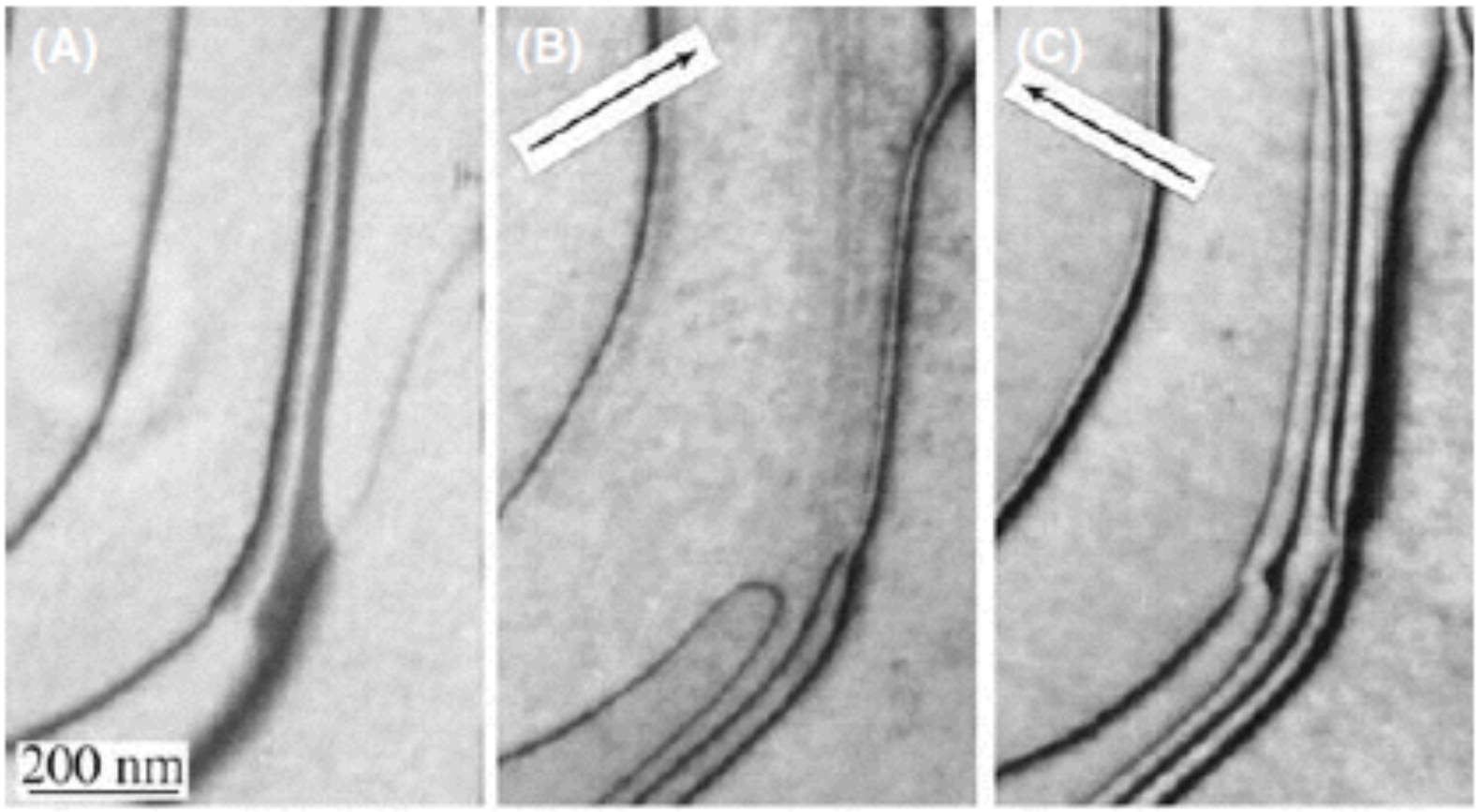


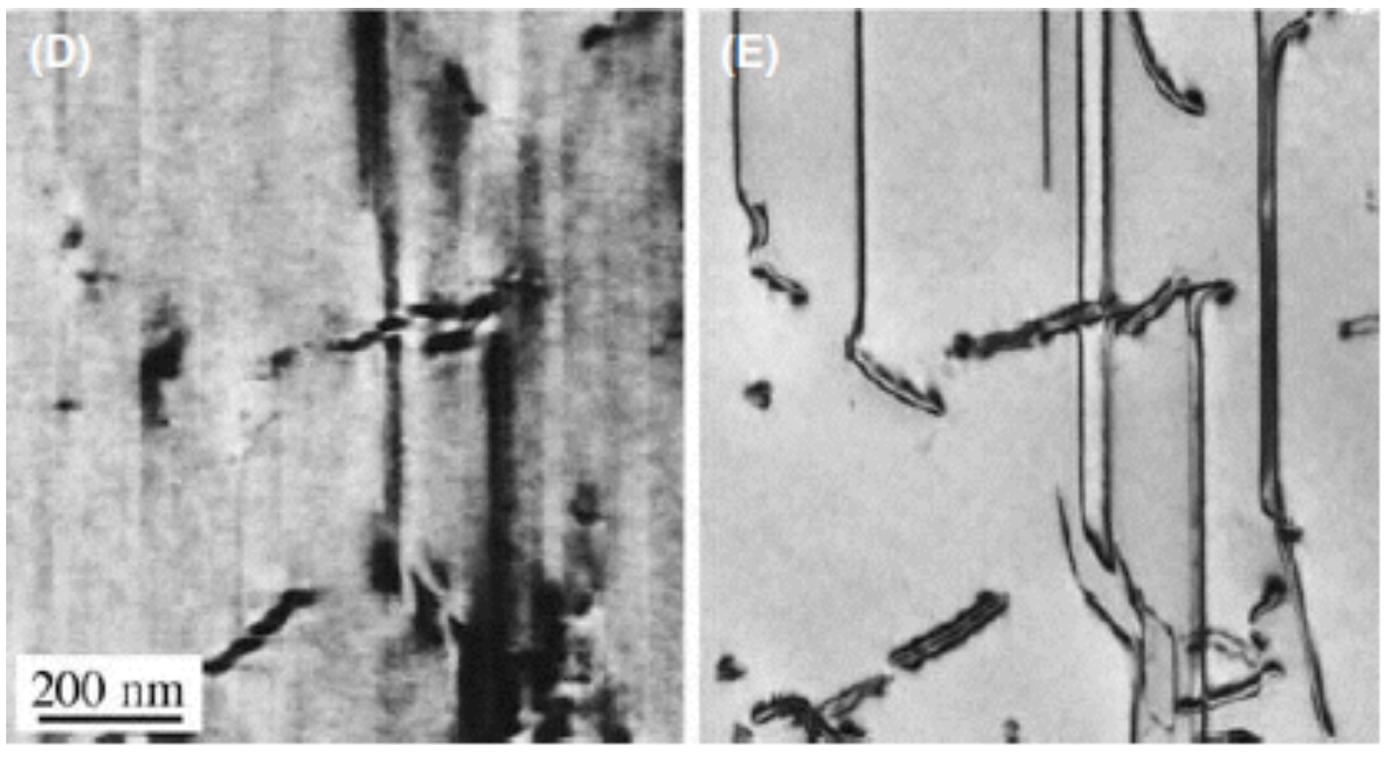


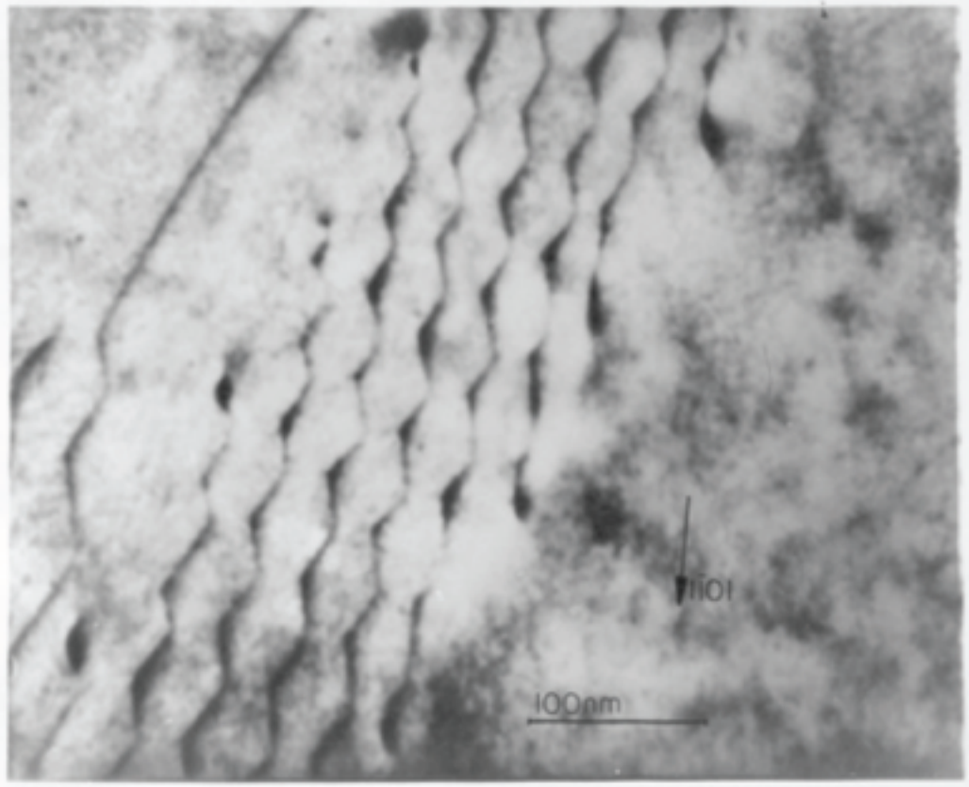

- 繞射光偵測不到差排應變場對晶格的扭曲所以dislocation沒有對比

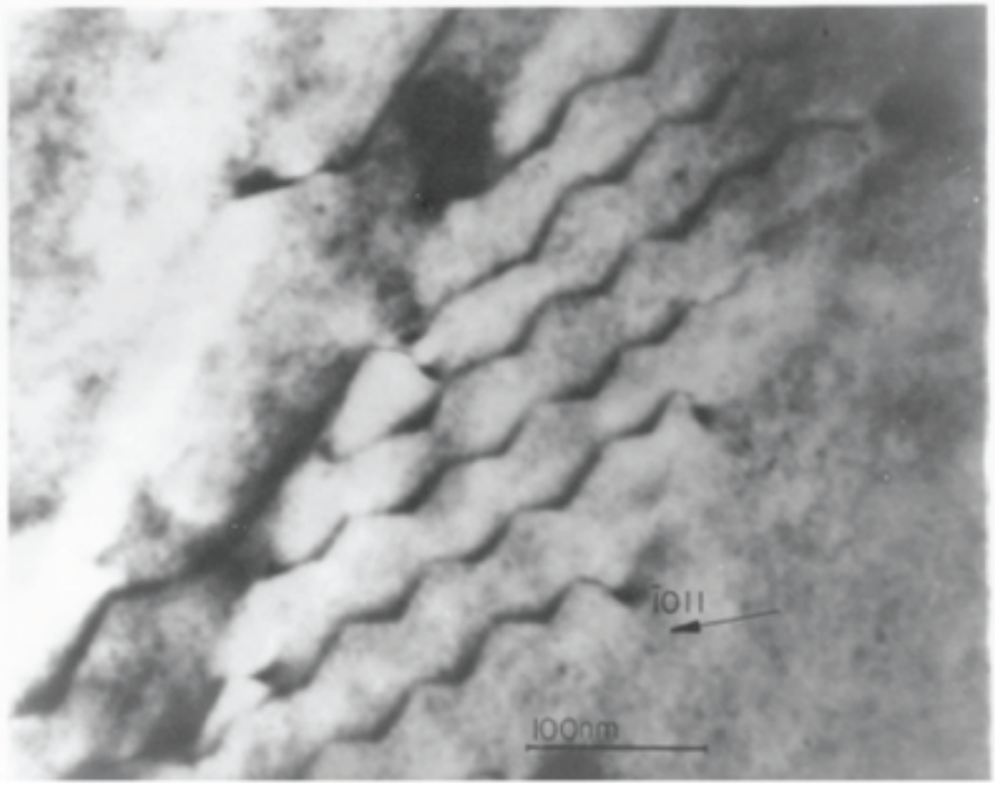
$g \cdot b( g \cdot R= 0)$是用來測定 dislocation Burgers Vector 的準則

