

Data Table 30 K_2PtCl_6

Cubic, space group $Fm\bar{3}m$, No. 225; $a = 9.755 \text{ \AA}$; $Z = 4$, $V = 928.28 \text{ \AA}^3$

Atomic Positions

Pt in 4(*a*): $0,0,0$; fc

Cl in 24(*e*): $\pm(x,0,0; 0,x,0; 0,0,x)$; $x = 0.240$; fc

K in 8(*c*): $\pm\frac{1}{4},\frac{1}{4},\frac{1}{4}$; fc

Positions

 Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

		(0, 0, 0) +	(0, $\frac{1}{2}$, $\frac{1}{2}$) +	($\frac{1}{2}$, 0, $\frac{1}{2}$) +	($\frac{1}{2}$, $\frac{1}{2}$, 0) +	
192	<i>l</i> 1	(1) x, y, z (5) z, x, y (9) y, z, x (13) y, x, \bar{z} (17) x, z, \bar{y} (21) z, y, \bar{x} (25) $\bar{x}, \bar{y}, \bar{z}$ (29) $\bar{z}, \bar{x}, \bar{y}$ (33) $\bar{y}, \bar{z}, \bar{x}$ (37) \bar{y}, \bar{x}, z (41) \bar{x}, \bar{z}, y (45) \bar{z}, \bar{y}, x	(2) \bar{x}, \bar{y}, z (6) z, \bar{x}, \bar{y} (10) \bar{y}, z, \bar{x} (14) $\bar{y}, \bar{x}, \bar{z}$ (18) \bar{x}, z, y (22) z, \bar{y}, x (26) x, y, \bar{z} (30) \bar{z}, x, y (34) y, \bar{z}, x (38) y, x, z (42) x, \bar{z}, \bar{y} (46) \bar{z}, y, \bar{x}	(3) \bar{x}, y, \bar{z} (7) \bar{z}, \bar{x}, y (11) y, \bar{z}, \bar{x} (15) y, \bar{x}, z (19) $\bar{x}, \bar{z}, \bar{y}$ (23) \bar{z}, y, x (27) x, \bar{y}, z (31) z, x, \bar{y} (35) \bar{y}, z, x (39) \bar{y}, x, \bar{z} (43) x, z, y (47) z, \bar{y}, \bar{x}	(4) x, \bar{y}, \bar{z} (8) \bar{z}, x, \bar{y} (12) \bar{y}, \bar{z}, x (16) \bar{y}, x, z (20) x, \bar{z}, y (24) $\bar{z}, \bar{y}, \bar{x}$ (28) \bar{x}, y, z (32) z, \bar{x}, \bar{y} (36) y, z, \bar{x} (40) y, \bar{x}, \bar{z} (44) \bar{x}, z, \bar{y} (48) z, y, x	
96	<i>k</i> . <i>m</i>	x, x, z \bar{z}, \bar{x}, x x, x, \bar{z} $\bar{x}, \bar{z}, \bar{x}$	\bar{x}, \bar{x}, z \bar{z}, x, \bar{x} $\bar{x}, \bar{x}, \bar{z}$ x, \bar{z}, x	\bar{x}, x, \bar{z} x, z, x x, \bar{x}, z z, x, \bar{x}	x, \bar{x}, \bar{z} x, \bar{z}, \bar{x} x, z, \bar{x} \bar{z}, x, x	z, x, x \bar{x}, \bar{z}, x \bar{x}, z, x $\bar{z}, \bar{x}, \bar{x}$
96	<i>j</i> <i>m</i> . .	$0, y, z$ $\bar{z}, 0, y$ $y, 0, \bar{z}$ $0, \bar{z}, \bar{y}$	$0, \bar{y}, z$ $\bar{z}, 0, \bar{y}$ $\bar{y}, 0, \bar{z}$ $0, \bar{z}, y$	$0, y, \bar{z}$ $y, z, 0$ $y, 0, z$ $z, y, 0$	$0, \bar{y}, \bar{z}$ $\bar{y}, z, 0$ $\bar{y}, 0, z$ $z, \bar{y}, 0$	$z, 0, y$ $y, \bar{z}, 0$ $0, z, \bar{y}$ $\bar{z}, y, 0$
48	<i>i</i> <i>m</i> . <i>m</i> 2	$\frac{1}{2}, y, y$ $\bar{y}, \frac{1}{2}, y$	$\frac{1}{2}, \bar{y}, y$ $\bar{y}, \frac{1}{2}, \bar{y}$	$\frac{1}{2}, y, \bar{y}$ $y, y, \frac{1}{2}$	$\frac{1}{2}, \bar{y}, \bar{y}$ $\bar{y}, y, \frac{1}{2}$	$y, \frac{1}{2}, y$ $y, \bar{y}, \frac{1}{2}$
48	<i>h</i> <i>m</i> . <i>m</i> 2	$0, y, y$ $\bar{y}, 0, y$	$0, \bar{y}, y$ $\bar{y}, 0, \bar{y}$	$0, y, \bar{y}$ $y, y, 0$	$0, \bar{y}, \bar{y}$ $\bar{y}, y, 0$	$y, 0, y$ $y, \bar{y}, 0$
48	<i>g</i> 2 . <i>m</i> <i>m</i>	$x, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, x, \frac{3}{4}$	$\bar{x}, \frac{3}{4}, \frac{1}{4}$ $\frac{3}{4}, \bar{x}, \frac{3}{4}$	$\frac{1}{4}, x, \frac{1}{4}$ $x, \frac{1}{4}, \frac{3}{4}$	$\frac{1}{4}, \bar{x}, \frac{3}{4}$ $\bar{x}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, x$ $\frac{1}{4}, \frac{1}{4}, \bar{x}$
32	<i>f</i> . <i>3m</i>	x, x, x x, x, \bar{x}	\bar{x}, \bar{x}, x $\bar{x}, \bar{x}, \bar{x}$	\bar{x}, x, \bar{x} x, \bar{x}, x	x, \bar{x}, \bar{x} \bar{x}, x, x	
24	<i>e</i> 4 <i>m</i> . <i>m</i>	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	$0, 0, x$ $0, 0, \bar{x}$
24	<i>d</i> <i>m</i> . <i>m</i> <i>m</i>	$0, \frac{1}{4}, \frac{1}{4}$	$0, \frac{3}{4}, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\frac{1}{4}, 0, \frac{3}{4}$	$\frac{1}{4}, \frac{1}{4}, 0$ $\frac{3}{4}, \frac{1}{4}, 0$
8	<i>c</i> $\bar{4}$ <i>3m</i>	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$			
4	<i>b</i> <i>m</i> $\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$				
4	<i>a</i> <i>m</i> $\bar{3}m$	$0, 0, 0$				

Table 4.17. The rock salt structure, sodium chloride, B1 .

Formula unit NaCl, sodium chloride

Space group: Fm $\bar{3}$ m (no. 225)

Cell dimensions: a5.6402 Å

Cell contents: 4 formula units

Atomic positions: Na in (4a) m $\bar{3}$ m (0, 0, 0) FCT

Cl in (4b) m $\bar{3}$ m (1/2, 1/2, 1/2) FCT

Examples:

compound	a (Å)	compound	a (Å)	compound	a (Å)	compound	a (Å)
MgO	4.213	MgS	5.200	LiF	4.0270	KF	5.347
CaO	4.8105	CaS	5.6948	LiCl	5.1396	KCl	6.2931
SrO	5.160	SrS	6.020	LiBr	5.5013	KBr	6.5966
BaO	5.539	BaS	6.386	LiI	6.00	KI	7.0655
TiO	4.177	MnS	5.224	LiH	4.083	RbF	5.6516
MnO	4.445	MgSe	5.462	NaF	4.64	RbCl	6.5810
FeO	4.307	CaSe	5.924	NaCl	5.6402	RbBr	6.889
CoO	4.260	SrSe	6.246	NaBr	5.9772	RbI	7.342
NiO	4.1769	BaSe	6.600	NaI	6.473	AgF	4.92

$I\bar{4}c2$

No. 120

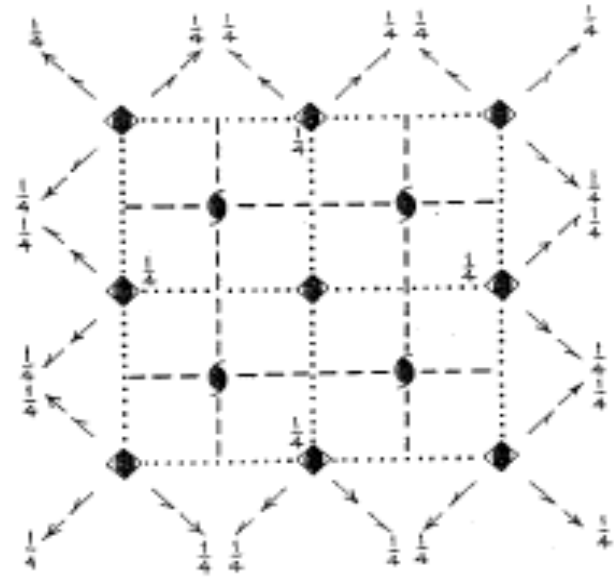
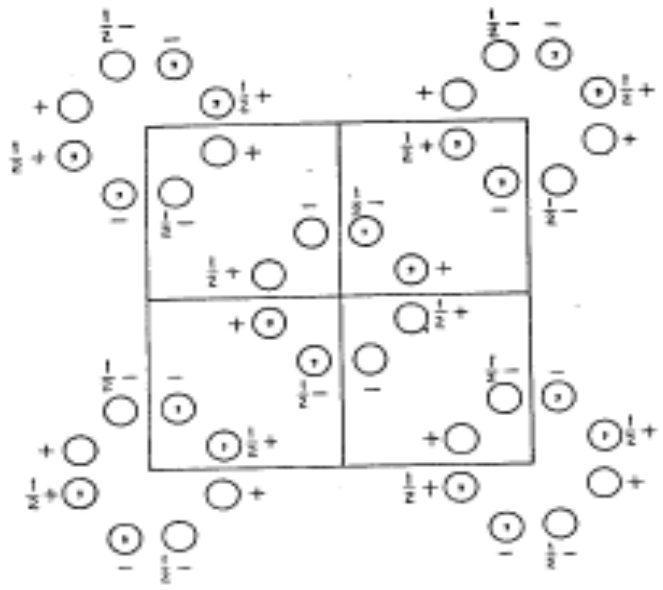
D_{2d}^{10}

