半導體材料分析技術與應用

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Feature of a MOS

Matel silicide

Poly(n)

Gate oxide (1.5 nm)

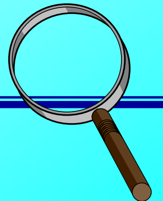
S(n)

CD

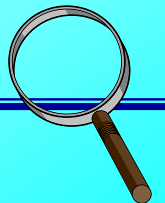
D(n)

Substrate(p)

CD = 0.18, 0.15, 0.13 μm; 90, 65 , …. nm



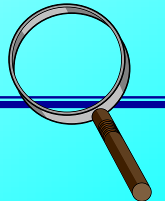
Schematic IC Structure



Techniques to Characterize IC Microstructure

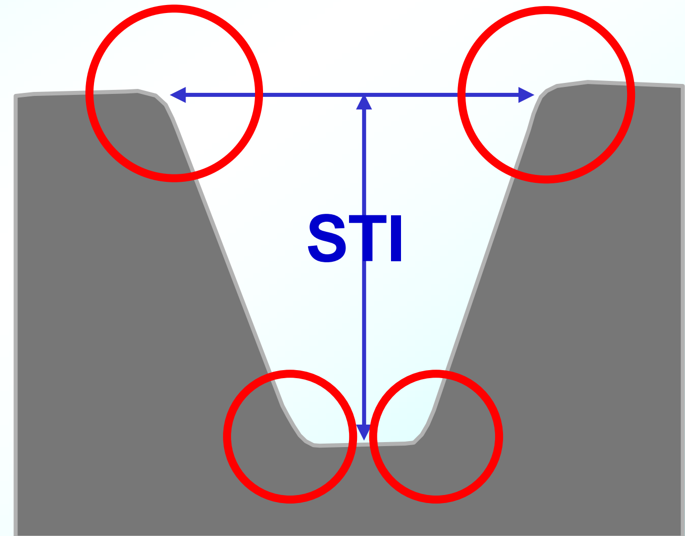
IC Microstructure

Microscopy	Spectroscopy	Diffraction
Images	Spectra	Diff. Patterns



影像提供的訊息

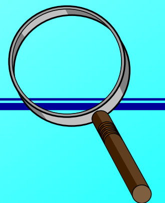
- 圖案(pattern) 卍 卐
- 尺寸(dimension)
- 輪廓(profile)



Typical tools :

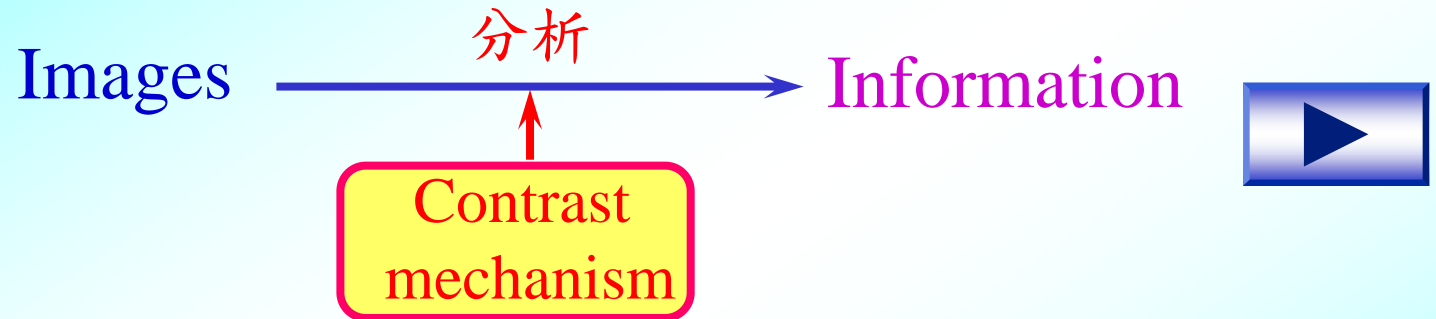
OM ➔

PV-SEM (in-line)
FIB (defects) ➔ **TEM**
XSEM (off-line)



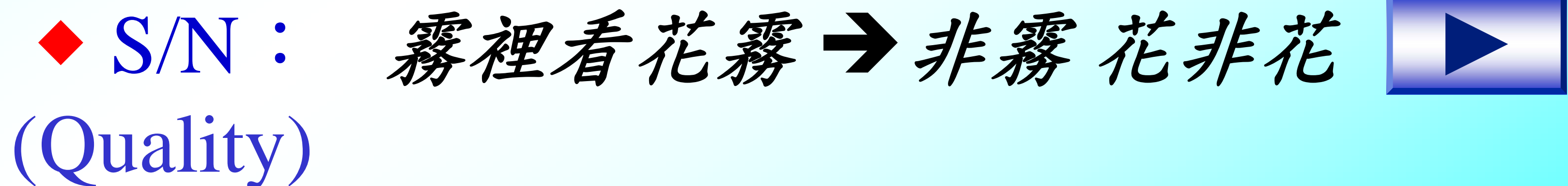
影像三要素

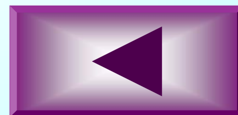
◆對比：***No contrast, No information!***

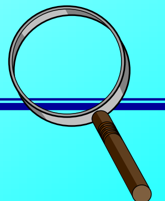


◆倍率：

◆ S/N：
(Quality)

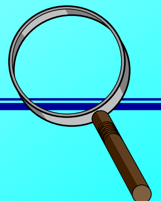






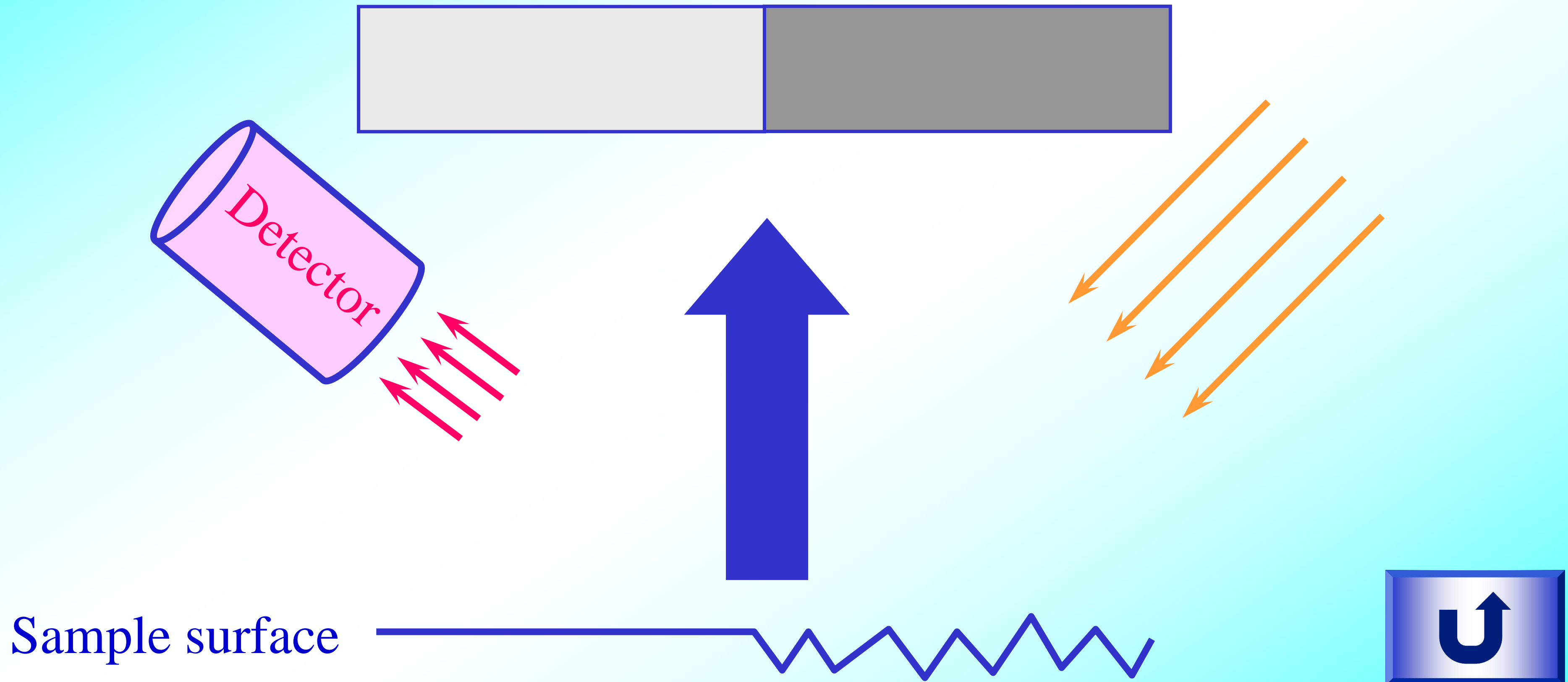
Mechanism of Image Contrast

What is the color of polar bear fur ?



Information in an Image

- B&W in an OM image



Puzzles Caused by Partial Images

An images showing only partial image of a feature may conduct misunderstanding and wrong conclusions.

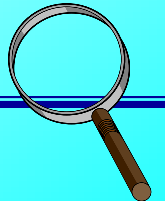
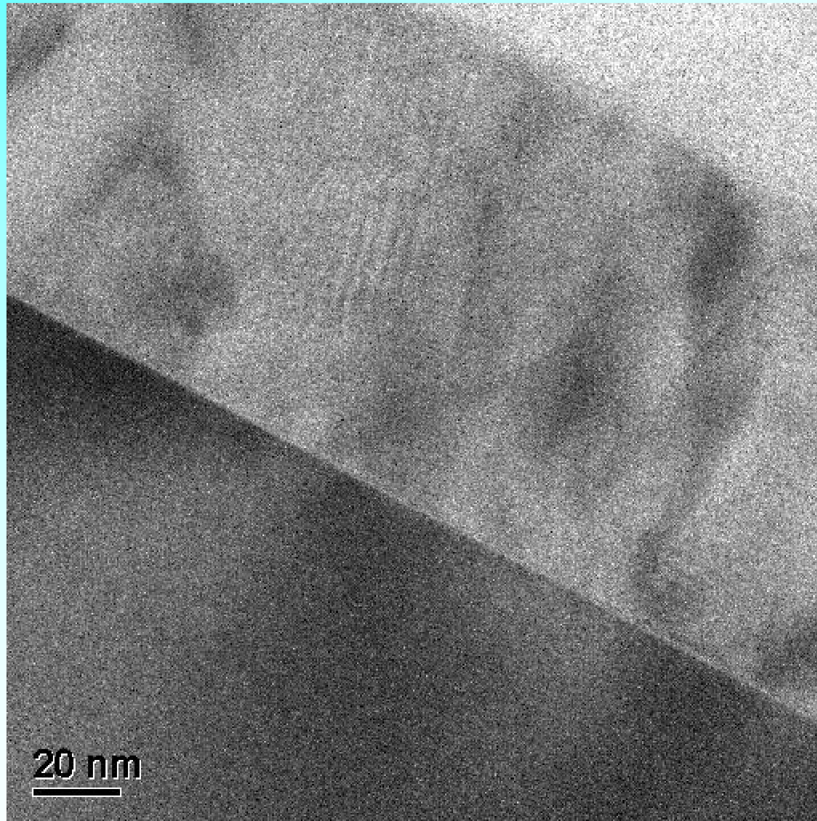
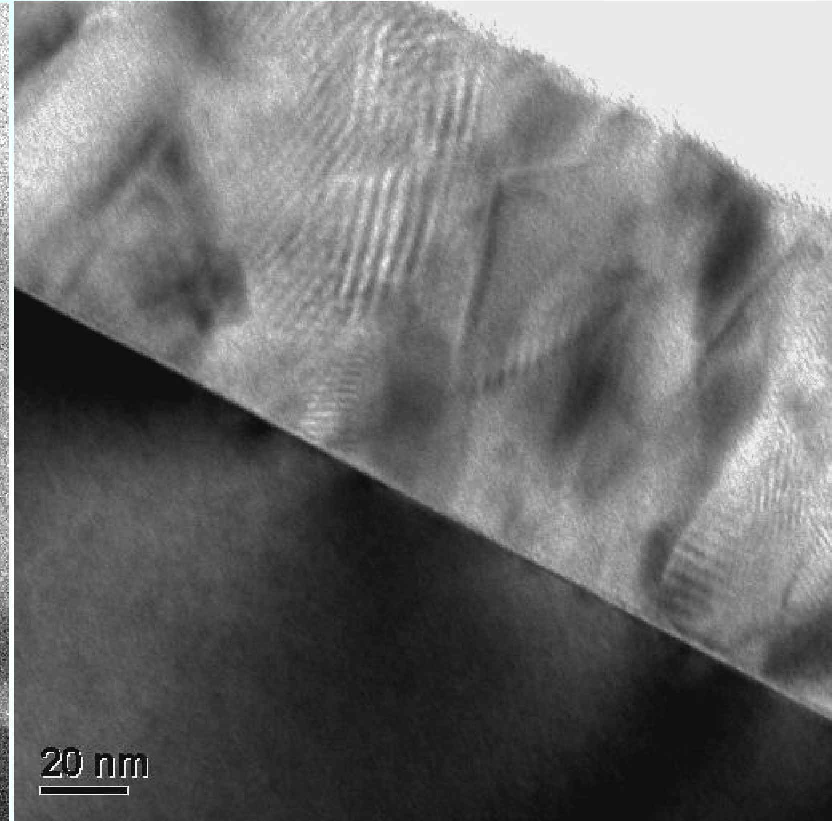
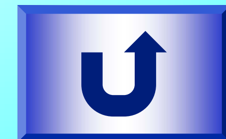
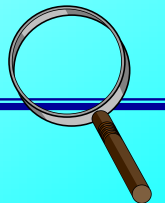


Image Quality – Dose









Composition Analysis

Live Time: 120 seconds Real Time: 136 seconds

2047

Counts

Pb

Pb

N

Sn

Sn

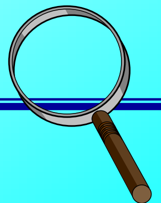
Cu

0

0.000 KeV 10.230

20KV 35° 11:53 8-Jan-1999

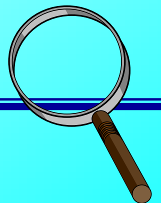
For a Sn-Pb alloy, is composition analysis required to identify the dark phase and the bright phase?



Objects of Composition Analysis

- What kind of elements are included in the sample?
- What is the ratio of constituent elements?
- What is the chemical bonding:
  (CoSi and $CoSi_2$)

- What are the distributions of specified elements?
  - Across the interface or boundary
  - Depth profiles



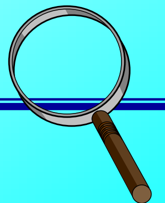
Composition Analysis -- Spectroscopes

質譜儀：Such as SIMS，用質荷比鑑定元素種類

能譜儀：用電子或X-射線的能量鑑定元素種類

Electron type: Auger, EELS, ESCA(XPS)

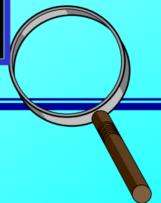
X-ray type: EDS, XRF



Composition Analysis – Factors concerned

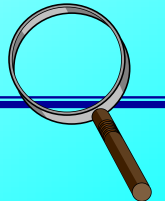
- Spatial resolution
- Energy resolution
- Detection limit: ppm or wt%
- Conductive sample or not

Spectroscope	Source	Signal	Spatial resolution	Energy or mass	Sample conductivity	Detection limit	Features
Auger	electons	electons	15 nm	7 eV	V	0.1 wt%	Signal emerges from $t \leq 5$ nm
EDS	electons	X-ray	1 ~ 20 nm	130 eV	V	0.1 wt%	
EELS	electons	electons	1 ~ 3 nm	1 eV	V	0.1 wt%	
ESCA(XPS)	X-ray	electons	5 mm 200um	0.2 eV	X	0.1 wt%	
SIMS	ions	ions	xy: 150 um; z : < 1nm	500 ~ 10000	V	ppm	High dynamic range ~ 10^7
XRF	X-ray	X-ray	200 um		X	0.01 wt%	Fast, automation & quantitative



To be or Not to be

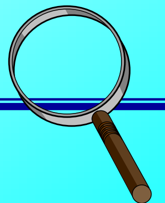
- No signal for a specific element does not absolutely means it does not exist, but
  - Below detection limit
  - Improper operation condition
    - For EDS, $E < 0.5\ E_{th}$
  - Energy peak overlap
  - The specific phase is blocked



Crystallography

They are all carbon products

They are all SiO_2 products

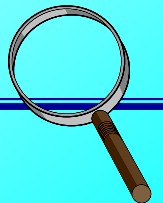


Crystallography

Are isomers in the micro and/or sub-micro world so easy to be identified ?

- How to distinguish glass quartz (SiO_2) ?
- How many kinds of Al_2O_3, $TiSi_2$, TiO_2 ?

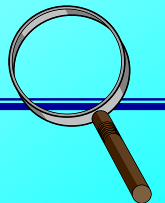
Composition	JCPDS No.	Crystall structure	a/b/c (Å)
Al_2O_3	族繁不及備述		
$TiSi_2$	10-225	Orthorhombic	3.62/13.76/3.60
	35-785	Orthorhombic	8.27/8.55/4.8
TiO_2	21-1236	Orthorhombic	4.531/5.498/4.900
	21-1272	Tetragonal	3.785/ /9.514
	21-1276	Tetragonal	4.593/ / 2.959
	29-1360	Orthorhombic	5.456/9.182/5.143
	33-1381	Hexagonal	9.22/ /5.685



如何選擇正確的分析儀器

- **影像**
  - 解析度：μm 、 nm 、Å
- **成份**
  - 精確度： ± 10% 、 ± 5% 、 ± 2% 、.....
  - 偵測極限： 1 wt% 、0.01 wt% 、ppm
- **晶相**
  - 塊材(Bulk)
  - 薄膜：100 nm 、 10 nm
  - 局部：μm 、 nm

Trade off : Higher resolution will cost more and take longer

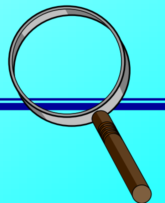


Something Before Go to a Scope

No ticket! No enter!

What is your ticket to MA?

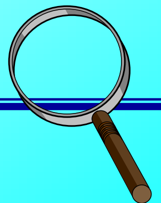
A Good Sample



Difficulty in Sample Preparation

Technique	Difficulty in Sample Preparation
TEM	1, 8 ~ 10
SEM	1 ~ 4
AES	1 ~ 3 **(Don't touch with a metal ??)**
ESCA	1 **(Don't touch with a metal ??)**
SIMS	1
AFM	1
SCM	7 ~ 8

More difficult takes more time and higher cost.