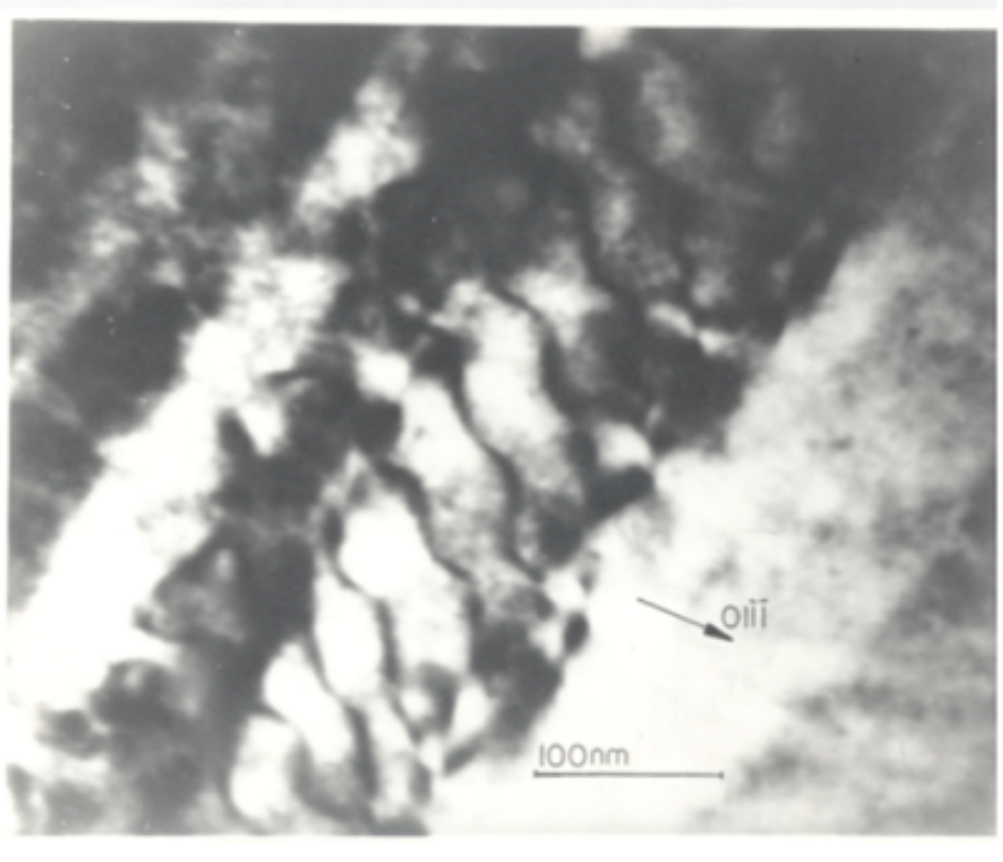
No contrast

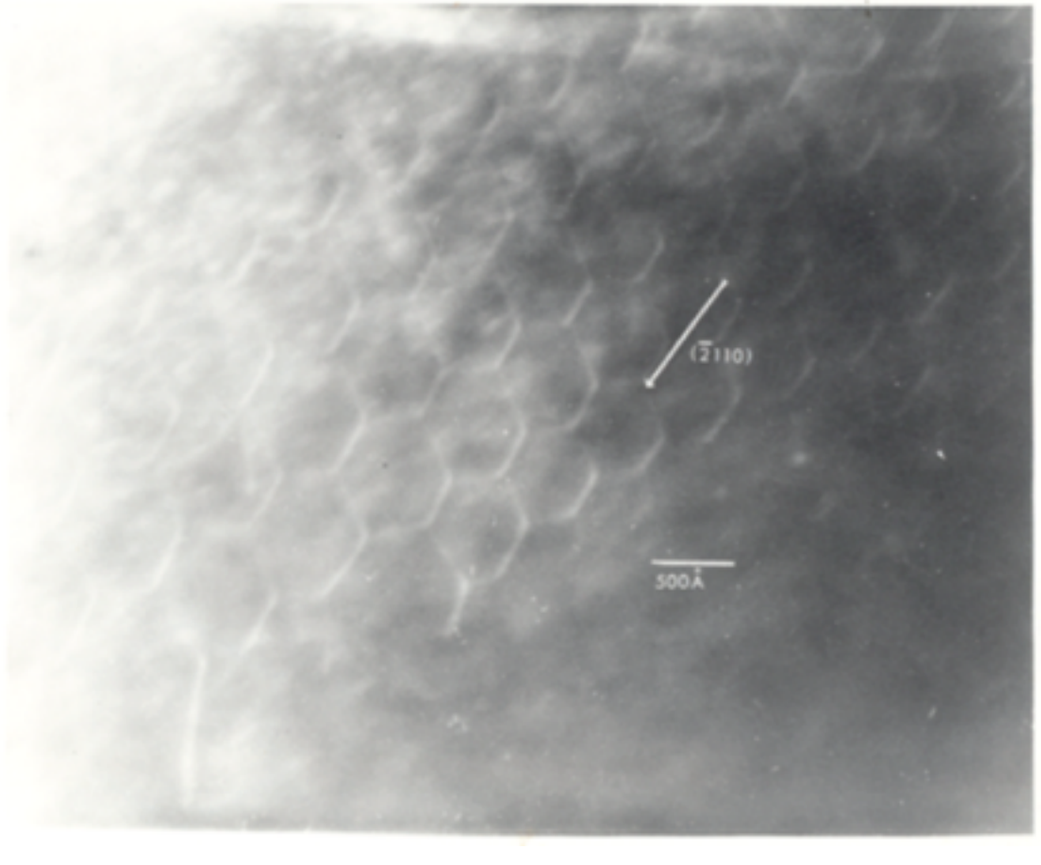

(A)
(B)
(C)
200 nm

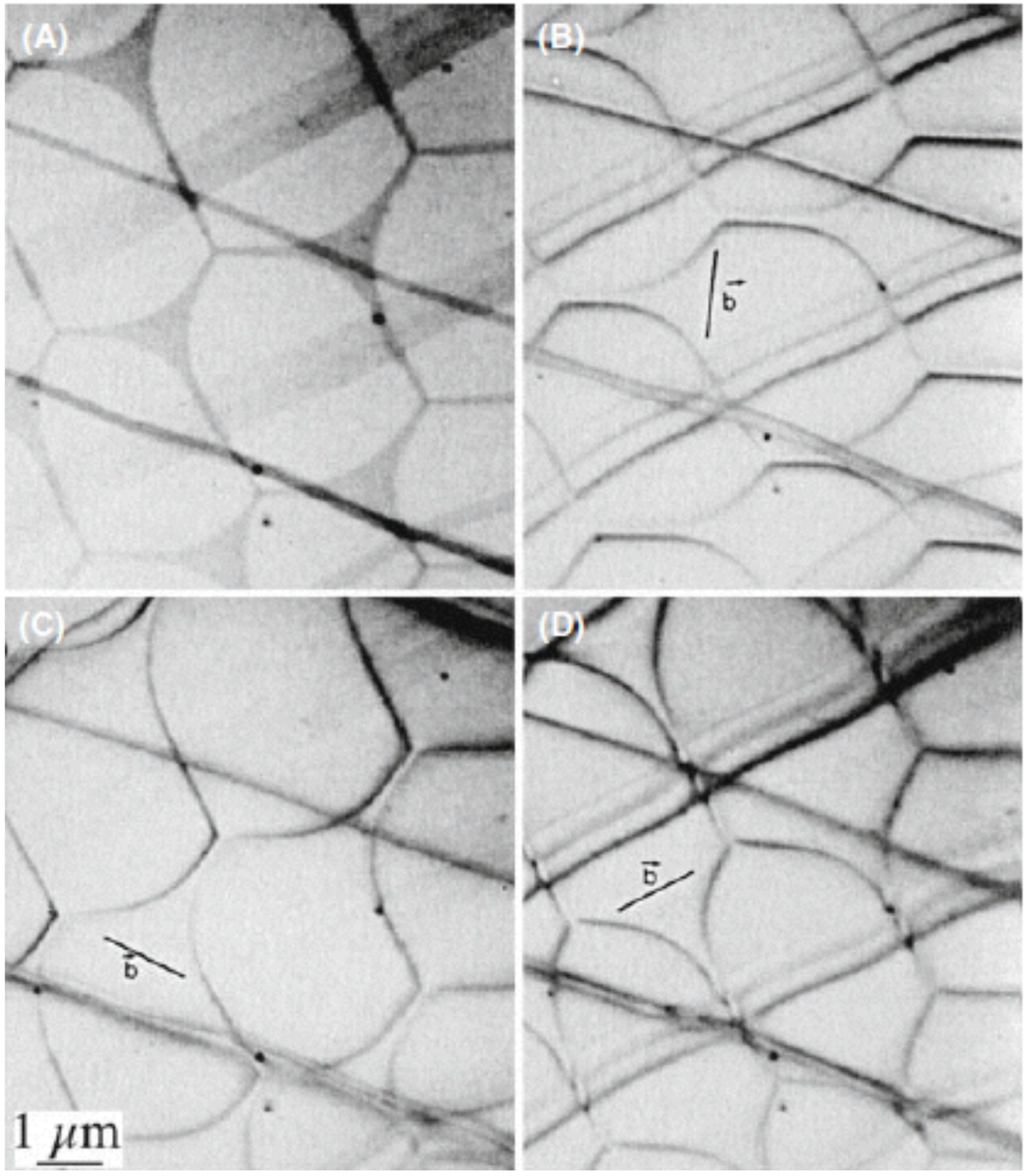

(D)
(E)
200 nm


$\bar{1}101$
100nm


$\bar{1}011$
100nm


$01\bar{1}\bar{1}$
100nm


$(\bar{2}110)$
500 Å

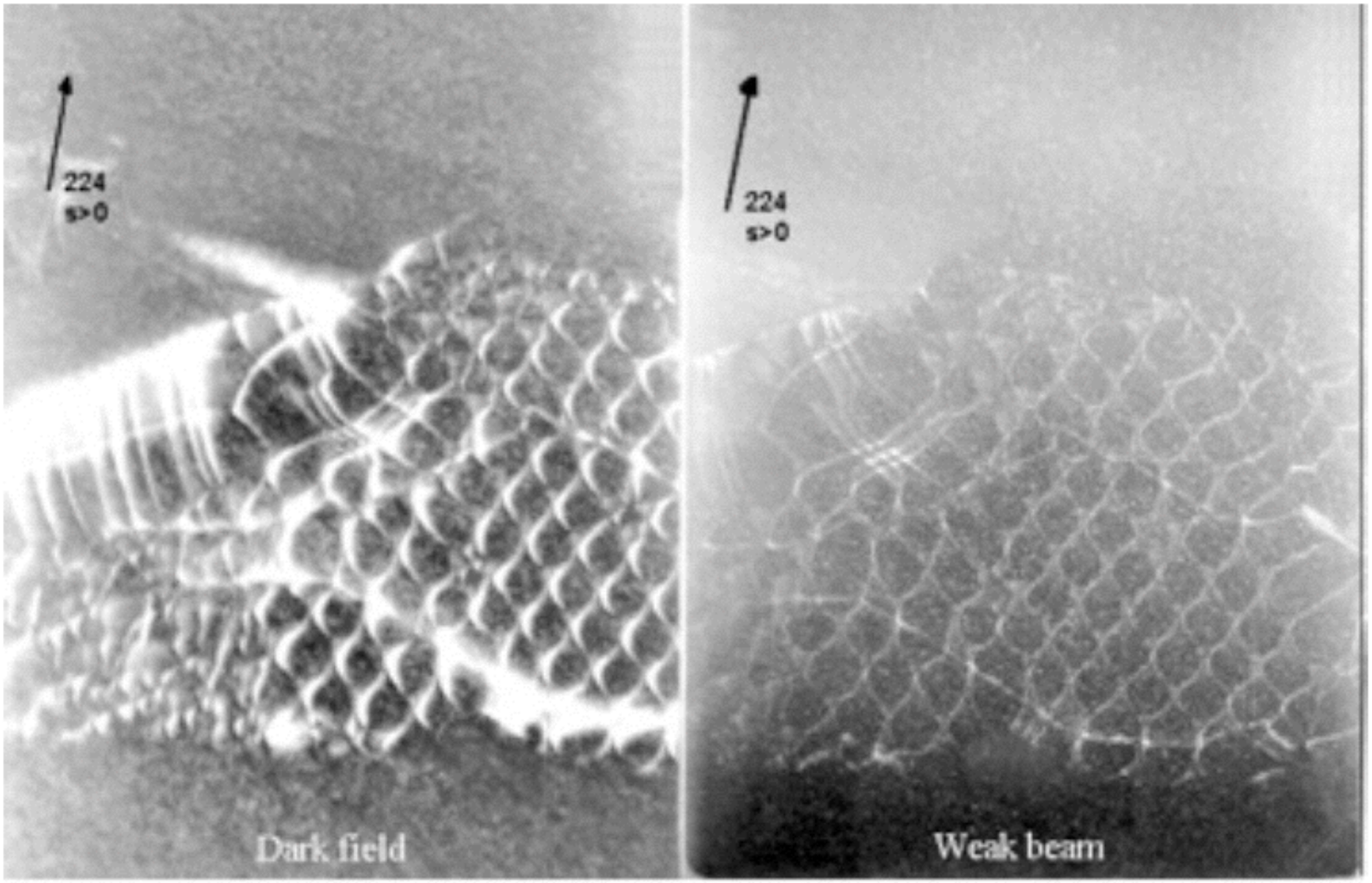

(A)
(B)
b
(C)
b
1 μm
(D)
b

Perfect dislocation 完美差排之鑑定Truth Table fcc

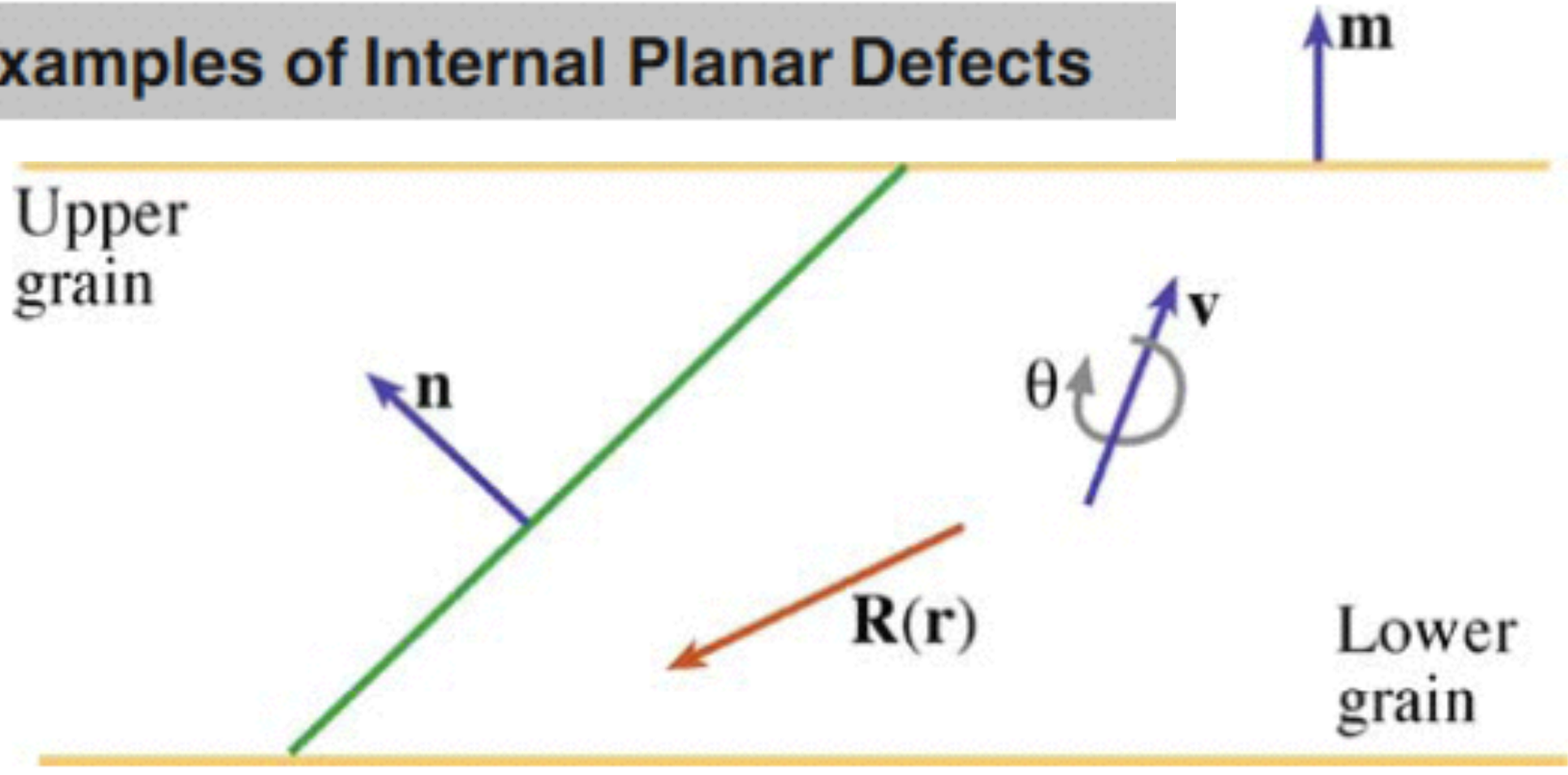
可能之Burgers Vector

| b \ g | 200 | 020 | 1-11 | -1-11 |
|---|---|---|---|---|
| ½[110] | 1 | 1 | 0 | -1 |
| ½[101] | 1 | 0 | 1 | 0 |
| ½[110] | 0 | 1 | 0 | 0 |
| ½[011] | 1 | -1 | 1 | 0 |
| ½[10-1] | 1 | 0 | 0 | -1 |
| ½[01-1] | 0 | 1 | 1 | -1 |