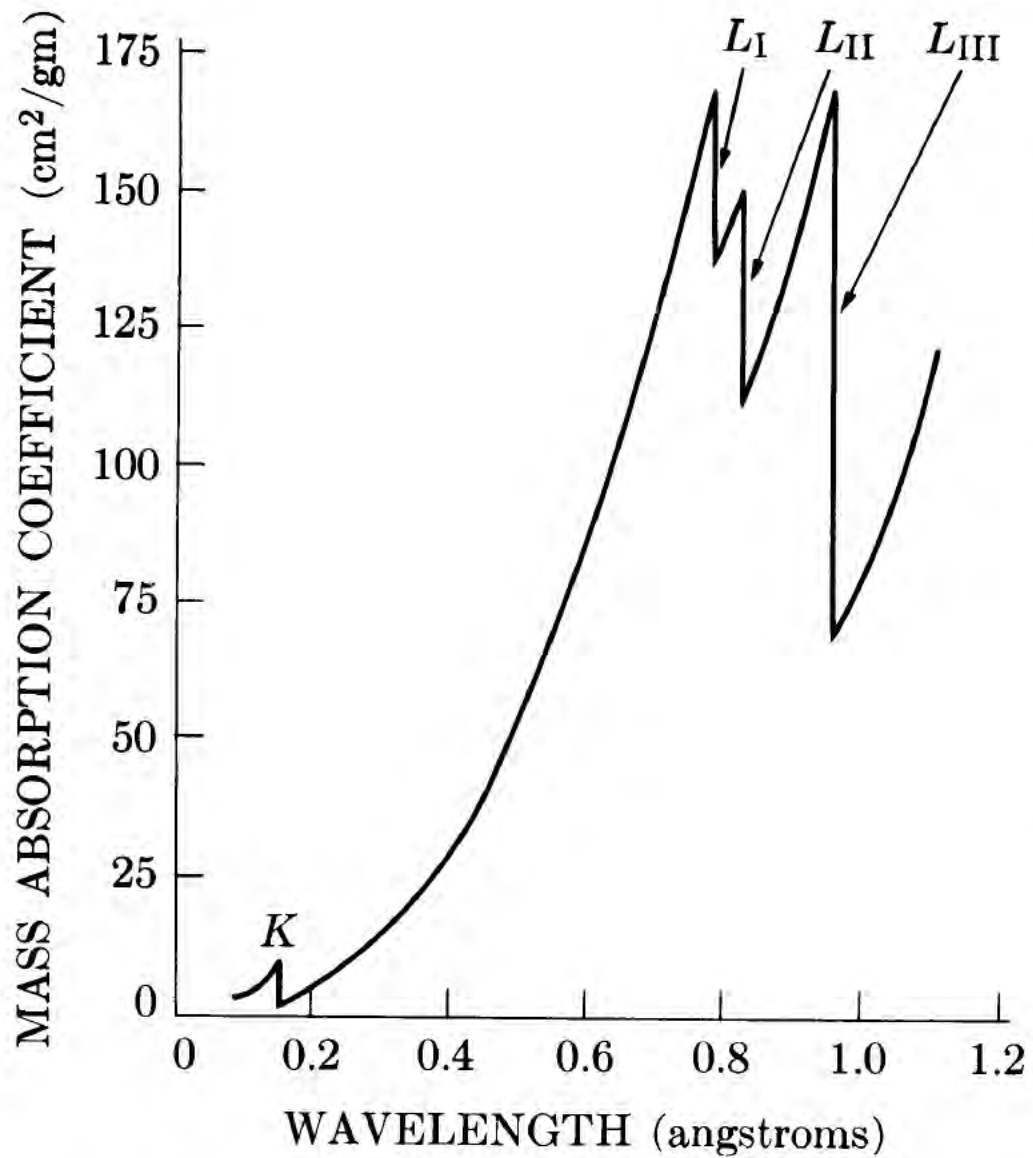
$I\bar{4}c2$

$\bar{4}m2$

Tetragonal

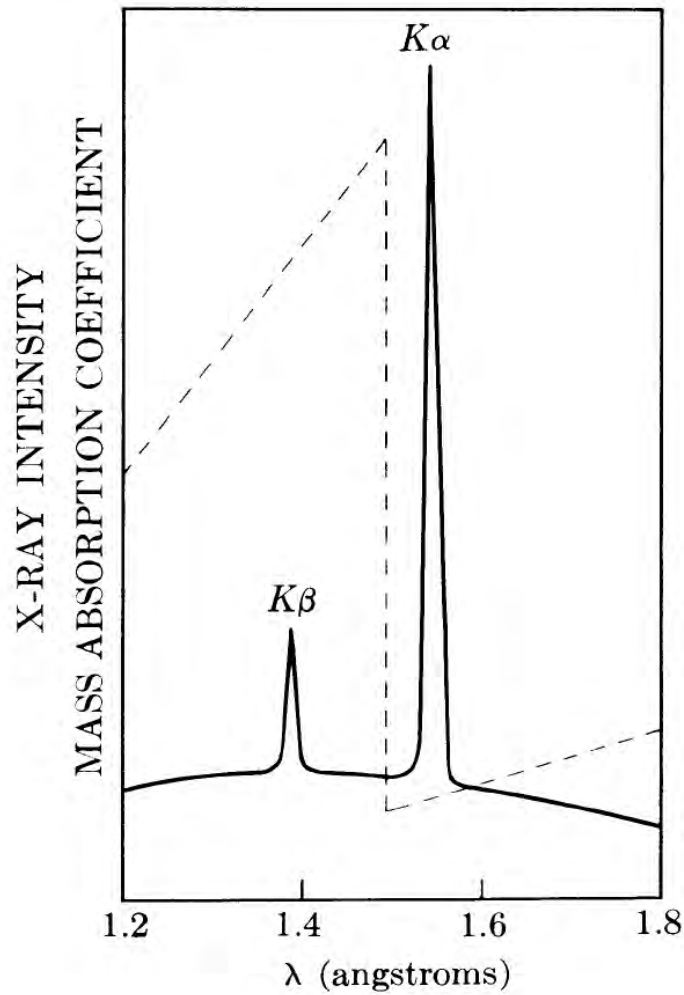
Patterson symmetry $I4/mmm$



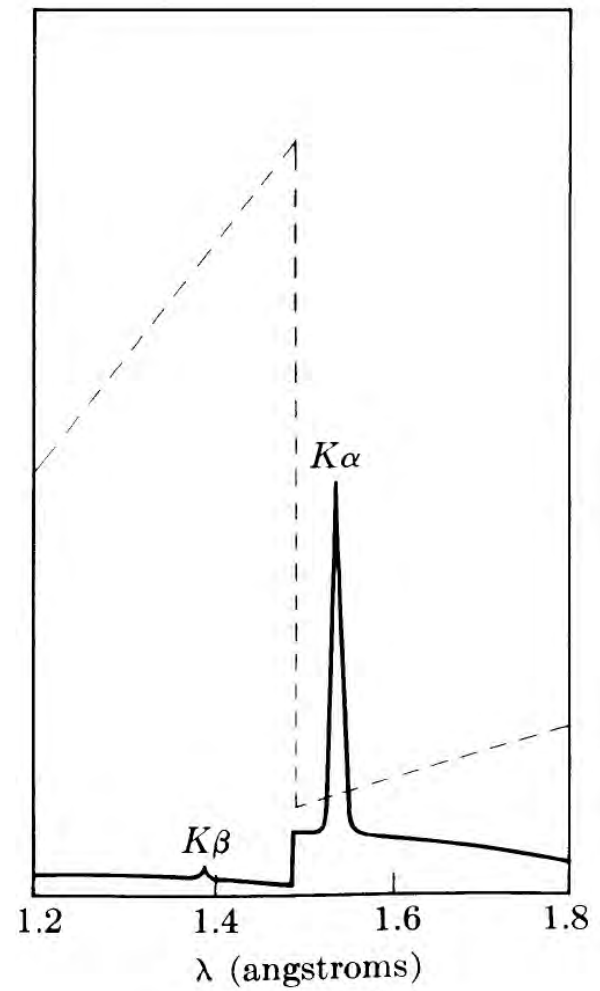


Absorption coefficients of lead

Cu radiation



No Filter



Ni Filter

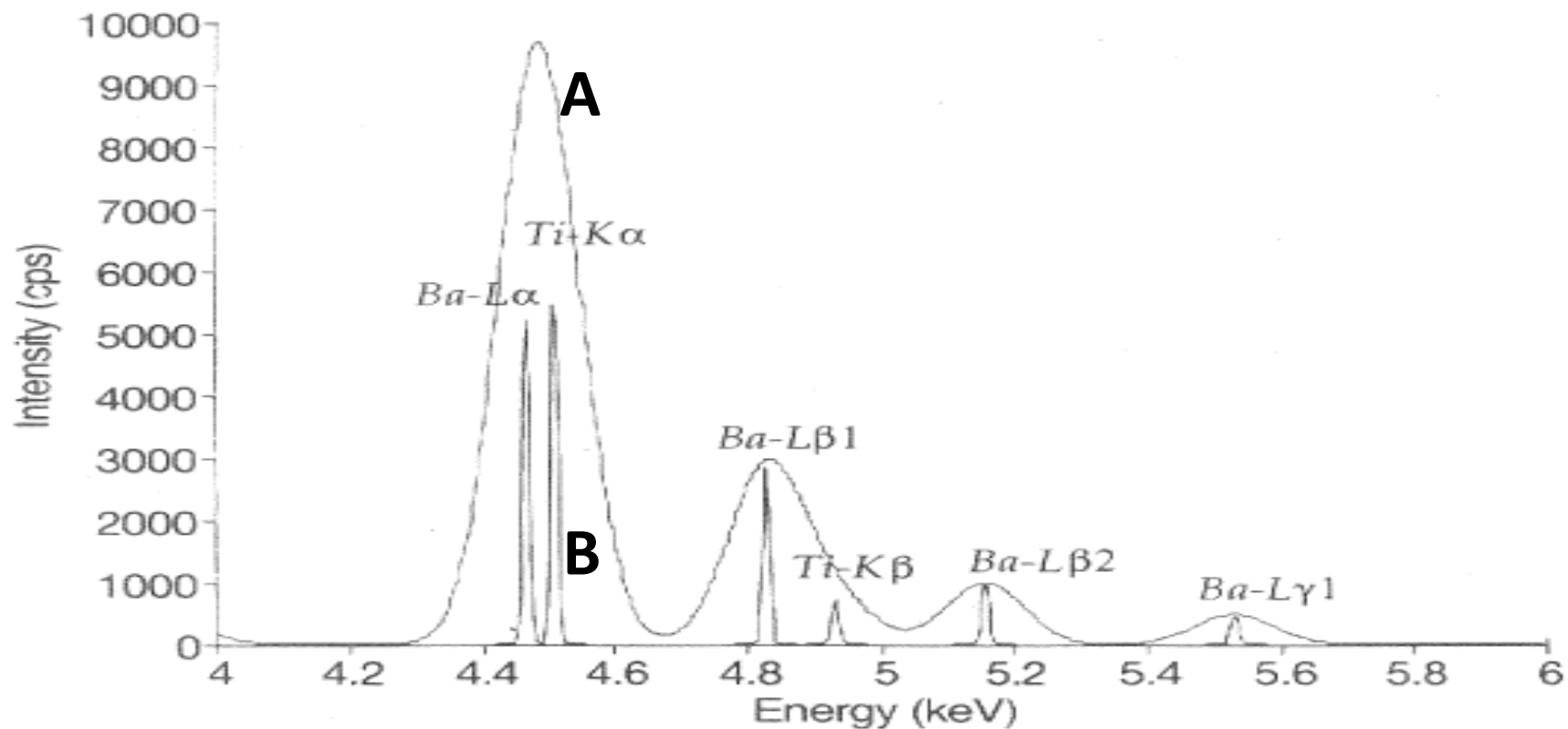


Figure 4

Superposed EDS and WDS spectra from BaTiO₃. The EDS spectrum was obtained with a detector having 135-eV resolution, and shows the strongly overlapped Ba L α ₁-Ti K α and Ba L β ₁-Ti K β peaks. The WDS spectrum from the same material shows the peaks to be completely resolved.