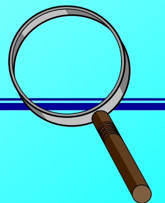
Steps of Material Analysis

- To determine what kind of information required?
- To determine how to analyze the sample (choose tools)
- To make an adequate sample
- To set up the instrument parameters in best conditions
- To run the experiment carefully and record data
- To analyze data
- To draw a conclusion by knowledge and experience
- To reconfirm the data if necessary
- **To submit a solution for a problem**

Importance of MA in Semiconductor Industry

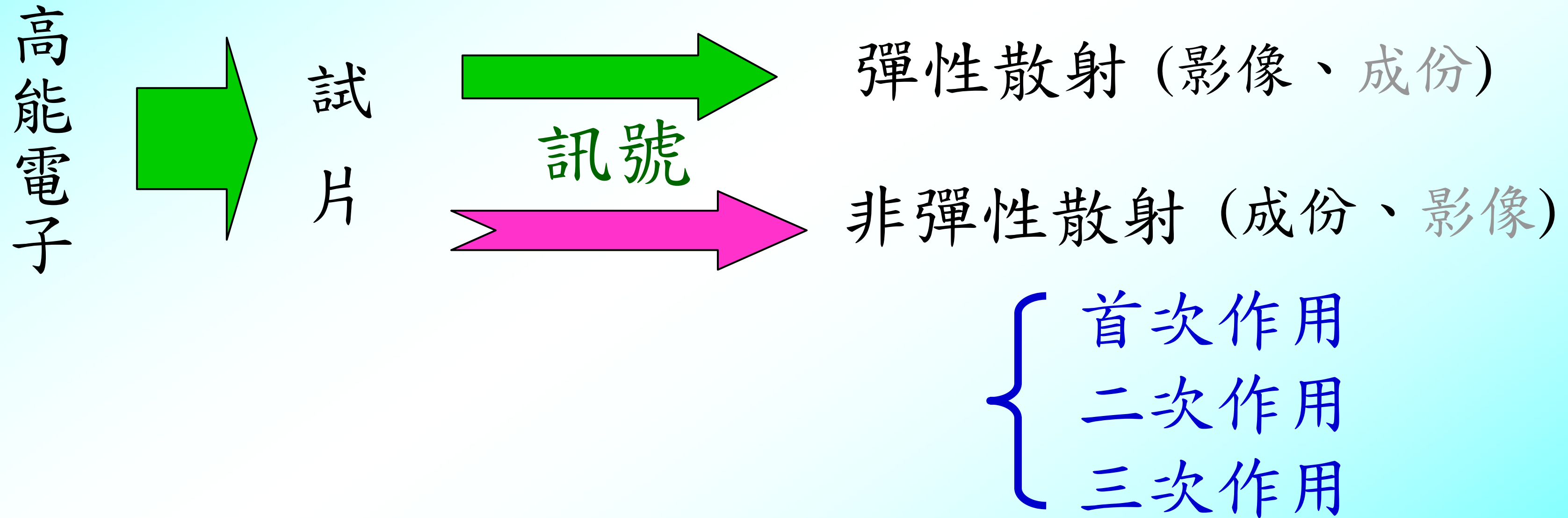
- Check process proper or not in time.
- Reduce the cycle time of R&D
- Reduce the turn around time of defect analysis

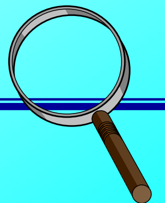
Systematic MA database ← Planned MA



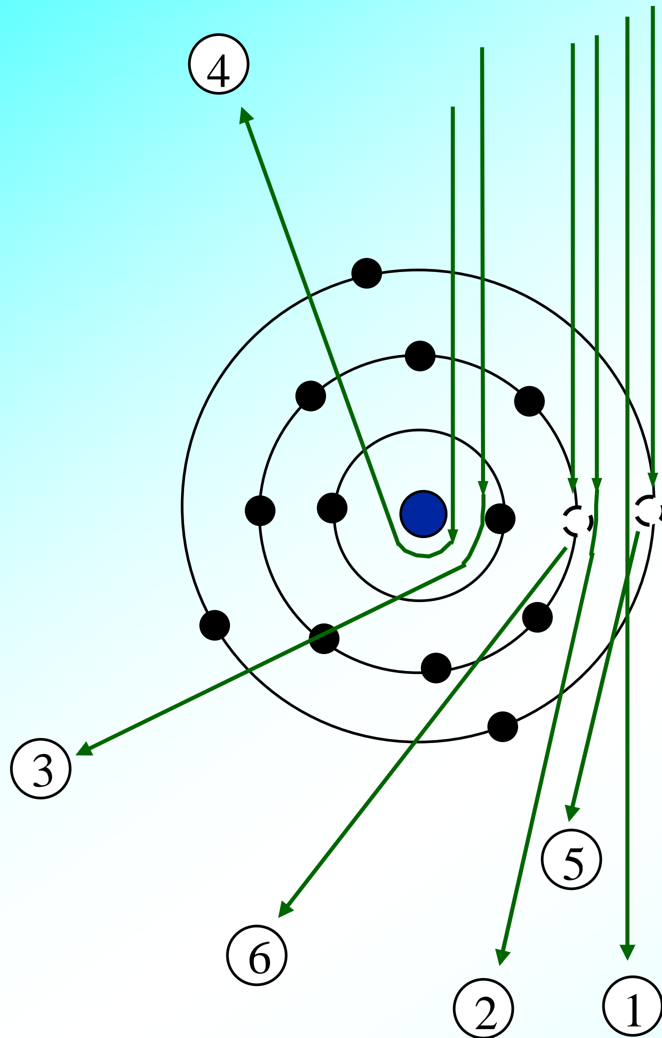
電　鏡　分　析 基　本　原　理

基本原理：用高能電子撞擊待測物，再用適當的偵測器偵測作用後發出的訊號。

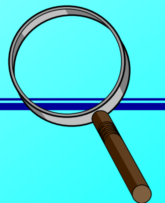




電鏡工作原理 : Primary Interactions



1. Unscattered
2. Low angle elastically scattered
3. High angle elastically scattered
4. Back scattered
5. Outer shell inelastically scattered
6. Inner shell inelastically scattered



電鏡工作原理：2nd and 3 rd Interactions

入射電子
(主電子)

反射電子

歐傑電子

光電子
(ESCA)

入射X-ray

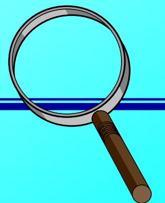
特性
X-ray

二次電子

未散射
電子

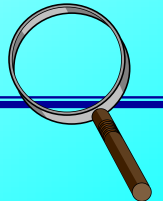
彈性散射
電子

非彈性散射
電子



Volume of Signal Generated v. s. Probe Size

Secondary Electrons (SEM)
e^-
Auger Electrons (AES)
0.5 ~ 5.0 nm
Backscattered Electrons (SEM)
Characteristic X-rays
(EDS/SEM)
0.5 ~ 4 μm



穿透式電鏡工作原理

入射電子
(主電子)

二次電子 (< 100 eV)

C. L.

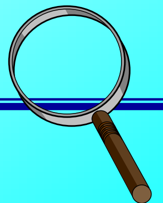
特性X-ray

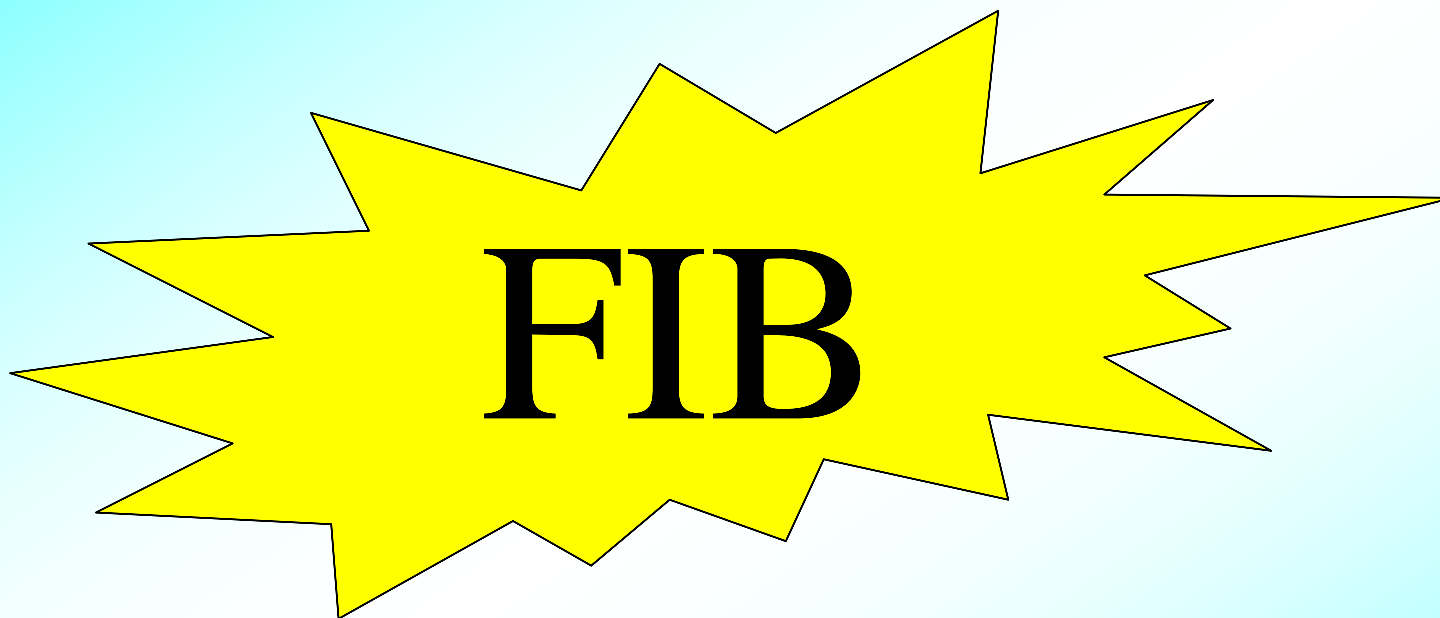
試　　片

彈性
散射電子

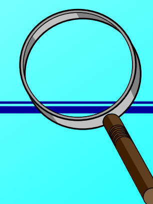
穿
透
電
子

非彈性
散射電子



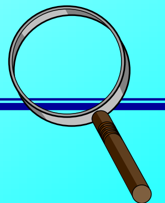


Focus Ion Beam

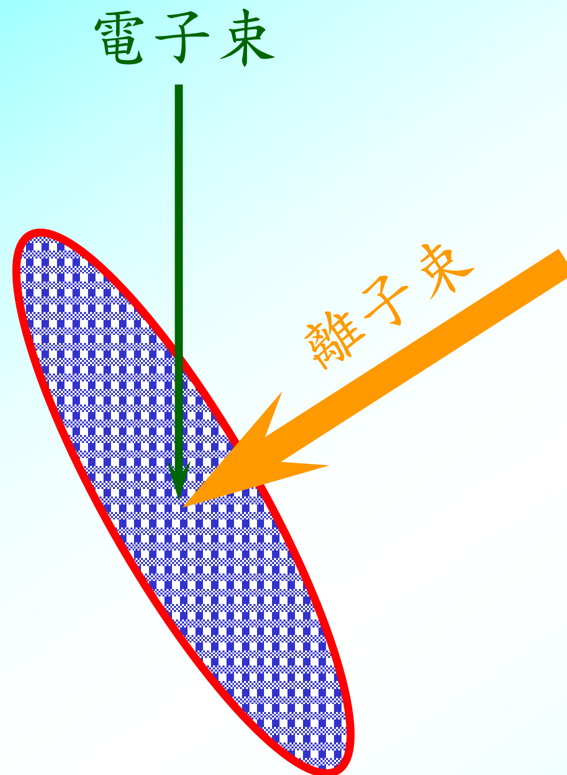


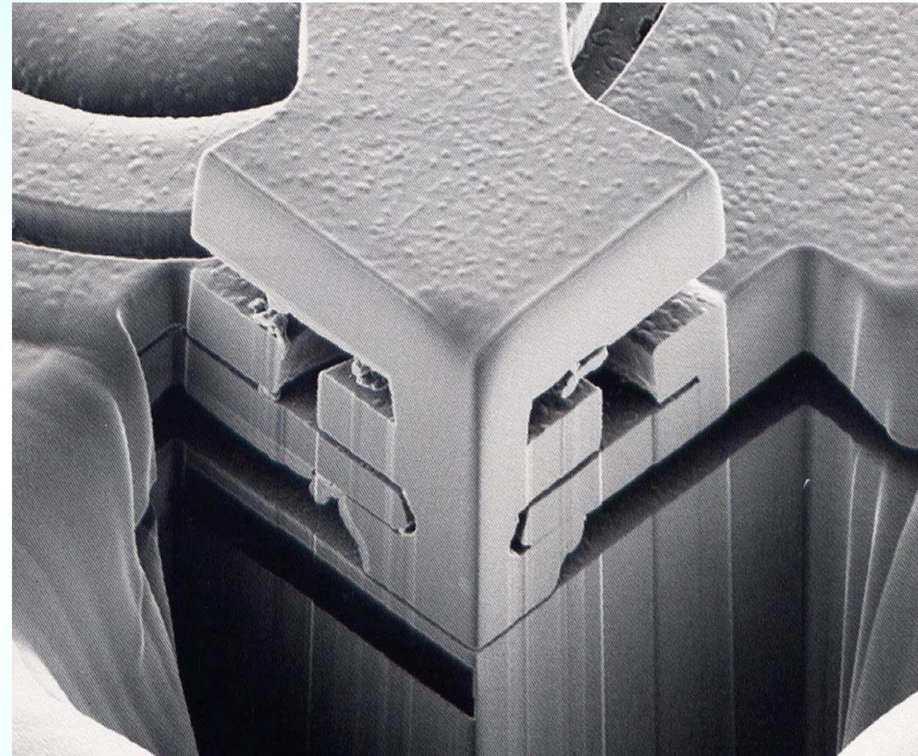
聚焦離子束簡介

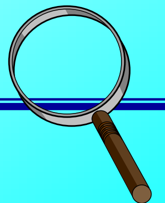
- 有Single beam (ion beam only) 和 Dual beam (ion beam + electron beam) 二種。
- For SEM SEI images，1.4 nm resolution can be available。
- 材料分析儀器中，唯一俱備現場切割能力的儀器。
- 利用適當的切割技術，可以剖析元件的3D結構，是逆向工程最有力的工具之一。
- 俱有in-line分析缺陷的能力。
- 利用Voltage contrast技術，可做半導體元件電性故障分析中open類故障的定位與缺陷分析。
- 常被使用來製作深次微米半導體元件的**TEM試片**。



FIB Configuration and Applications

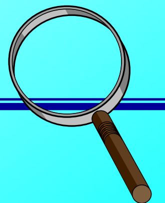






SEM

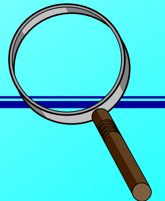
Scanning Electron Microscopy



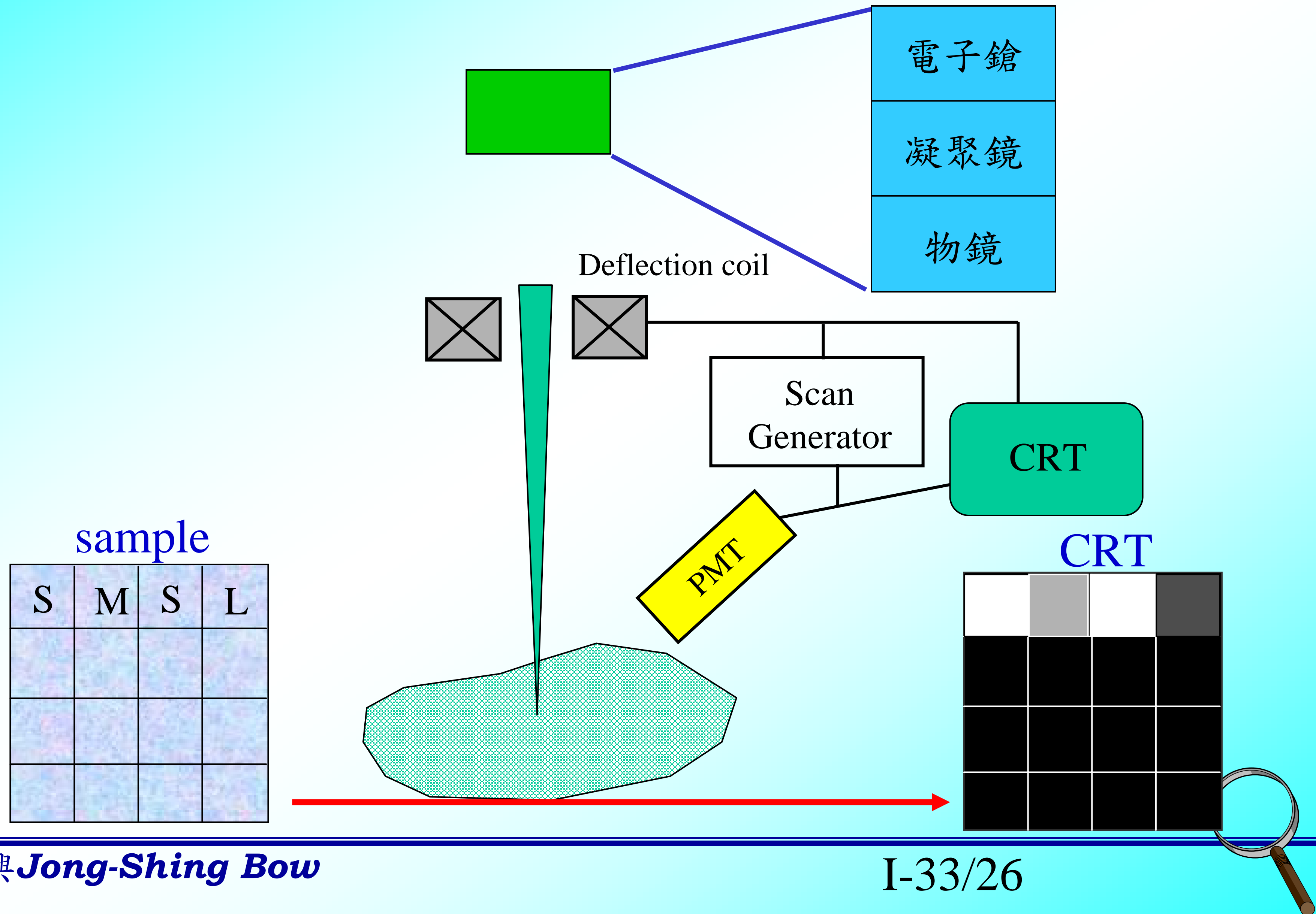
掃瞄式電鏡簡介

- The most used electron microscope (EM) in IC industry
- 有SEI、BEI、mapping 三種成像法。
- 最重要的分析工具，操作電壓10 ~ 30 kV ，近年來則走向低電壓 (=> 1 kV or less)的趨勢。
- 供應表面層的形態、微結構、和成份訊息。
- 橫截面觀察供應薄膜結構整體結構關係、薄膜厚度。、和成份訊息。
- 自動化量測。
- 表面下的空孔(BEI) 。*What is the color of voids in a BEI?*
  - Interface broadening by
    - -- beam broadening
    - -- chemical etching

==> 當待測物的尺寸小於10 nm時，此效應造成的誤差變的非常明顯。

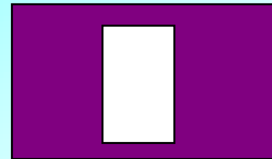


How the SEM Produce an Image – (1)

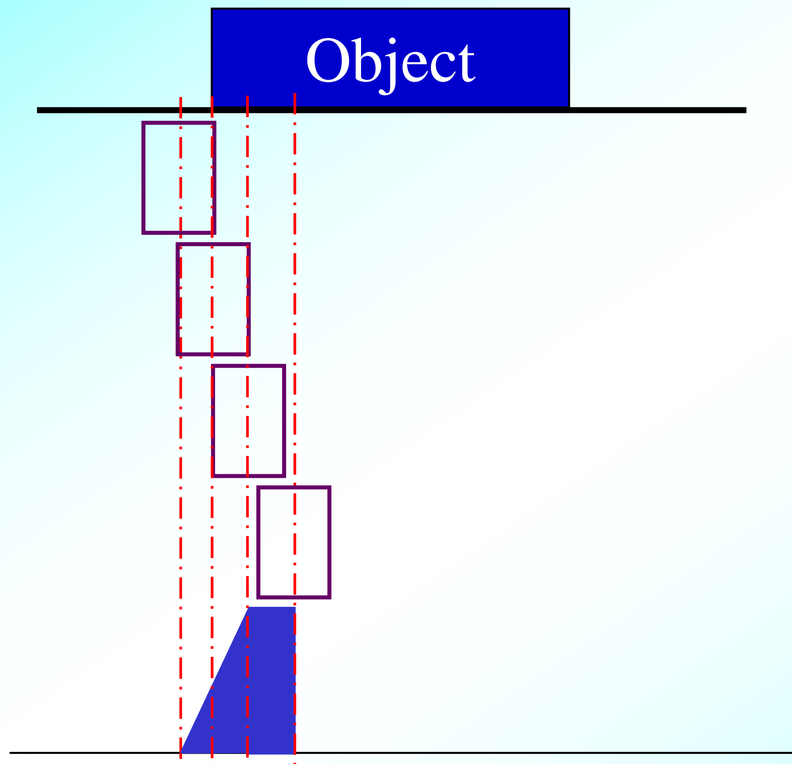


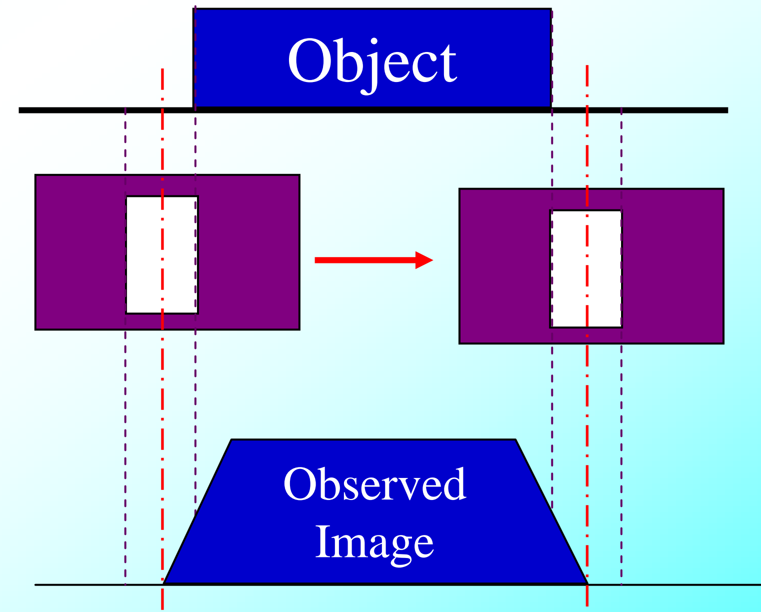
How the SEM Produce an Image – (2)

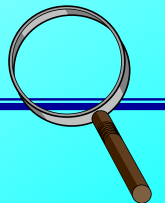
Observed Image = Probe $*$ Object



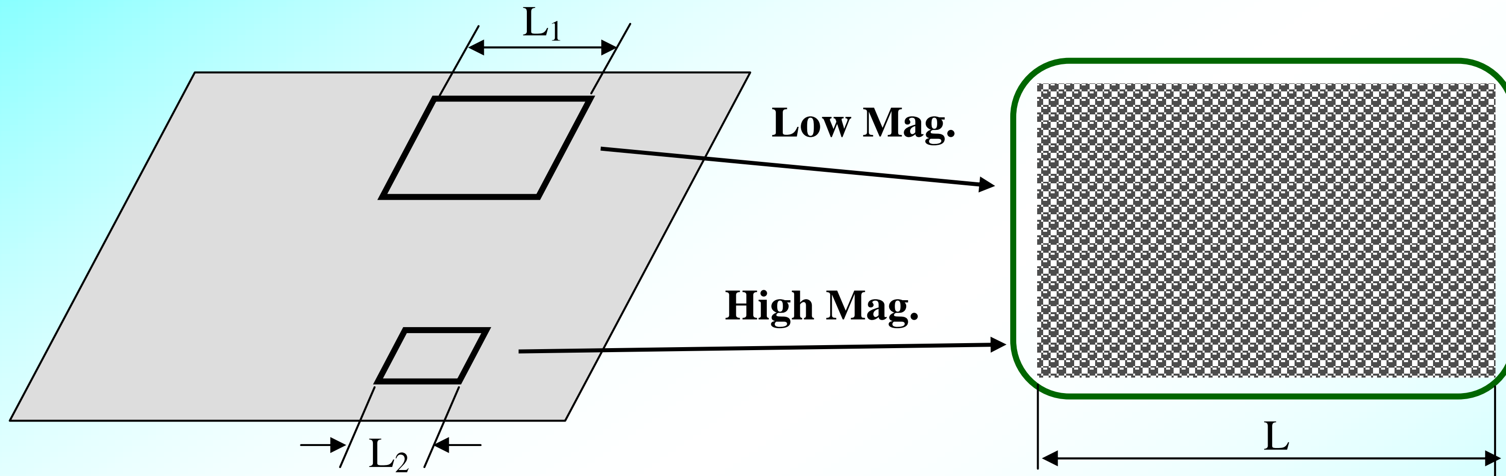
“Probe”