# Dark field and Weak beam



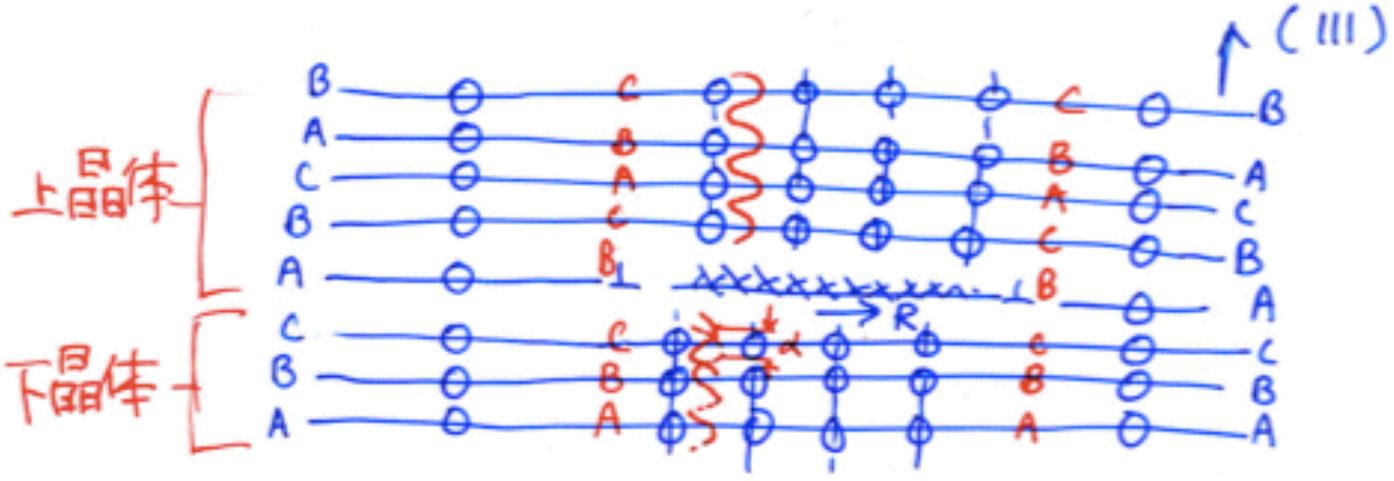
# Examples of Internal Planar Defects




| Planar defect | Structure | Example | Example |
|---|---|---|---|
| SF | Diamond-cubic, fcc, zinc blende | Cu, Ag, Si, GaAs | $\mathbf{R} = \frac{1}{3}[111]$ or $\mathbf{R} = \frac{1}{6}[112]$ |
| APB/IDB | Zinc blende, wurtzite | GaAs, AlN | Inversion |
| APB | CsCl | NiAl | $\mathbf{R} = \frac{1}{2}[111]$ |
| APB/SF | Spinel | $MgAl_2O_4$ | $\mathbf{R} = \frac{1}{4}[110]$ |
| GB | All materials | Often denoted by $\Sigma$ where $\Sigma^{-1}$ is the fraction of coincident lattice sites | Rotation plus **R** |
| PB | Any two different materials | Sometimes denoted by $\Sigma_1, \Sigma_2$ which are not equal | Rotation plus **R** plus misfit |
| RB | Extra translation | {112} Twin boundary in Al | **R** not related to lattice |

① 疊差 (Stacking Fault)：上,下晶体位移3-個向量 $\vec{R}$

- 面心立方 (fcc metal), dimond, HCP)




- 在實空間的位移
→倒空間相位差

$\alpha = 2\pi g \cdot R$

- 注意 $g \cdot R = 0$

Stacking Fault out of contrast
沒看到缺陷，並不代表它不在那兒.
"電子束看到完美的晶体"

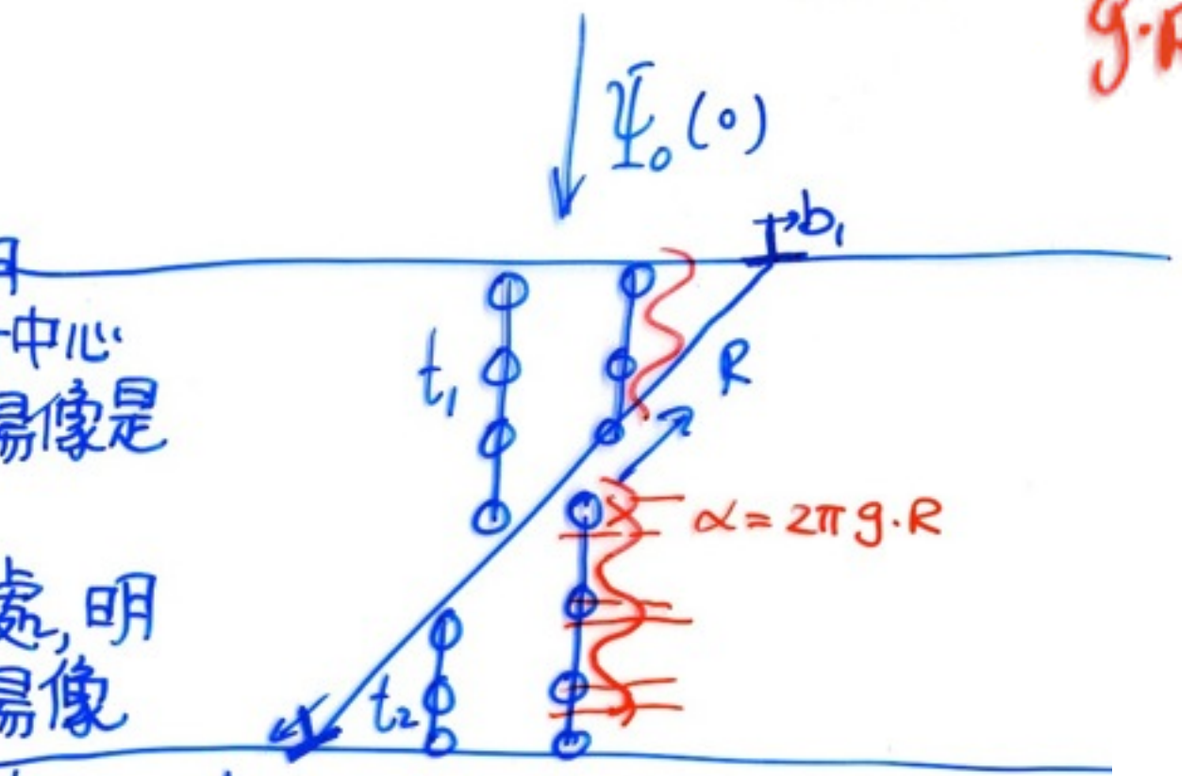
| | R | g | $\alpha = 2\pi\, g.R$ (mod $2\pi$) |
|---|---|---|---|
| SF in fcc | $\frac{1}{3}[111]$ | (111), (220), (113) | $2\pi/3$ |
| SF in fcc | $\frac{1}{3}[111]$ | (113) | $4\pi/3$ |
| Translation at APB in $Fe_3Al$ | $\frac{1}{2}[110]$ | (100) | $\pi$ |
| Small **R**, e.g., NiO | Any | **g** or **s** or $\xi_g$ differ slightly | $\delta$ |

- $g\cdot R>0$，明場第一條紋亮
  $g\cdot R<0$，明場第一條紋暗

- 明場像的明暗條紋是對中心對稱，而暗場像是非對稱

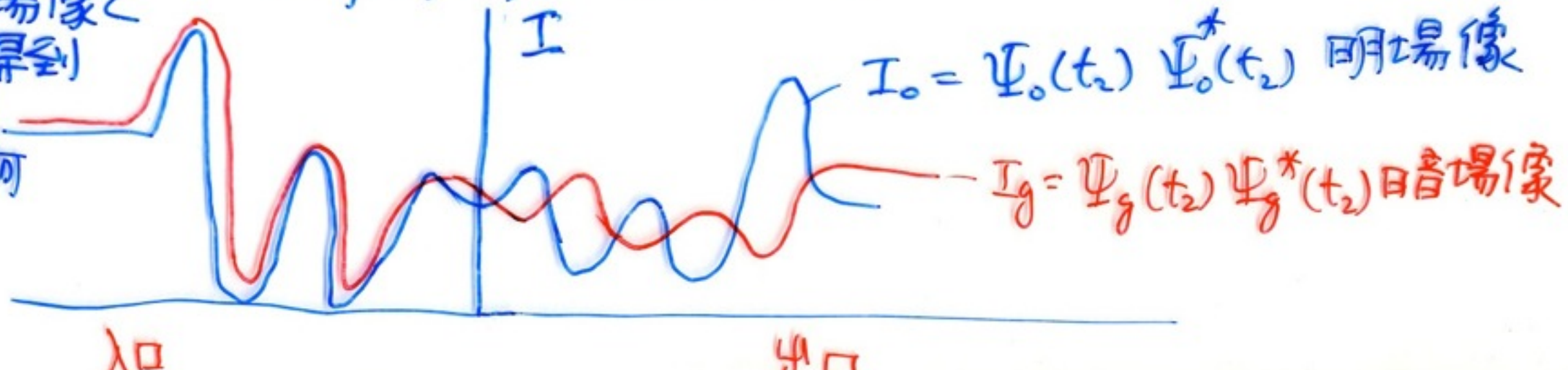
- 在試片入口處，明場像和暗場像都是相同對比而在出口處是相反對比

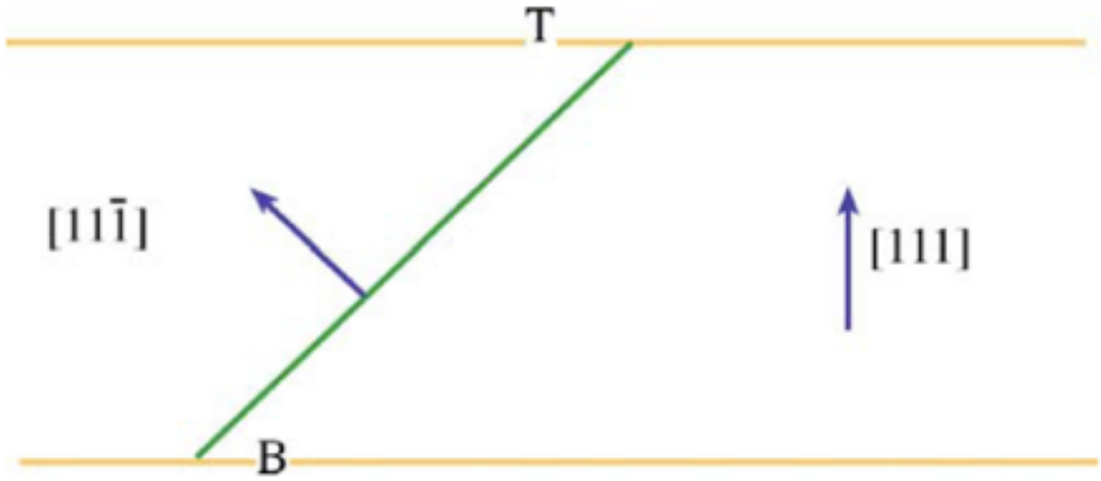
③ 可由明場像與暗場像之比較得到 Stacking Fault 如何位移.




$\Psi_0(t_2)$ $\Psi_g(t_2)$

(Bright field) (Dark Field)