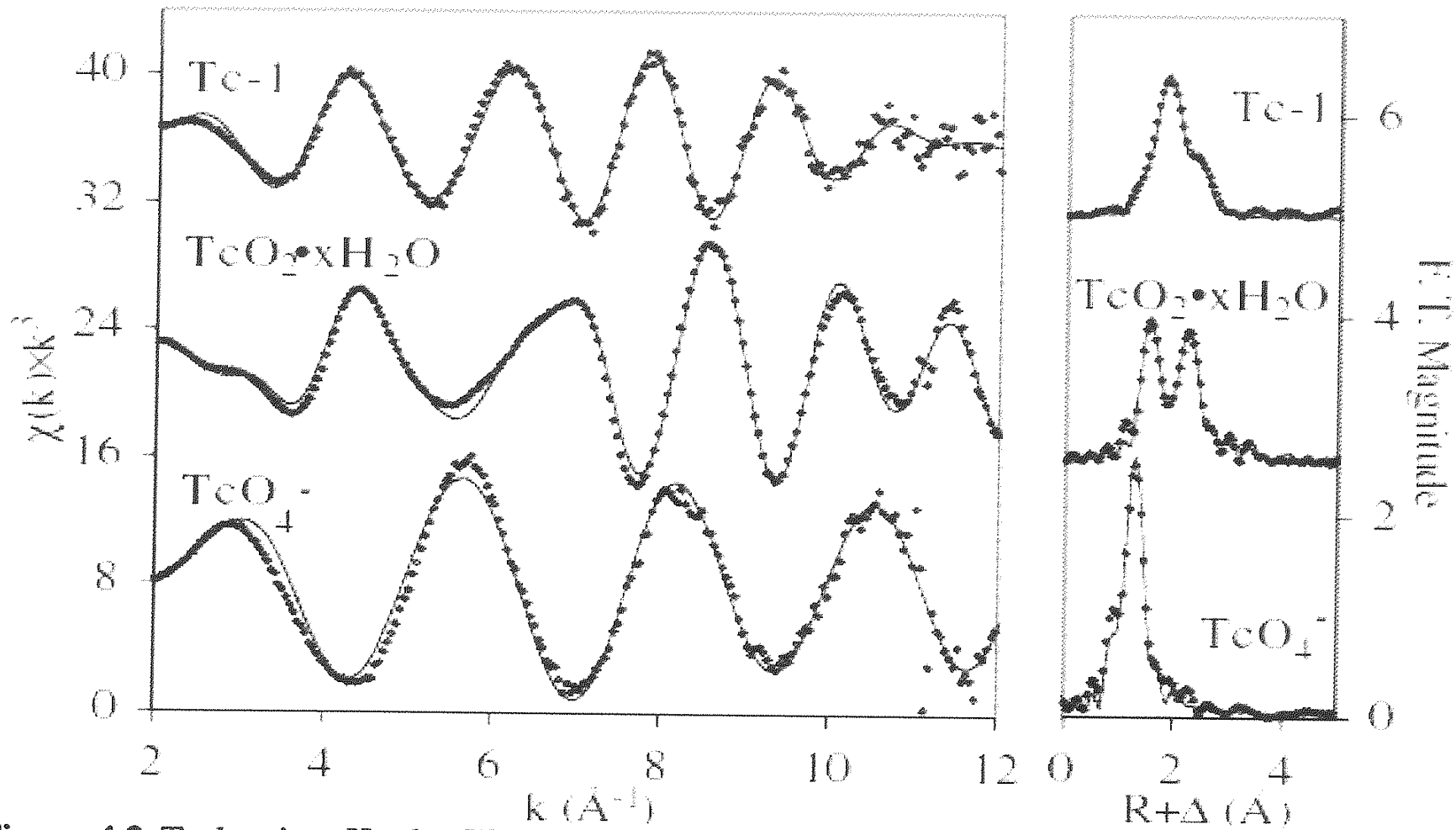
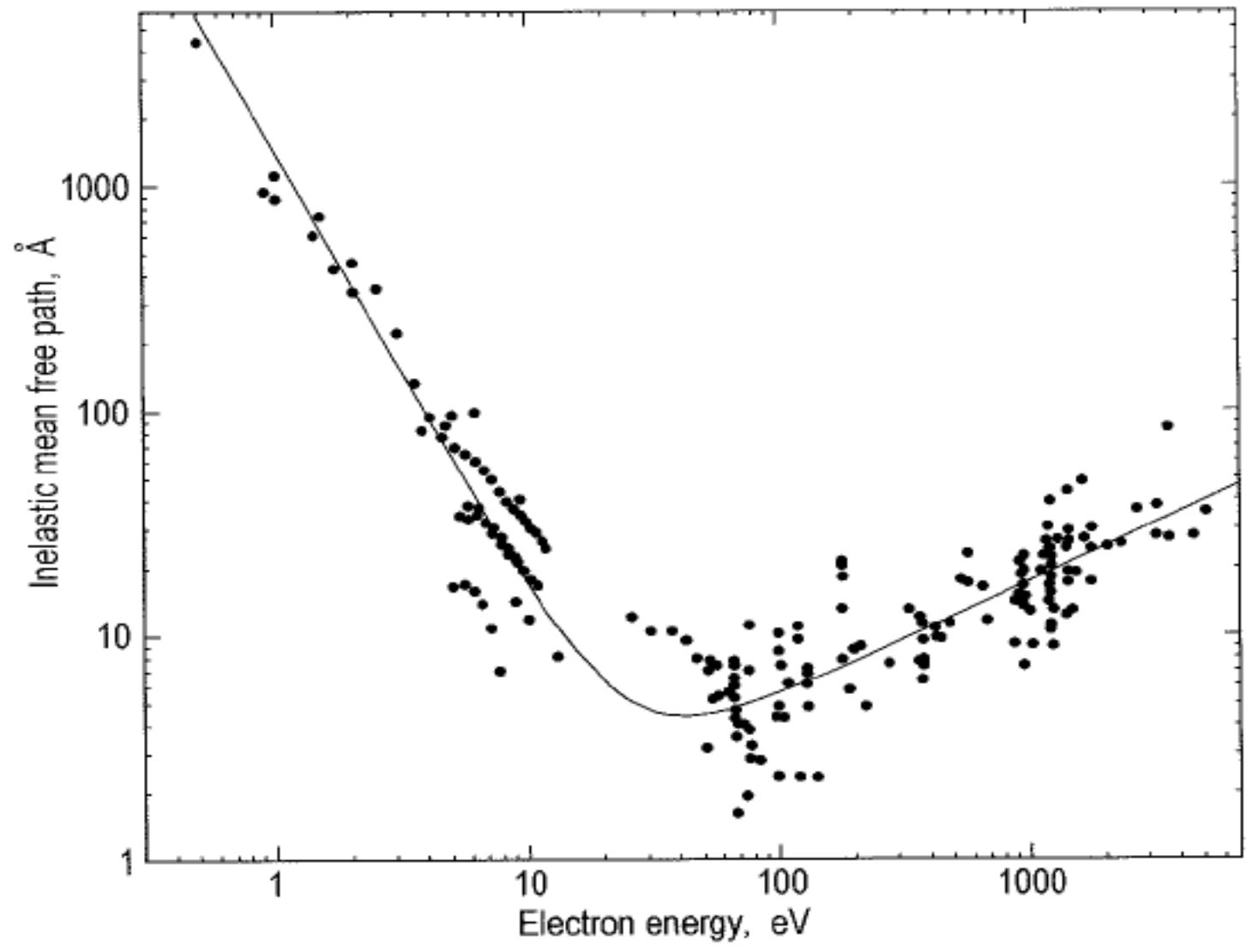
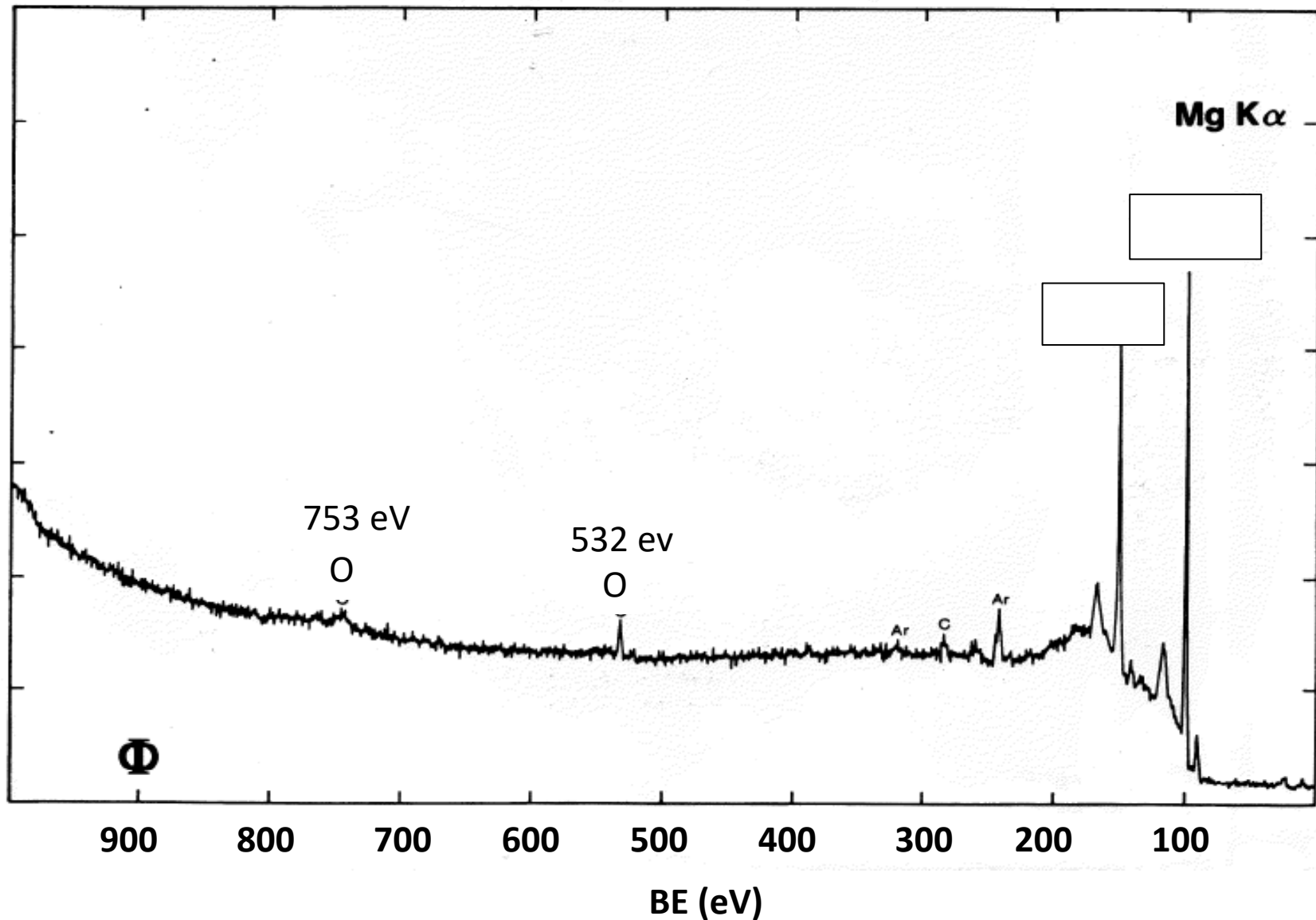


