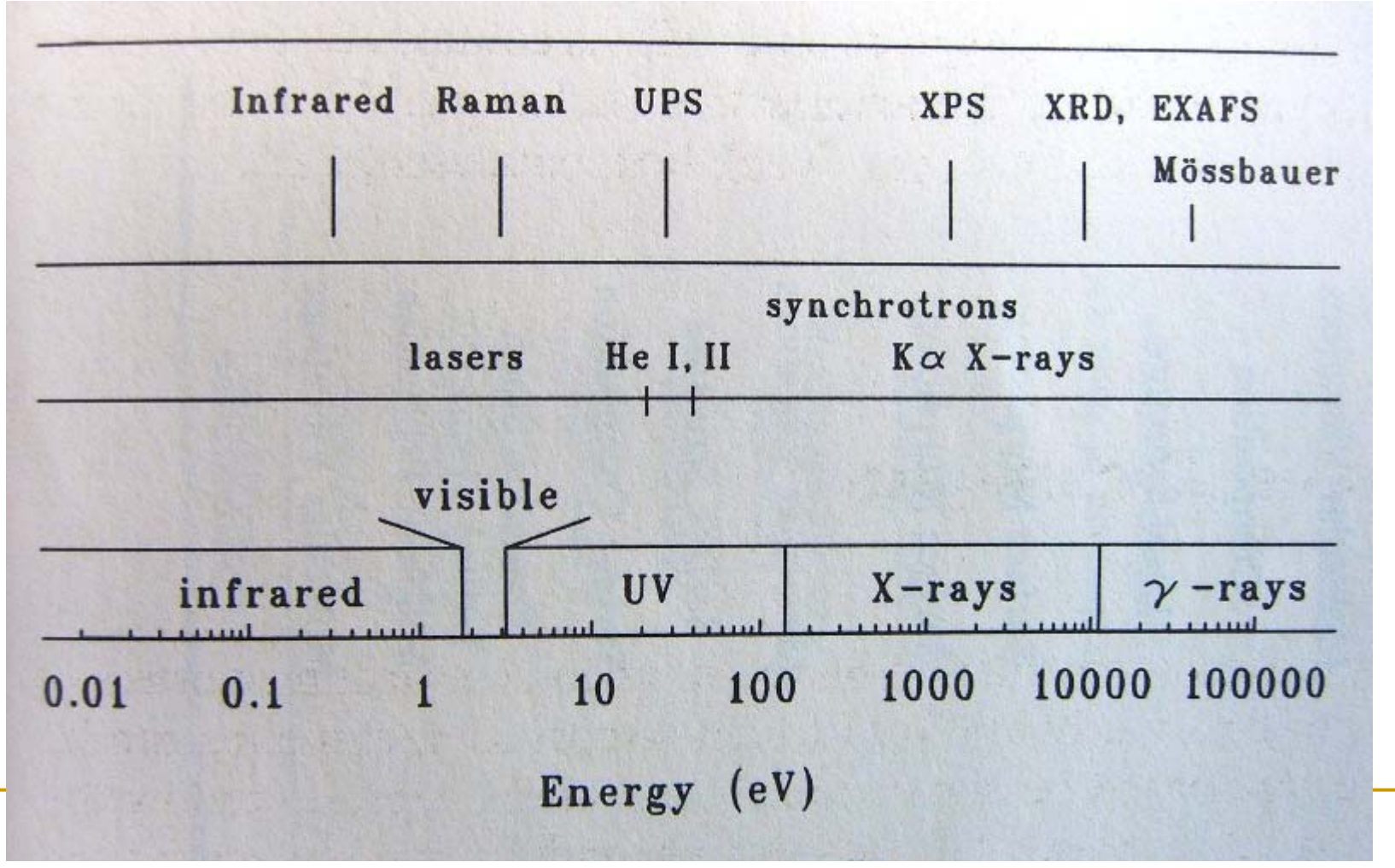
XPS
X-ray Photoelectron Spectroscopy

連興隆

光譜儀之使用範圍

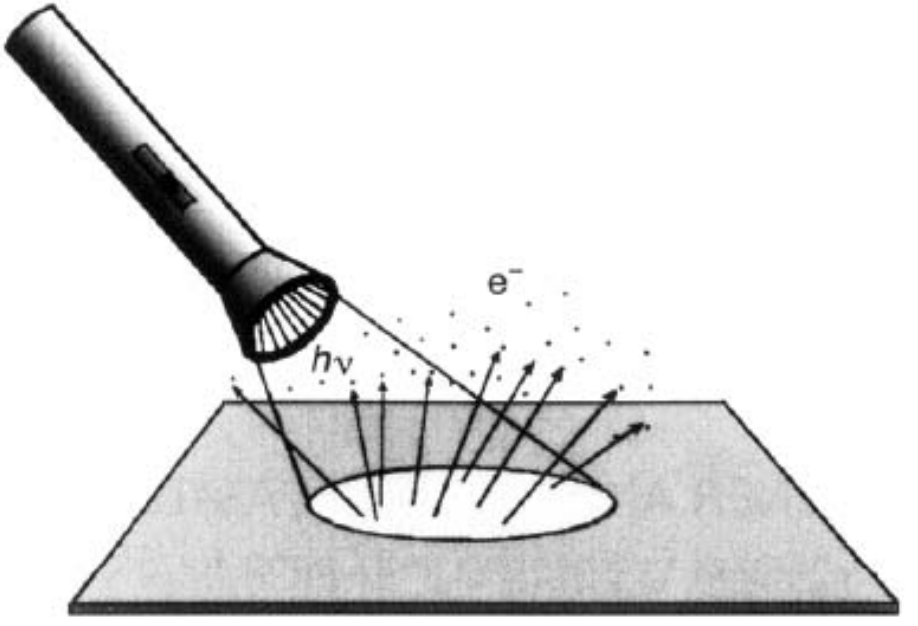

Infrared
Raman
UPS
XPS
XRD, EXAFS
Mössbauer
synchrotrons
lasers
He I, II
Kα X-rays
visible
infrared
UV
X-rays
γ-rays
0.01
0.1
1
10
100
1000
10000
100000
Energy (eV)