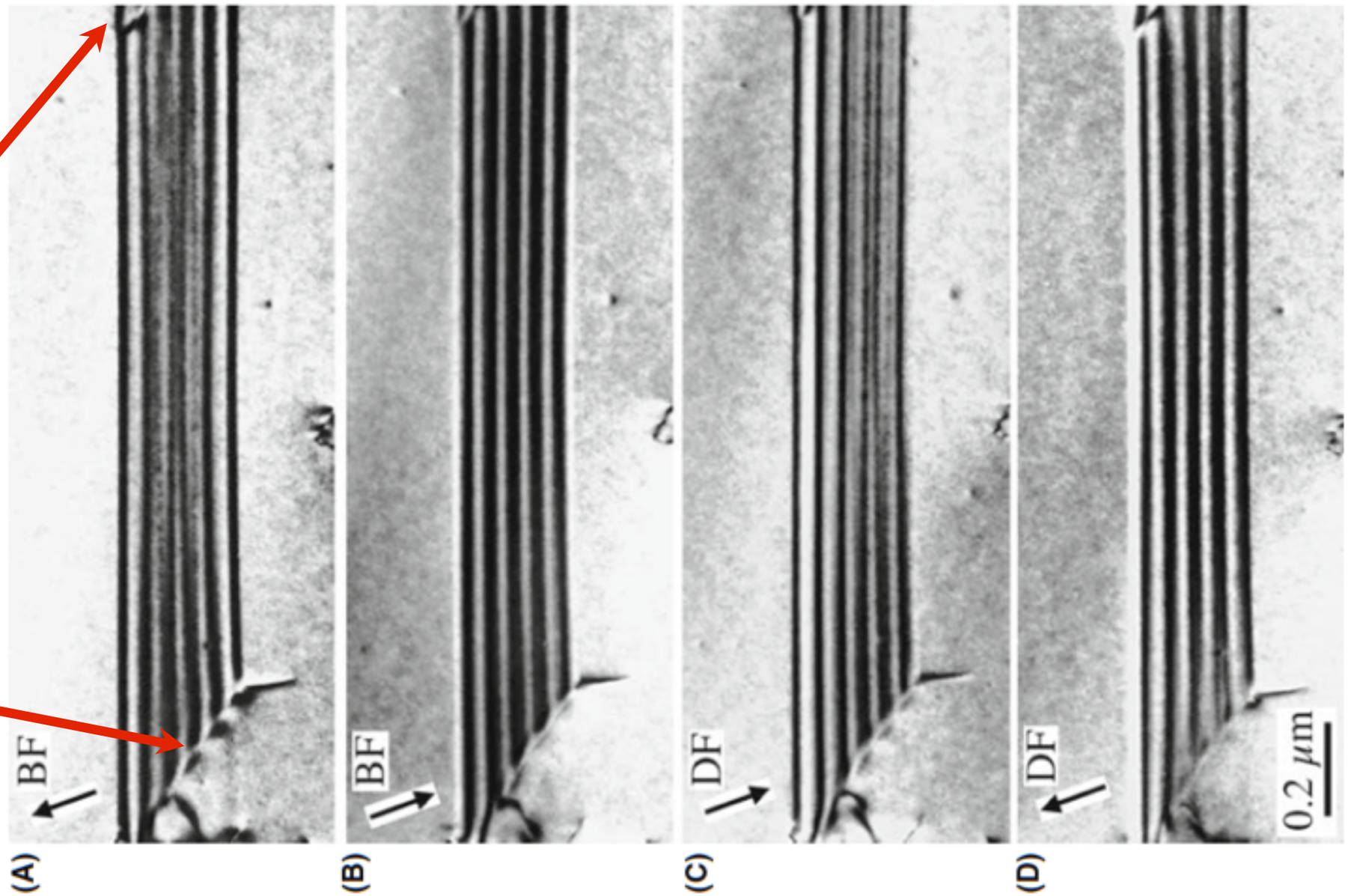


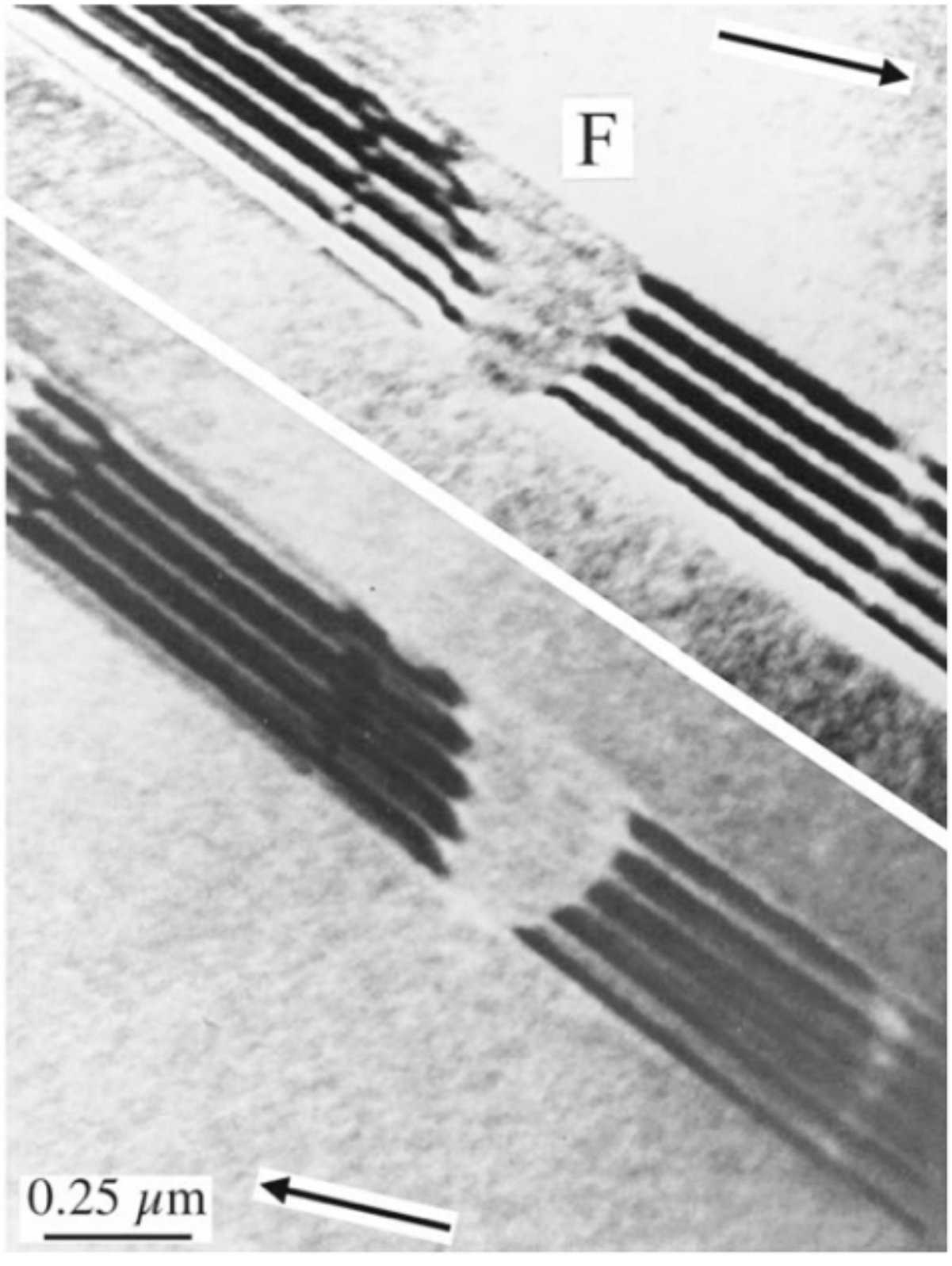



At the bottom surface: the contrast in BF and DF are complementary

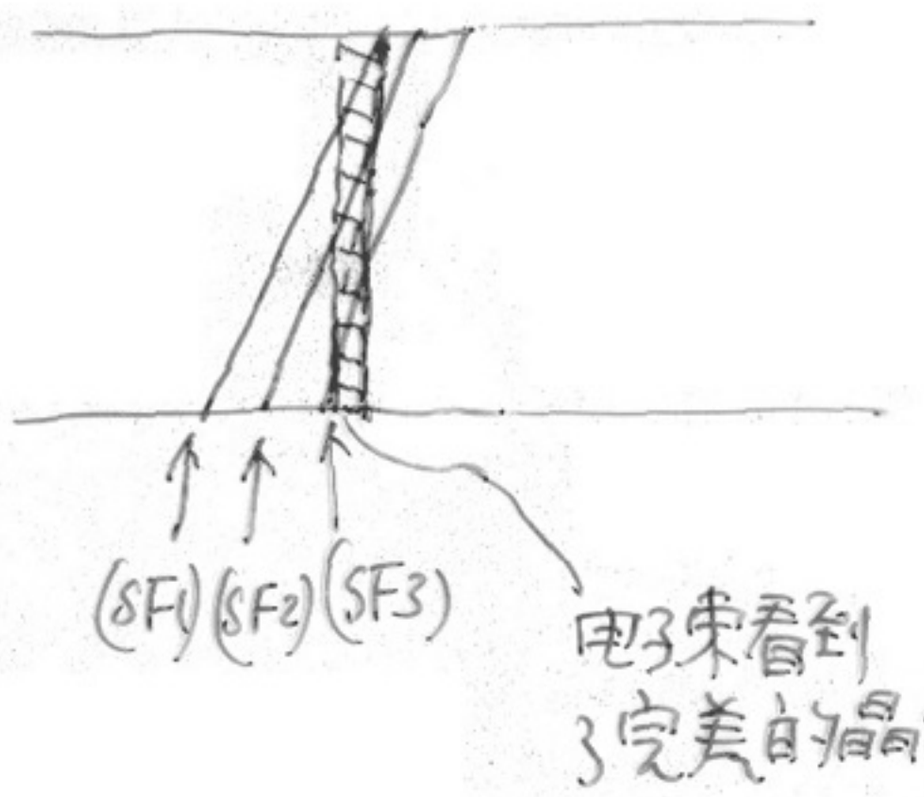
At the top surface: the contrast in BF and DF are same