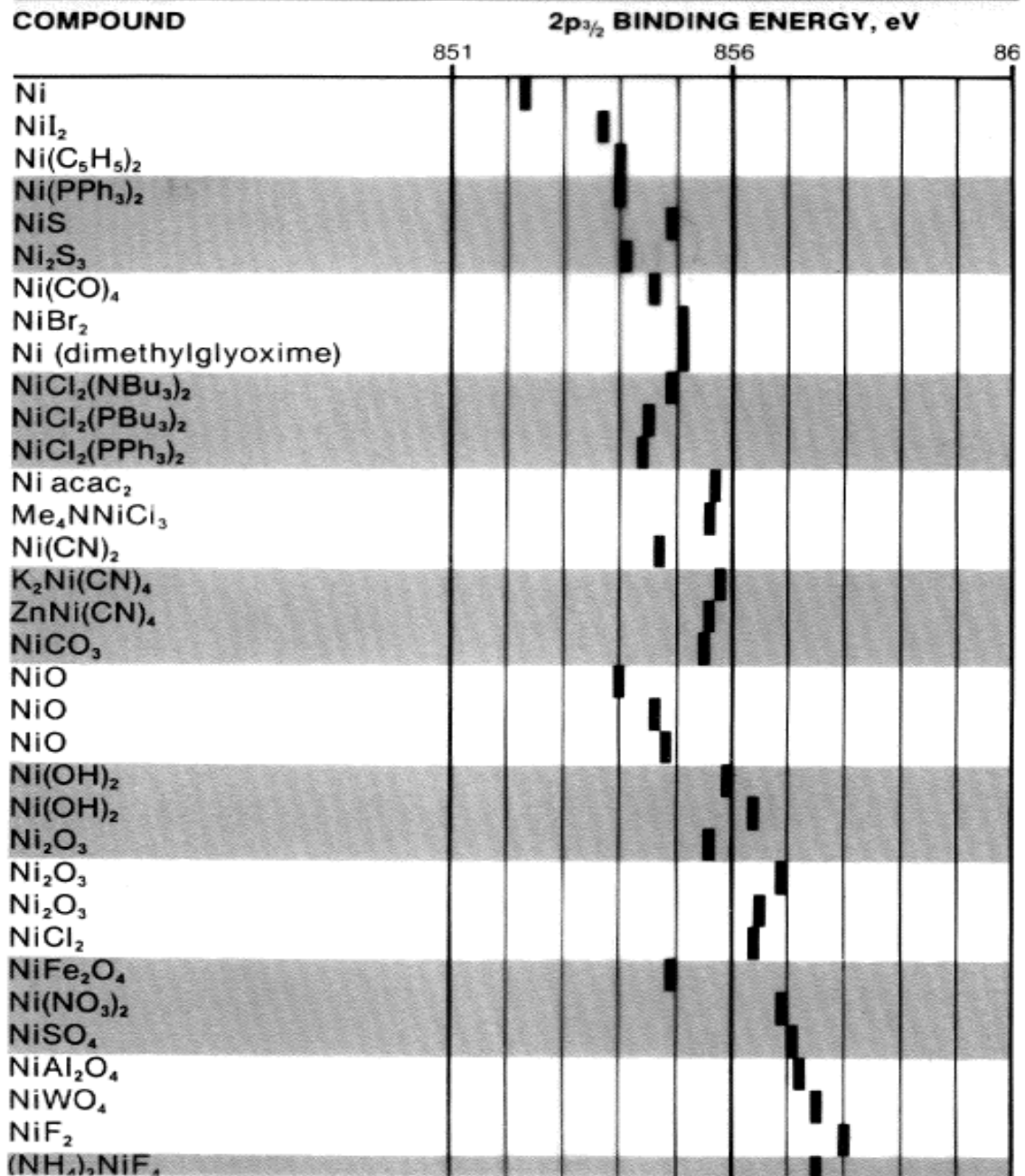
Figure 4.0 Tc-1, TcO₂·xH₂O, and TcO₄⁻ neutron diffraction data.





Nickel, Ni

Atomic Number **28**



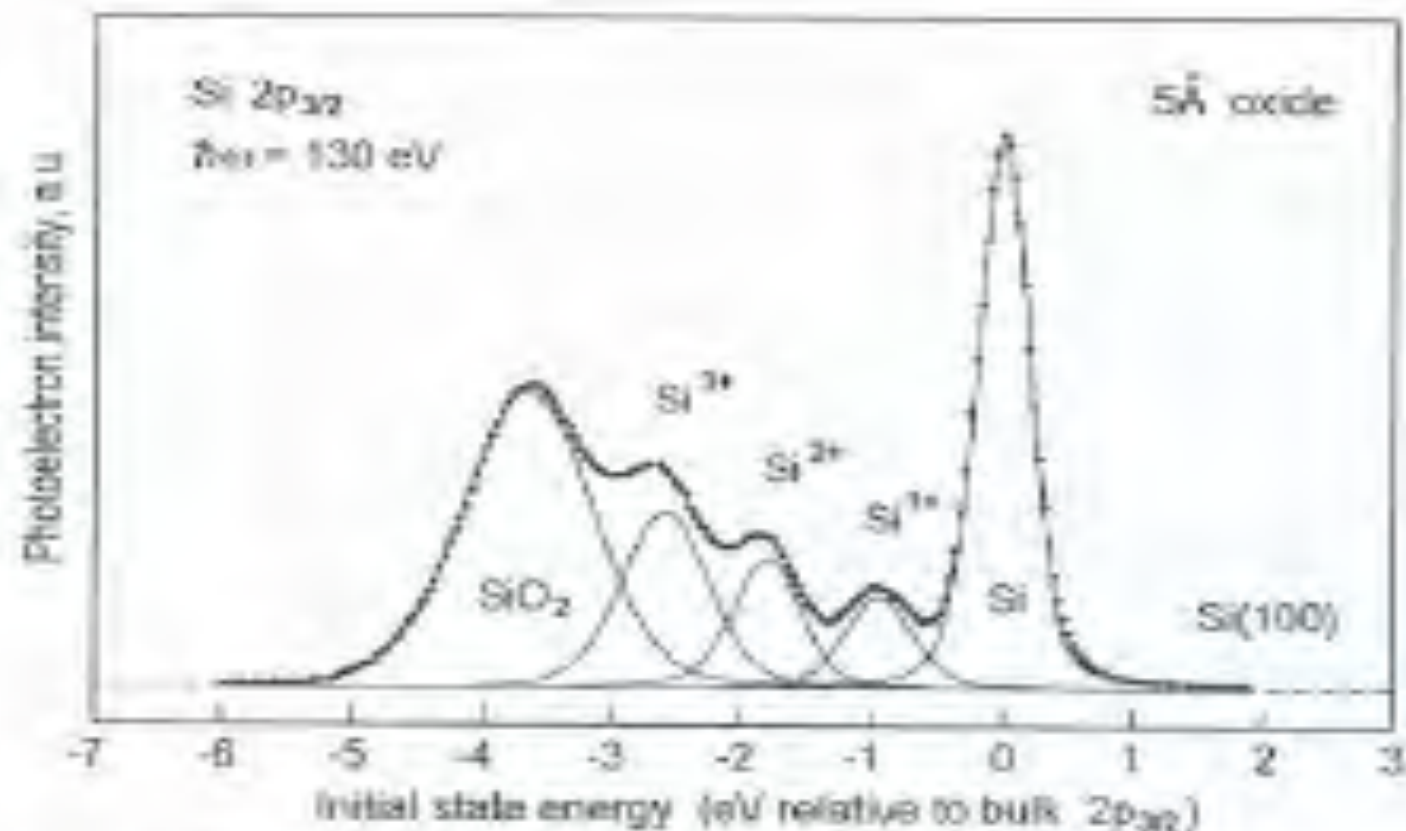
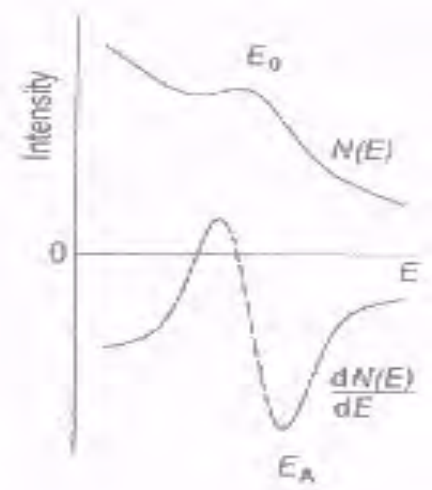
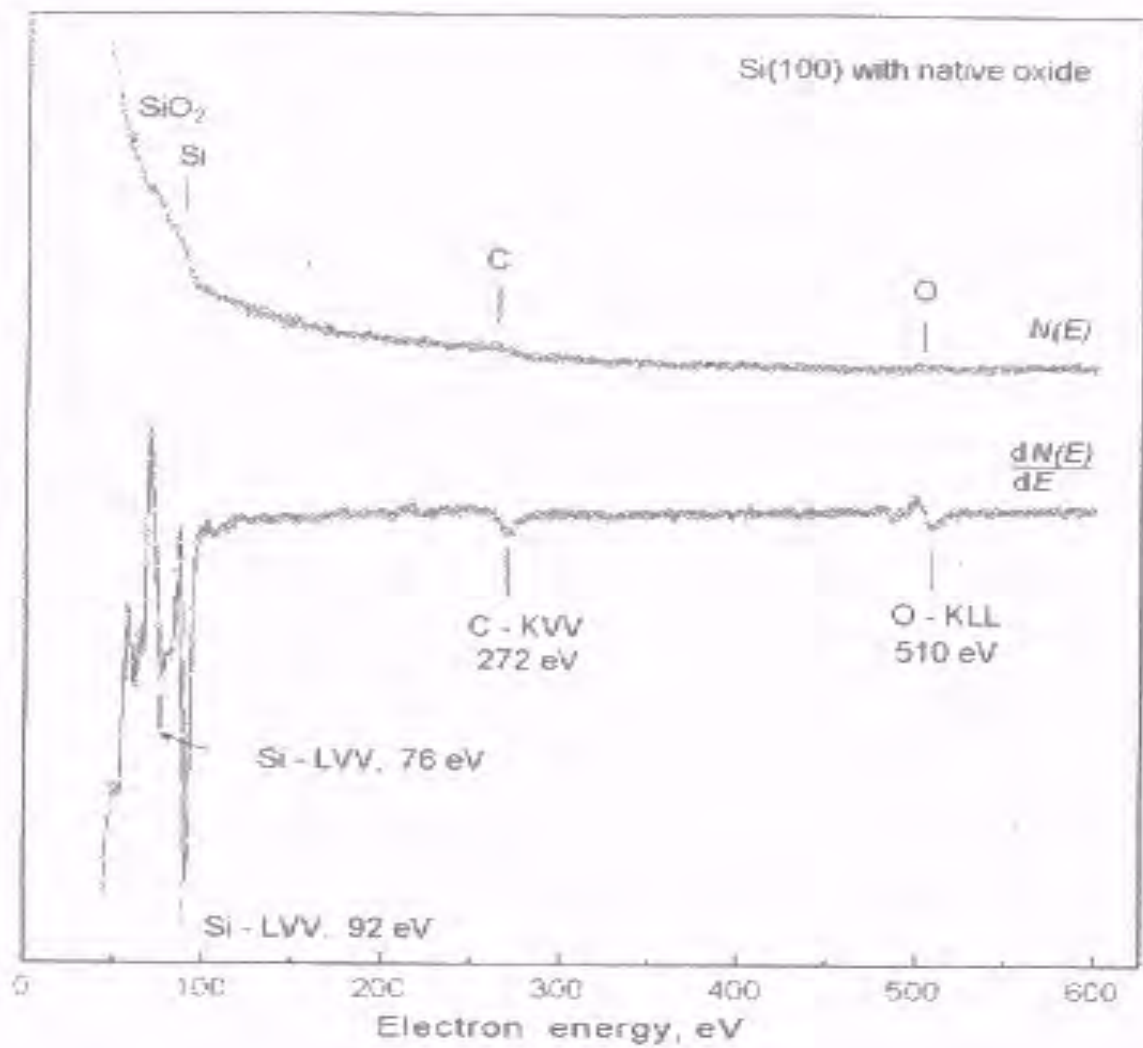