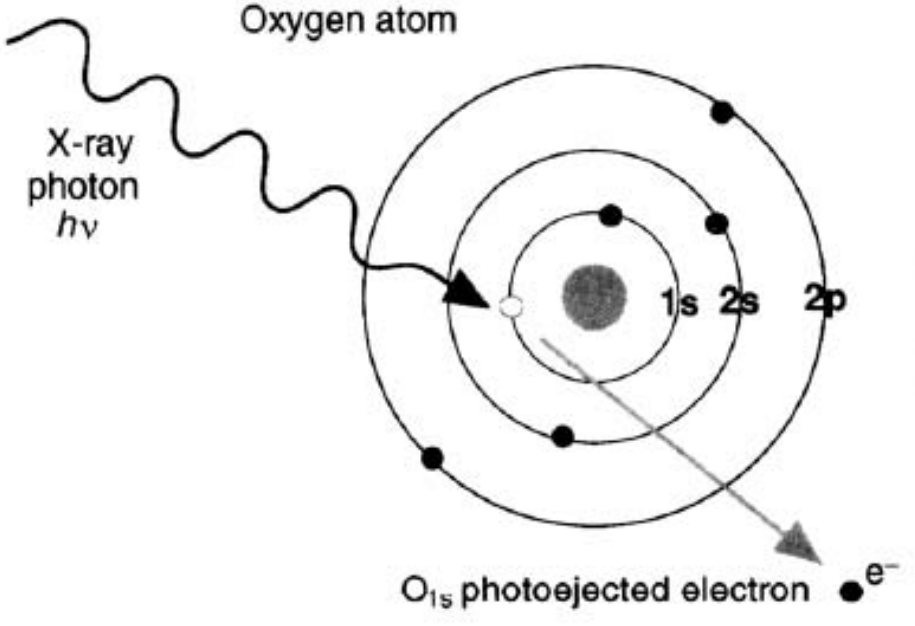
Introduction

Photoelectric effect

Photoelectric effect

Einstein, Nobel Prize 1921



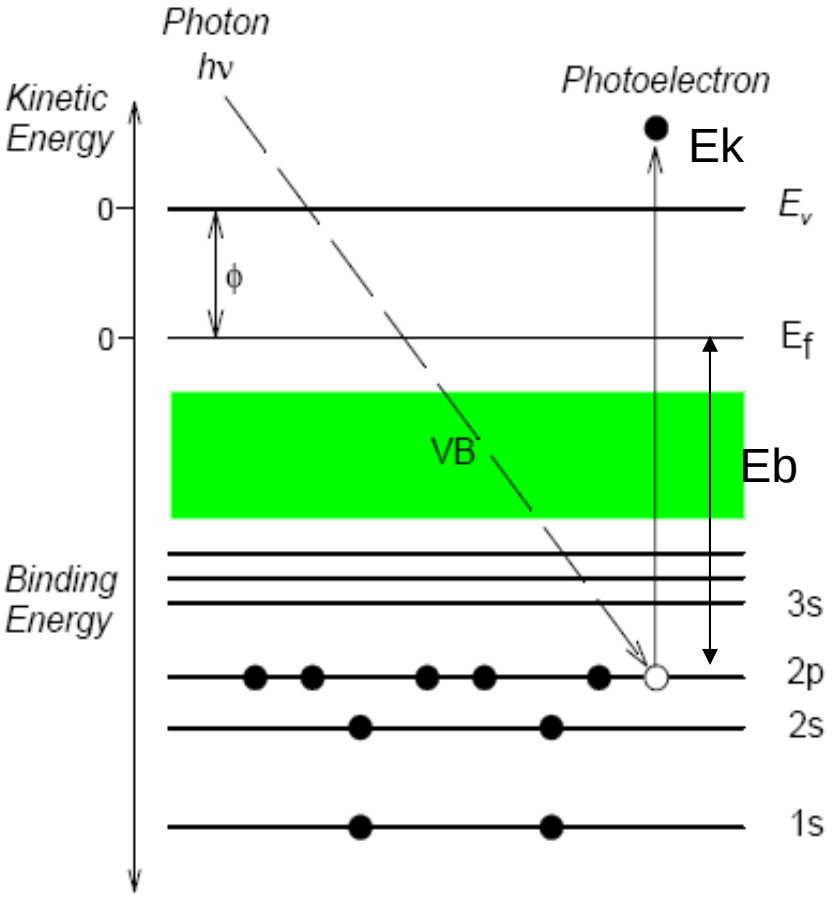


Photoemission as an analytical tool

Kai Siegbahn, Nobel Prize 1981

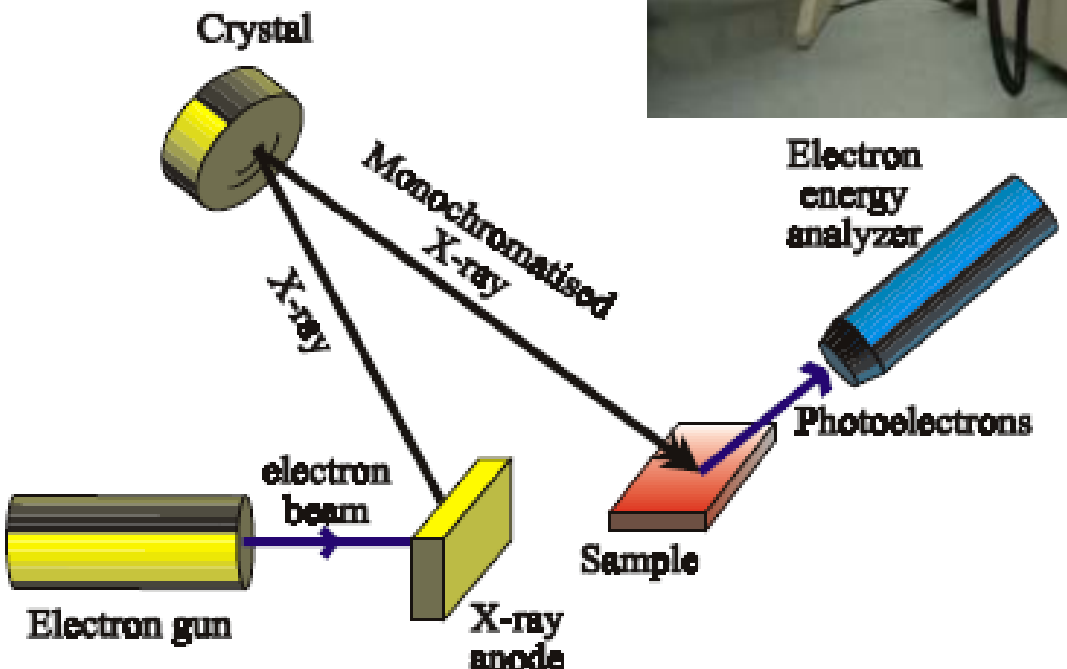
主要功能與原理

- 了解分析物之化學鍵結(價態)



Ek = *hν*-Eb-φ

ne	Energy, eV	Width, eV
$M\zeta$	132.3	0.47
$M\zeta$	151.4	0.77
$M\zeta$	171.4	1.21
$M\zeta$	192.3	1.53
$L\alpha$	395.3	3.0
$L\alpha$	572.8	3.0
$L\alpha$	851.5	2.5
$L\alpha$	929.7	3.8
$K\alpha$	1253.6	0.7
$K\alpha$	1486.6	0.85
$K\alpha$	1739.5	1.0
$L\alpha$	1922.6	1.5
$L\alpha$	2042.4	1.7
$K\alpha$	4510.0	2.0
$K\alpha$	5417.0	2.1
$K\alpha$	8048.0	2.6