partial dislocations





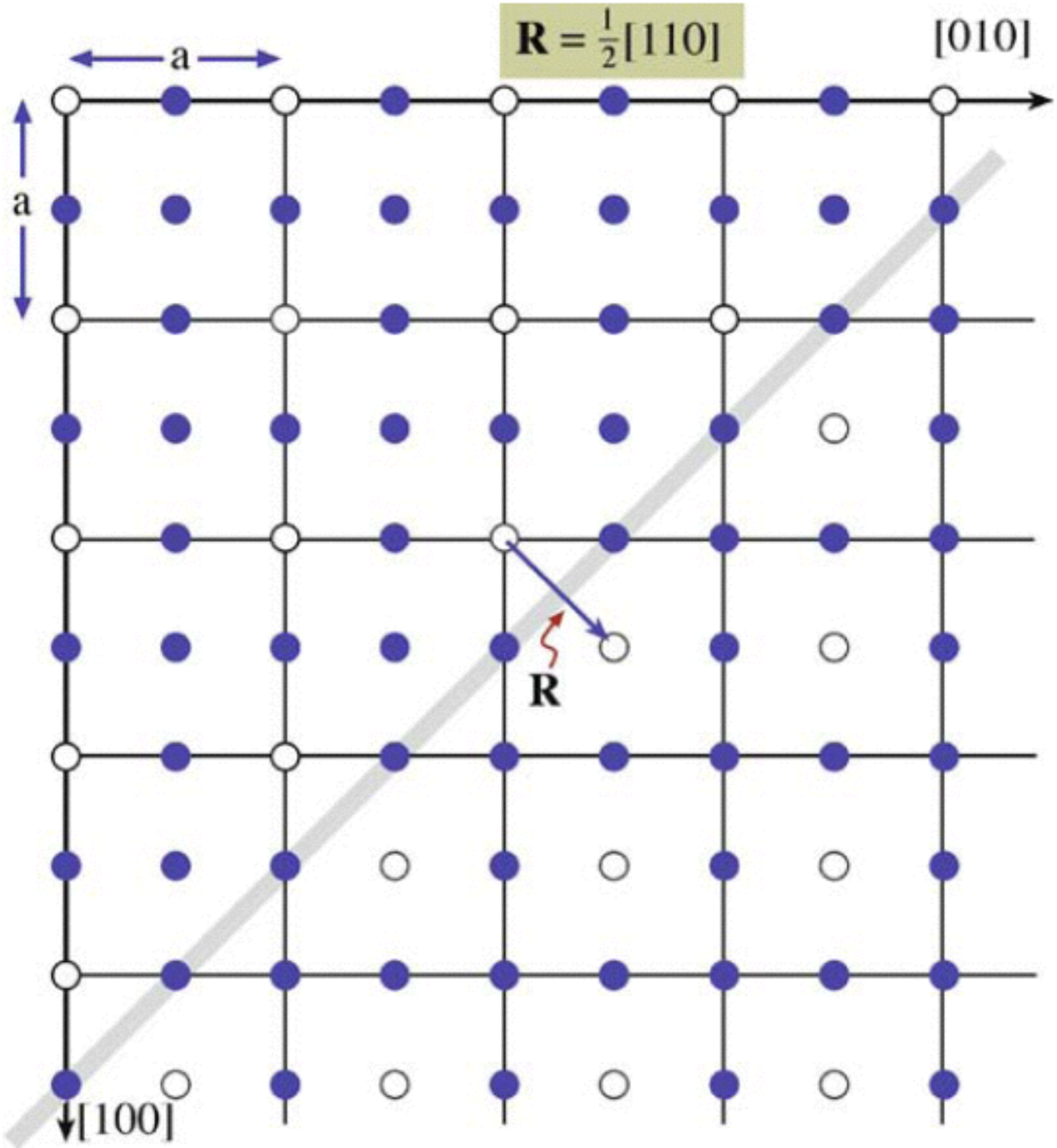

# 重疊"疊差"



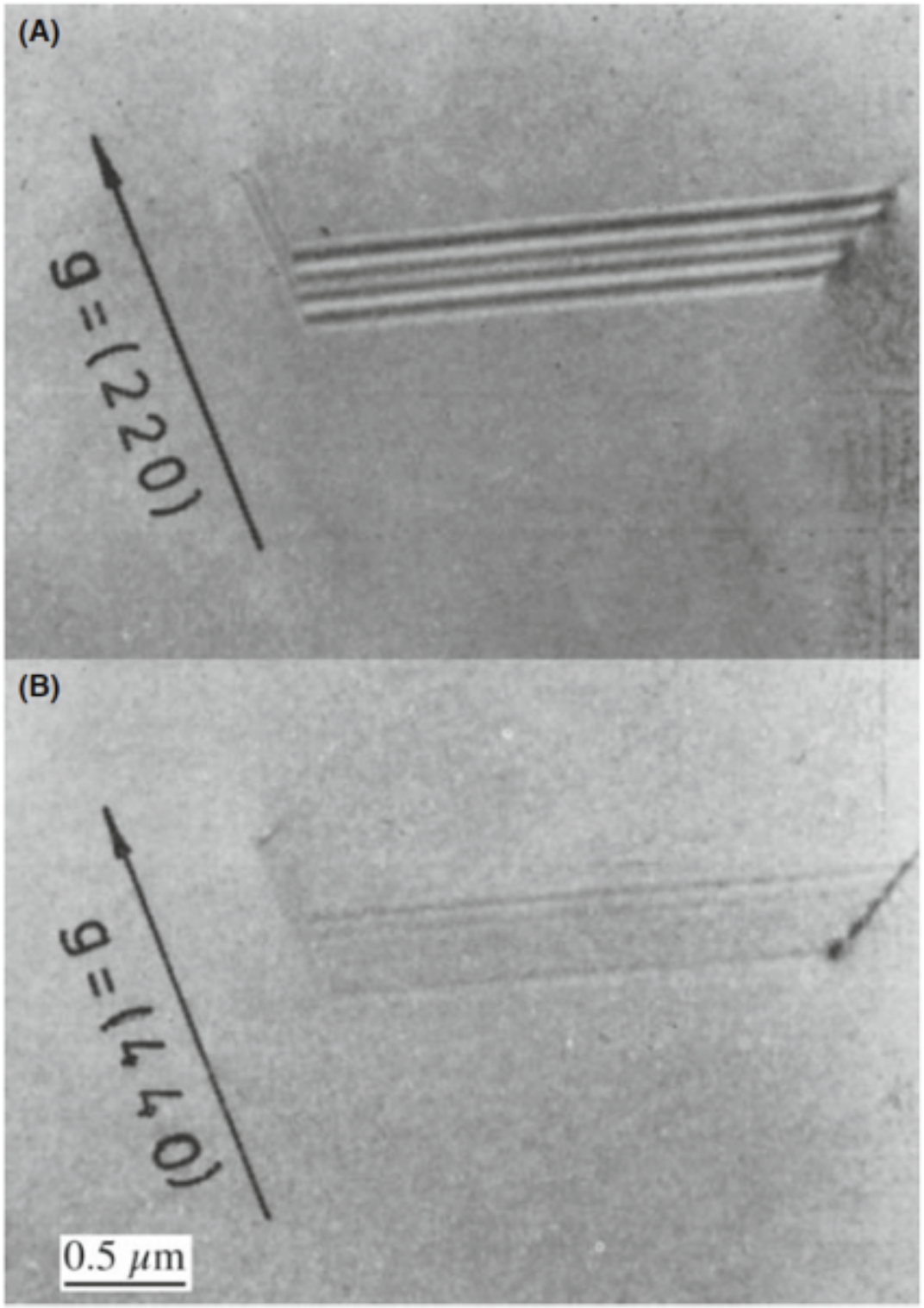

$R_t = 3 \cdot \frac{1}{6}[112] = \frac{1}{2}[112]$

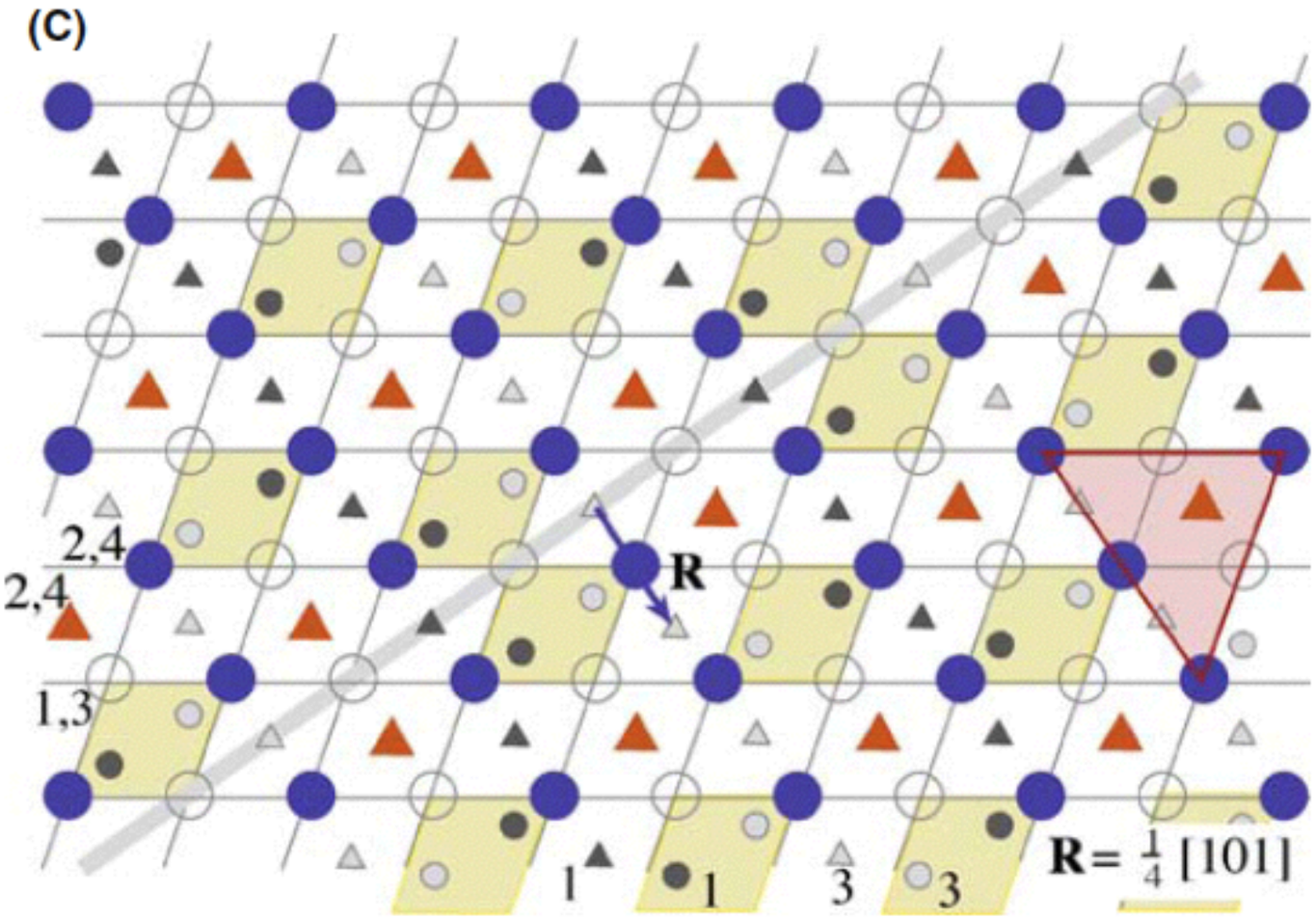
$R_t = 3 \cdot \frac{1}{3}[111] = \frac{1}{3}[111]$

# OTHER TRANSLATIONS: π AND δ FRINGES

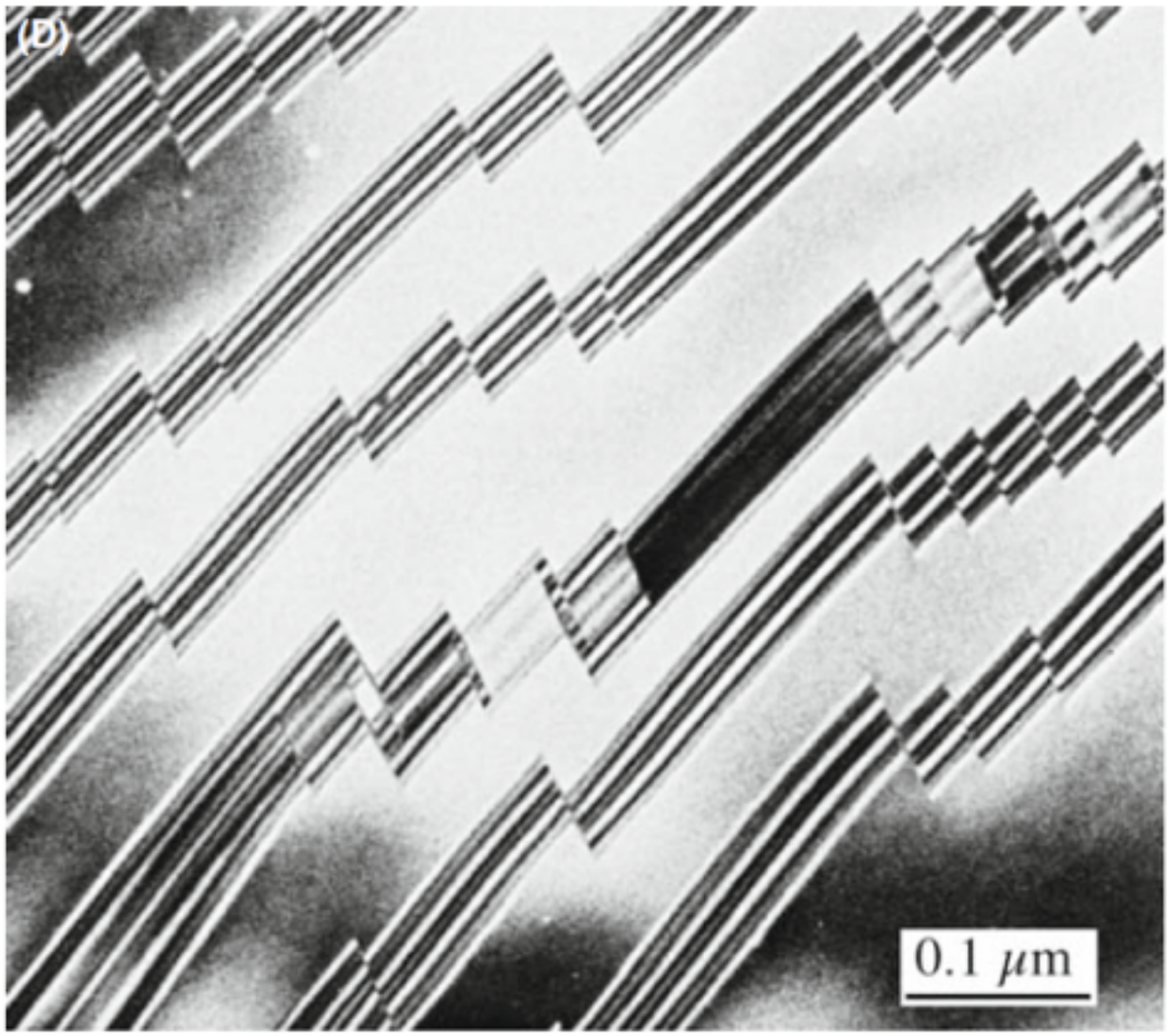


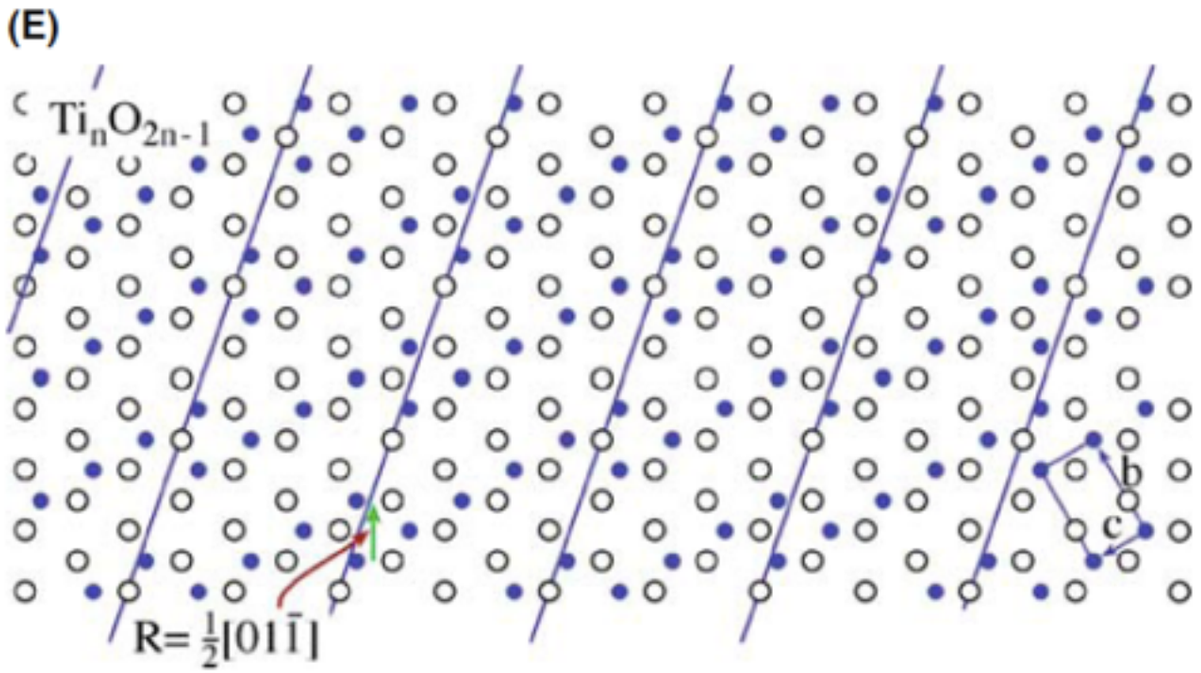
# APBs in $TiO_2$.