Fig. 5.23. Si 2p_{3/2} core-level spectrum from an ultrathin SiO₂ on Si(100) surface (note that the Si 2p_{1/2} partner line is already subtracted). The peak due to clean Si, the peaks due to Si in different oxides are so clearly resolved. The peaks shift to lower energies with increasing oxidation states [after Hümpfer et al., 1984].



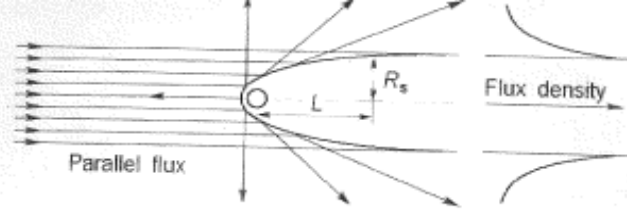


Fig. 6.6. Shadow cone formed from trajectories of projectile ions scattered from a target atom

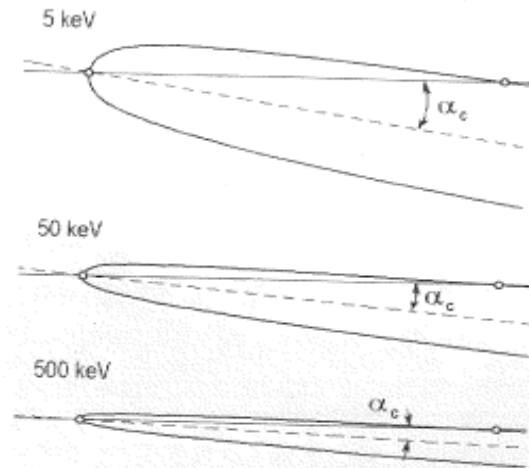


Fig. 6.7. Calculated shadow cones for Li^+ ions with energy of 5 keV, 50 keV, and 500 keV scattering from Ag atoms. The critical angles of shadowing α_c are indicated. The shadow cone width and critical angle decrease substantially with increasing ion kinetic energy (after Williams [6.3])

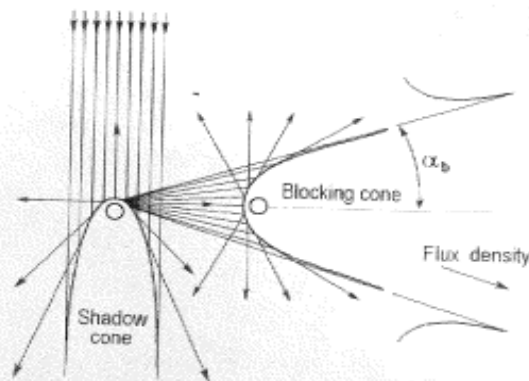


Fig. 6.8. Shadow and blocking cones for scattering from a pair of atoms

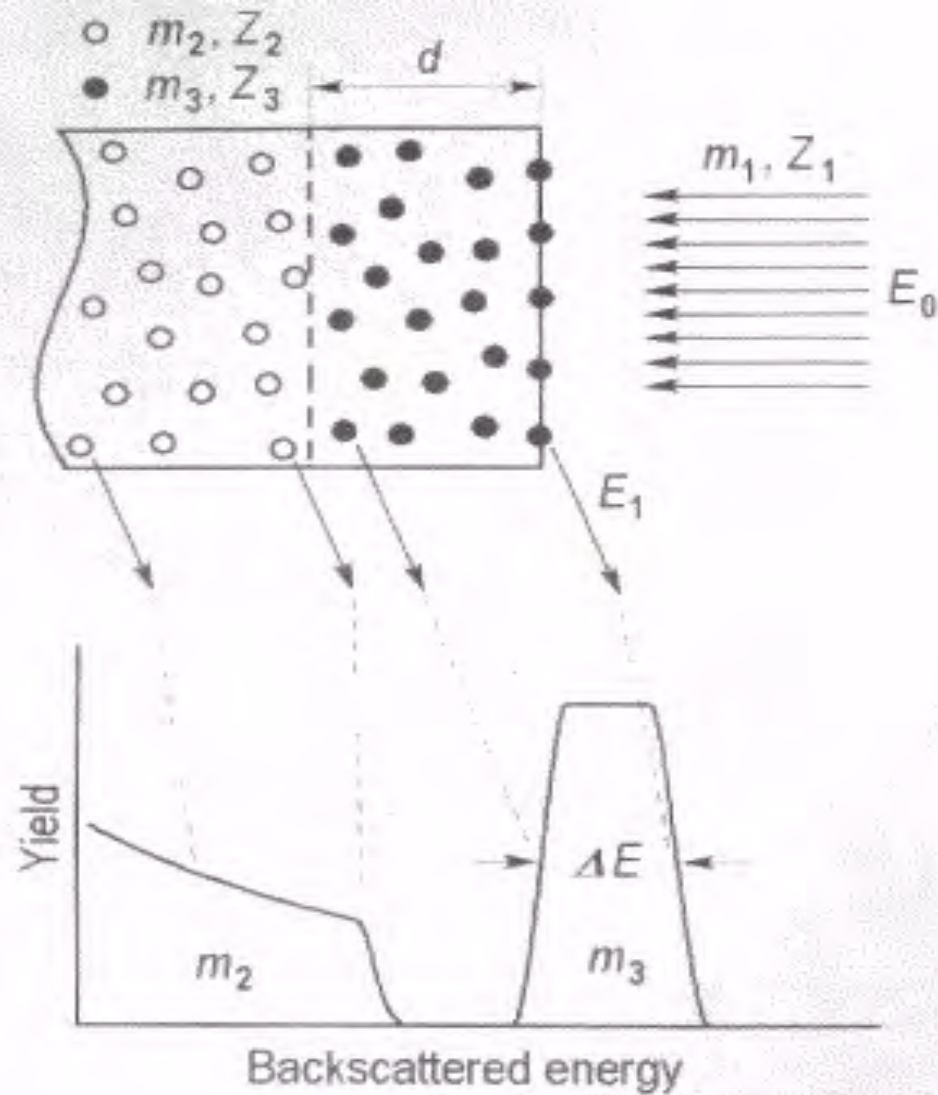


Fig. 6.28. Schematic diagram of the energy spectrum of ions (m_1, Z_1, E_0) scattered from a sample composed of a substrate (m_2, Z_2) and a film (m_3, Z_3) of thickness d . For simplicity, both film and substrate are assumed to be amorphous to neglect the structural effects. (after Feldman et al. [6.6])

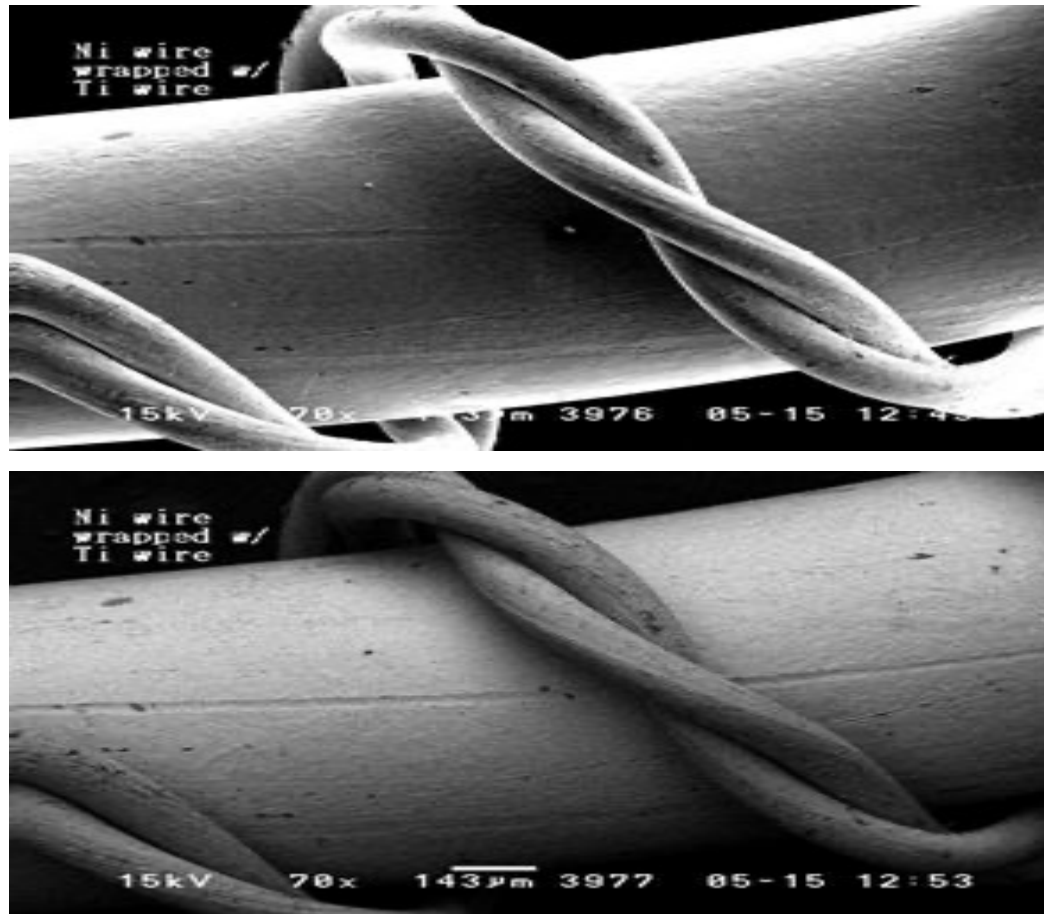
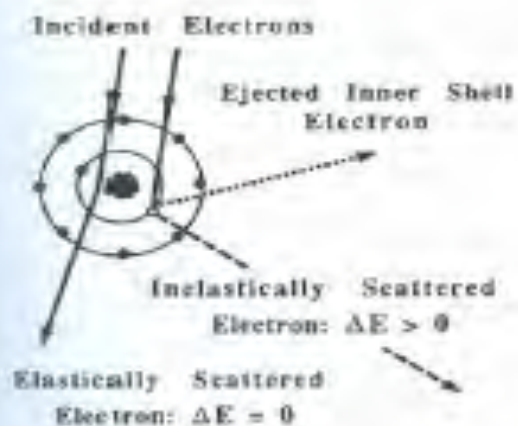