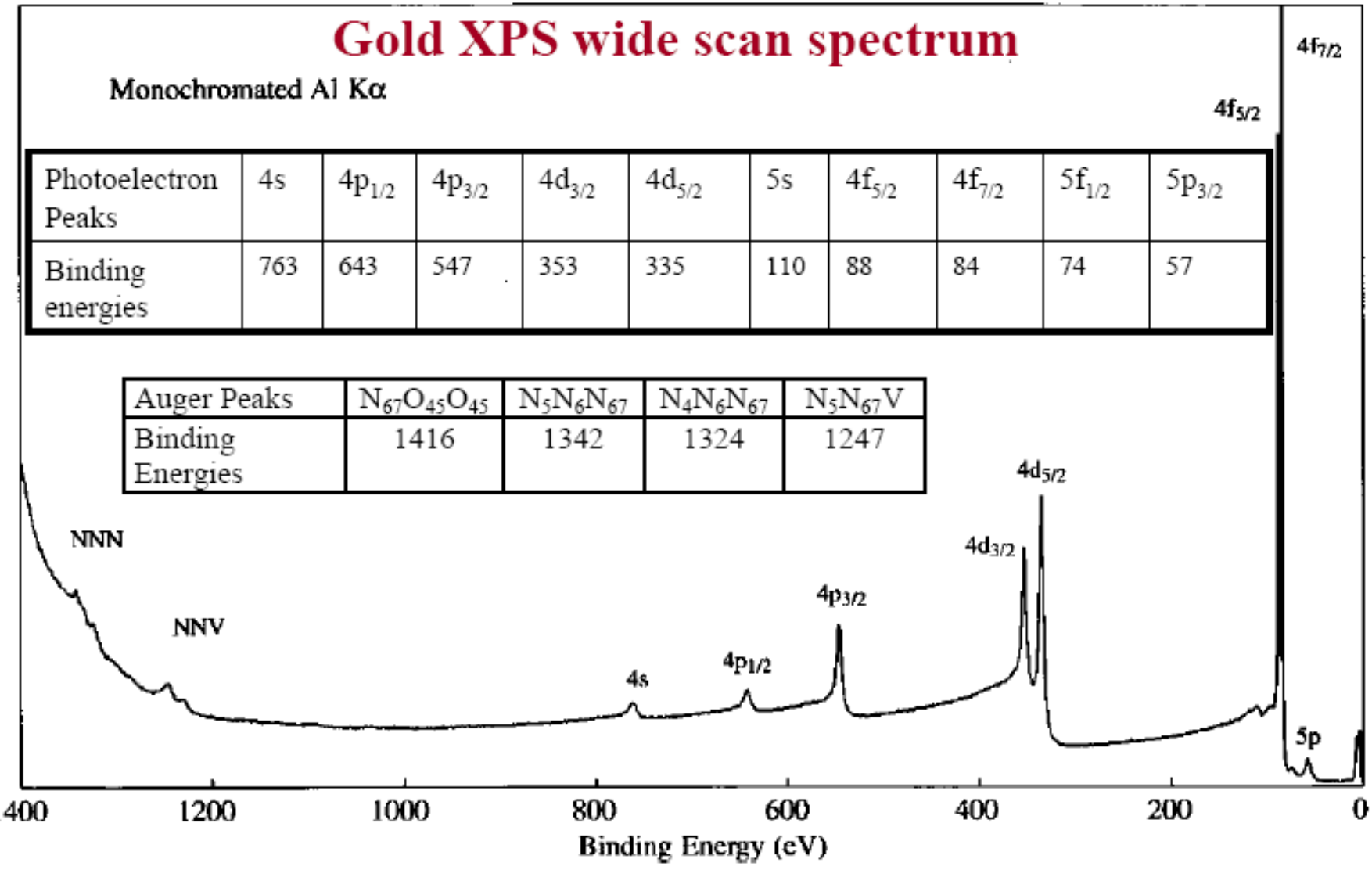
Qualitative analysis

Gold XPS wide scan spectrum

Monochromated Al Kα

Photoelectron Peaks	4s	$4p_{1/2}$	$4p_{3/2}$	$4d_{3/2}$	$4d_{5/2}$	5s	$4f_{5/2}$	$4f_{7/2}$	$5f_{1/2}$	$5p_{3/2}$
Binding energies	763	643	547	353	335	110	88	84	74	57

Auger Peaks	$N_{67}O_{45}O_{45}$	$N_5N_6N_{67}$	$N_4N_6N_{67}$	$N_5N_{67}V$
Binding Energies	1416	1342	1324	1247

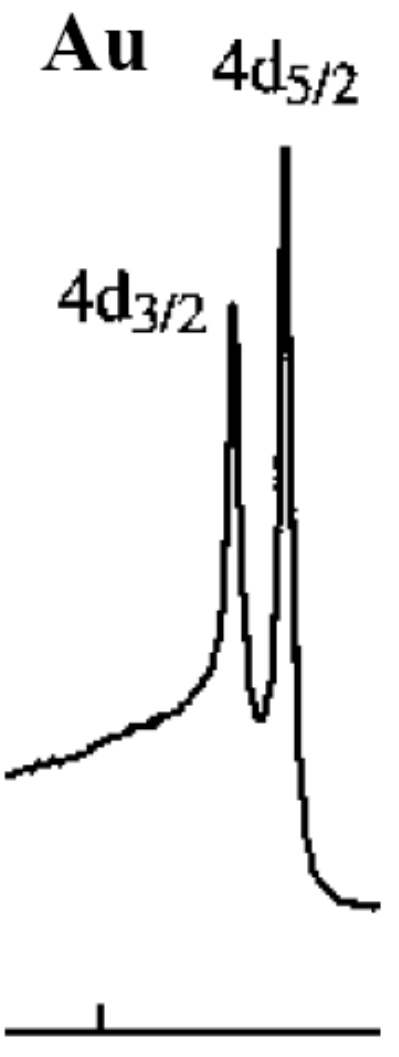


Orbital momentum (l) and spin momentum (s)

For p, d and f peaks, two peaks are observed.

The separation between the two peaks are named **spin orbital splitting**. The values of spin orbital splitting of a core level of an element in different compounds are nearly the same.

The **peak area ratios** of a core level of an element in different compounds are also nearly the same.