掃描區域與放大倍率



$$\text{Magnification} = \frac{\text{Length of raster line on CRT}}{\text{Length of raster line on the specimen}}$$

$$M = \frac{L}{L_i}$$

$L_1 > L_2 \Longrightarrow M_1 < M_2$

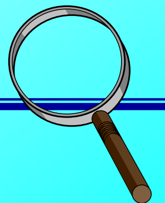
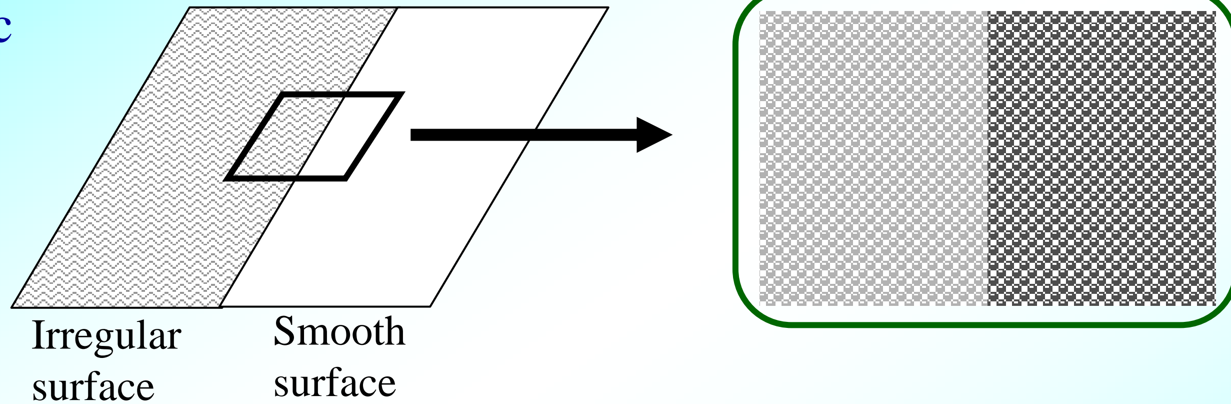
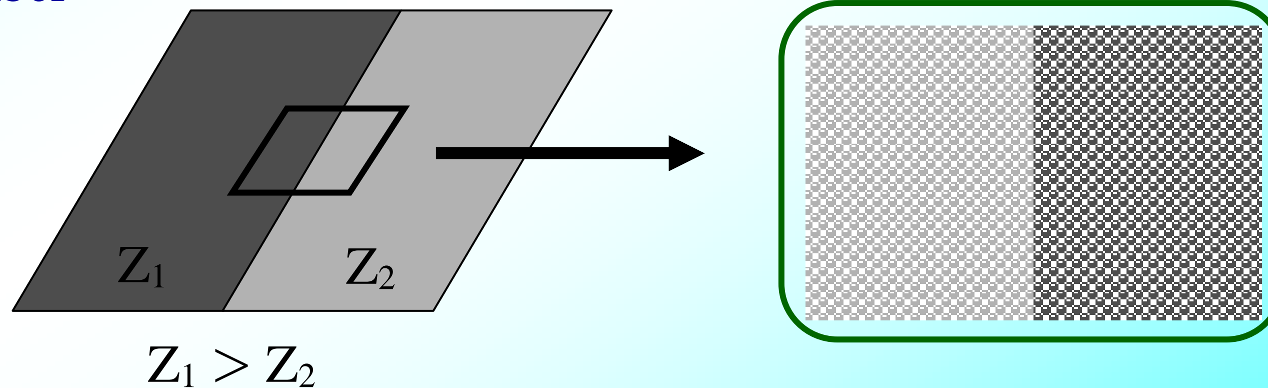


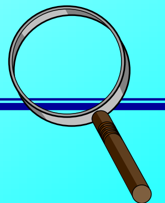
Image Contrast

- Topographic contrast

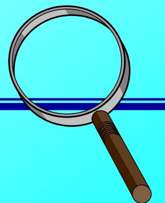


- Atomic number contrast





Coefficient of BE and SE

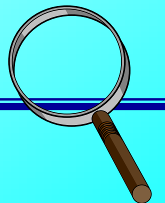


Topographic Contrast

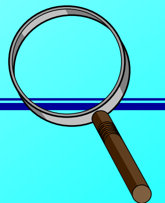
e⁻

e⁻

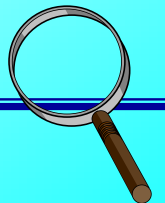
e⁻



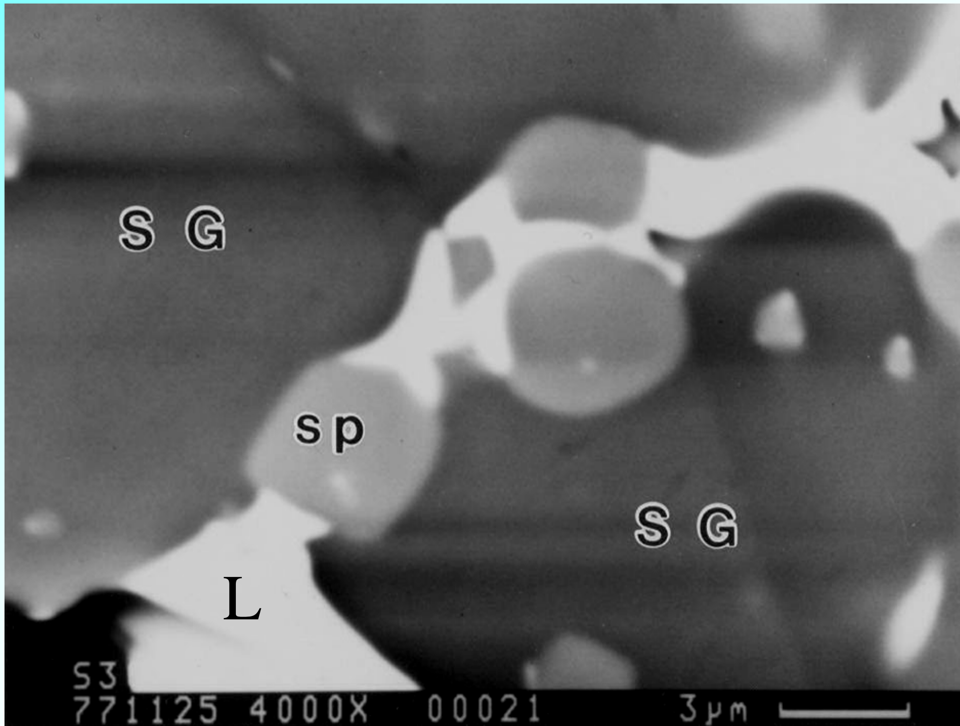
Generation of Secondary Electrons



Effect of SEI Detector Position



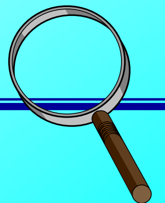
SEM BEI Image



SG = ZnO grain
sp = Spinel (Sb_2O_3) grain
Liquid phase: Bi-rich

Atomic number (Z):

O = 8 Zn = 30
Sb = 51 Bi = 83



Resolution of SEM Images

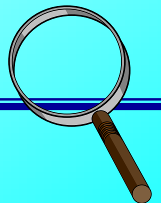
? High magnification gives higher resolution

Resolution of normal naked eyes @ 25 mm = 0.1 mm

D x M > 0.1 mm can be resolved

M	D
10KX	10 nm
100KX	1 nm
200KX	0.5 nm

So, we can get a 0.20 nm resolution at 500KX , can we?



Effect of Spot Size on Image - 1

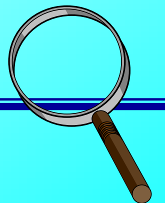
Spot size = 10 nm

Spot size
= 5 nm

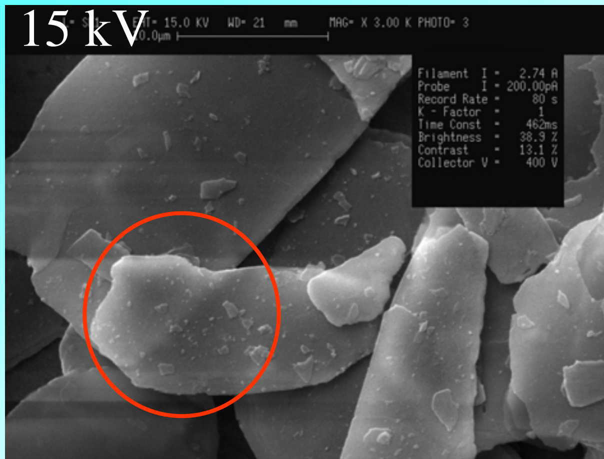
Spot size = 2 nm

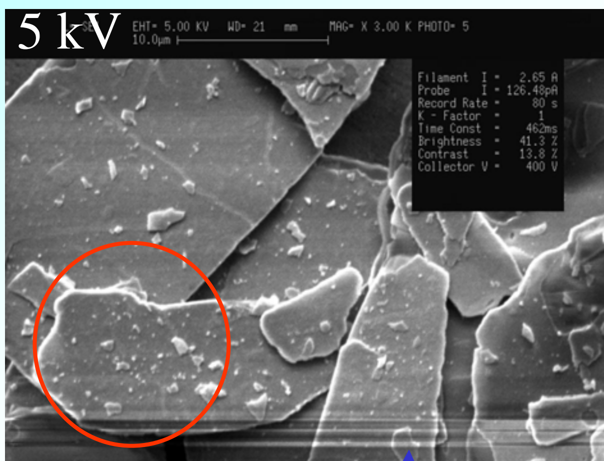
5 nm

5 nm



SEM Image vs. Acc. Voltage





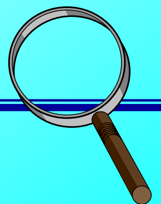
Charging

高電壓時，有些二次電子來自距表面0.2 µm (雲母片厚度)以下。

所以觀察奈米材料，需用較低的電壓，以免失去最上表面的訊息。

但是非導體試片要注意放電效應。

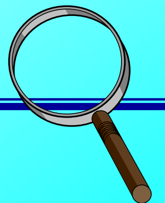
資料提供: 陳世昌先生



Limits of SEM

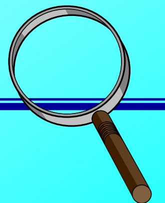
There is no single instrument or technique that can solve all problems!

- If z-dimension is required ➔ ***AFM***
- If the structure of a very precisely specific site is required ➔ ***FIB***



TEM

Transmission Electron Microscopy



TEM Techniques

CTEM

- Diffraction
  - SADP
  - Nano Diff.
  - CBED
- Image
  - BF
  - WB
  - CDF
  - HREM

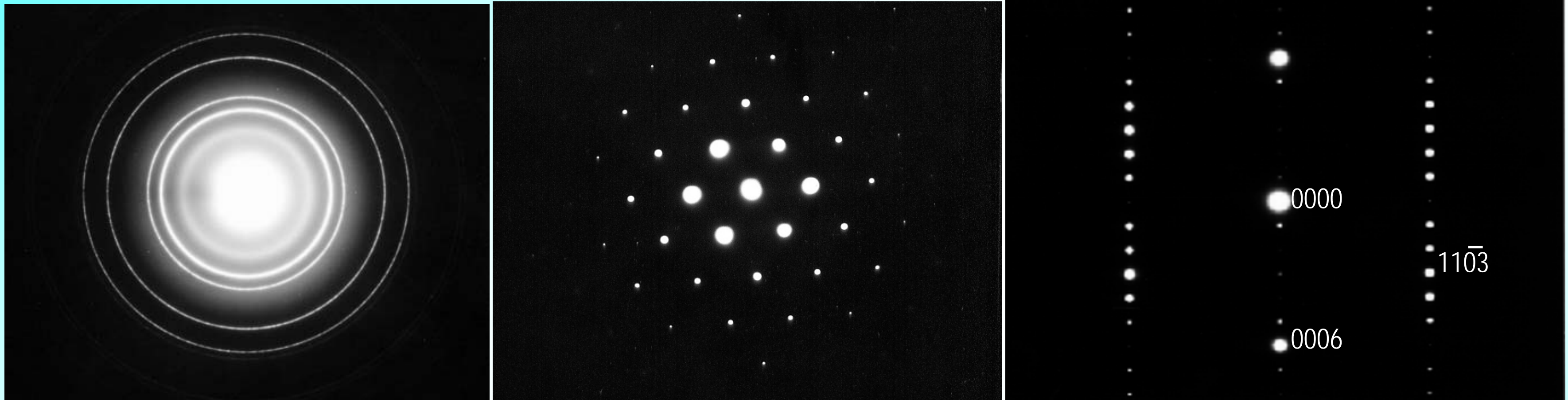
($s < 0$, $s = 0$, $s > 0$)

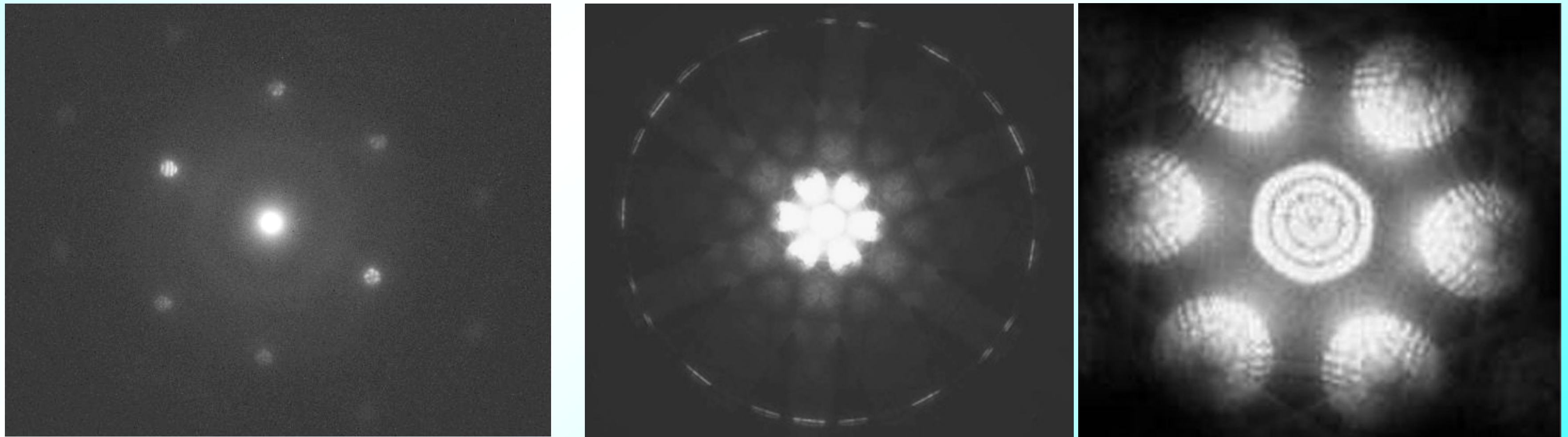
AEM

- Composition
  - EDS
    - Mapping
  - EELS
    - ESI
      - Mapping
      - Jump R mapping
      - Pre-/Post- edge image
    - EFI

Information offered by TEM-- Crystallography

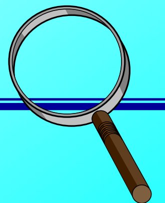
SADP



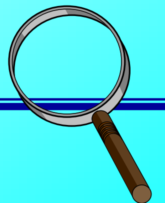


Nano-diffraction

CBED



SADP : Crystalline vs. Amorphous



Information offered by TEM-- Images

BF

CDF

HREM

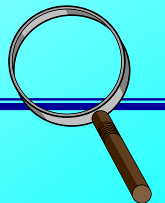


Image Contrast Mechanism

$$C = f\,(A, t, s)$$

A: composition

A phase consisted of high z elements shows dark contrast.

t: specimen thickness

The thick region shows dark contrast.

s: diffraction condition

Grains closed to zone axes show darker contrast.

Electron scattering & Absorption

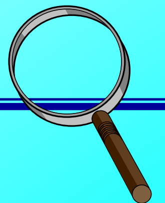
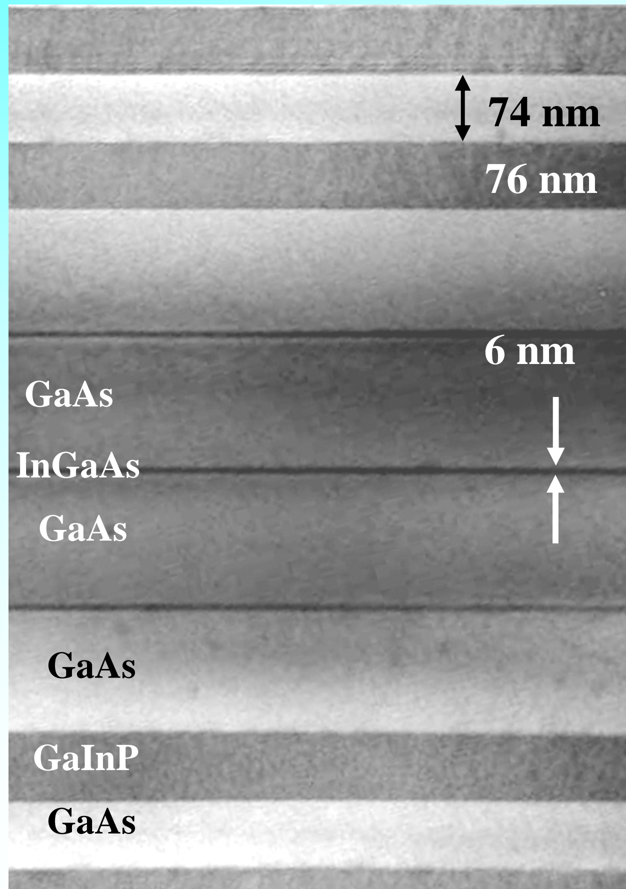
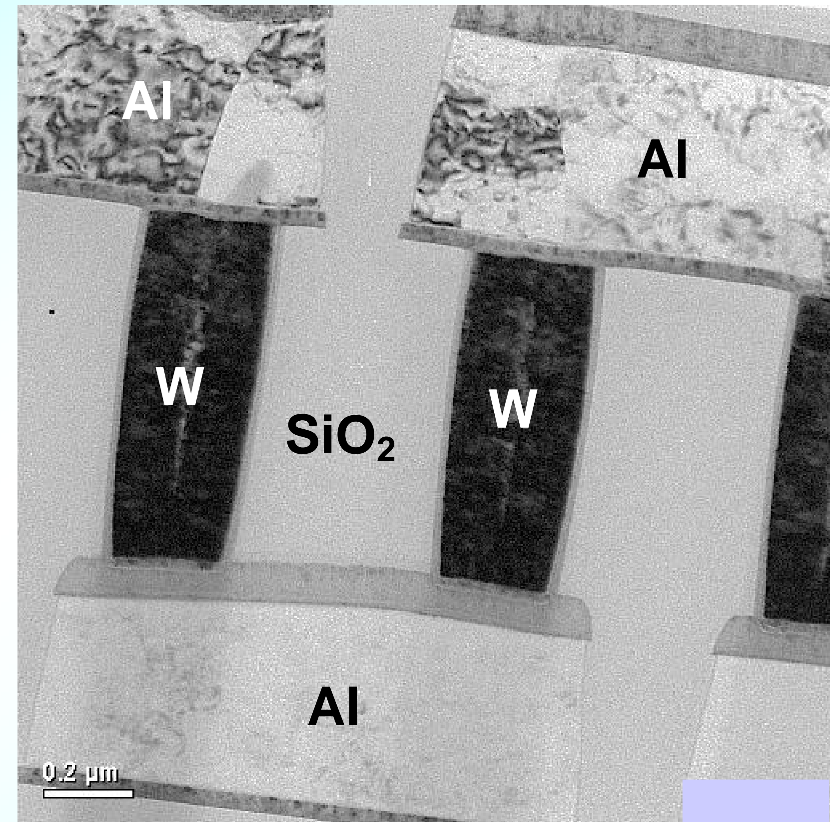