Figure 1: (Top) Secondary electron image of a twisted pair of Ti wires wrapped around a thicker Ni wire is shown. (Bottom) The same specimen is shown in back scatter mode. The two metals can now be differentiated based on contrast; elements of greater atomic mass (Ni in this case) appear brighter in a back scattered electron image. Both images were collected at magnification 70x and show the advantage of great depth of focal field in a SEM.



b

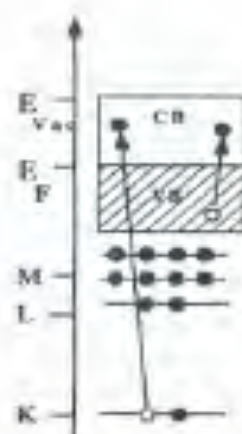
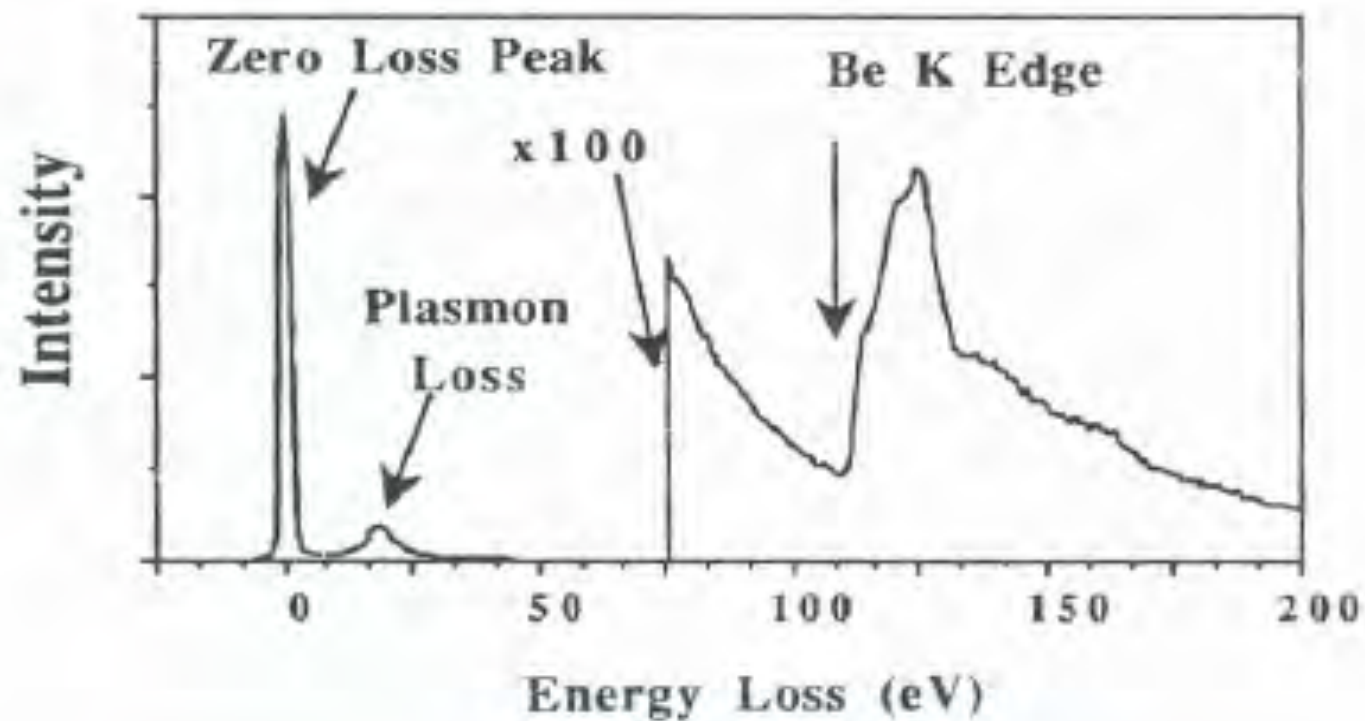
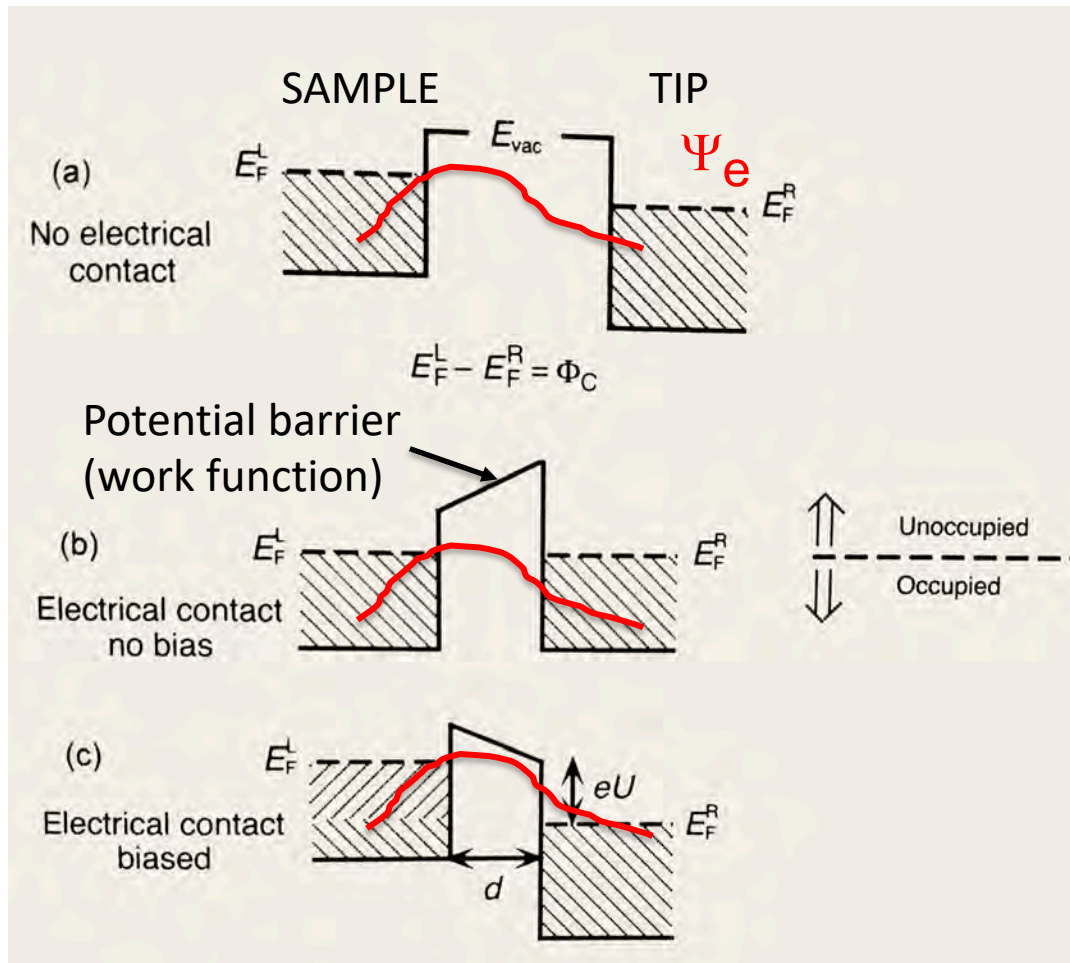


Figure 1 (a) Excitation of inner shells by Coulombic interactions. (b) Energy level diagram illustrating excitation from inner shell and valence band into the conduction band and the creation of a corresponding vacancy.