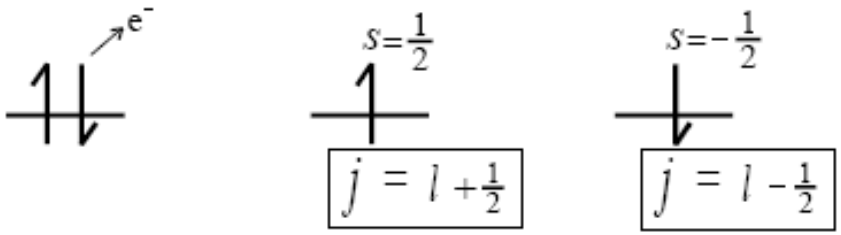


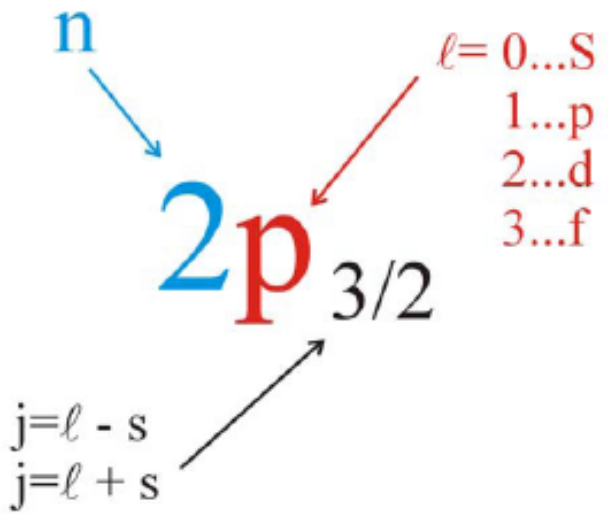
Spin orbital splitting and peak area ratios assist in element identifications.

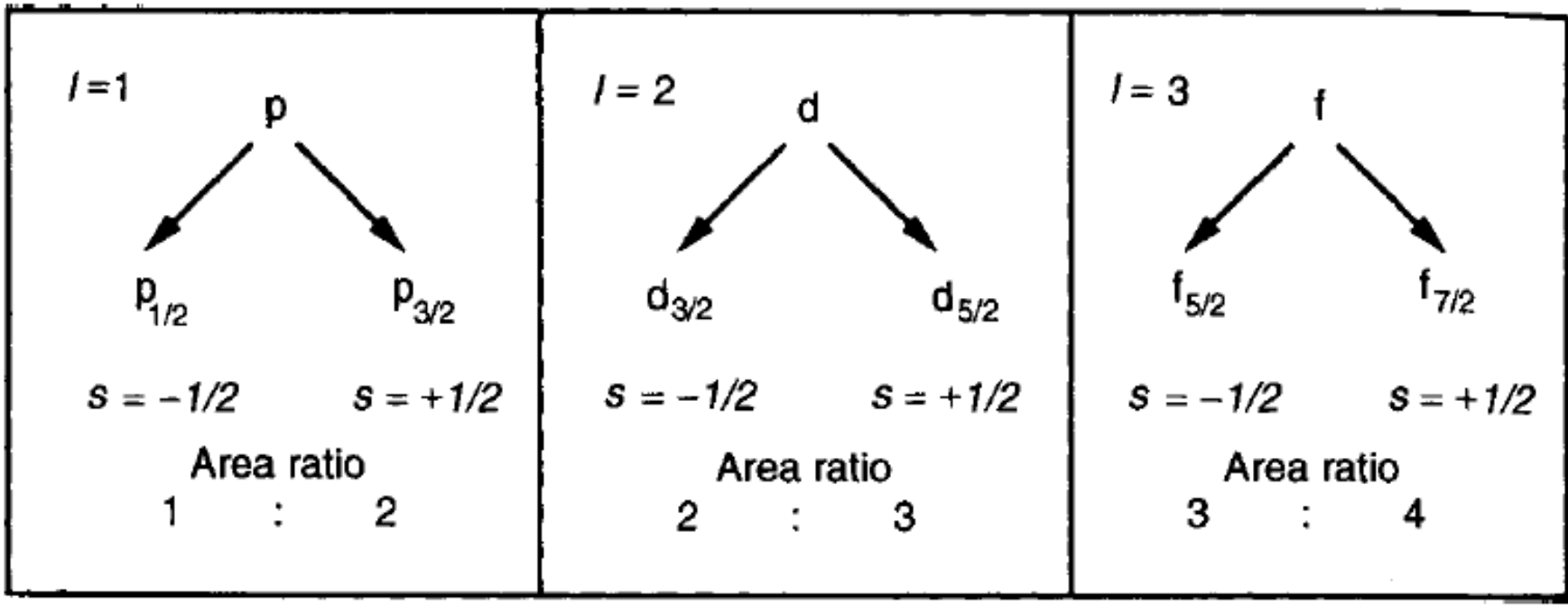
Spin-orbital splitting

Peak Notations

L-S Coupling ($j = l \pm s$)