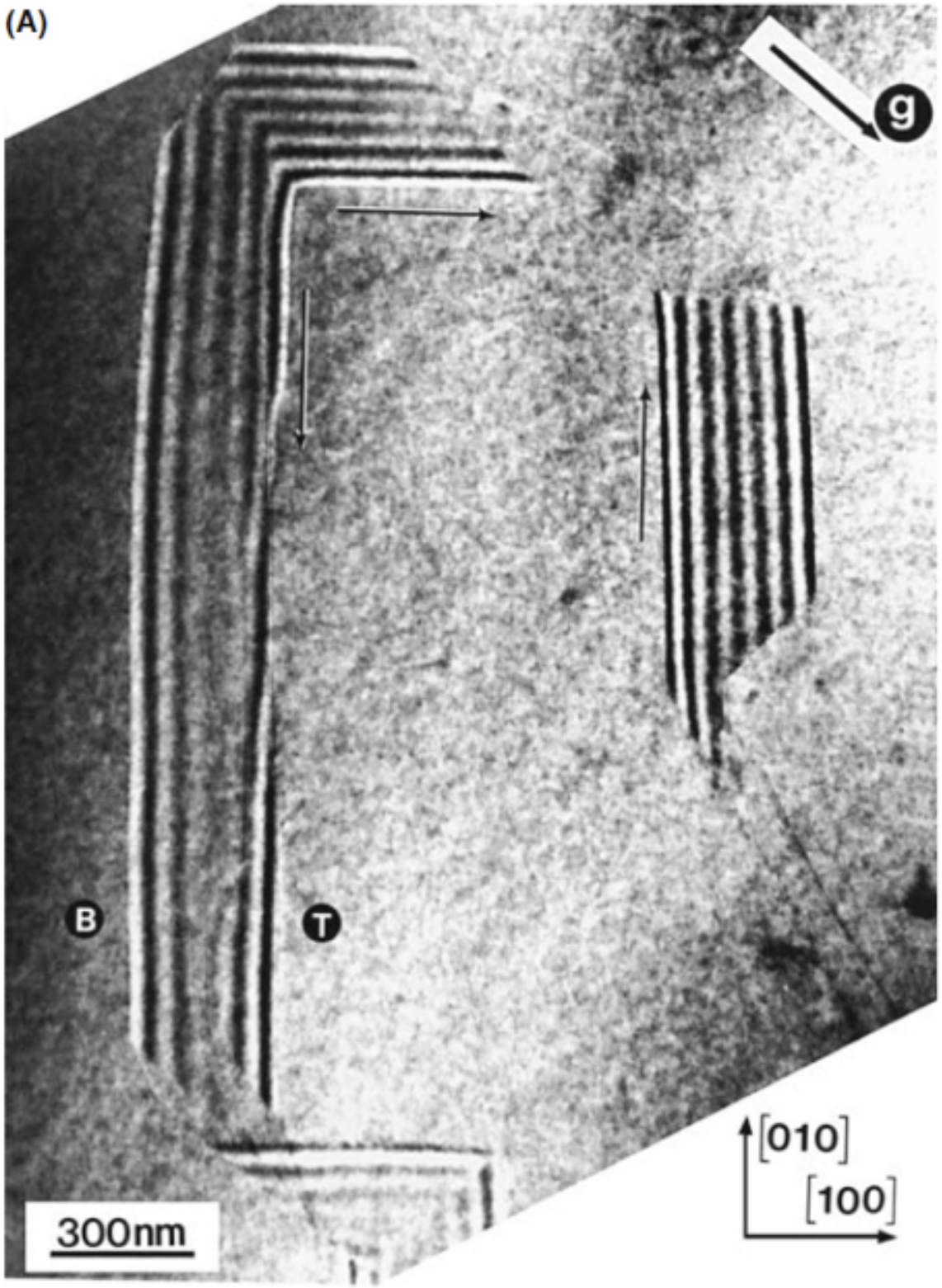



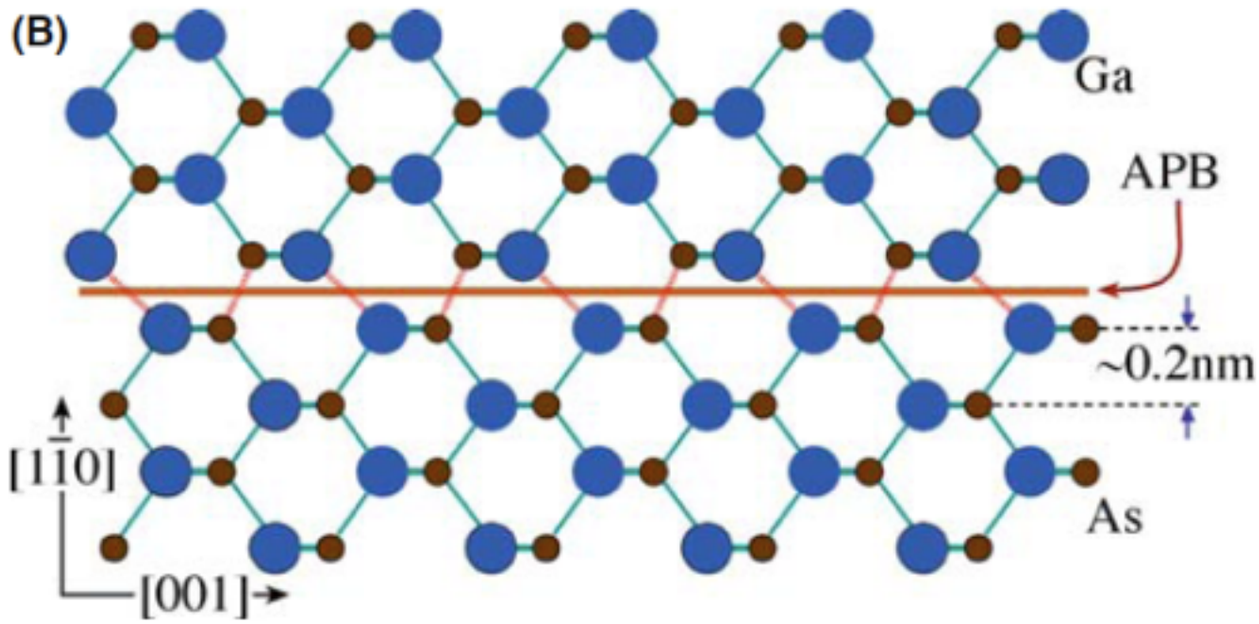
# APBs in $TiO_2$



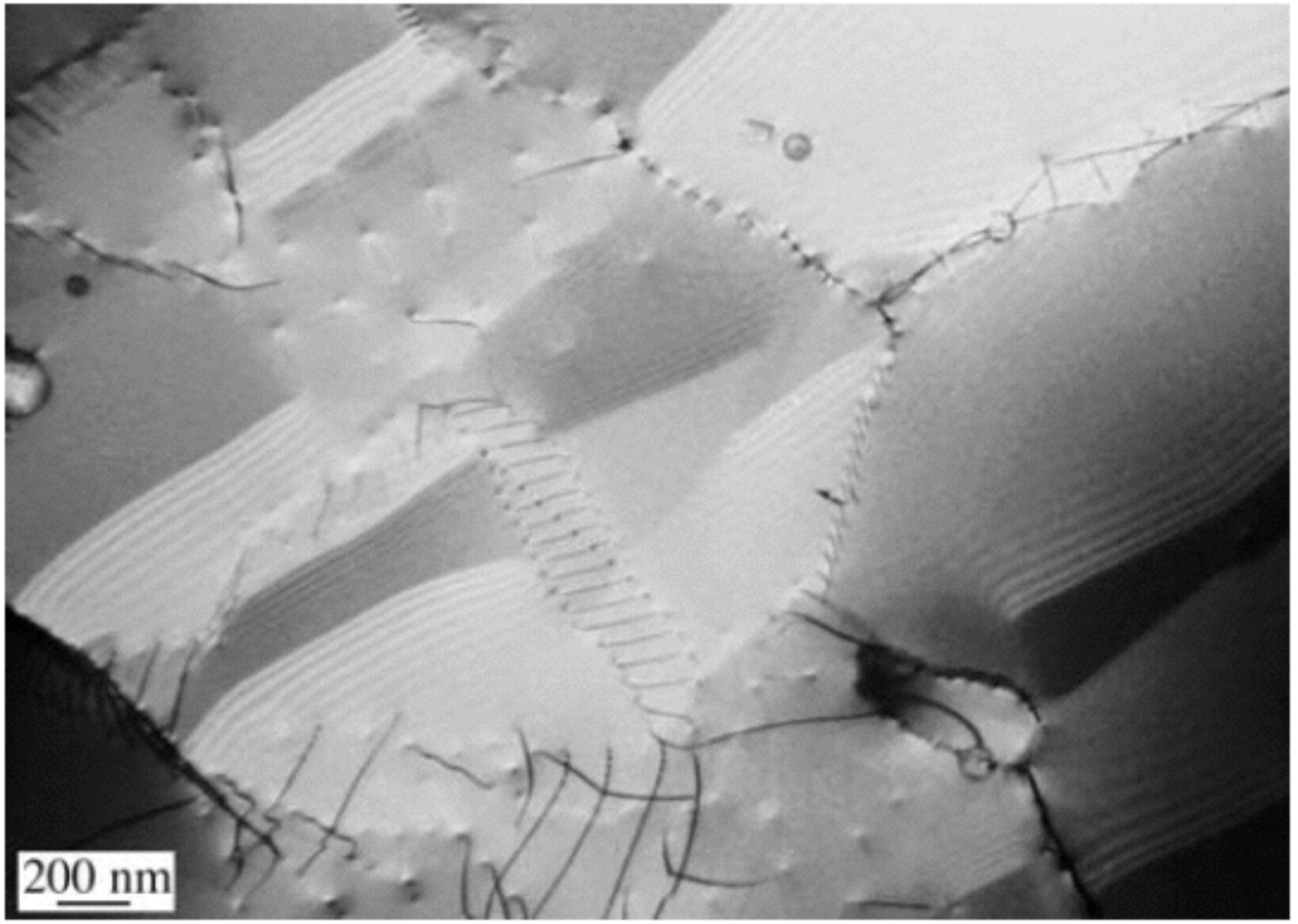
# APB (or IDB) of GaAs



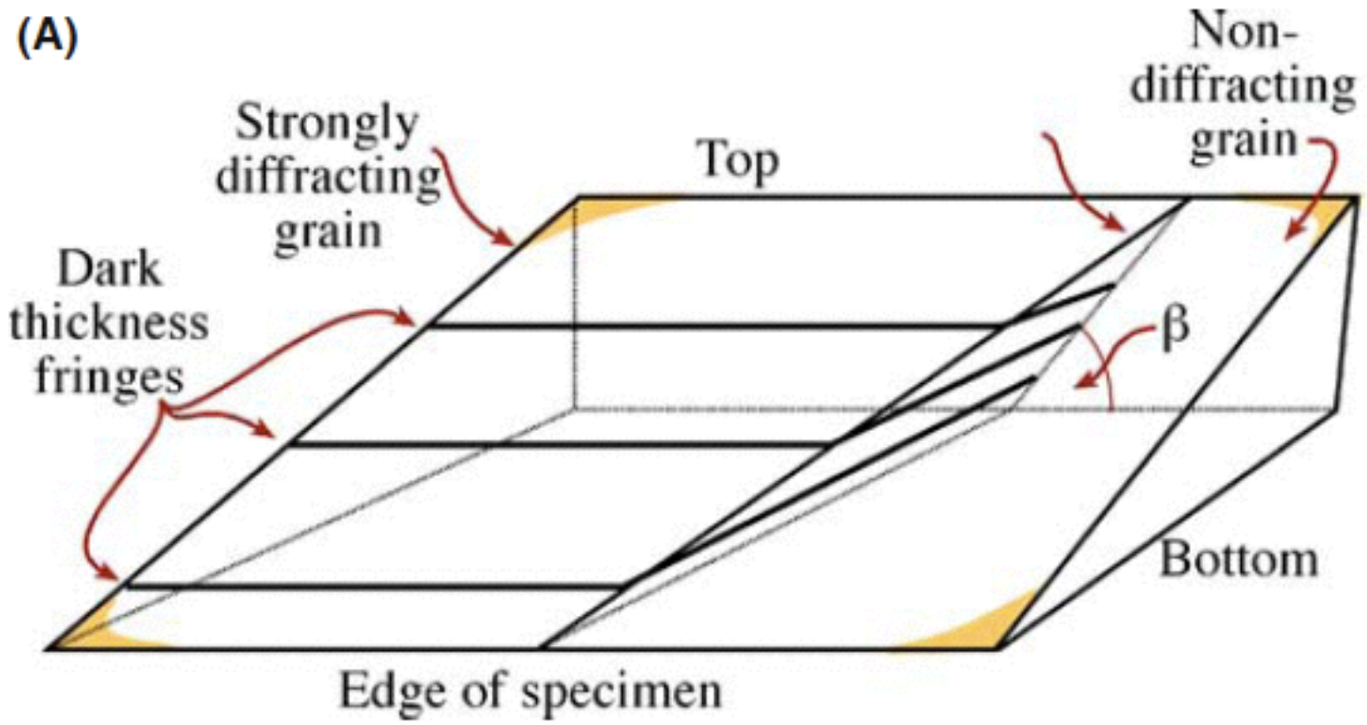
# Examples of Special Phase Boundaries

| Boundary | Example of material | Features |
|---|---|---|
| Ferromagnetic domain boundaries | NiO | |
| Ferroelectric and piezoelectric boundaries | $BaTiO_3$ | Small tetragonal distortion |
| Composition boundary | GaAs/AlGaAs | $\xi_g$ is different on two sides of boundary, even for perfect lattice matching |
| Structure boundaries | $\alpha$-SiC/$\beta$-SiC | |
| | hcp-Co/fcc-Co | |
| Composition/structure | NB/$Al_2O_3$ | |
| | Al/Cu | |
| | $\alpha$-Fe/$Fe_3C$ | |

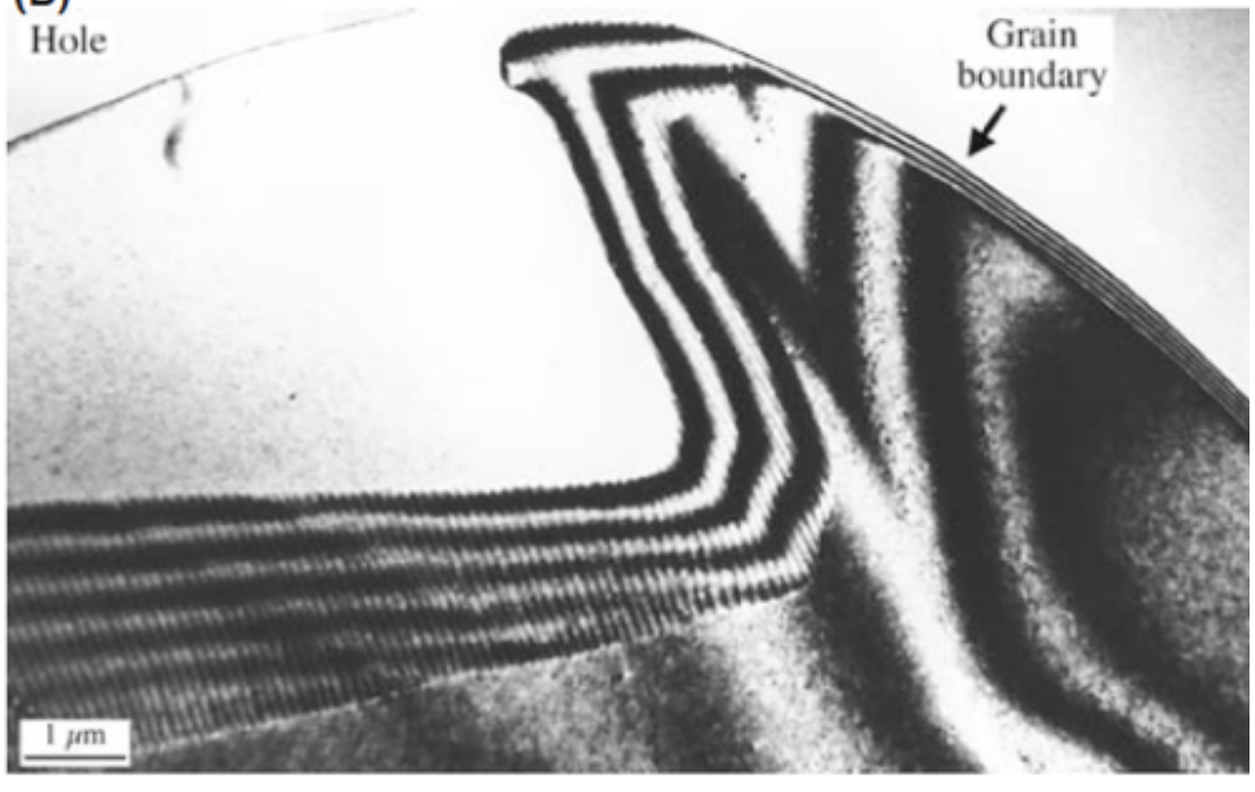



The ferroelectric material NiO undergoes a structural change from cubic to distorted rhombohedral at the Curie temperature. Although the distortion in the rhombohedral structure is very small, it does cause a detectable rotation of the lattice planes that results in the $\delta$ fringes in the image.

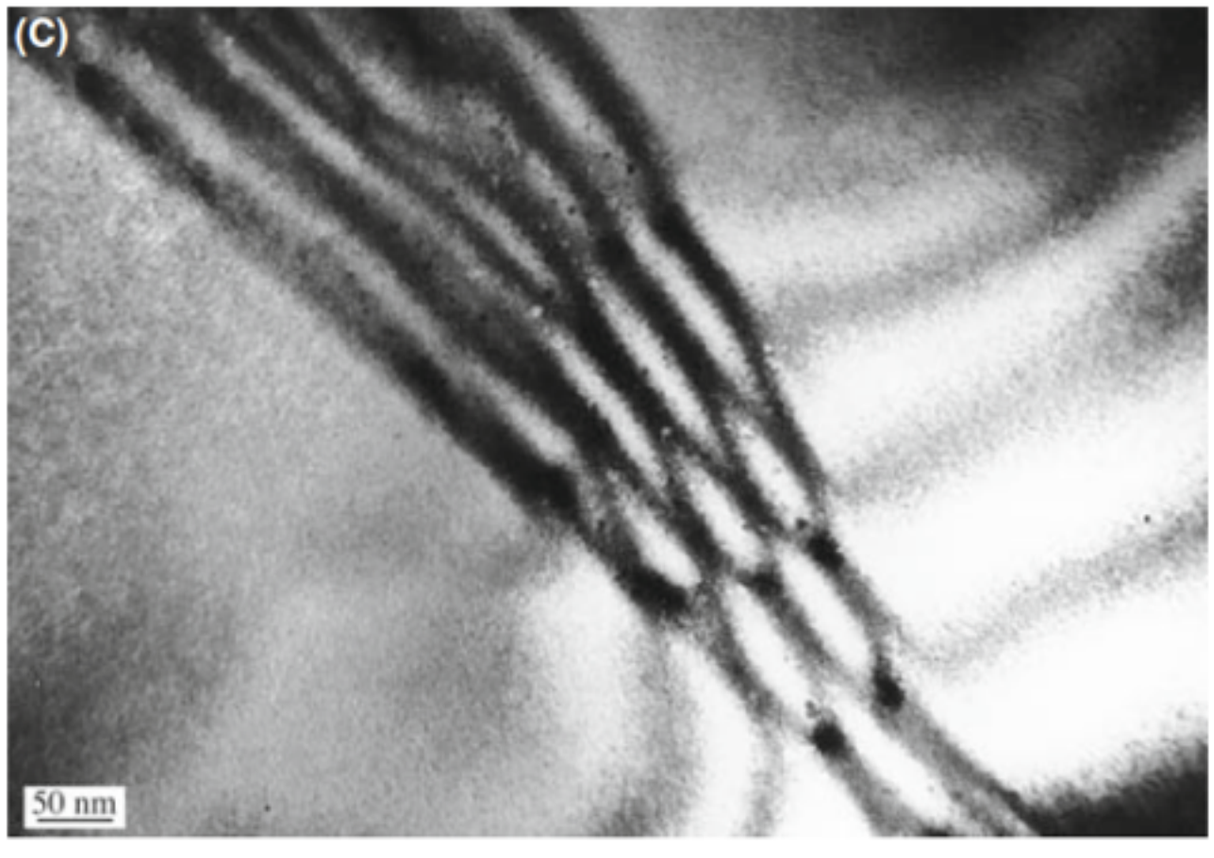
(A)