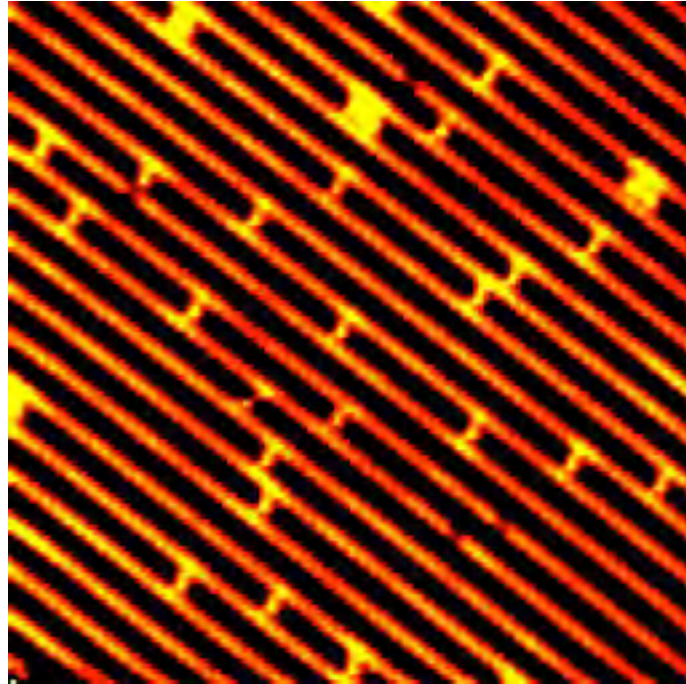
EELS mechanism



EELS

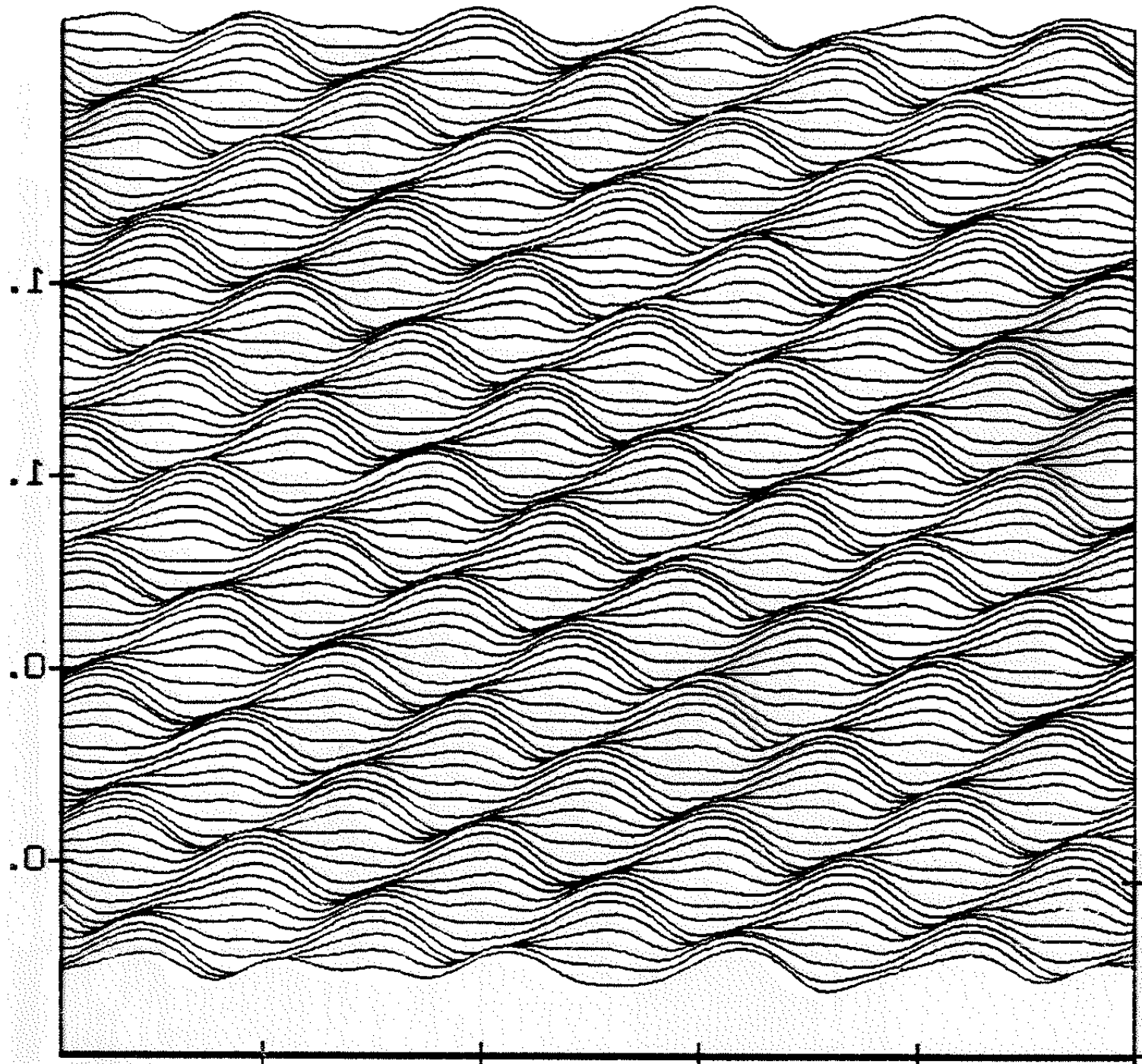


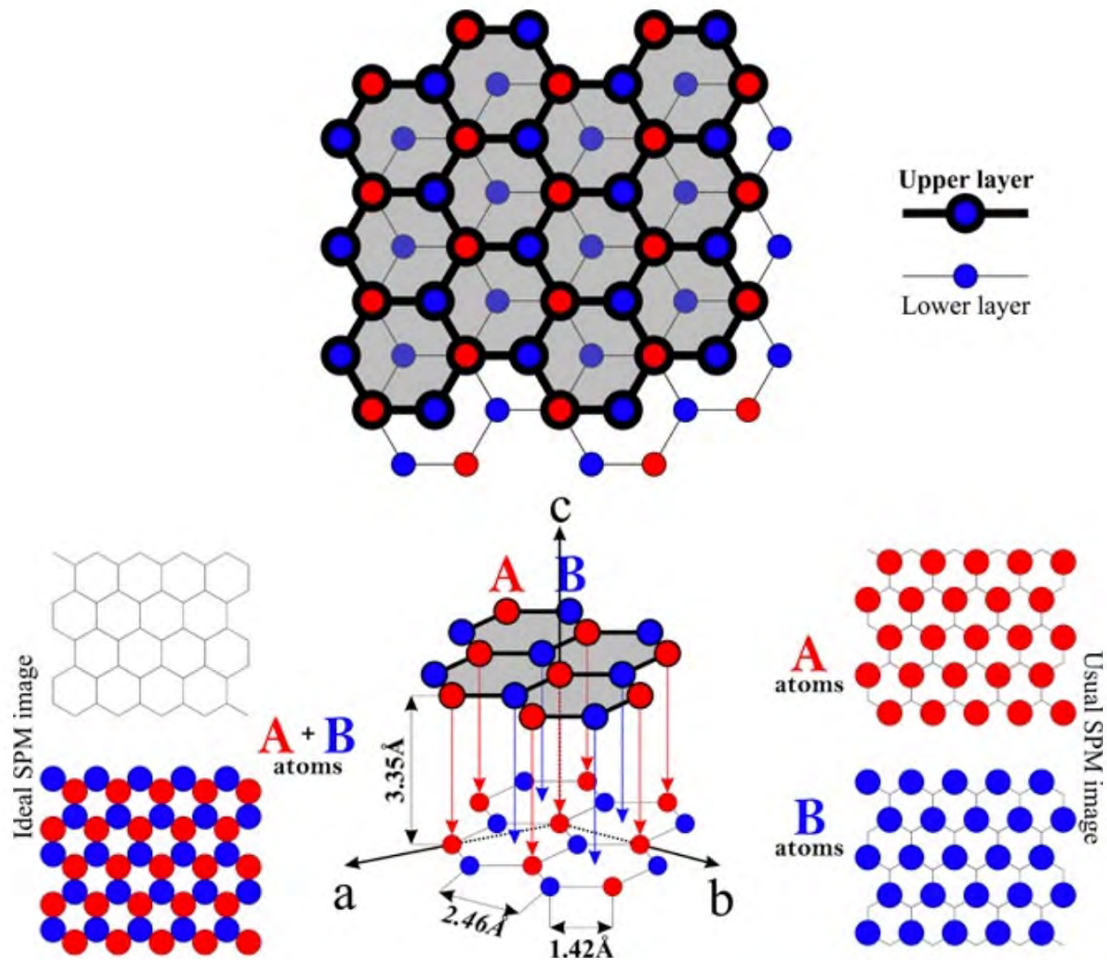
- (a) with no elec contact, get different fermi levels for 2 metals (contact potential = Φ_C). Work functions shown as E_{vac} . Notice work func on tip is larger here.
- (b) electrical contact, fermi levels are equal and still higher work func on tip which acts as a barrier to electron migration.
- (c) with bias so that tip lower (more+) by voltage U (we use V , so eV). Fermi level in sample higher than tip, so electrons in sample (right slanted lines) can lower energy by moving to tip, but still that solid line=work function barrier exists. But electrons tunnel from sample to tip because of wave function of the electrons.





AFM tip





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6 carbons in a ring can be classified into 3 A (α) and a B (β) atoms according to their positions relative the lower layer of graphene. **B (β) atoms**, not sitting atop an atom underneath, gives high tunneling current (“**visible**”) when imaged under constant height mode, as seen from above result.