Image Contrast from Atomic Conditions





$Z_p = 15$, $Z_{Ga} = 31$,
$Z_{As} = 33$, $Z_{In} = 49$,

$Z_N = 7$, $Z_{Al} = 13$,
$Z_{Ti} = 22$, $Z_W = 74$,

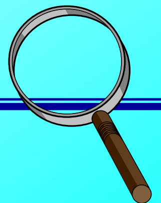
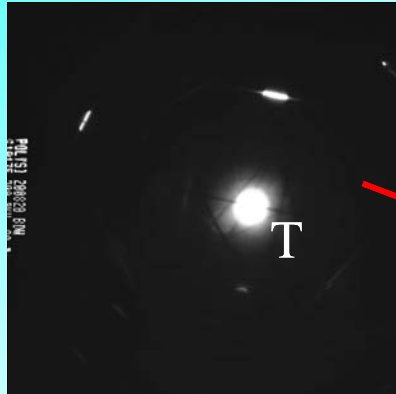
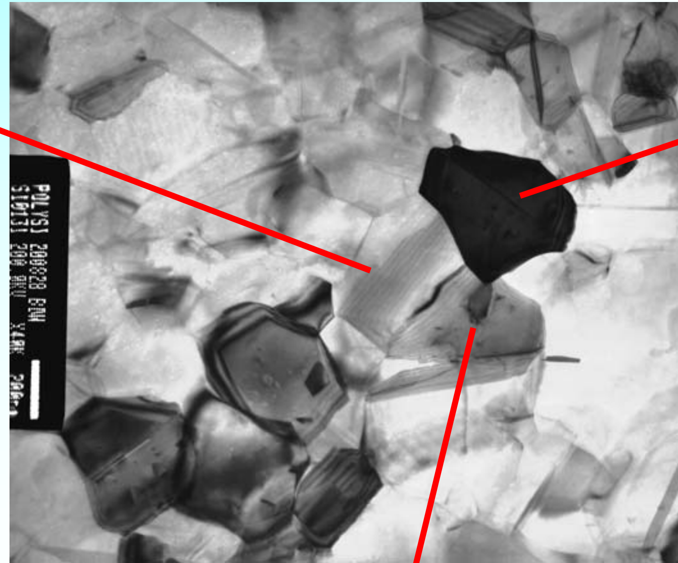
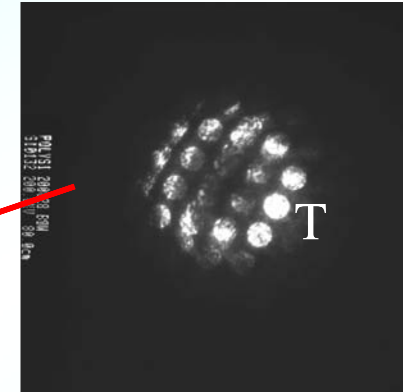
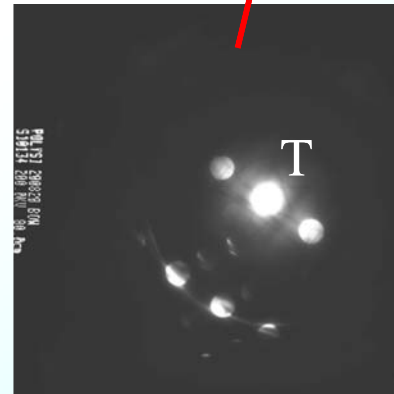


Image Contrast from Diffraction Conditions









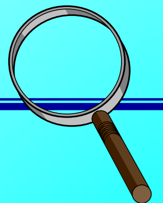
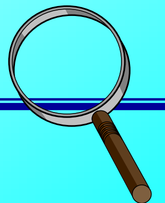


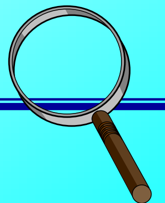
Image Contrast Mechanism

Loose vs Dense
Diffraction condition

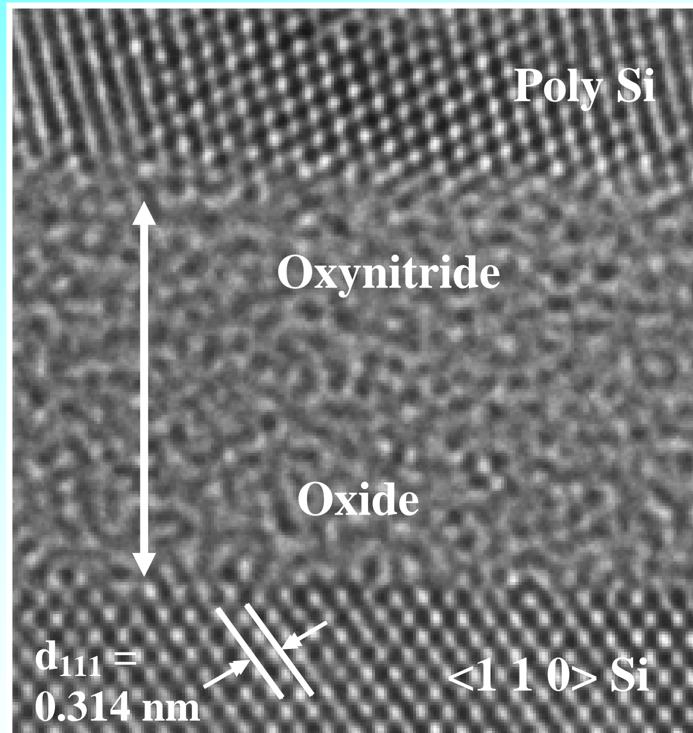
OBJ aperture

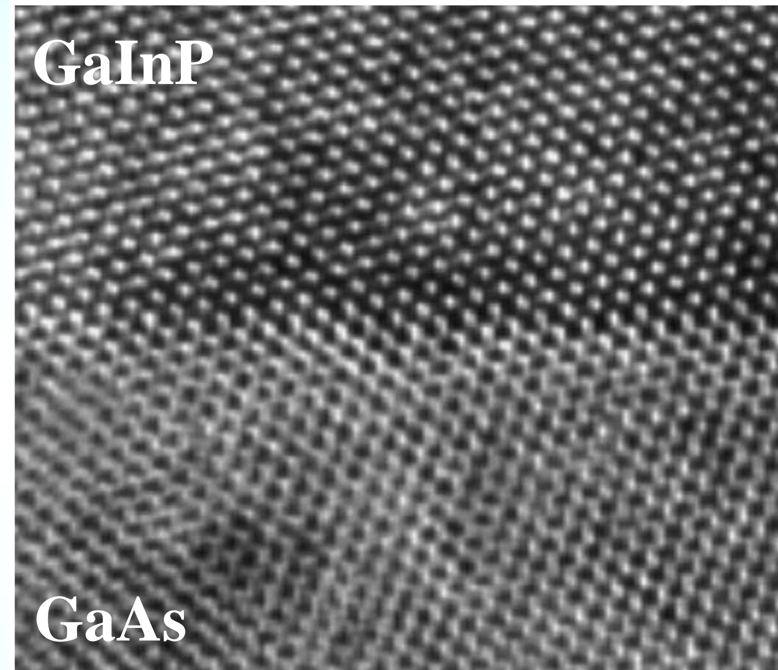


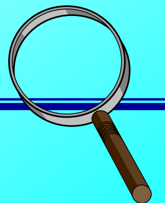
TEM—影像：Defects



HREM Image — Interface (1)

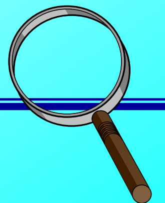






Some Puzzles in TEM Images

- Defocus
  - In focus has the highest resolution but poor contrast.
  - Optimum under-focus is usually used in TEM imaging.
- Sample local bending
- 3D to 2D projection



聚焦值對影像的影像 – (1)

a
1.9 nm

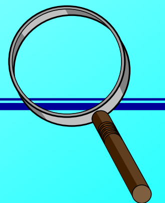
b
1.6 nm

c
2.6 nm

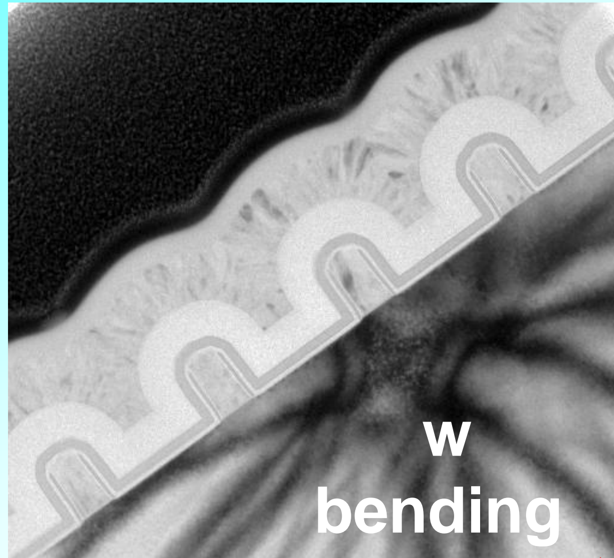
d
3.3 nm

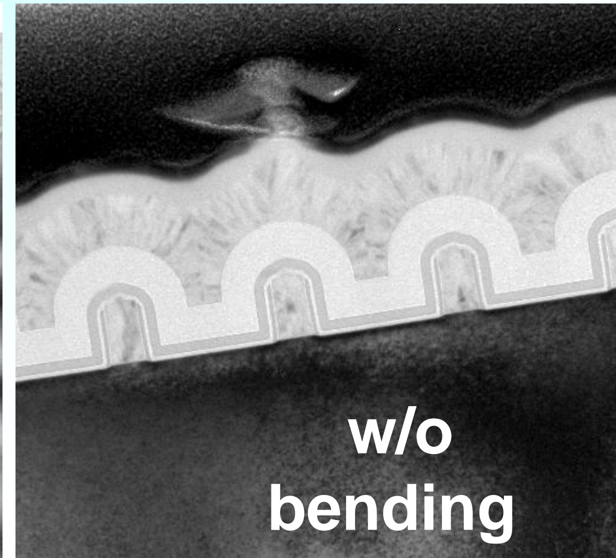
e
4.1 nm

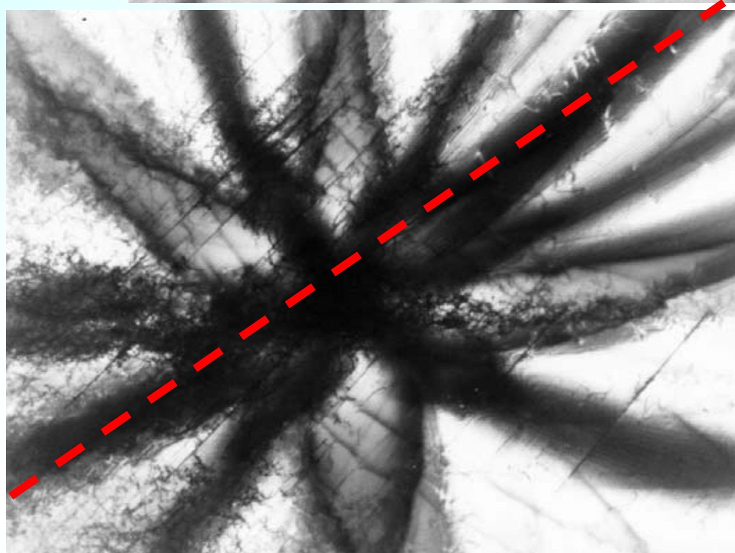
(a) underfocus 167 nm; (b) underfocus 74 nm; (c) overfocus 19 nm
(d) overfocus 112 nm; (e) overfocus 205 nm.

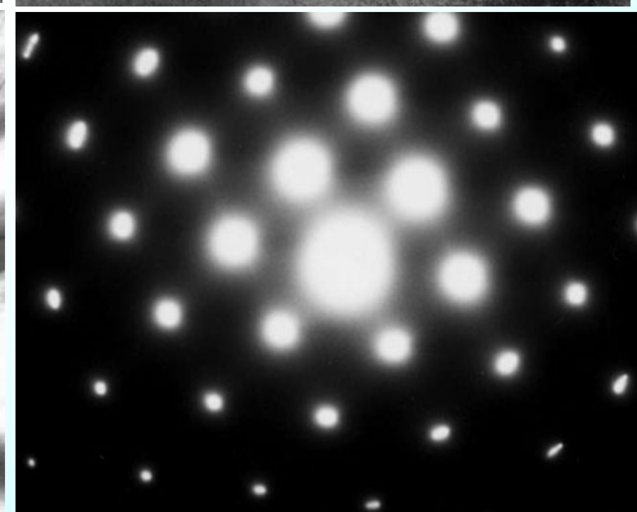


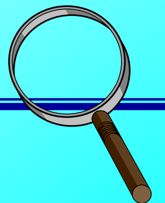
Bend Contours





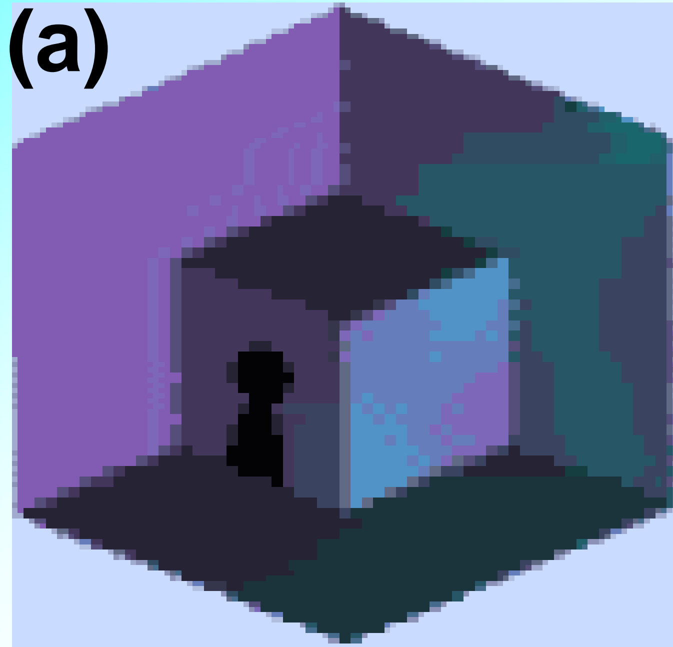






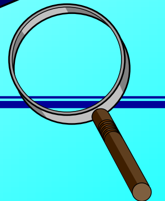
Artifact in TEM Images

(a)的影像是一個大立方體缺了一角(b)？或是一個小立方體放在三面板中(c)呢？

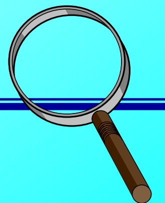


(b)

(c)



Puzzles of 3D Objects to 2D Projections



Artifacts in HRTEM images

e^-

t_1

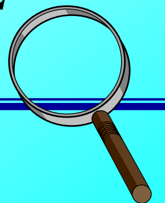
Δt_1

Δt_2

t_1

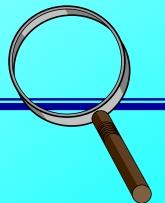
$t_2 = t_1 - \Delta t_1$

$t_3 = t_1 - \Delta t_1 - \Delta t_2$



AFM/SCM

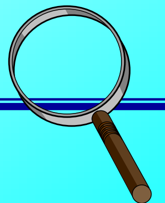
Atomic Force Microscopy
Scanning Capacitance Microscopy



AFM簡介

SPM(scanning probe microscope)是一群研究樣品表面性質(形態、磁性、電性、.......等等)的顯微鏡的總稱，AFM是SPM家族的一員。

AFM則是藉由探針尖端和樣品表面的原子吸力或斥力的作用，使懸桿彎曲或偏折，進而產生AFM 影像。AFM可在空氣中使用，而且可分析非導體樣品，因此成為目前最方便，而且使用最廣泛的SPM。



AFM基本結構

mirror

Laser diode

PSPD
detector

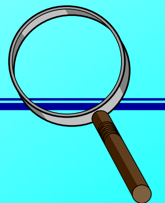
A local mirror surface

cantilevel

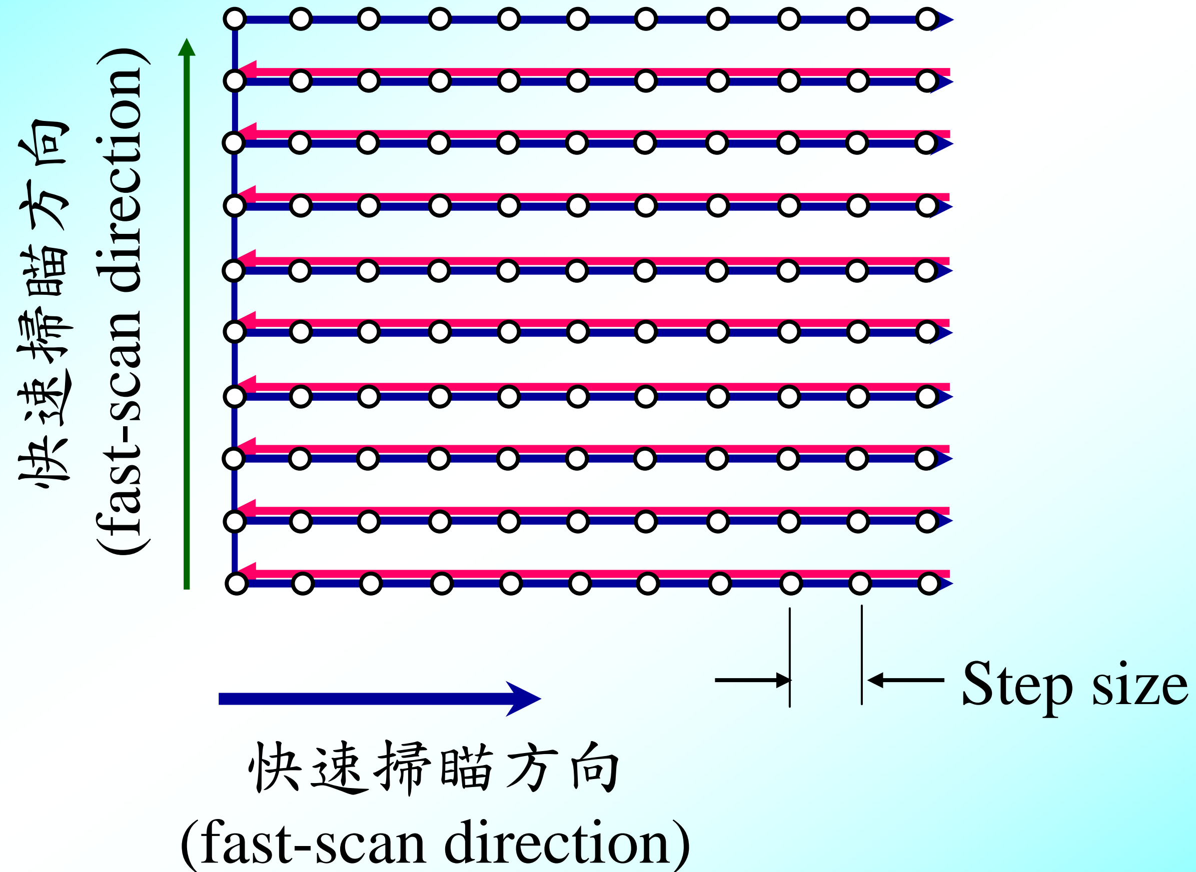
sample

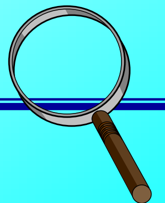
PZT
scanner

PSPD: position sensitive photodetector



Scanner Motion





AFM : Surface Topograph & Profile

Å
800
400
0
A
0 1 2 3 µm

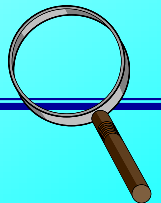
Topography, 10010017.HDF
µm
9.17
4.58
0.00
6 4 µm 2 0
6 4 µm 2 0

Height Profile [A]
Å
800
400
0
0 0.5 1 1.5 2 µm

27° 28° 27° 28°

0.47 µm
0.73 µm
0.79 µm
1.20 µm

資料提供: 陳思澐小姐



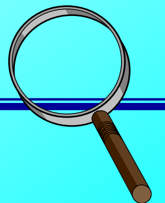
AFM to SCM

Thin oxide

well

$$C = k\frac{A}{d}$$

$$k = k(\text{Conc.}_{doping})$$

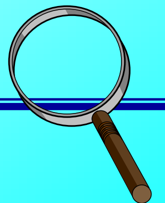


Scanning Capacitance Microscope (SCM)

$$\Delta C = K \, \Delta q$$

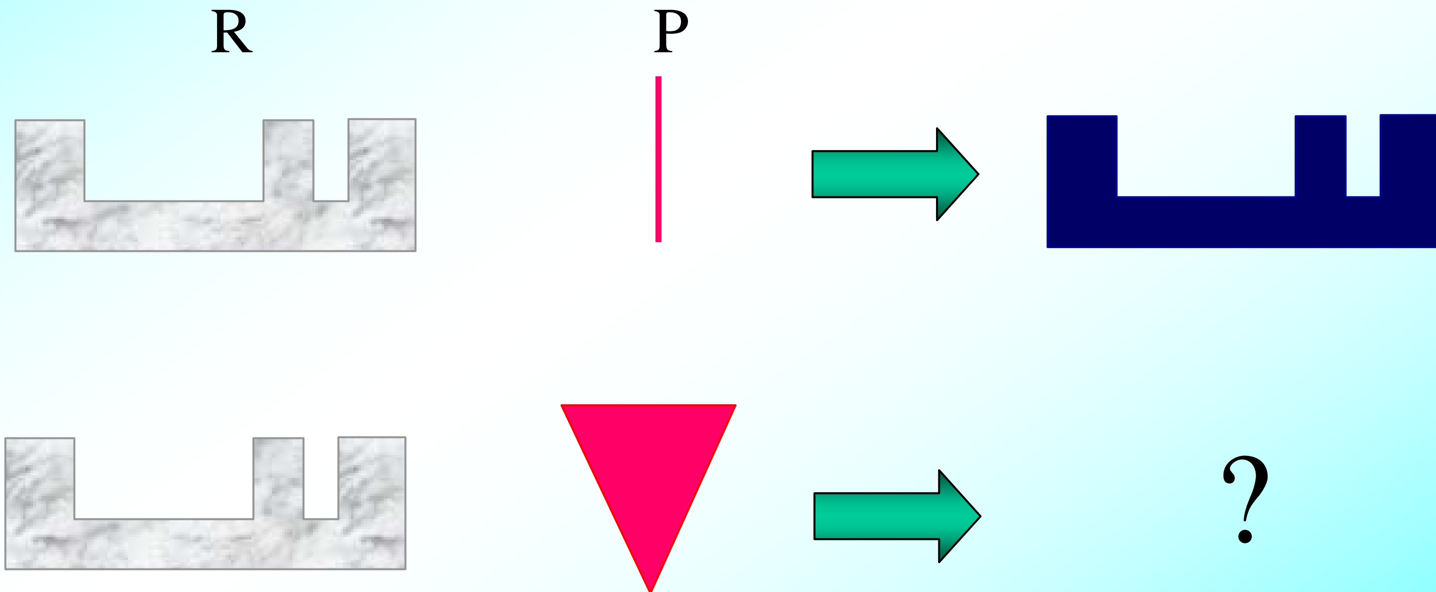
$K = f(k, A, d)$ is a magnifying factor

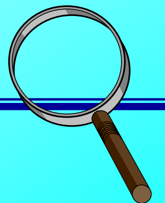
- Increase A ➔ reduce rsolution。
- Because SiO_2 is the dielectric layer, so a dense SiO_2 layer has a higher K value
- Reduce d ➔ increase K
  Tunneling is the limit。