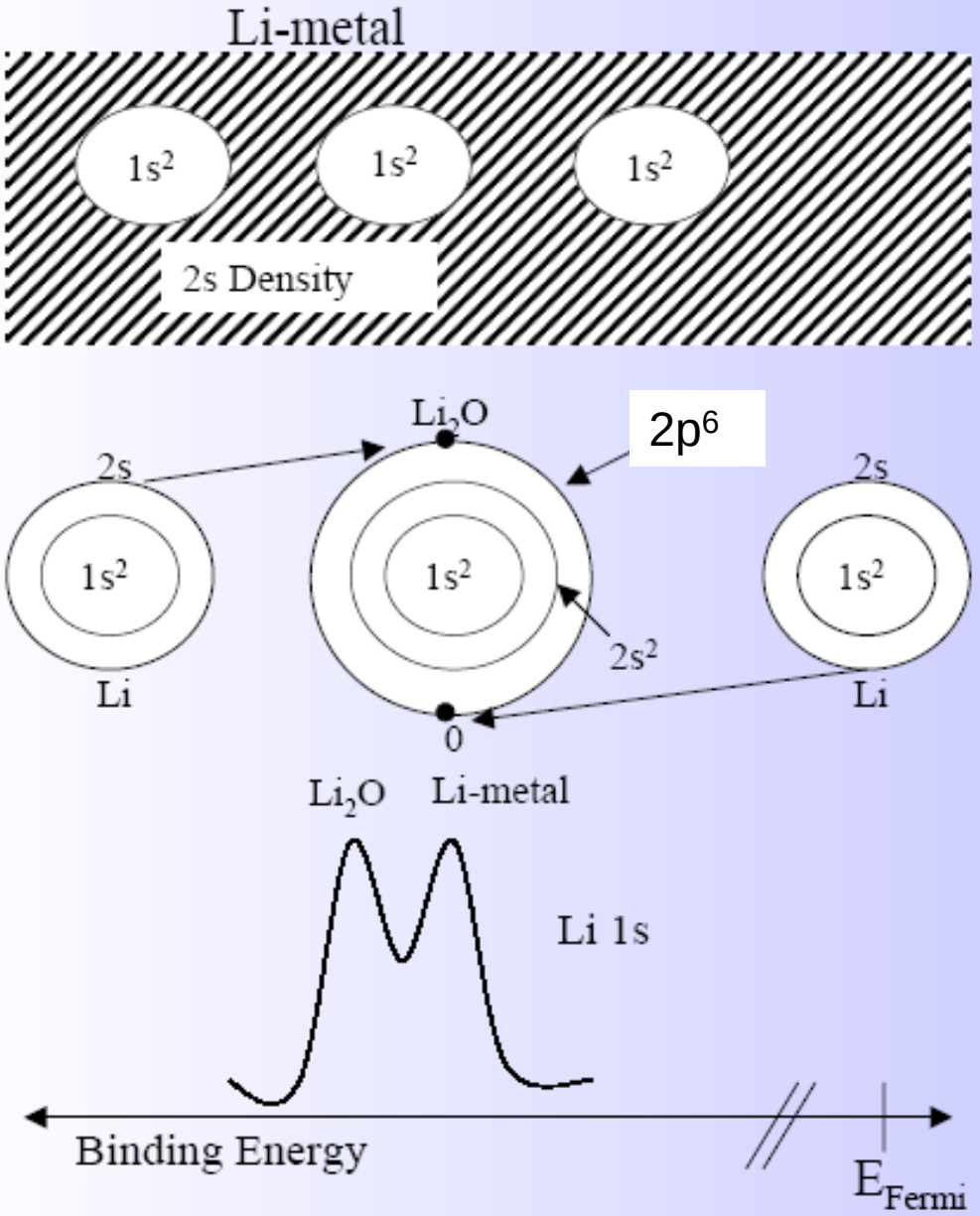




Binding Energy and Oxidation states

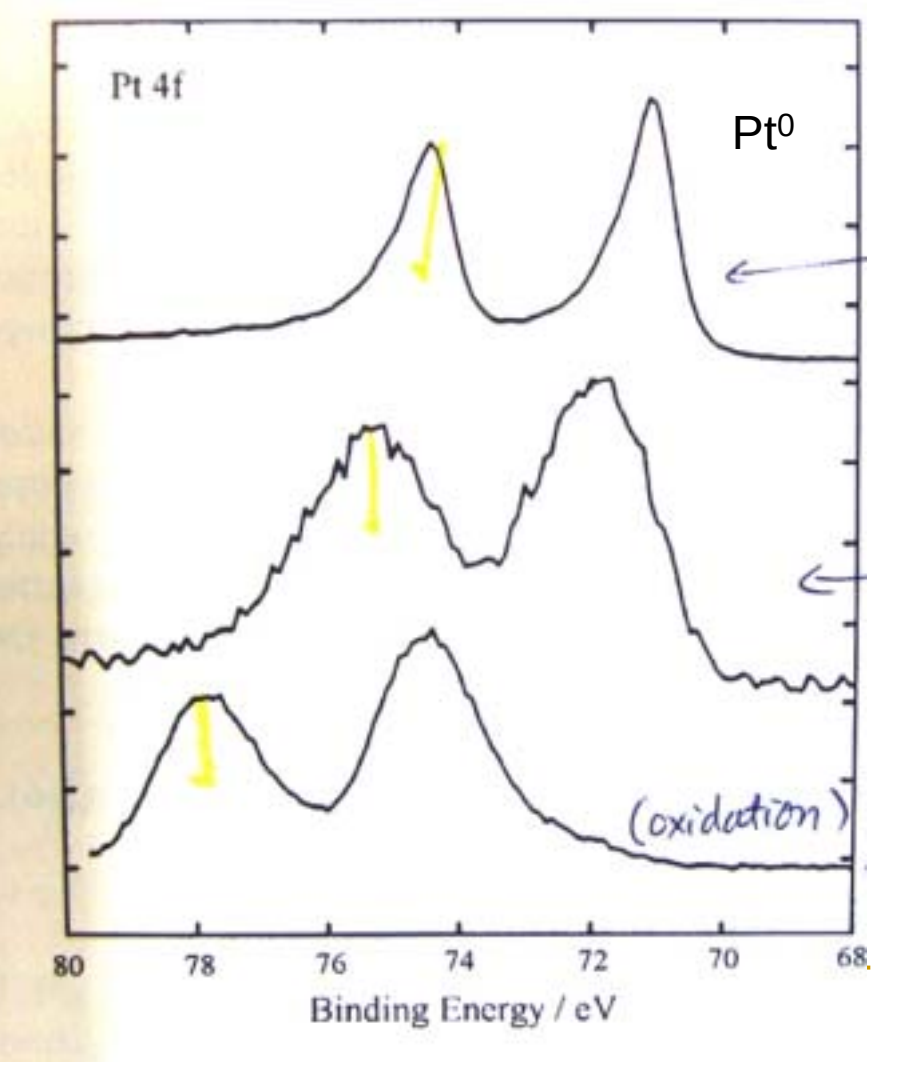
Li .:O: . Li

O—8
Li—3

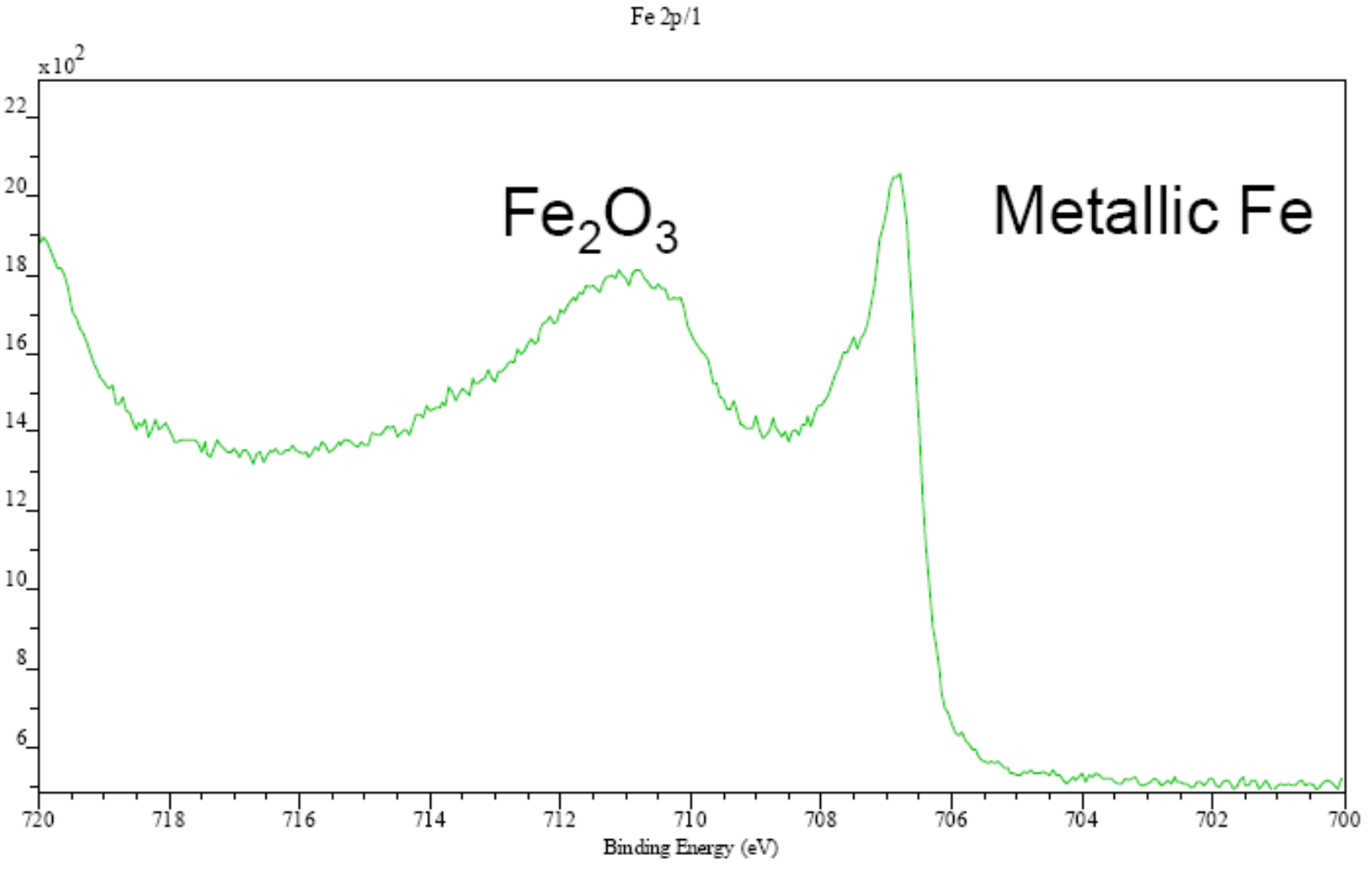