Strongly diffracting grain
Top
Non-diffracting grain
Dark thickness fringes
β
Bottom
Edge of specimen

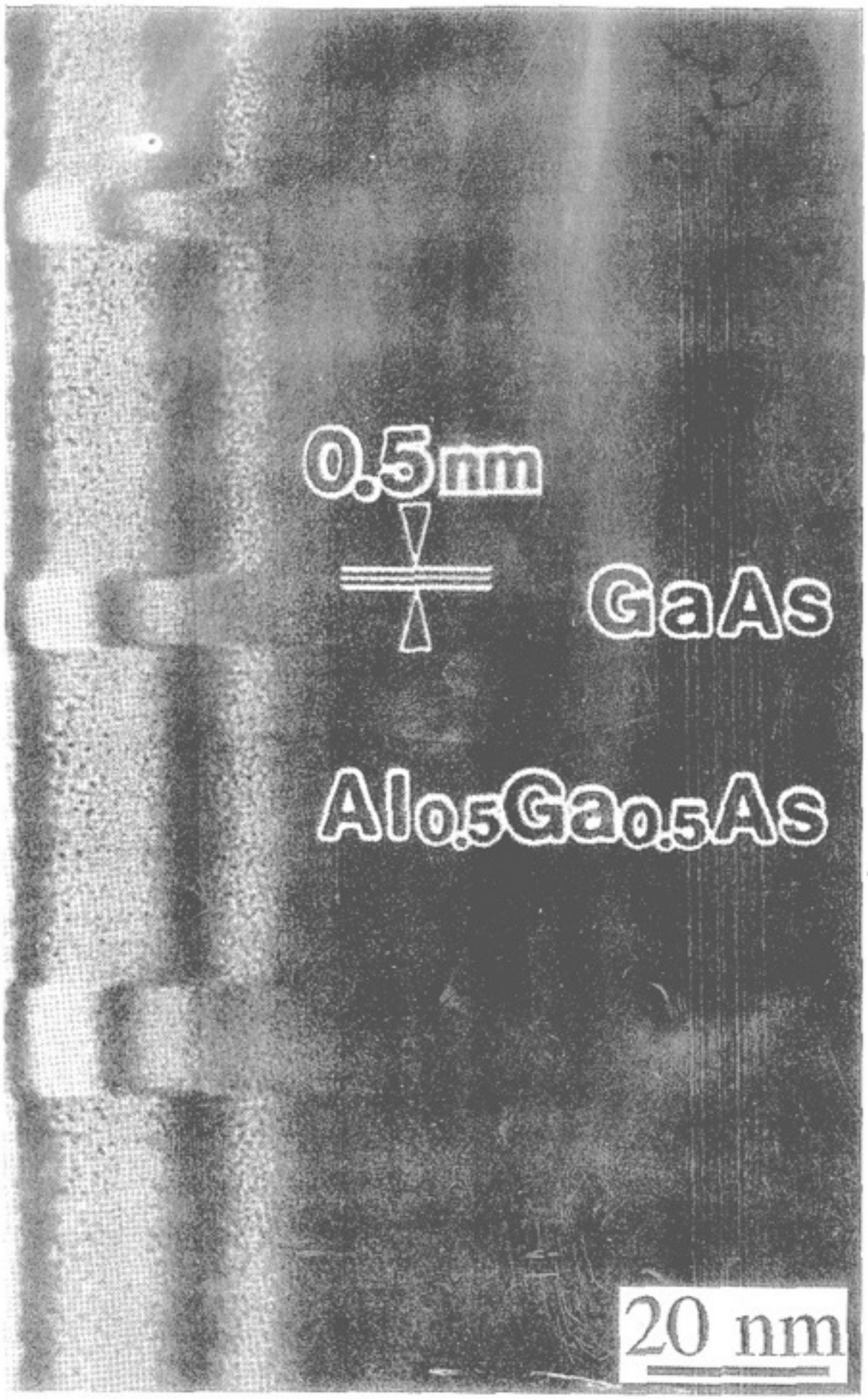
(B)


Hole
Grain boundary
1 μm

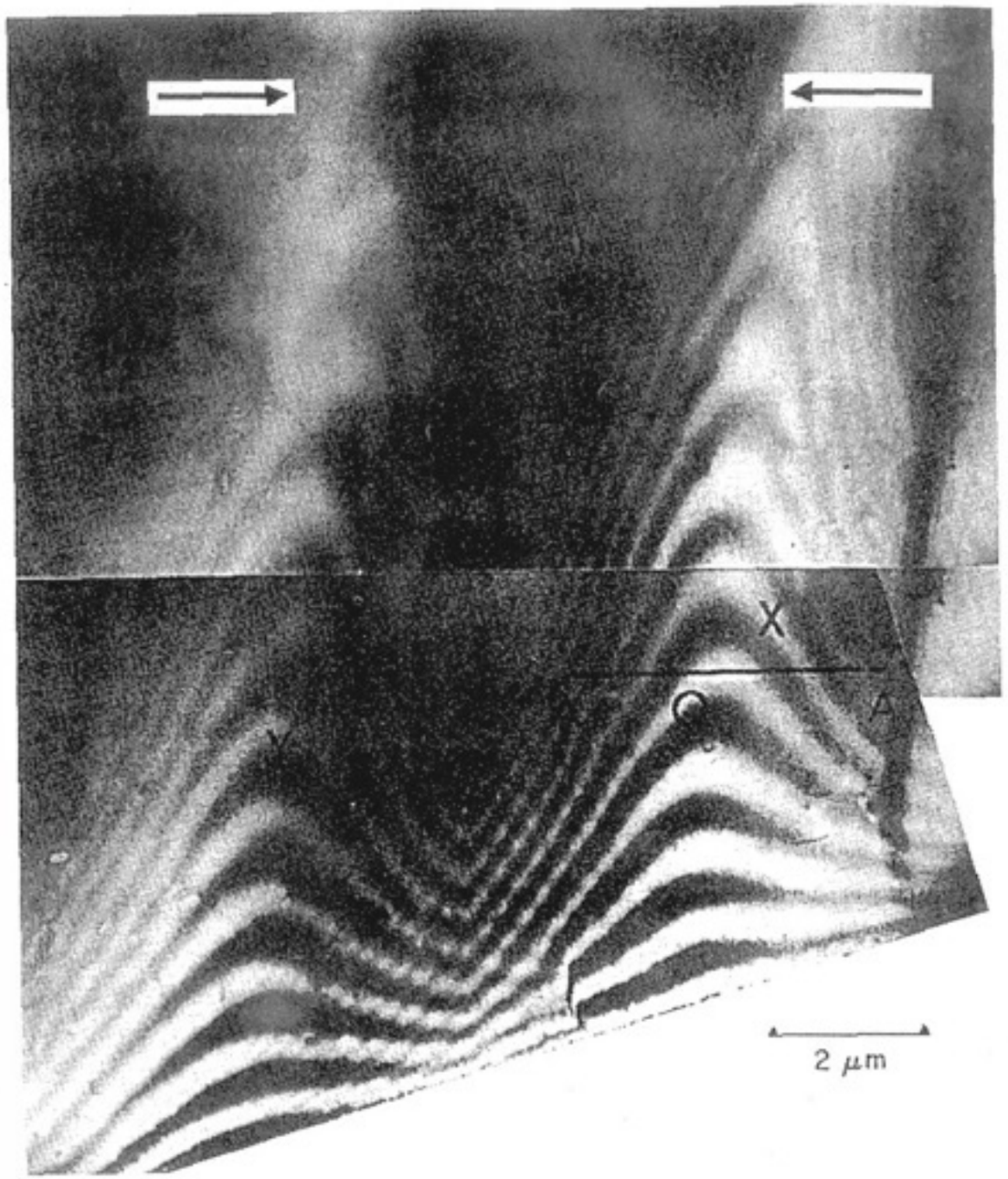
(C)


50 nm

A

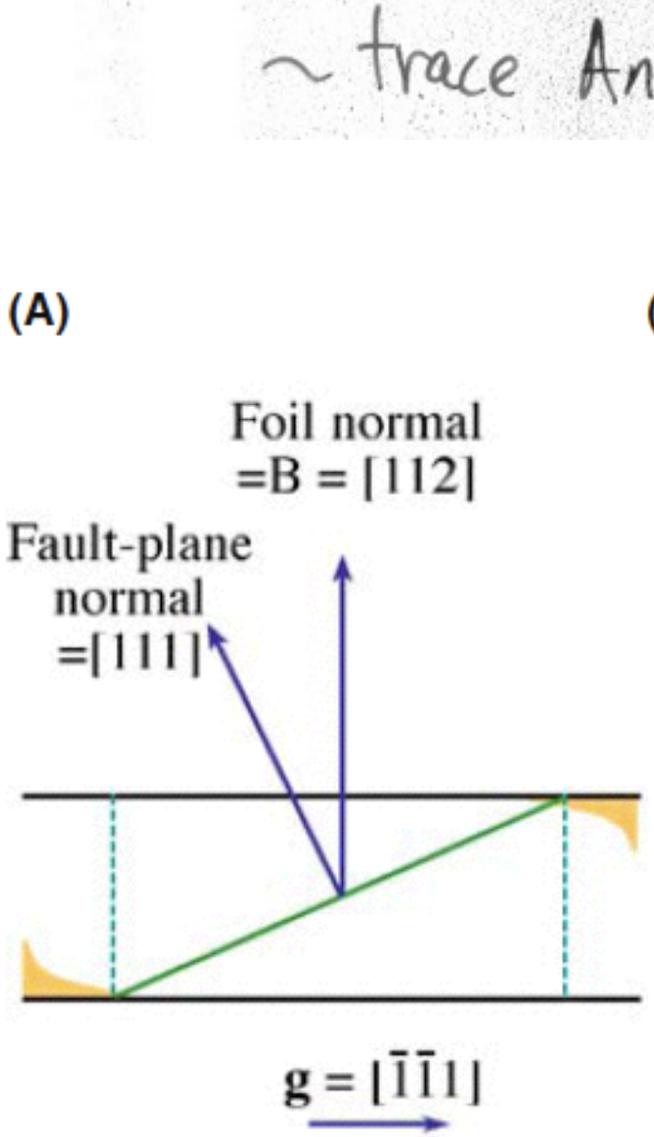


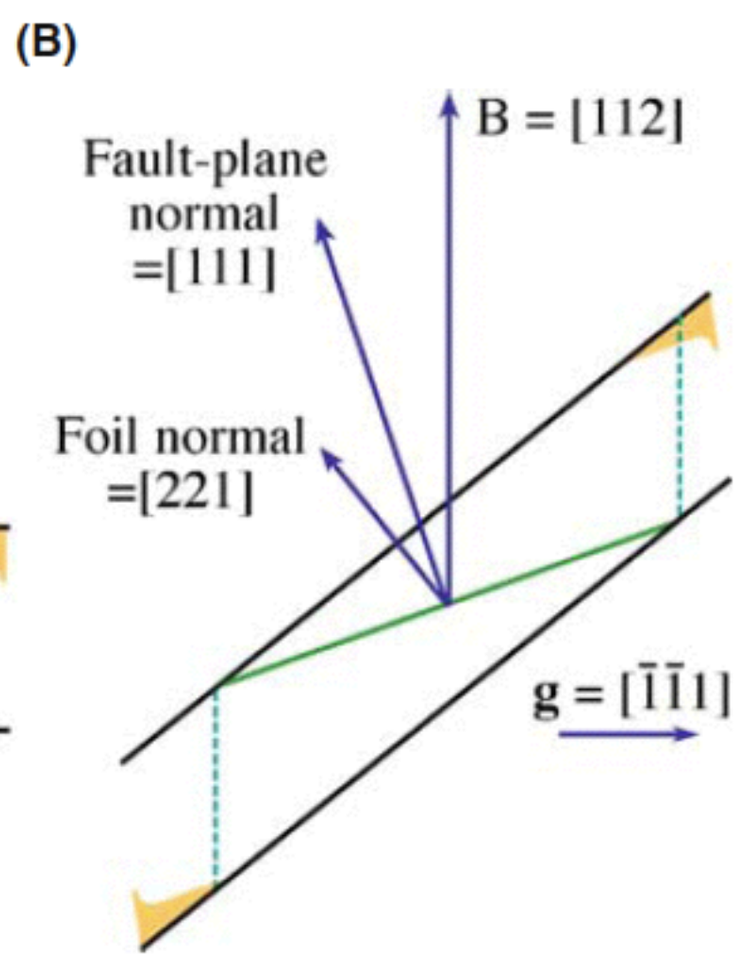


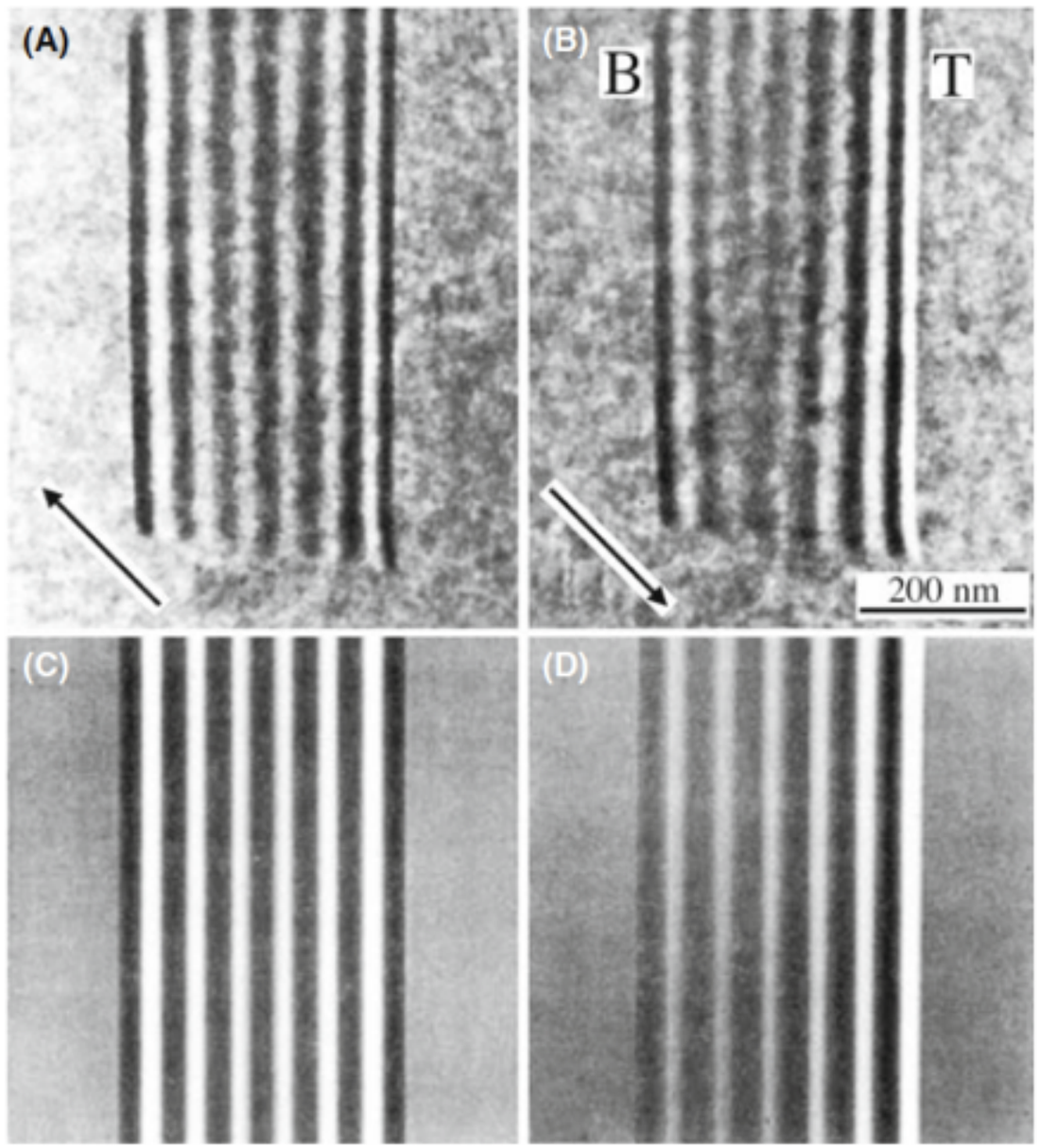



電腦模擬 (Computer Simulation)