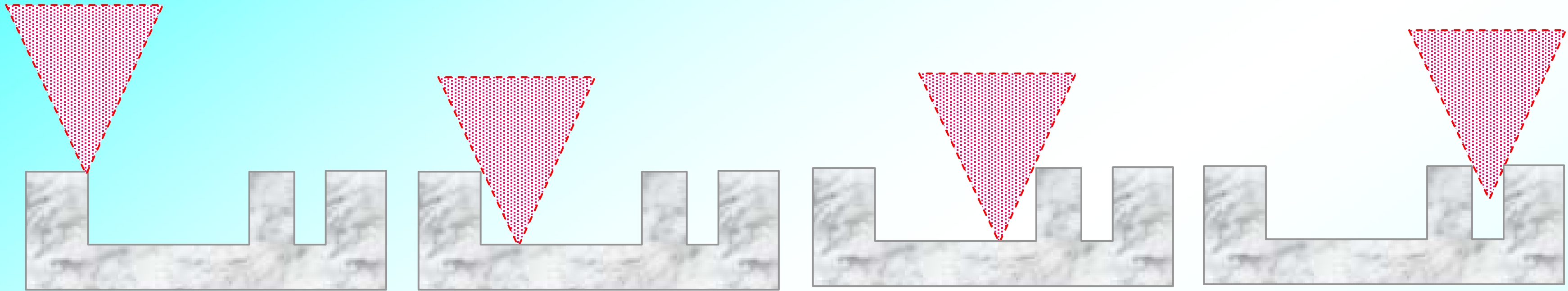
假像 (Artifacts)

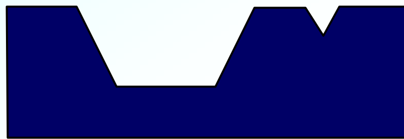
- 捲積(convolution)
  - 觀察影像 = 實際輪廓 (R) * 探針(P)

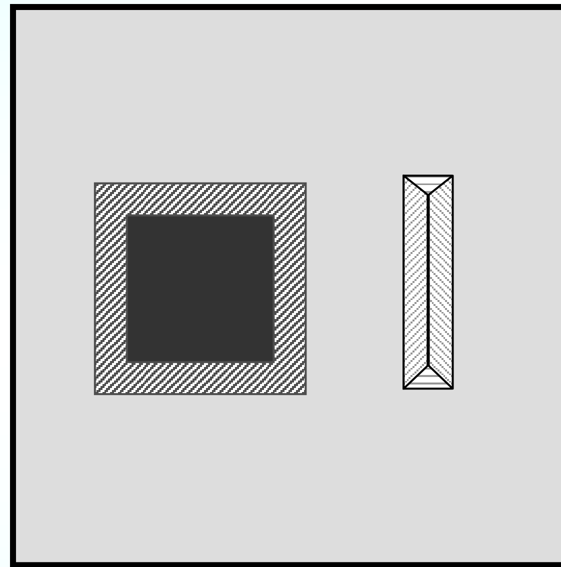


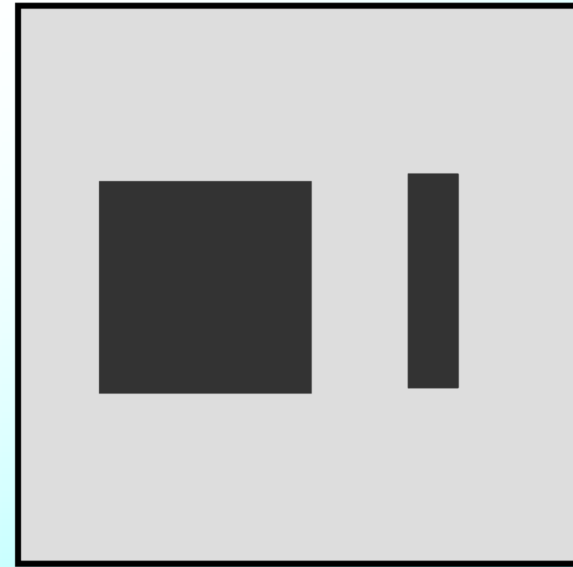


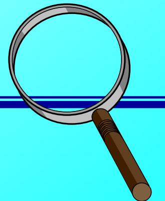
假像 (Artifacts) -- II











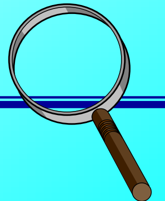
假像 (Artifacts) -- III

- **True Imaging vs Tip Imaging**

Tip imaging

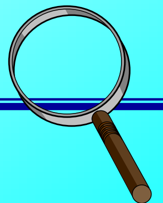
90° rotation of sample

True imaging



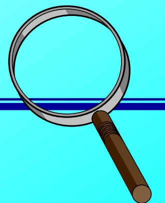
假像 (Artifacts) -- IV

- 如何偵測假像
  - 重新掃瞄一遍。
  - 改變掃瞄方向，重新掃瞄一遍。
  - 改變掃瞄倍率，重新掃瞄一遍。
  - 改變掃瞄速率，重新掃瞄一遍。
  - 旋轉試片，確認是true image or tip image。

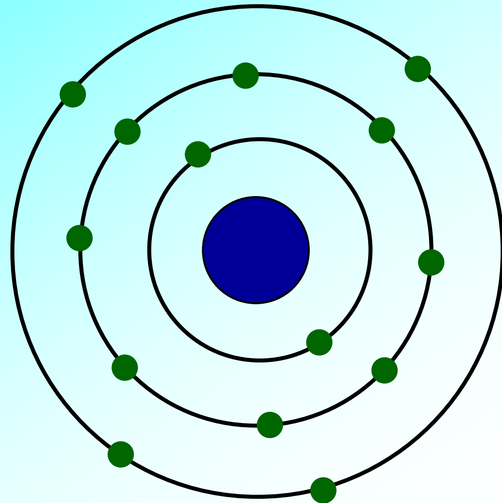


EDS

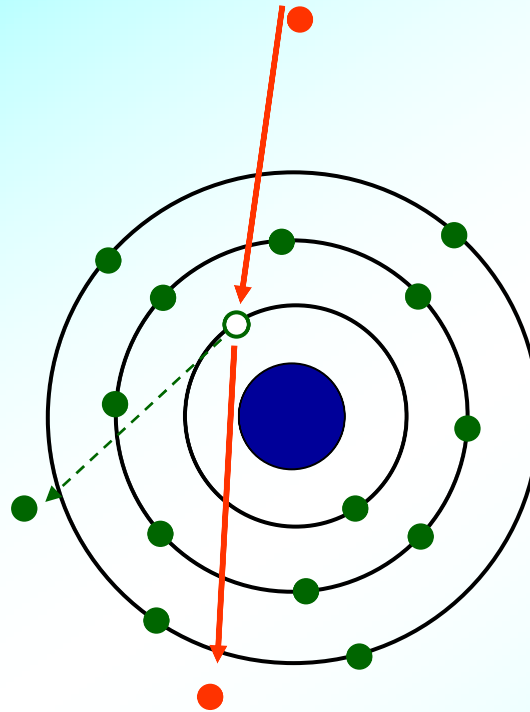
Energy Dispersive Spectroscopy



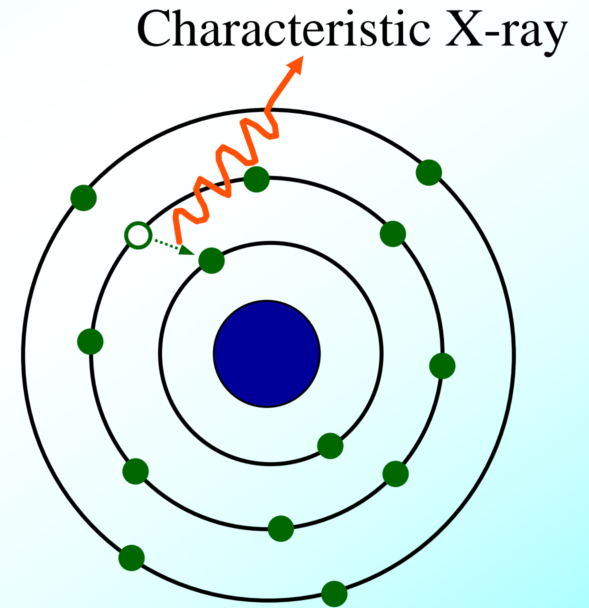
特性X-光的產生



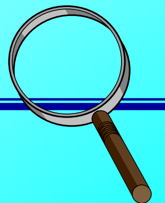
基態原子結構



內層電子被高能電子游離，原子處於激發狀態。

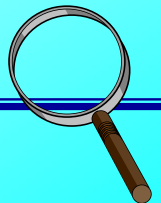


外層電子掉落內層軌域，多餘能量以特性x-光釋出。特性x-光能量等於兩能階差。

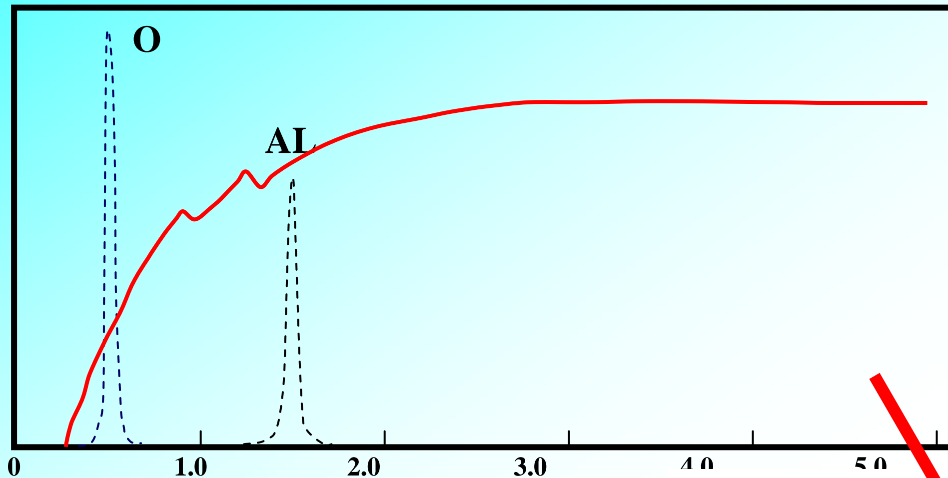


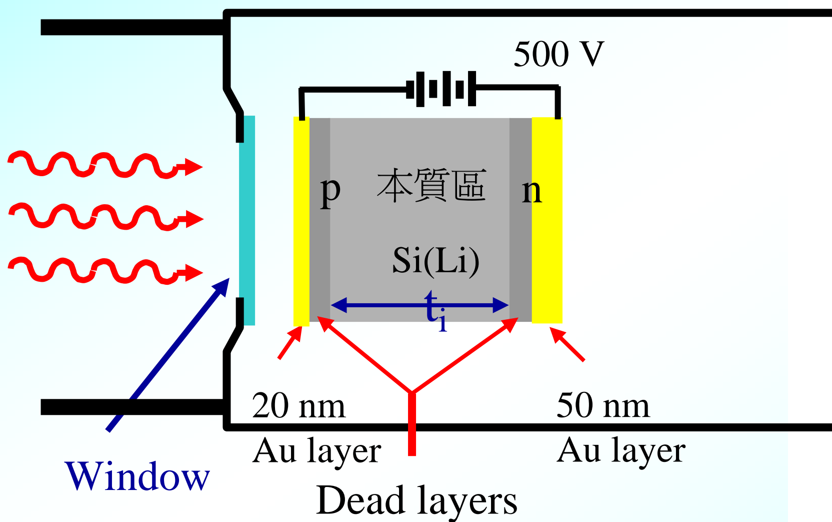
EDS 工作原理

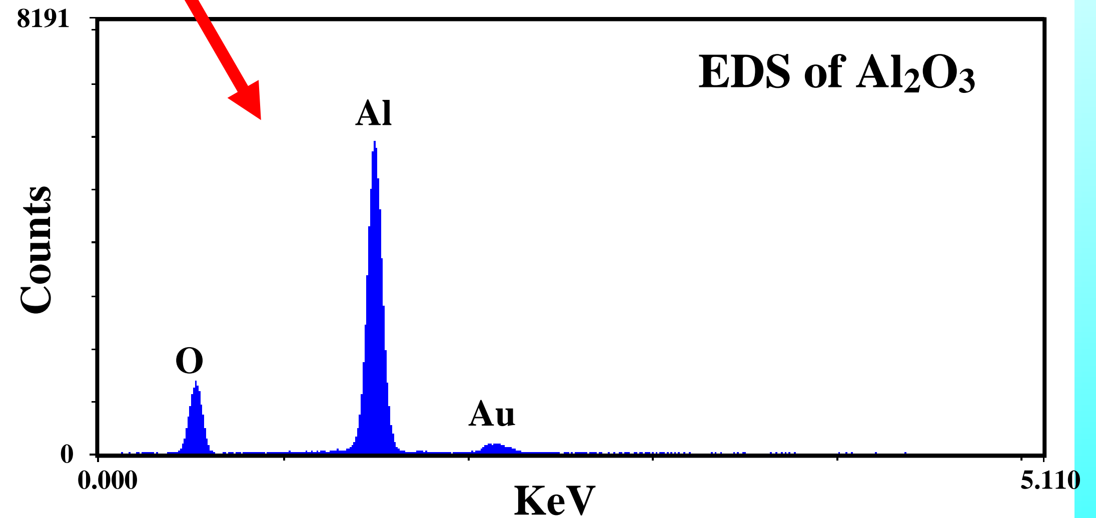
p
n
n x e^-
Pre-
amplifier
Main
amplifier
Pileup
Rejector
Display
Multichannel
Analyzer
Data
Output
Device
Computer
-500 V
Analog to
Digital
Converter
n
n + 5

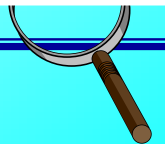


Convolution of Signal by Sensitivity









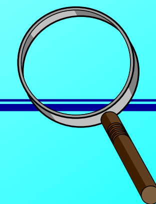
SEM加速電壓vs電子束/試片作用體積

20 KeV

10 KeV

5 KeV

e⁻ e⁻ e⁻



Volume of Signal Generated v. s. Probe Size

Secondary Electrons (SEM)

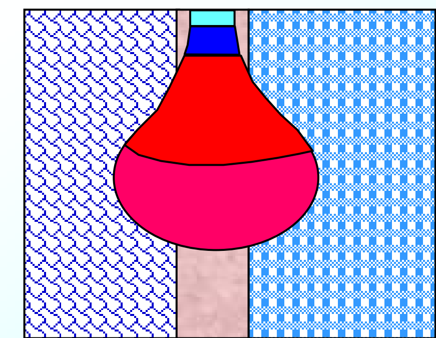
e^-

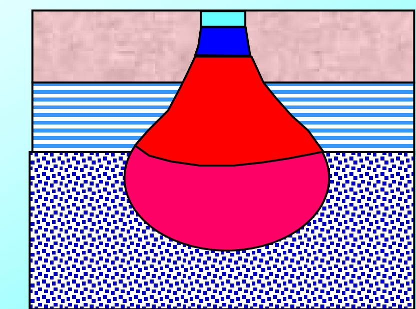
Auger Electrons (AES)
0.5 ~ 5.0 nm

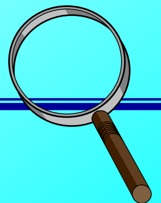
Backscattered Electrons
(SEM)

Characteristic X-rays
(EDS/SEM)

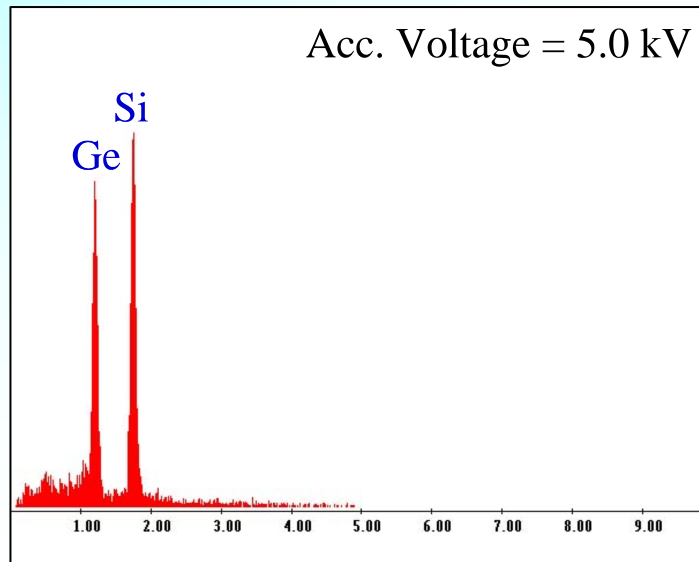
0.5 ~ 4 μm

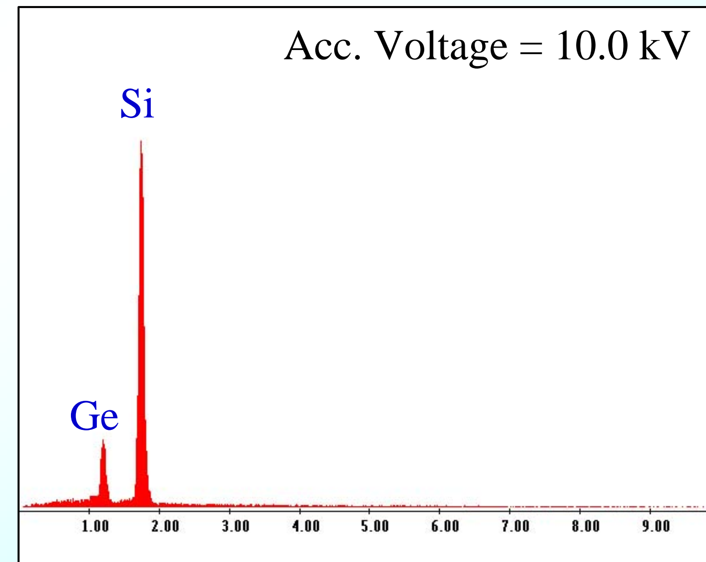


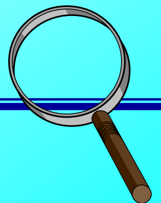




SEM EDS Analysis v.s. Acc. Voltage



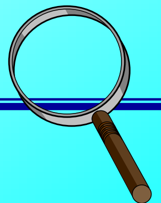




Pathological overlaps

- Energy resolution of EDS ~ 130 eV (0.13 keV)
  - Si K_α = 1.739 keV, Ta M_α = 1.709 keV, W M_α = 1.774 keV
  - Ti L_α = 0.452 keV, O K_α = 0.523 keV ; ΔE = 0.071 keV
    Ti K_α = 4.510 keV

Q: In-line SEM/EDS, Vacc = 5 keV, for a defect analysis
There is a peak at around 0.5 keV. It is labeled Ti/O by auto index.
How to judge it is Ti or O?