Binding Energy and Oxidation States

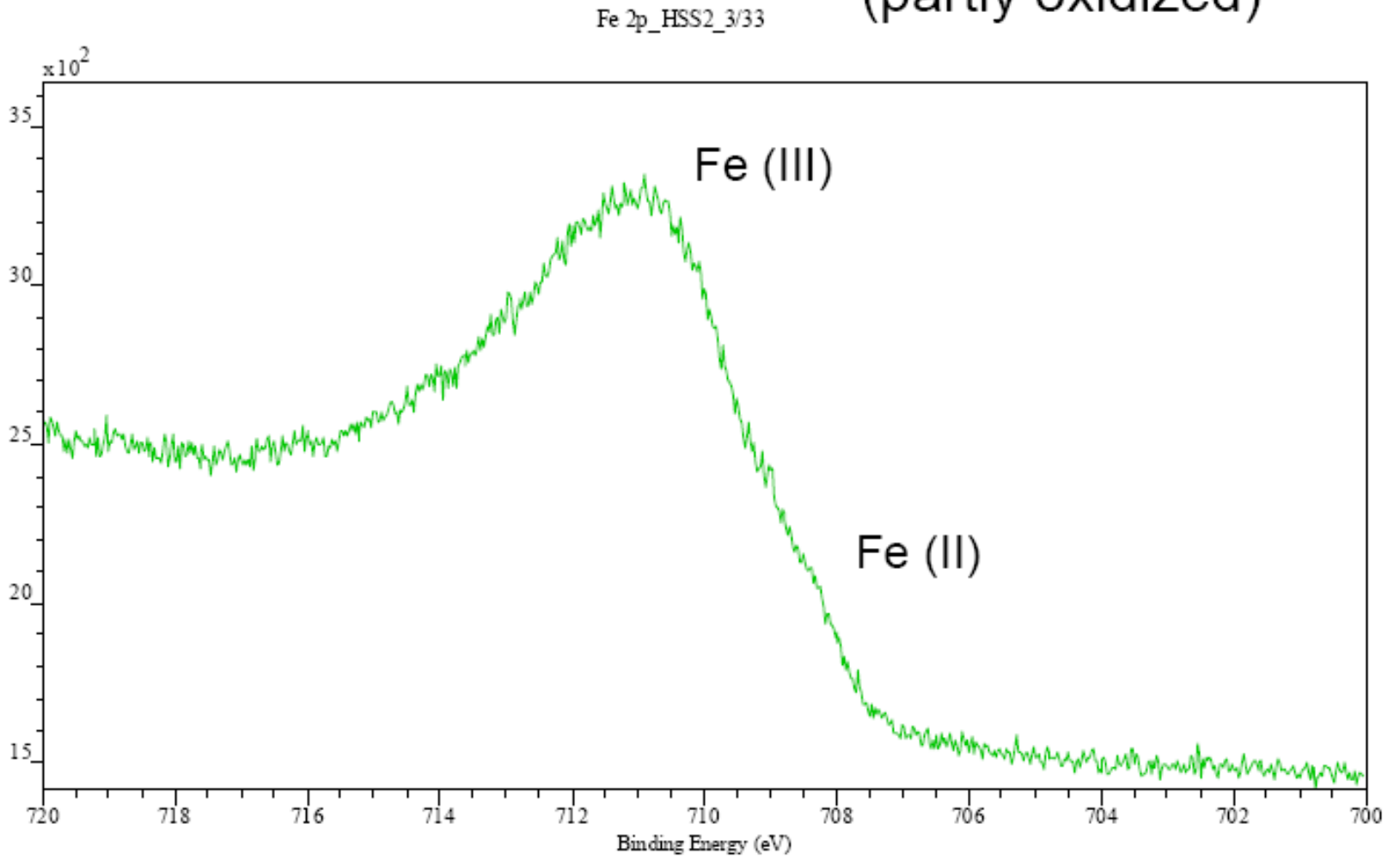
- BE隨著價數增加而提高



Detailed Iron 2p Spectrum of High Purity Iron



Detailed Spectrum of Fe 2p line for Magnetite (partly oxidized)



各項儀器之比較

儀器	分析內容	樣品量	優缺點
BET	表面積/孔隙大小	bulk	
Particle size analyzer	顆粒粒徑	bulk	
SEM	表面立體形狀	trace	
SEM-EDX	材料元素組成	bulk-trace	
TEM	材料的結構/晶型	trace; thin	
XRD	材料的化學組成/結構式	bulk	
XPS	材料的化學價數		