- $\vec{B}$, $\vec{g}$, $\vec{S}$ 由 Kikuchi pattern 求得
- Stacking plane normal, dislocation 方向
  ~ trace Analysis



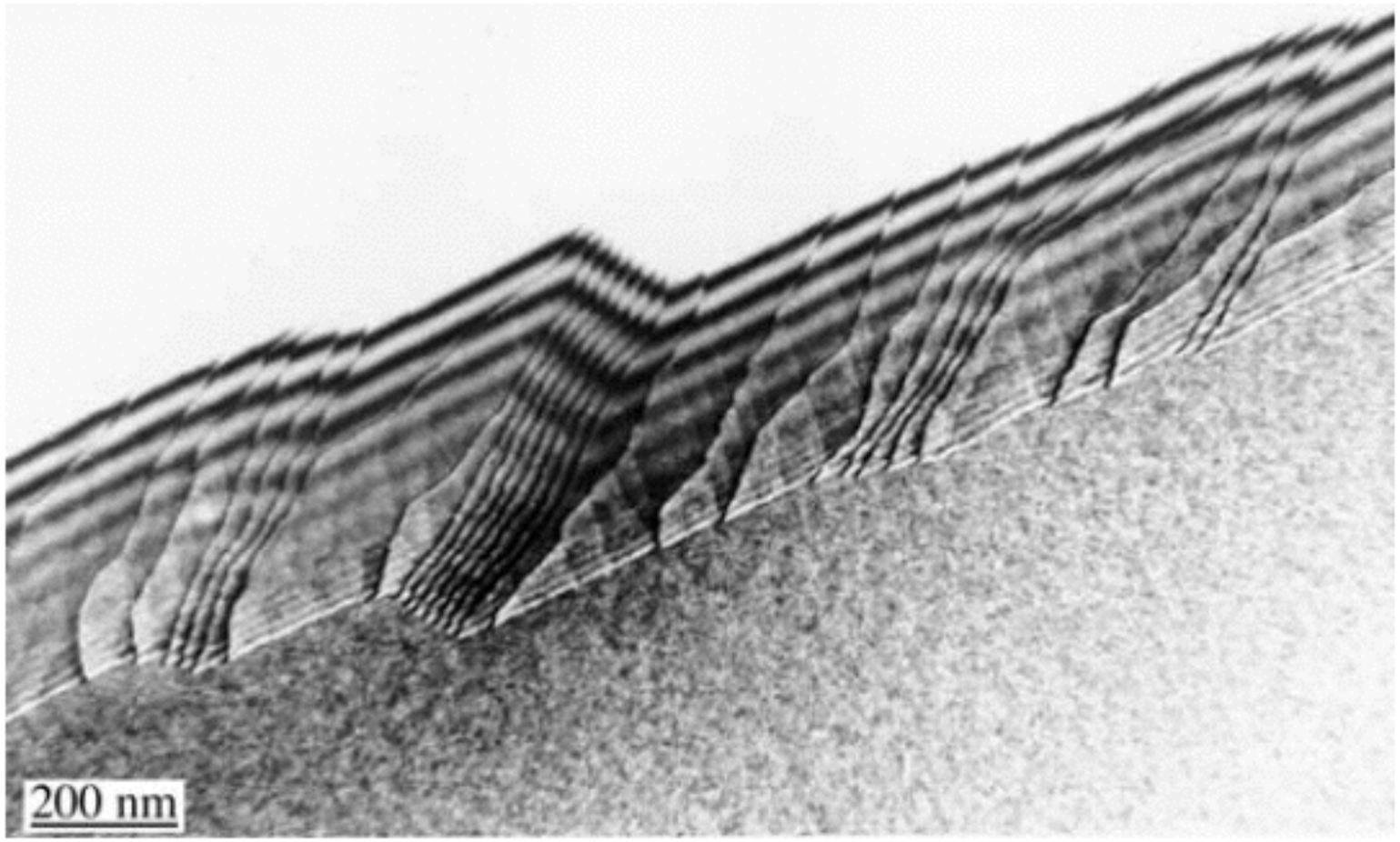
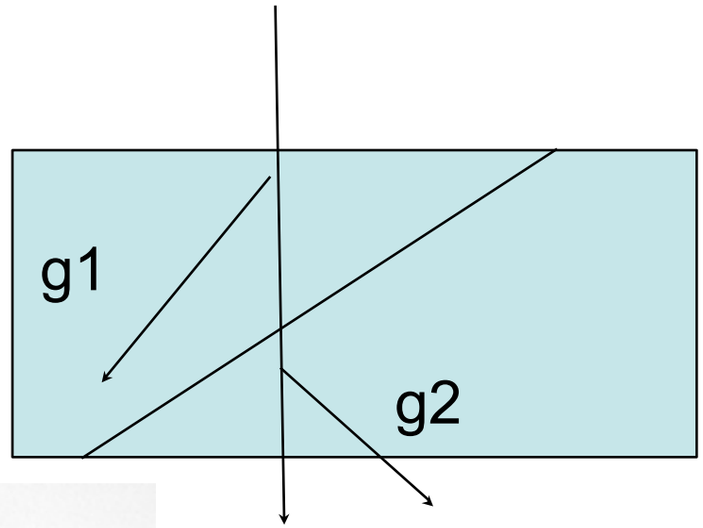
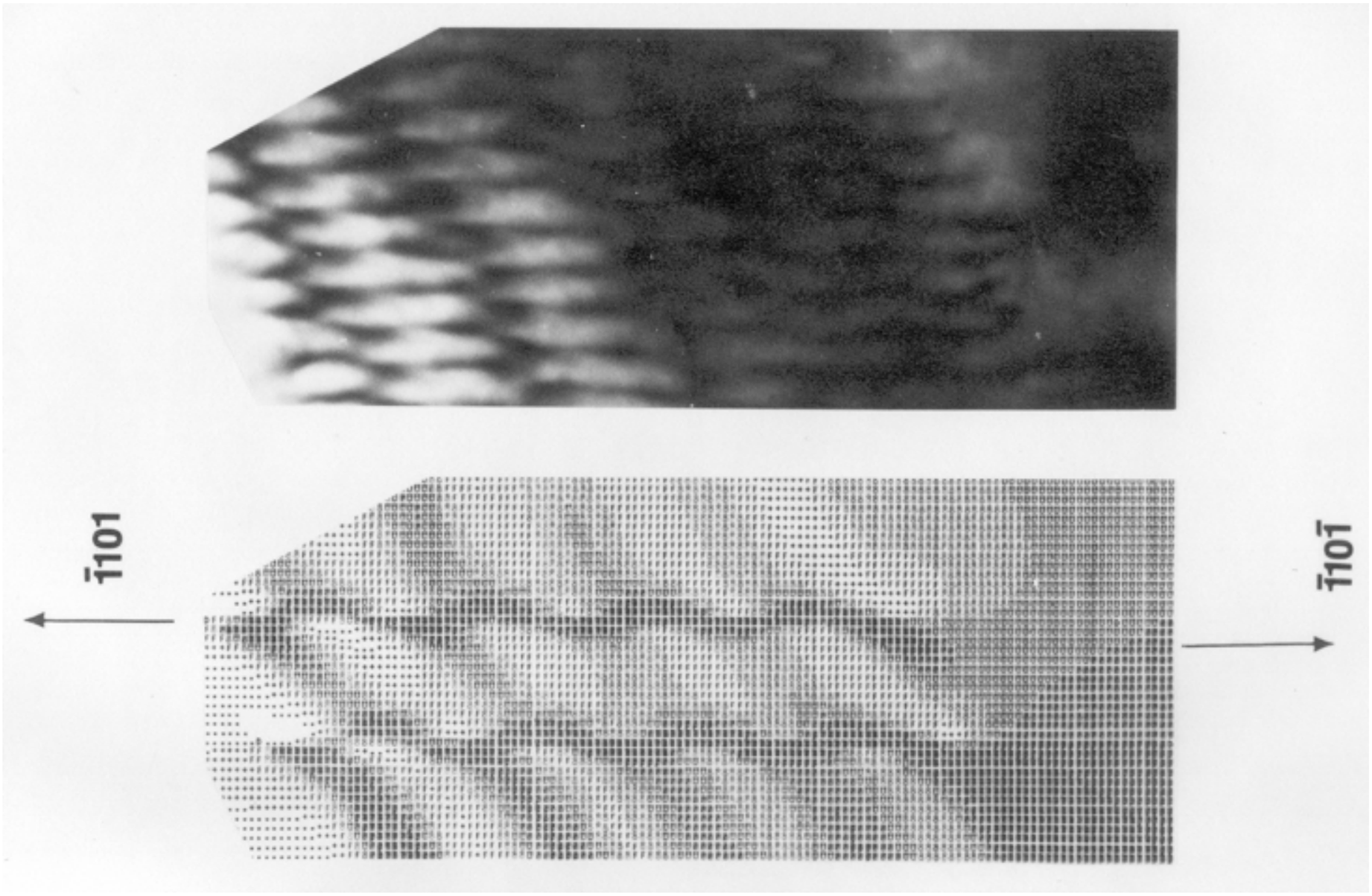
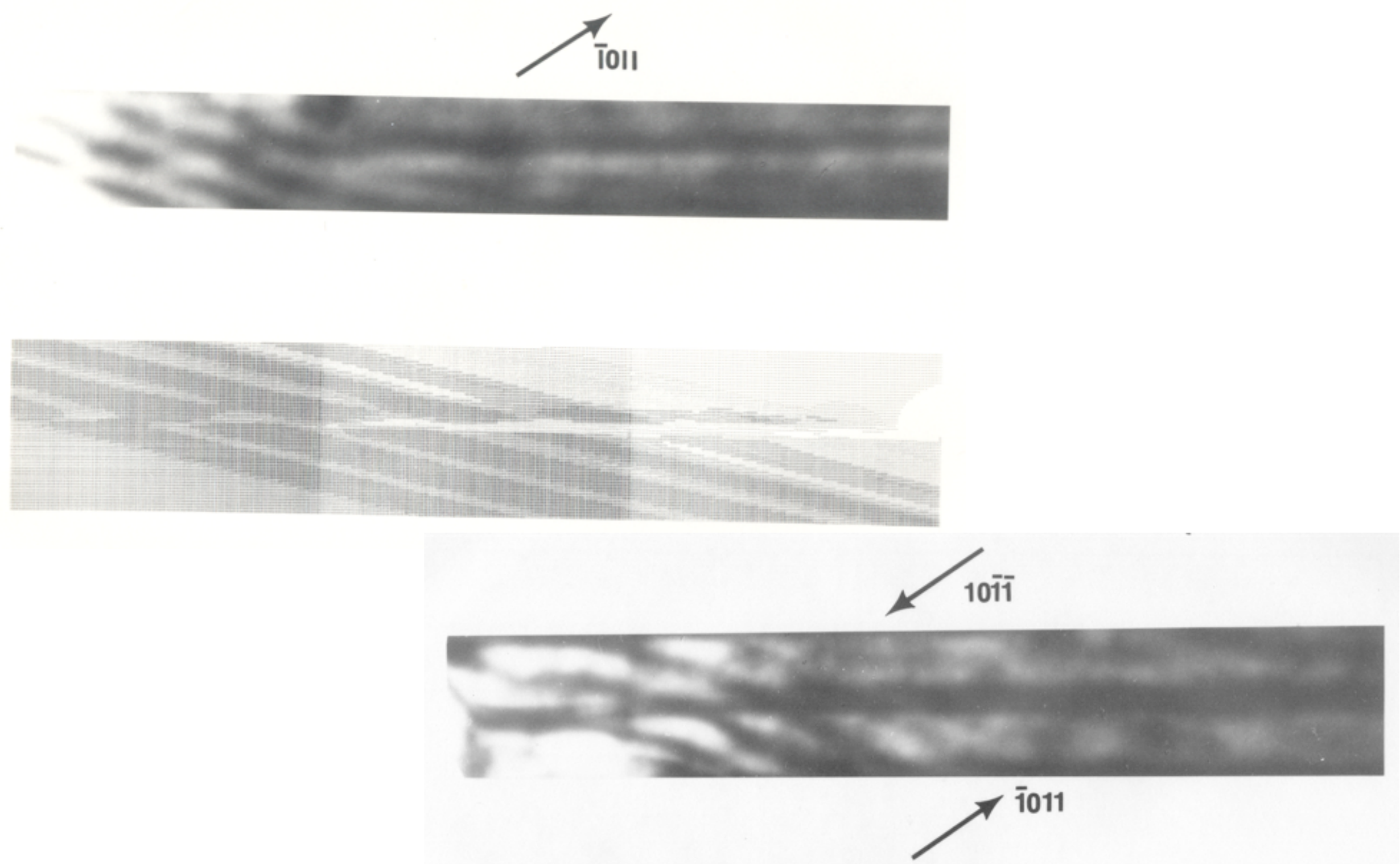



**FIGURE 26.21.** Steps at interfaces may also cause diffraction contrast when associated with strain. In this Ge specimen, the steps displace the thickness fringes in the GB so they are readily visible. The fringe spacing is different at the top and bottom of the boundary because the diffraction conditions are different at each grain.

# Dislocation in Σ13 Grain Boundary of Zn

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