SEM EDS Analysis v.s. Acc. Voltage

- For SEM/EDS analysis，要激發某一能量(E_x)的特性X-ray ，電子束的能量(E_o)最好大於等於$2E_x$，最少也要$1.5E_x$以上。

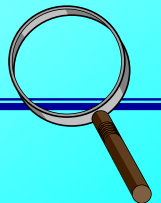
- Example
  - Vacc = 5 kV ie. = 5 keV

Si K_α = 1.739 keV

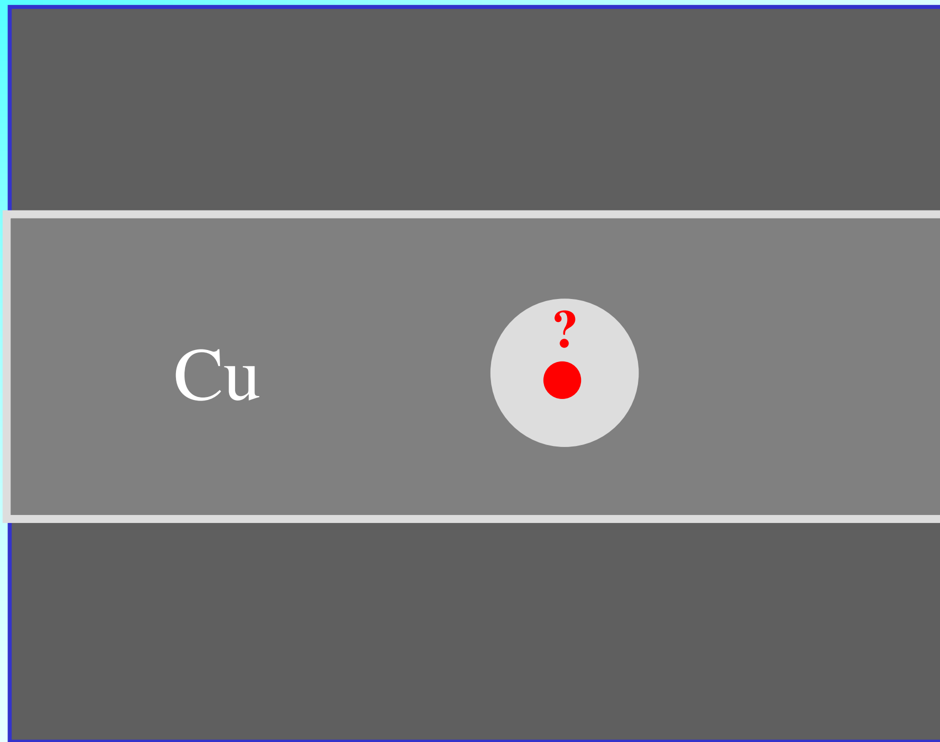
Ta M_α = 1.709 keV, L_α = 8.145 keV, $L_{\beta 1}$ = 9.342 keV, $L_{\beta 2}$ = 9.650 keV

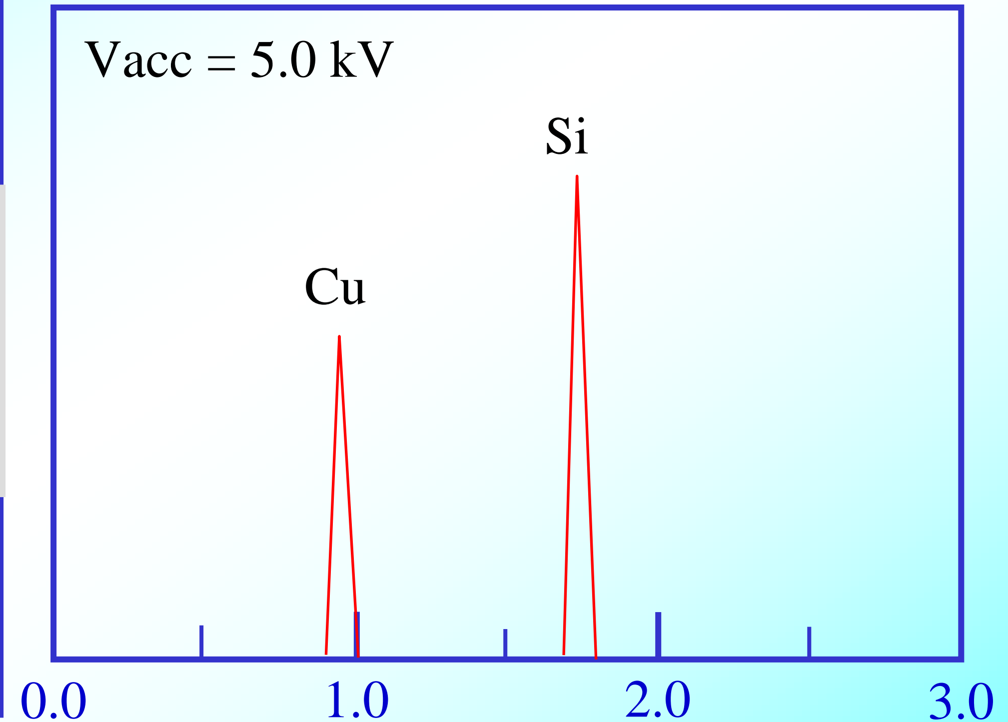
W M_α = 1.774 keV, L_α = 8.396 keV, $L_{\beta 1}$ = 9.671 keV, $L_{\beta 2}$ = 9.960 keV

Vacc = 20 kV should be used to separate Ta (or W) from Si.



Composition Analysis

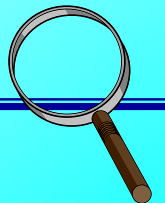




What is the particle?

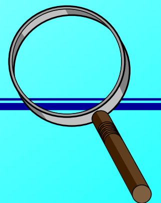
Is information in the image really not enough to tell it?

What does the EDS spectrum tell?



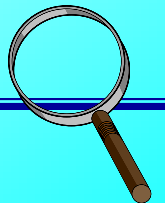
Limit of EDS/SEM

- Detection limit = 0.1 wt% ；
- Vacc = 5 keV is about the lowest operating volatage ；
- It is still not sensitive enough for a very thin layer ($t \leq 2$ nm) ；
- The vacuum of working chamber is another barrier ；
- AES has to be used for very thin layer analysis ；
- UHV working environment is used

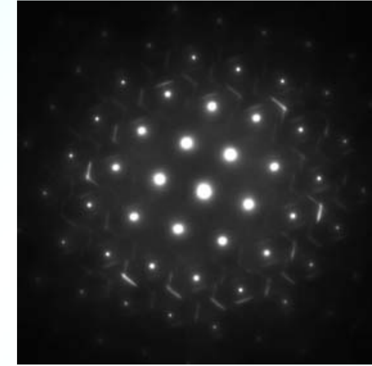


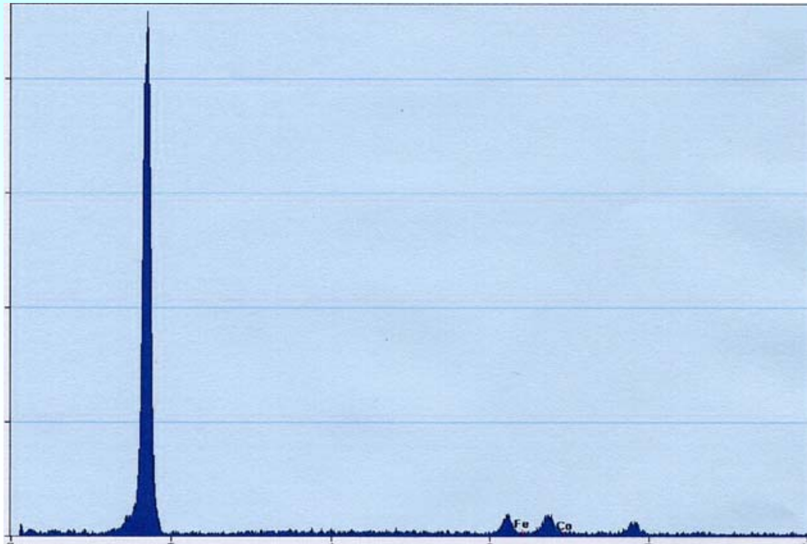
TEM-EDS

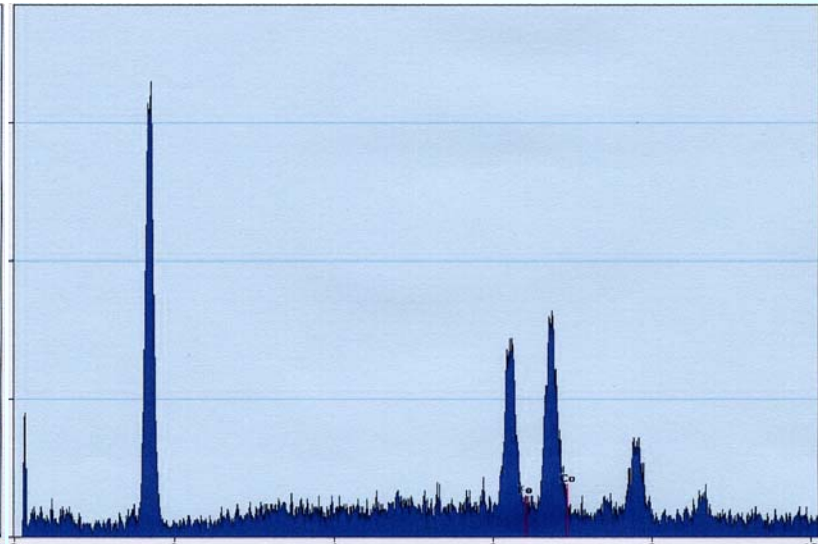
特性X-光的偵測可用波長分光儀(WDS)或能量分光儀(EDS) 。和SEM比較，在TEM分析中，產生特性X-光的體積非常小(見下圖)。加上試片漂浮效應在TEM中比較明顯，所以TEM只用EDS偵測特性X-光 。

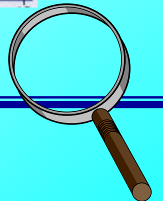


Effect of Diffraction Conditions



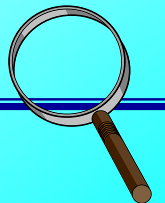






TEM/EELS

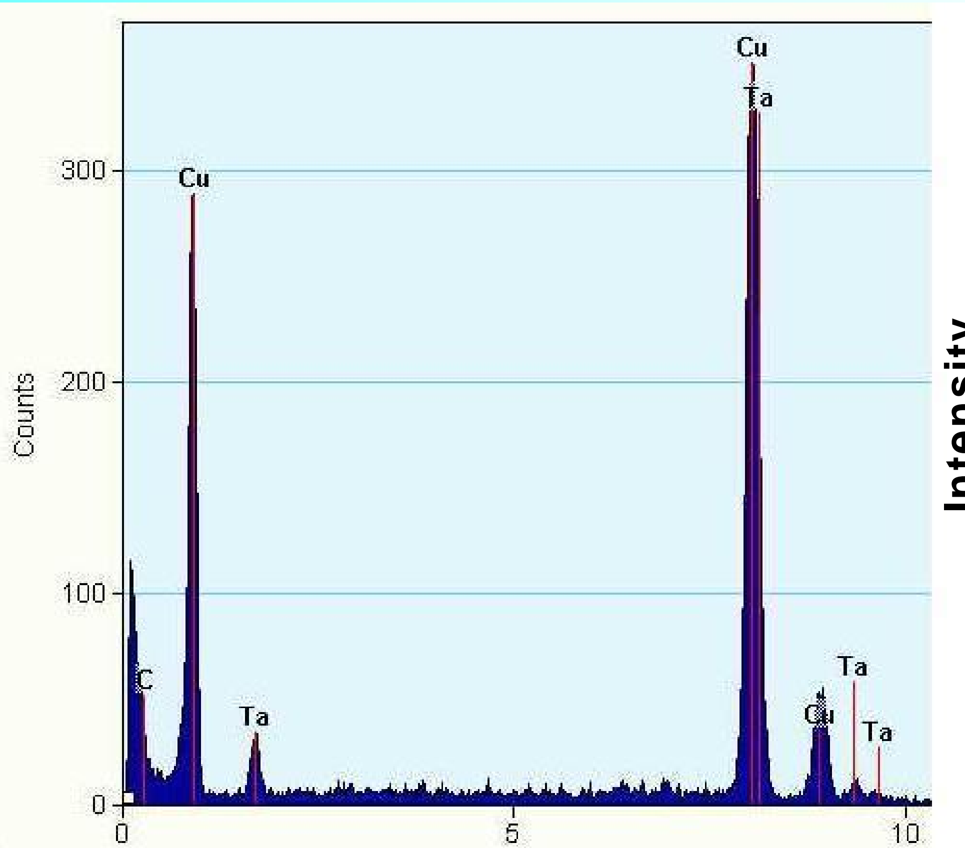
Electron Energy Loss Spectroscopy

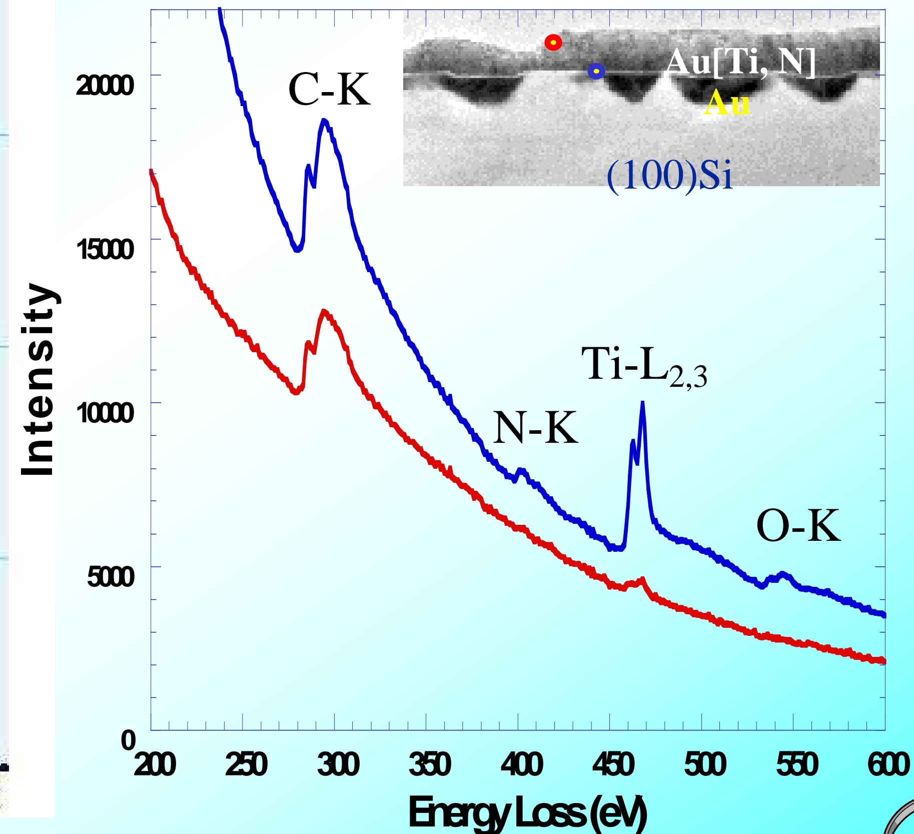


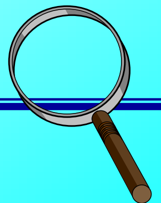
Information offered by TEM-- Composition

EDS

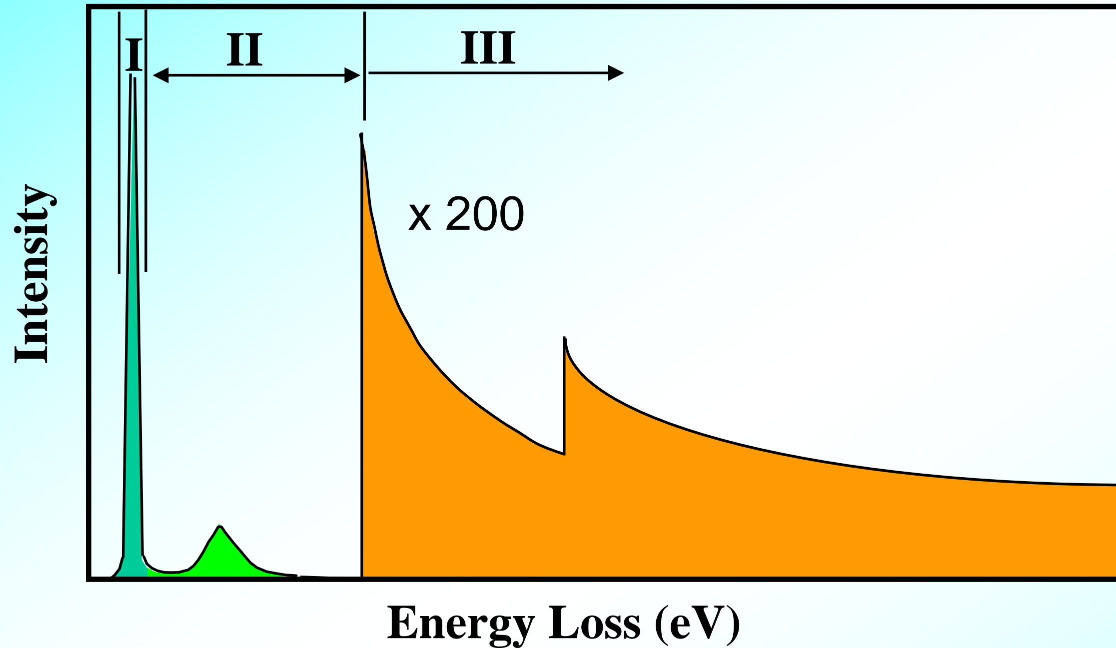
EELS







EELS-Basic



Energy Loss (eV)

I : 0 ~ 5 eV Zero Loss

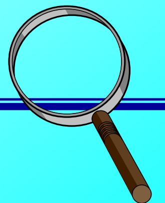
Unscattered + elastically scattered electrons

II : 5 ~ 50 eV Low Loss Region (Plasmons)

Electrons inelastically scattered by out-shell electrons

III : > 50 eV Core Loss Region

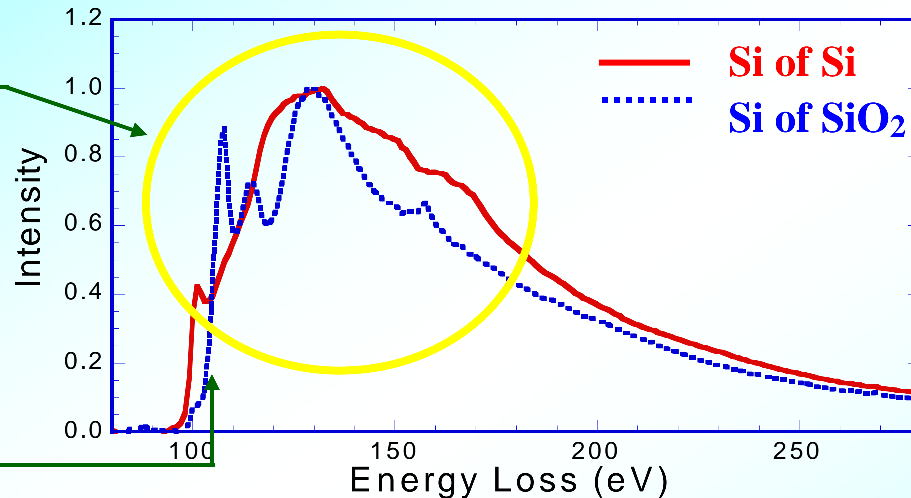
Electrons inelastically scattered by inner-shell electrons



EELS - Quantitative Analysis (II)

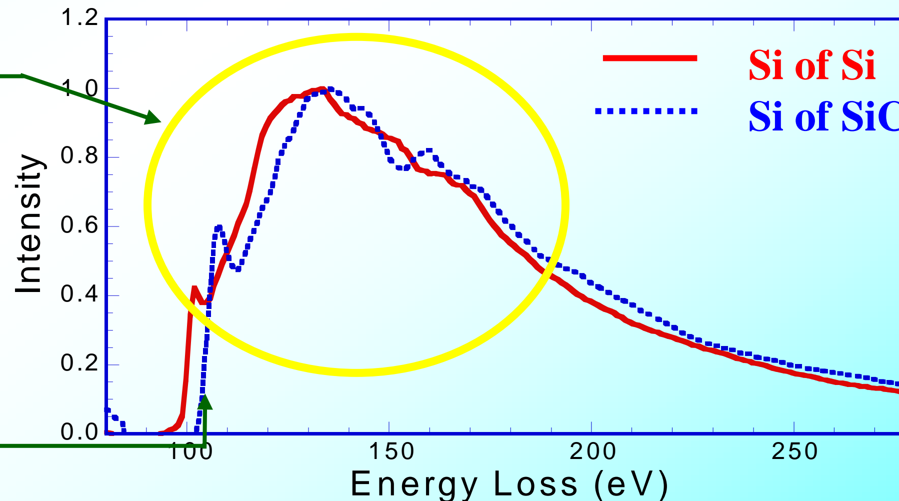
Near edge fine structure indicates different chemical bonding state

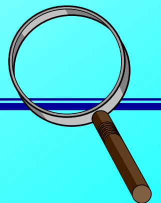
Threshold delay indicates higher bonding energy



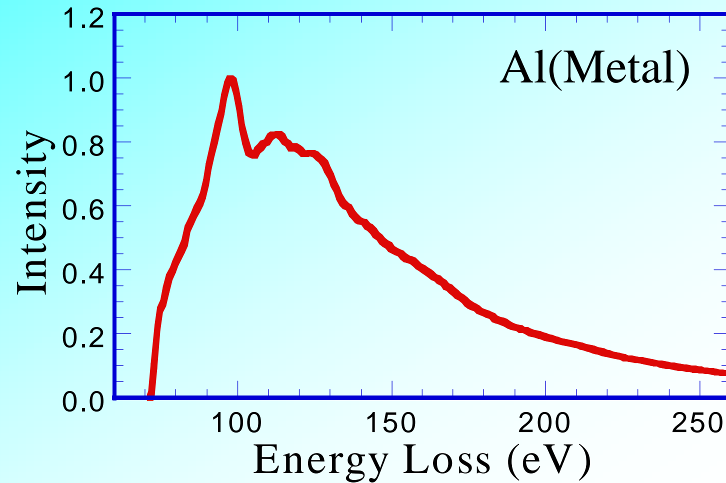
Near edge fine structure indicates similar chemical bonding state

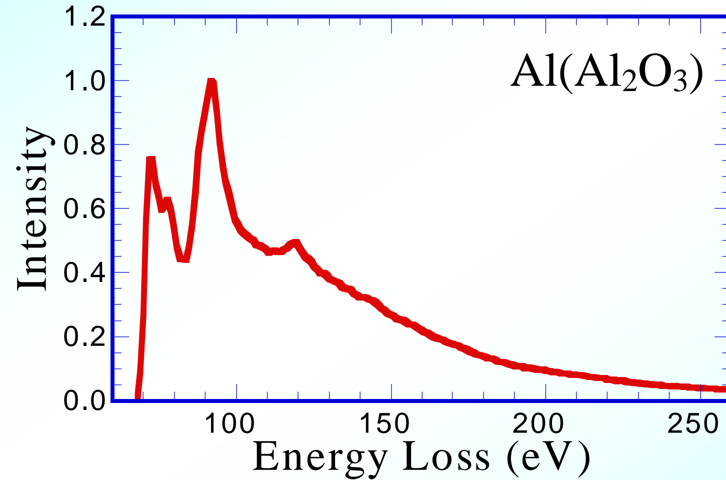
Threshold delay indicates higher bonding energy

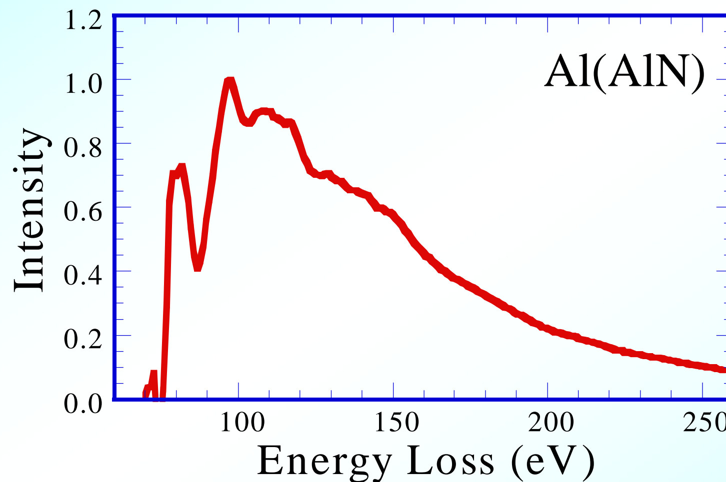


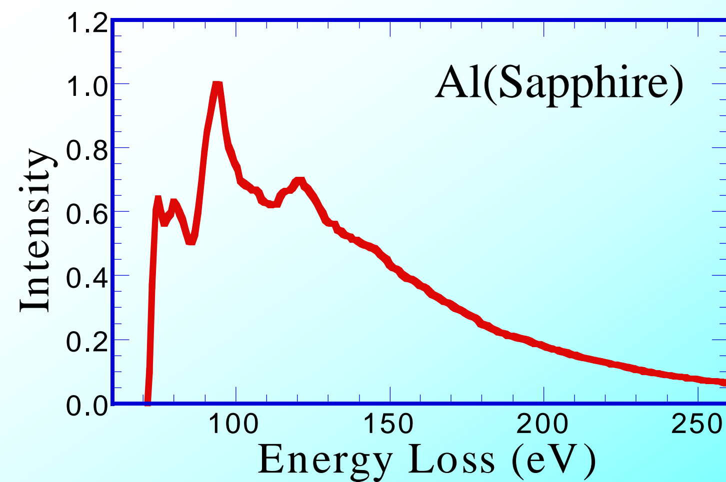


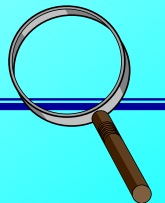
EELS - Quantitative Analysis (IV)











Energy Selected Imaging

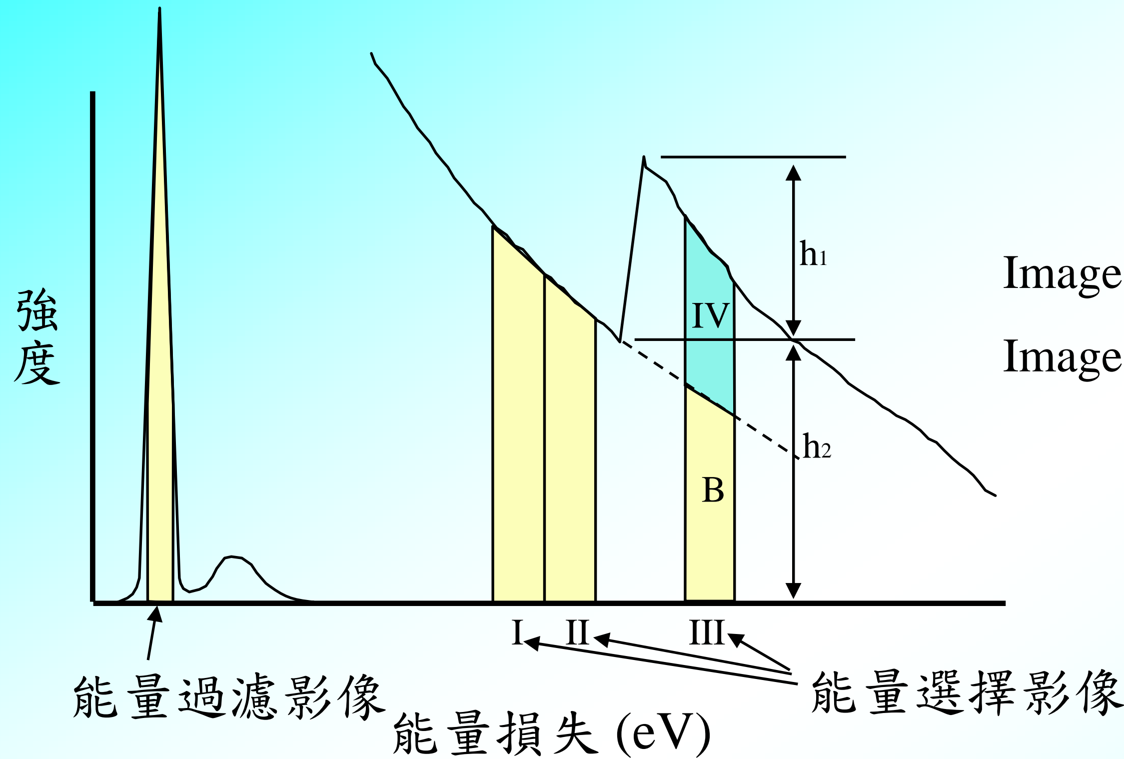


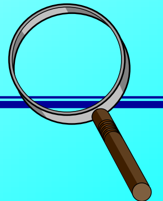
Image I and Image II = preedge images

Image III = Image B(background image) + image IV (the composition image)

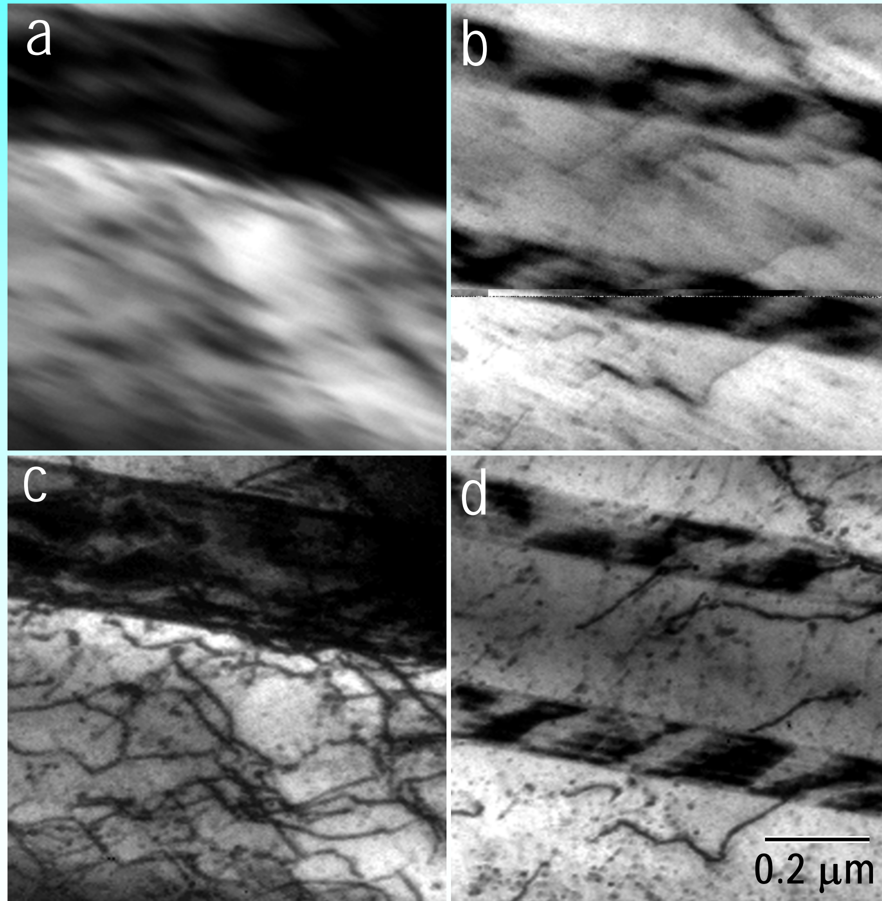
Linear approximation

$$imaB = imaI + \frac{imaI - imaI}{E_{II} - E_{I}} \times \left(E_{III} - E_{I}\right)$$

$$imaIV = imaIII - imaB$$



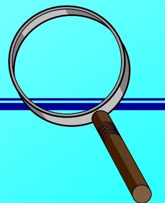
能量過濾影像(Energy Filtered Images)



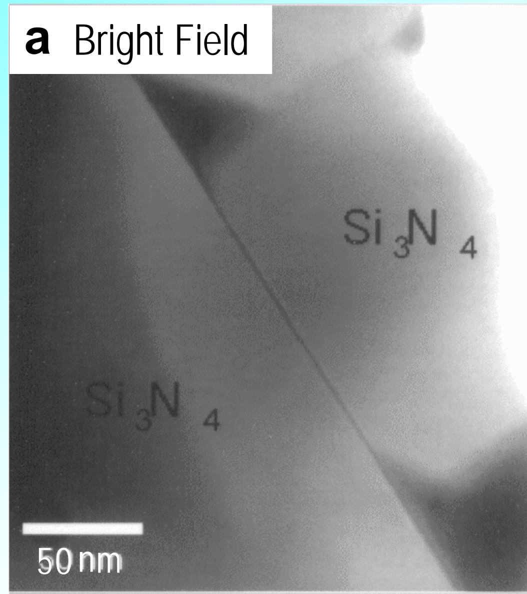
不銹鋼的能量過濾圖。
a 和 b是未過濾影像，
c 和 d 是過濾影像 ($\Delta E = 4$ eV)。

a 和 c 的試片厚度是 208 nm，
b和 d 的試片厚度是 88 nm ，
試片厚度由雙晶寬度求出。

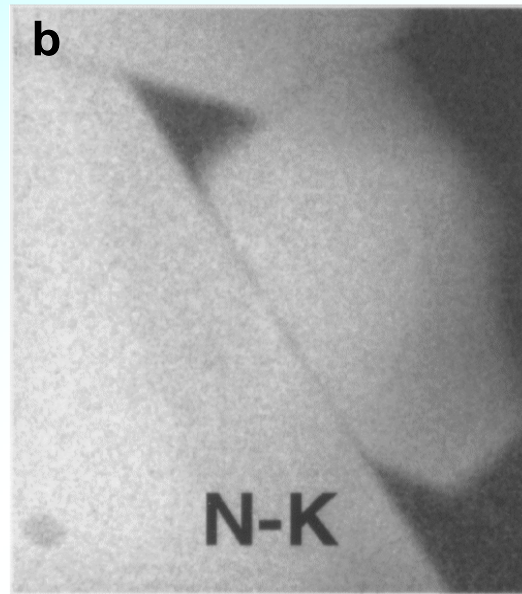
g = <111>•



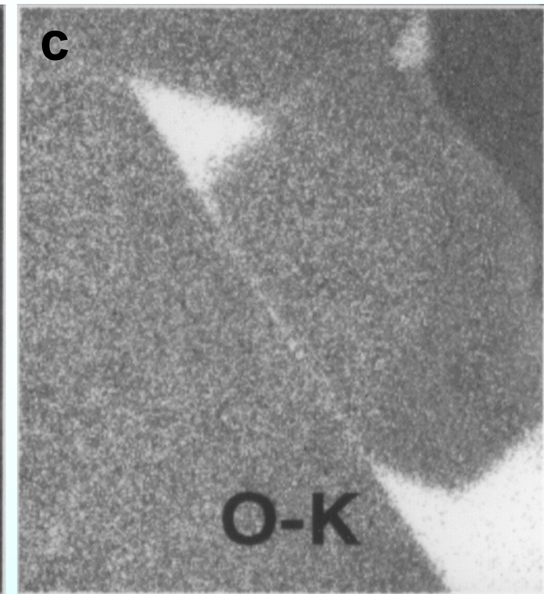
Energy Selected Image



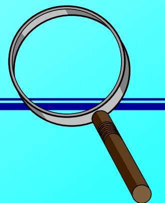
BF image



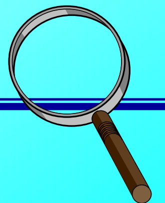
N mapping



O mapping



Auger Electron Spectroscopy



AES儀器原理

如下圖所示，被高能電子束激發的Auger電子自試片表面釋出，被電子能量分析器接收和分析，從其特性動能判斷元素的種類。接於能量分析器後面的電子檢測器則計算通過的電子數量，推算元素的濃度。

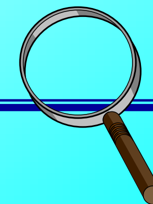
電子鎗

電子能量分析儀

電子檢測器

試片表面層

To訊號擷取暨數據處理系統



AES能譜中電子種類和其分佈

E₀

dN(E)/dE

微分能譜

O

Ag

N(E)×10

元素能峰

原始能譜

Ag

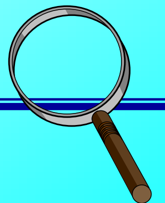
N(E)

非彈性背向散射電子

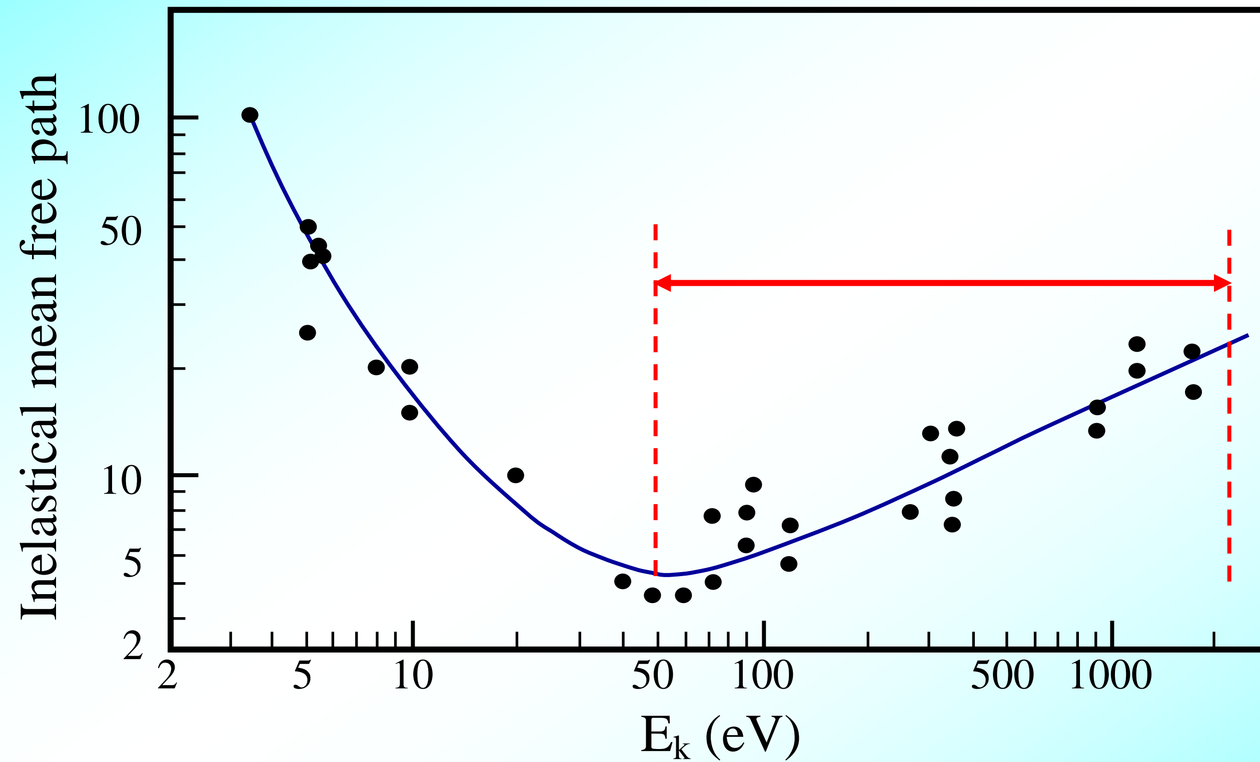
0 200 400 600 800 1000

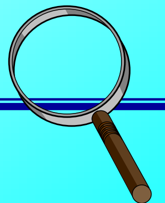
彈性反射電子

二次電子

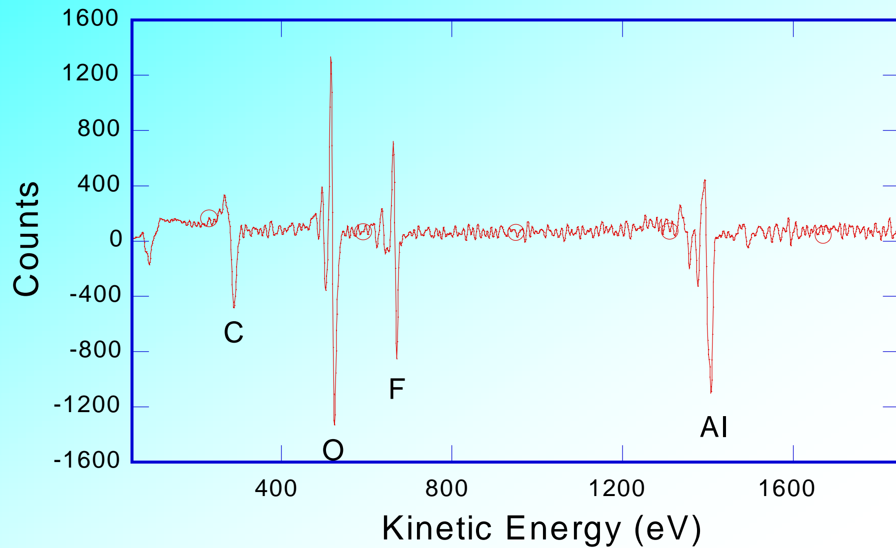


電子能量 vs 電子非彈性自由平均行程



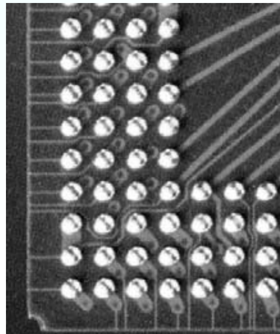


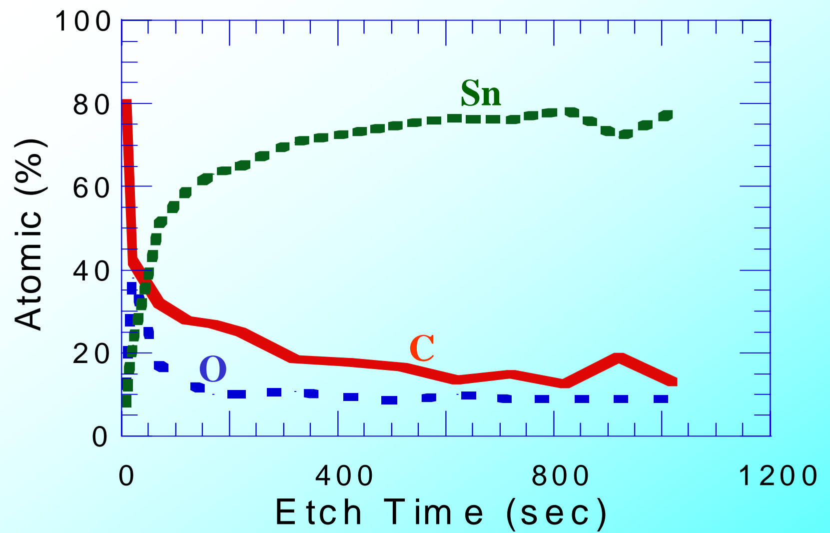
AES: Composition and Depth Profile



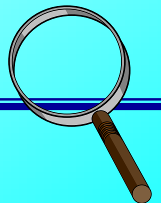
AES: $E_{KLM} = E_K - E_L - E_M$

Depth profile: $t \propto \tau$





資料提供: 田大昌先生&洪英傑先生



AES: Composition and Depth Profile

t = 0

e^-

Al

t = t_1

e^-

Al

t = t_2

e^-

Al

t = t_3

e^-

Al

t = 0

Oxide state

Au

t = t_1

C

Al

t = t_2

O

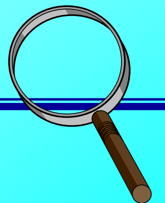
Metal state

t = t_3

500 1000 1500 2000

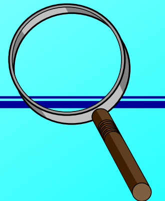
Kinetic Energy (eV)

資料提供: 黃啟貞小姐



SIMS

Secondary Ion Mass Spectroscopy



二次離子的生成機制 (II)

Primary ions

正離子

+

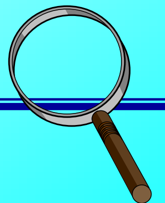
中性粒子

-

負離子

資訊深度 ~ 1 nm

植入離子



靜態SIMS能譜

O^{2+} , 8 KeVm 34.10 nA

Counts per second

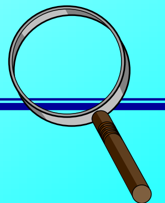
10^6
10^5
10^4
10^3
10^2
10^1
10^0

Si
Na
Si

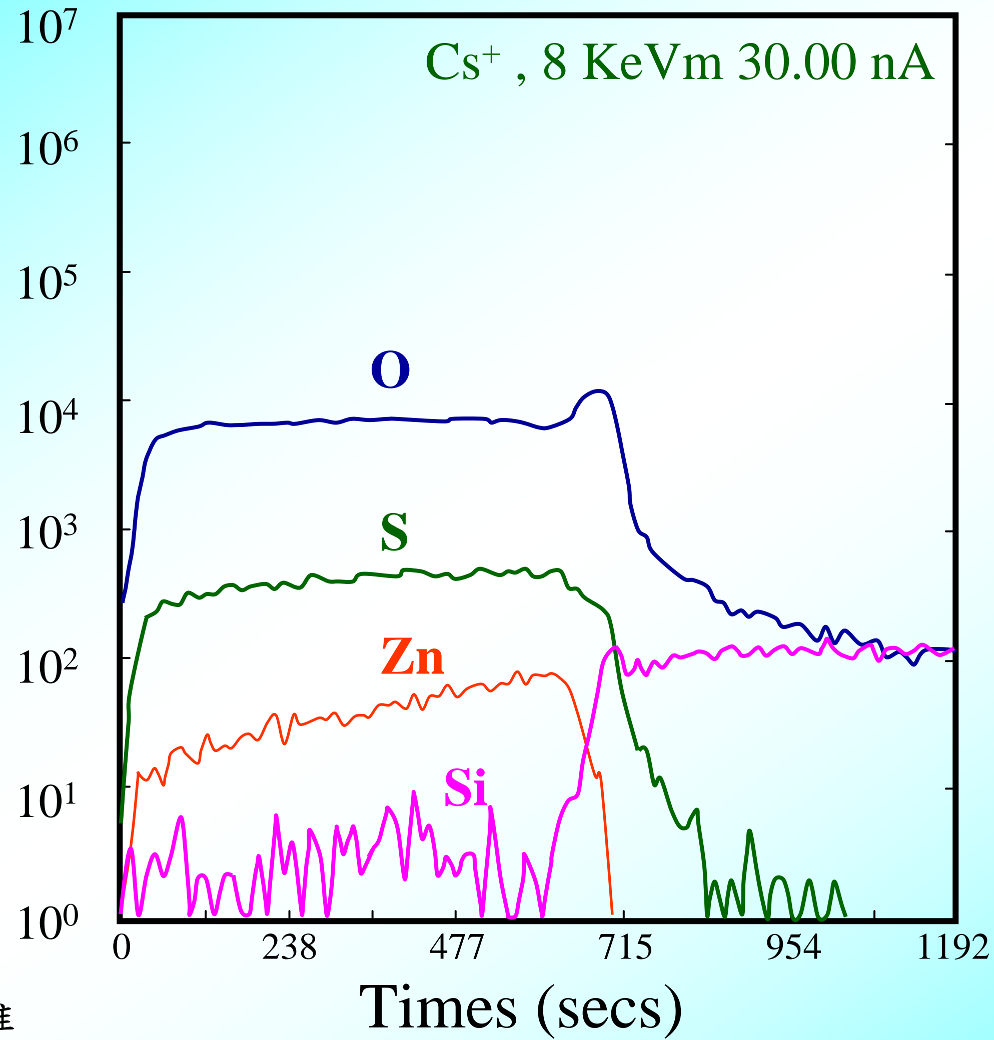
0 8.0 16 24 32 40 48 56 64 72 80

Atomic Mass Unites

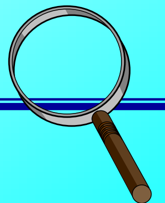
資料提供: Dr. 黃悉雅



縱深分析



資料提供: Dr. 黃悉雅



SIMS Measurement of N-well and P-well

[Atom/cm3] [c/s]

10^{22} 10^{21} 10^{20} 10^{19} 10^{18} 10^{17} 10^{16} 10^{15}

10^{8} 10^{7} 10^{6} 10^{5} 10^{4} 10^{3} 10^{2} 10^{1} 10^{0}

→28Si
←31P
←75As 28Si

NW (P)

0 500 1000 1500 2000 2500

Depth: [nm]

[Atom/cm3] [c/s]

10^{22} 10^{21} 10^{20} 10^{19} 10^{18} 10^{17} 10^{16} 10^{15}

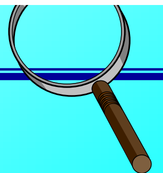
10^{8} 10^{7} 10^{6} 10^{5} 10^{4} 10^{3} 10^{2} 10^{1} 10^{0}

←11B
→28Si

PW (B)

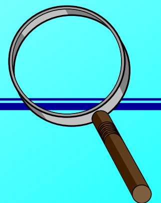
0 500 1000 1500 2000 2500

Depth: [nm]



SIMS在半導體分析的應用

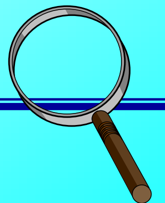
- Depth profile of implant dopants
  - 在半導體領域中應用最廣的分析
  - 尤其是B、P、As
  - 測定離子佈植機的機台特性和穩定性
- 污染元素分析
  - 高分子物質
  - Al、Fe、Co、Ni
- 元素擴散分析
- 硼磷矽玻璃
  - 必須利用電子束中和樣品表面電荷累積



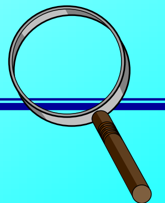
Crystallography

They are all carbon products

They are all SiO_2 products



XRD



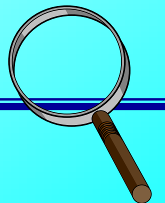
Characteristics of Crystals

Each crystal has a set of unique crystal planes.

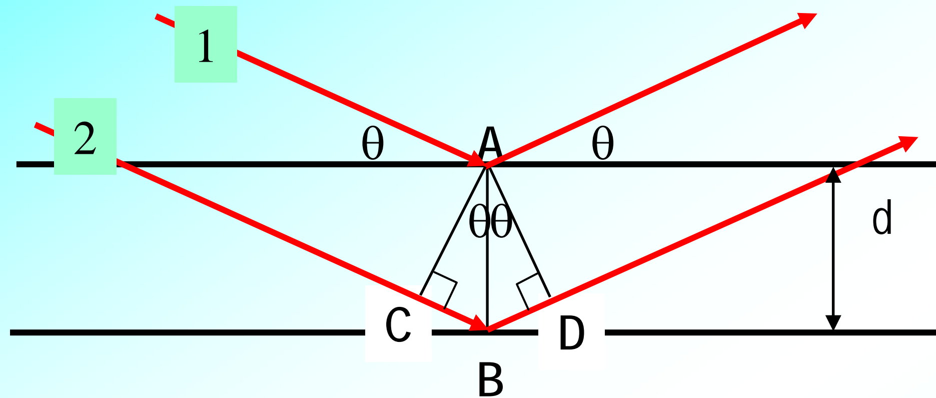
d_{hkl}

i.e. a unique set of {*hkl*}, as finger print

Eg.: fcc (*hkl*) = (111), (002), (022), (004)…..
bcc (*hkl*) = (011), (002), (022), (013), …..



Bragg's Law



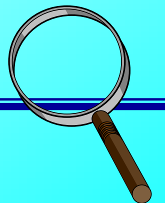
$$\Delta L = 2d\sin\theta = n\lambda$$

n=1, d = 2.5 Å

For x-ray

λ = 1.54 Å (Cu Kα)

$\theta = 17.7^{o}$



Phase Identification by XRD (1)

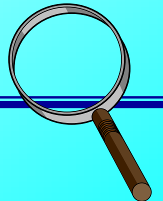
59.5°
49.3°
45.2°
36.5°
18.5°

Counts

30000
25000
20000
15000
10000
5000
0

10 20 30 40 50 60 70 80 90

2θ



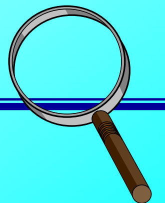
Phase Identification by XRD (2)

$\theta = 18.5^o, 36.5^o, 45.2^o, 49.3^o, 59.5^o$

$2d\sin\theta = \lambda$

$d = 2.427, 1.294, 1.085, 1.016, 0.894$ Å

Comparing this set of d-spacing with the XRD database



Phase Identification by XRD (3)

Counts

30000
25000
20000
15000
10000
5000
0

003
101
006
012
104
015
107
018
110

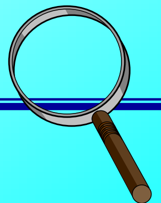
10 20 30 40 50 60 70 80 90

2θ

<77-1370> CoLiO2 (100%)

10 20 30 40 50 60 70 80 90

資料提供:林希哲博士



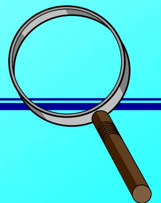
Phase Identification by XRD (4)

Advantages:

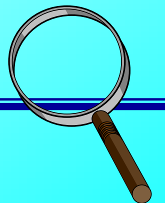
- Automatically
- Statistically
- Accurately

Disadvantages:

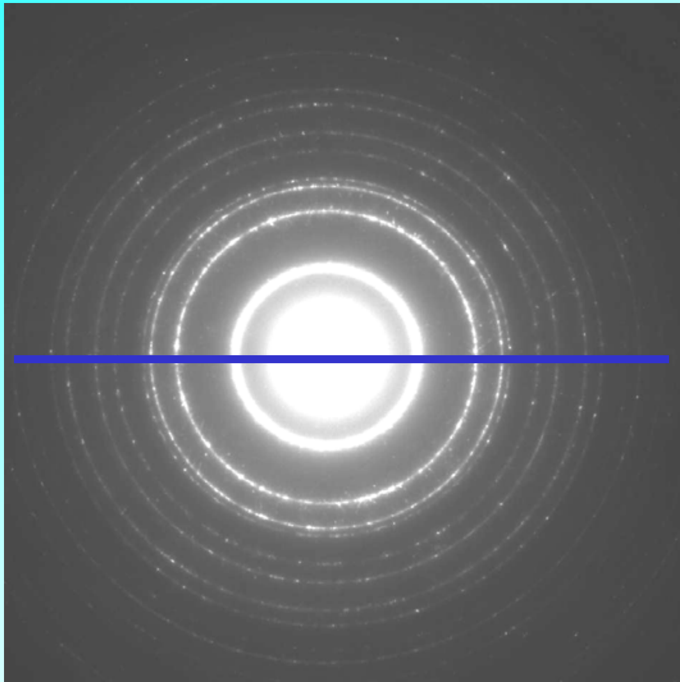
- Poor spatial resolution, several mm in diameter
- Need enough samples



Electron Diffraction



Phase Identification by SADP (2)



D_1

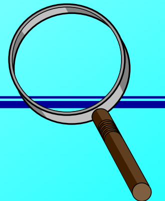
D_2

D_3

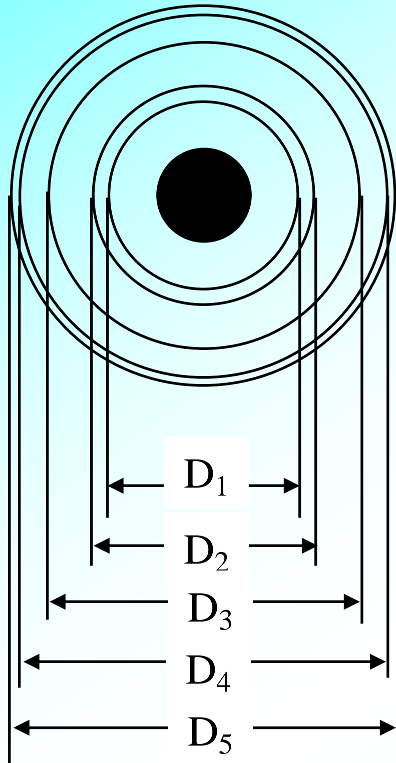
D_4

D_5

$$Rd = \lambda L$$



Phase Identification by SADP



(1) $R_1 : R_2 : R_3 : \ldots\ldots = 1 : X_2 : X_3 : \ldots\ldots$

==>crystal structure

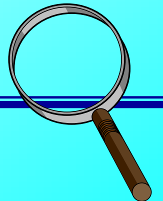
(2) if λL is known, $d = \dfrac{\lambda L}{R}$ ==> $d_1, d_2, d_3, \ldots$

(3) For cubic crystals

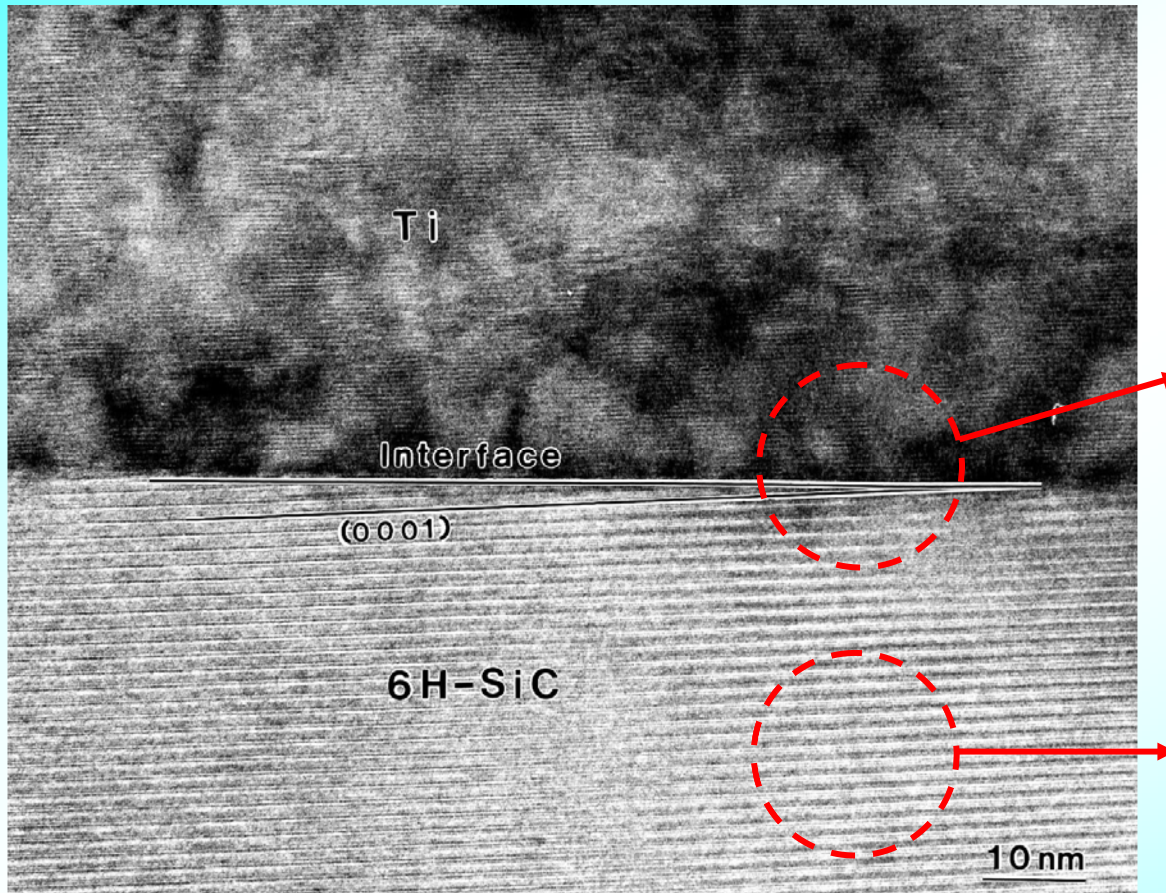
$$d_{hkl} = \frac{a_o}{(h^2 + k^2 + l^2)^{1/2}}$$

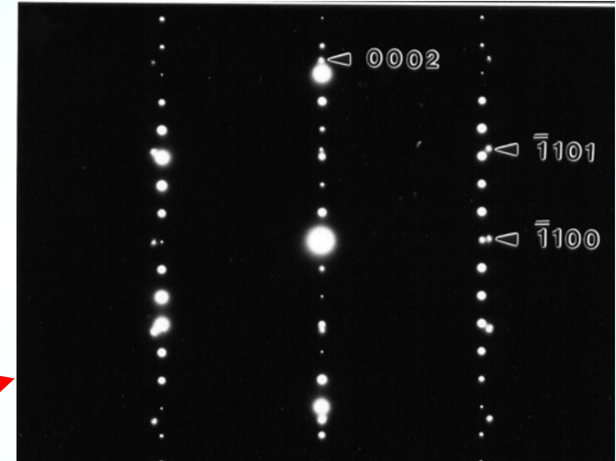
fcc 1:1.155:1.633:1.915:2.000

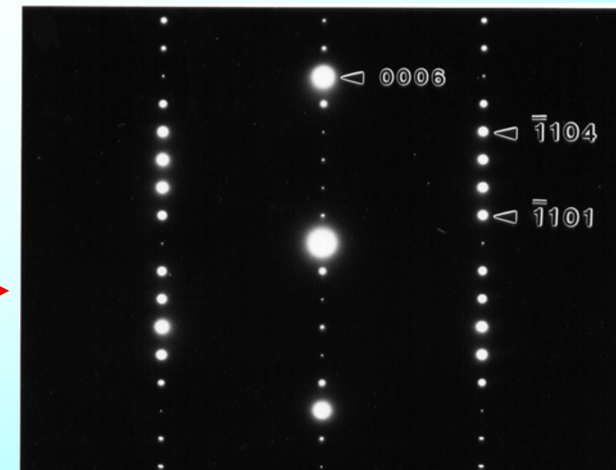
bcc 1:1.414:1.742:2.000:2.236

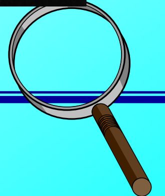


HREM and SADP of As-deposited Ti/6H-SiC



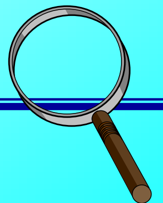




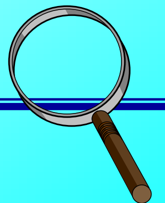


Converged Beam Electron Diffraction (CBED)

The fringes in the CBED (0 0 0) disc become blurred with increasing specimen thickness. An energy filtered CBED will help as an energy filtered image does.



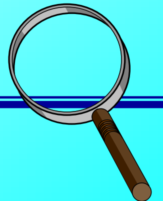
HREM Diffractogram



Fast Fourier Transform (FFT)

HREM → FFT → Inverse FFT

- Very High spatial resolution ~ 3 nm x 3 nm available
- Accurate measurement



Phase Identification by FFT (1)

a

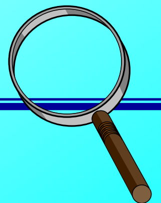
Ti

Ti_5Si_3

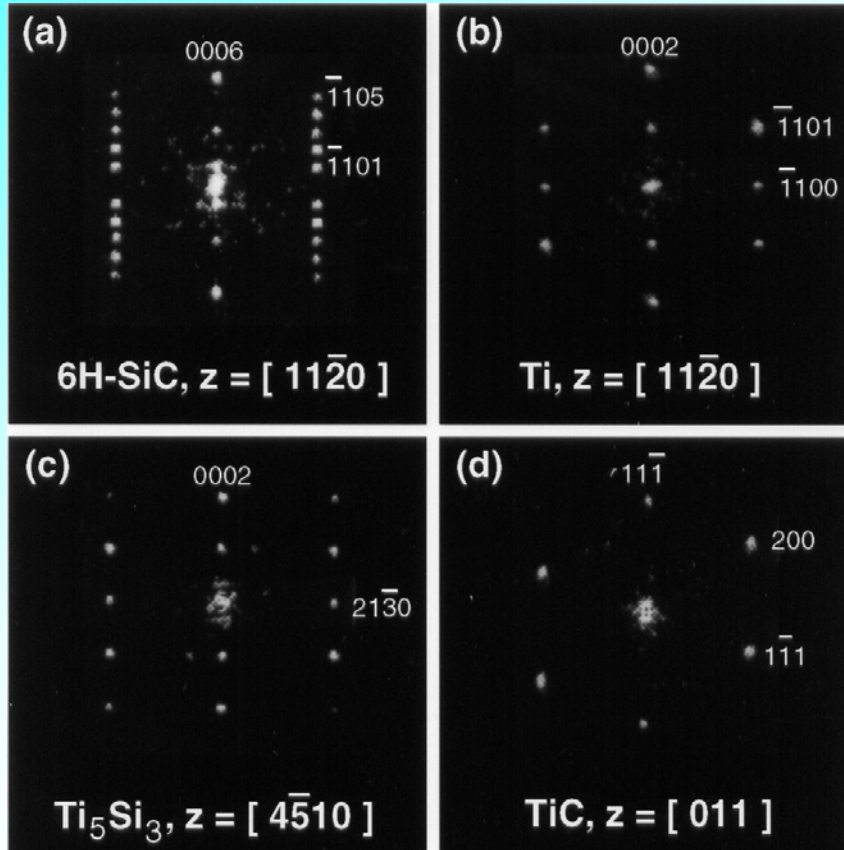
TiC

6H SiC

5 nm



Phase Identification by FFT (2)



	measured spacing(nm)	calculated spacing(nm)	error(%)	(h k . l)
700 °C/20 min. 6H-SiC	0.2513	0.2513	0.00	(0006)*
	0.2197	0.2174	1.08	$(1\bar{1}04)$
	0.2543	0.2511	1.29	$(1\bar{1}02)$
	0.2656	0.2621	1.33	$(1\bar{1}01)$
Ti_5Si_3	0.2572	0.2571	0.05	(0002)
	0.1770	0.1769	0.04	$(21\bar{3}2)$
	0.2205	0.2202	0.15	$(21\bar{3}1)$
	0.2432	0.2436	-0.14	$(21\bar{3}0)$
Ti	0.2353	0.2342	0.49	(0002)
	0.2254	0.2244	0.45	$(1\bar{1}01)$
	0.2567	0.2557	0.40	$(1\bar{1}00)$
TiC	0.2430	0.2499	-2.74	$(\bar{1}1\bar{1})$
	0.2460	0.2499	-1.54	$(11\bar{1})$
	0.2142	0.2164	-1.03	(200)