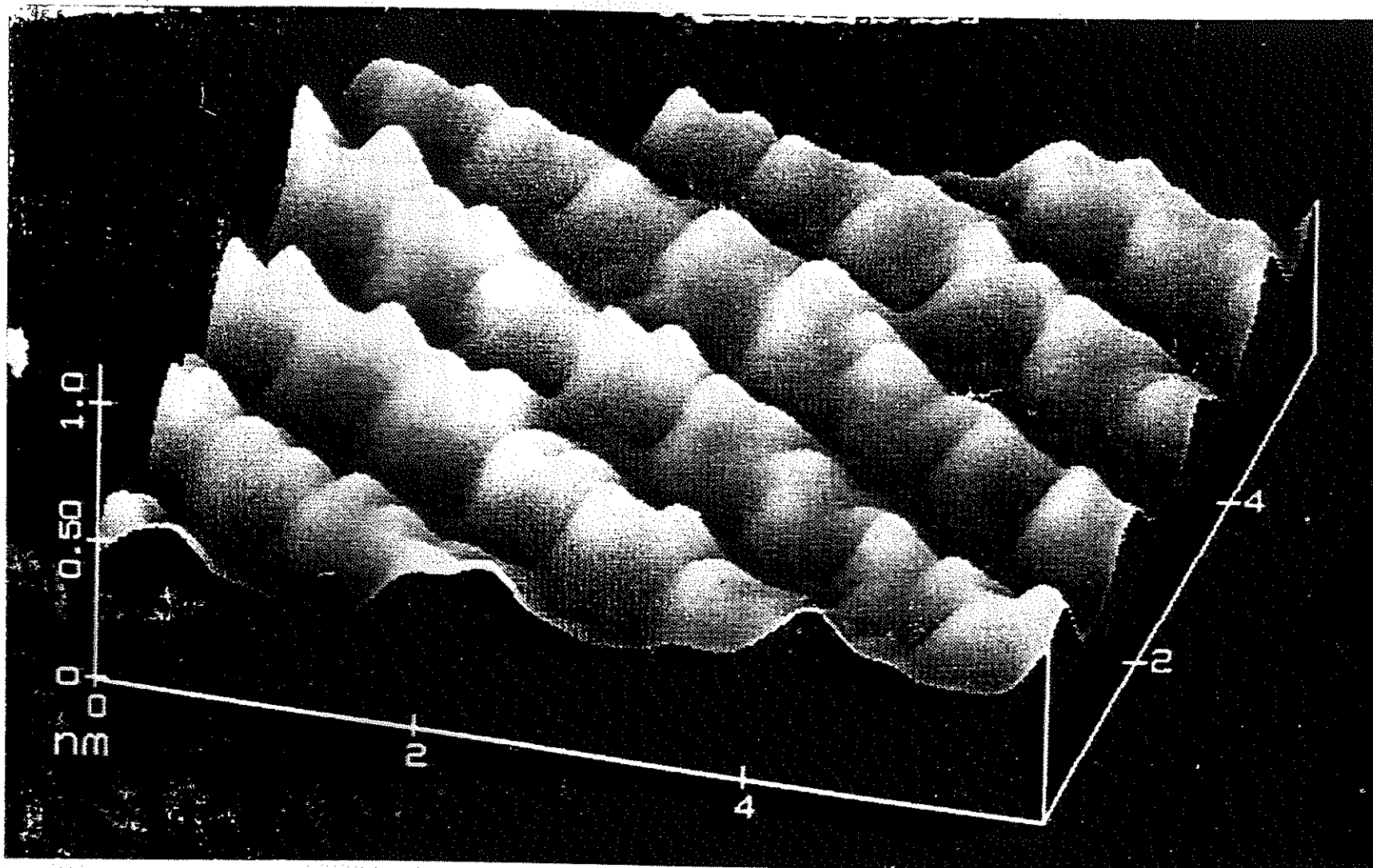
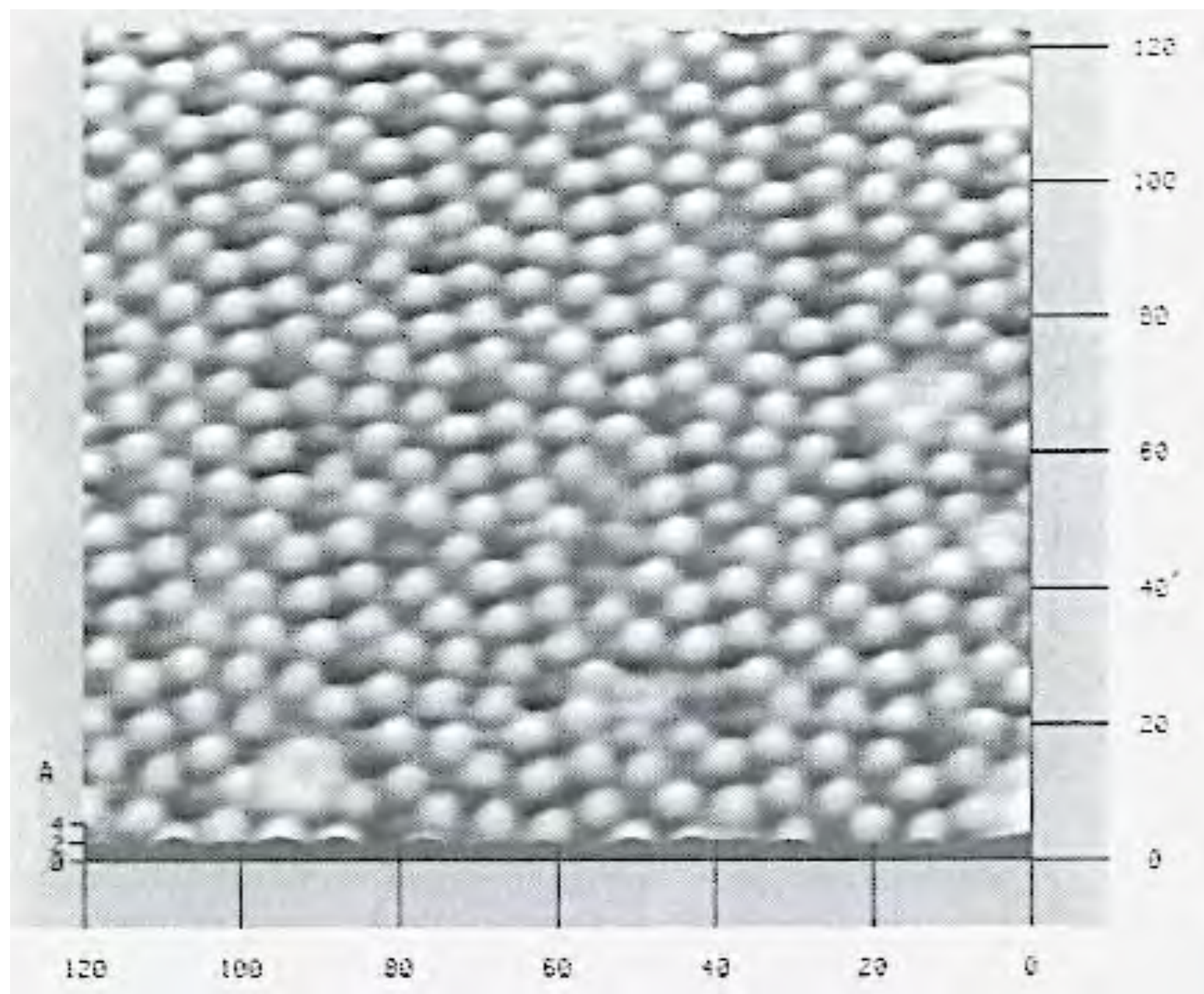
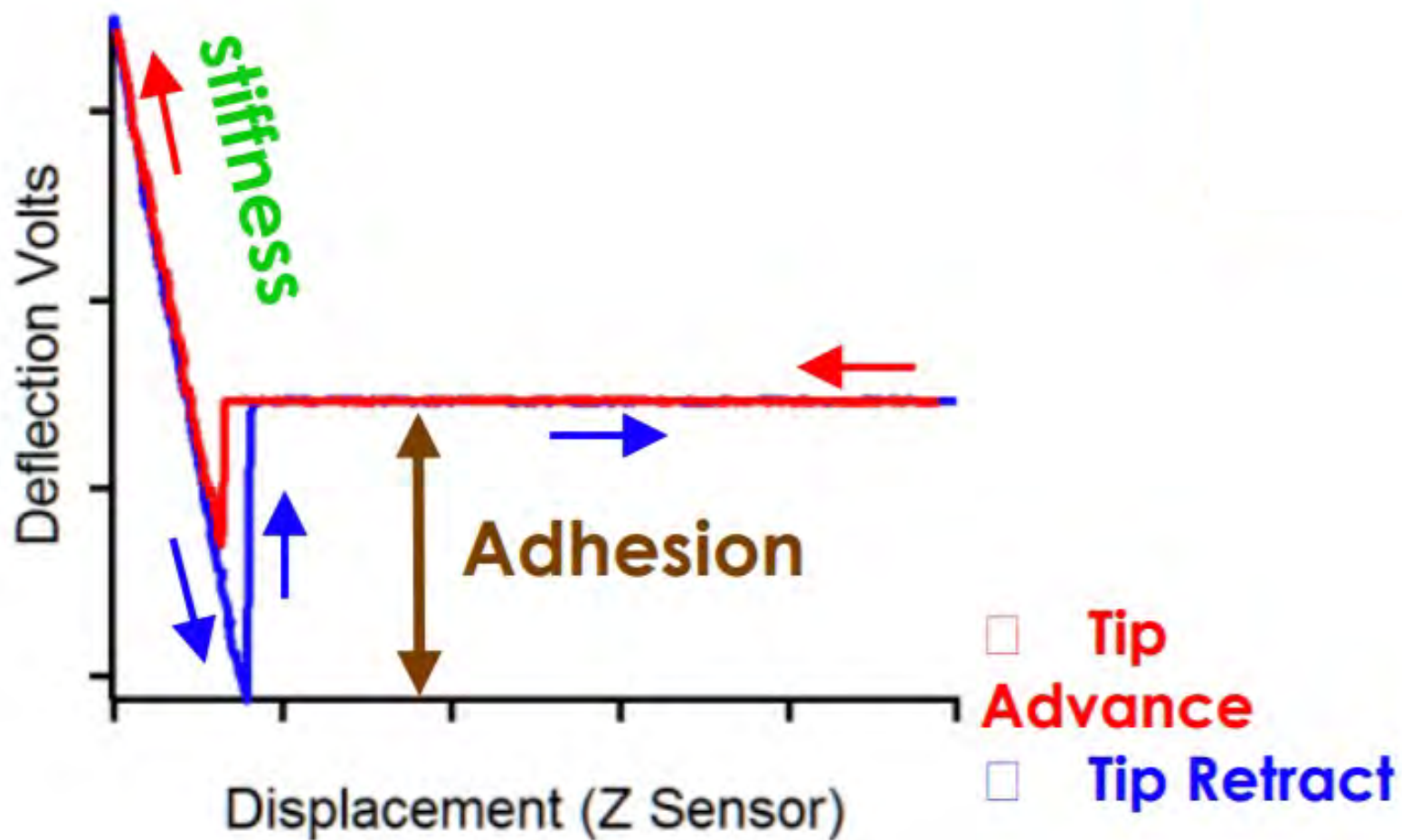


Figure 38.1 STM image of rows of molybdena octahedra on $\text{Rb}_{0.3}\text{Mo}_{0.7}\text{O}_3$, a "molybdenum bronze"
(G. Rudd and S. H. Garofalini, Rutgers University, 1992)





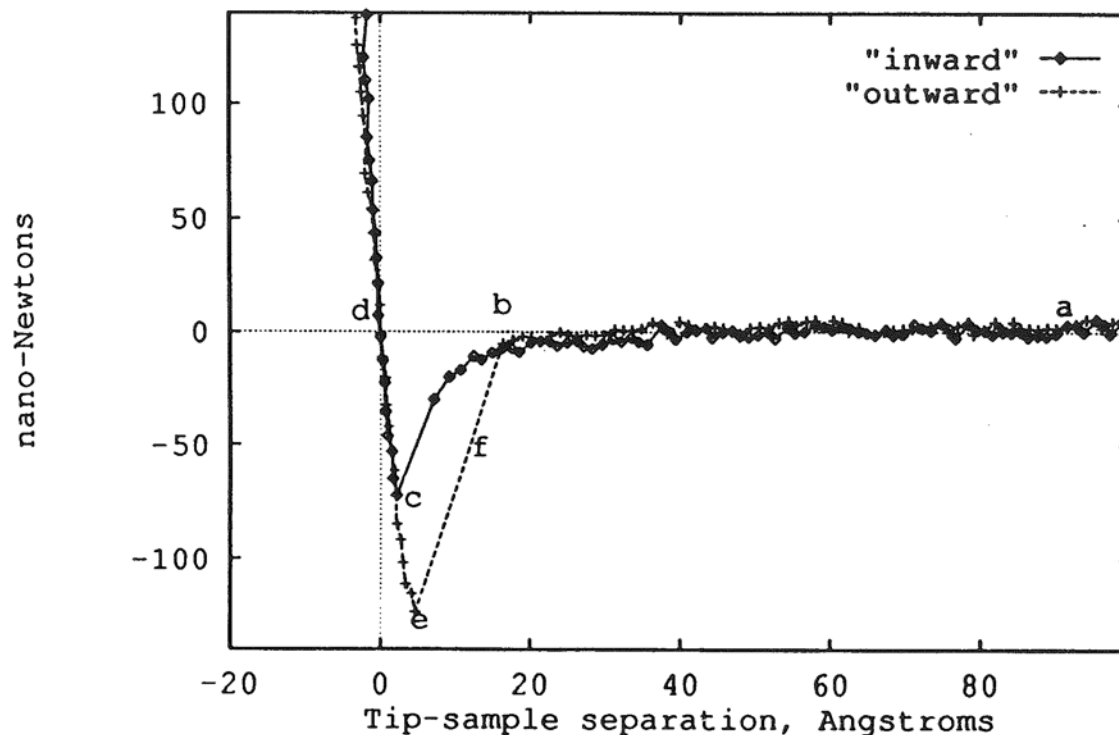


Fig. 1. Example of a F - D curve obtained on pure silica under vacuum. Repulsive forces are positive, attractive negative. "Inward" line traces the approach, "outward" withdrawal. At **a**, tip and sample are far apart and no force is measured. Around **b** onset of attraction begins, which is determined from the point where the slope of the attractive force crosses a threshold (about $1 \text{ nN}/\text{\AA}$). At **c** attractive force reaches a maximum and repulsive forces initiate. At point **d** net force is again zero, and we define this as zero tip-sample separation. On withdrawal, the attractive force goes through a maximum at **e** and is called the "adhesive force." Break-free occurs along **f** and, for discussions in this paper, is the point where the force returns to zero.

Rayleigh scattering

$$\bar{\nu}_0 = 20492 \text{ cm}^{-1}$$

$$\lambda_0 = 488.0 \text{ nm}$$

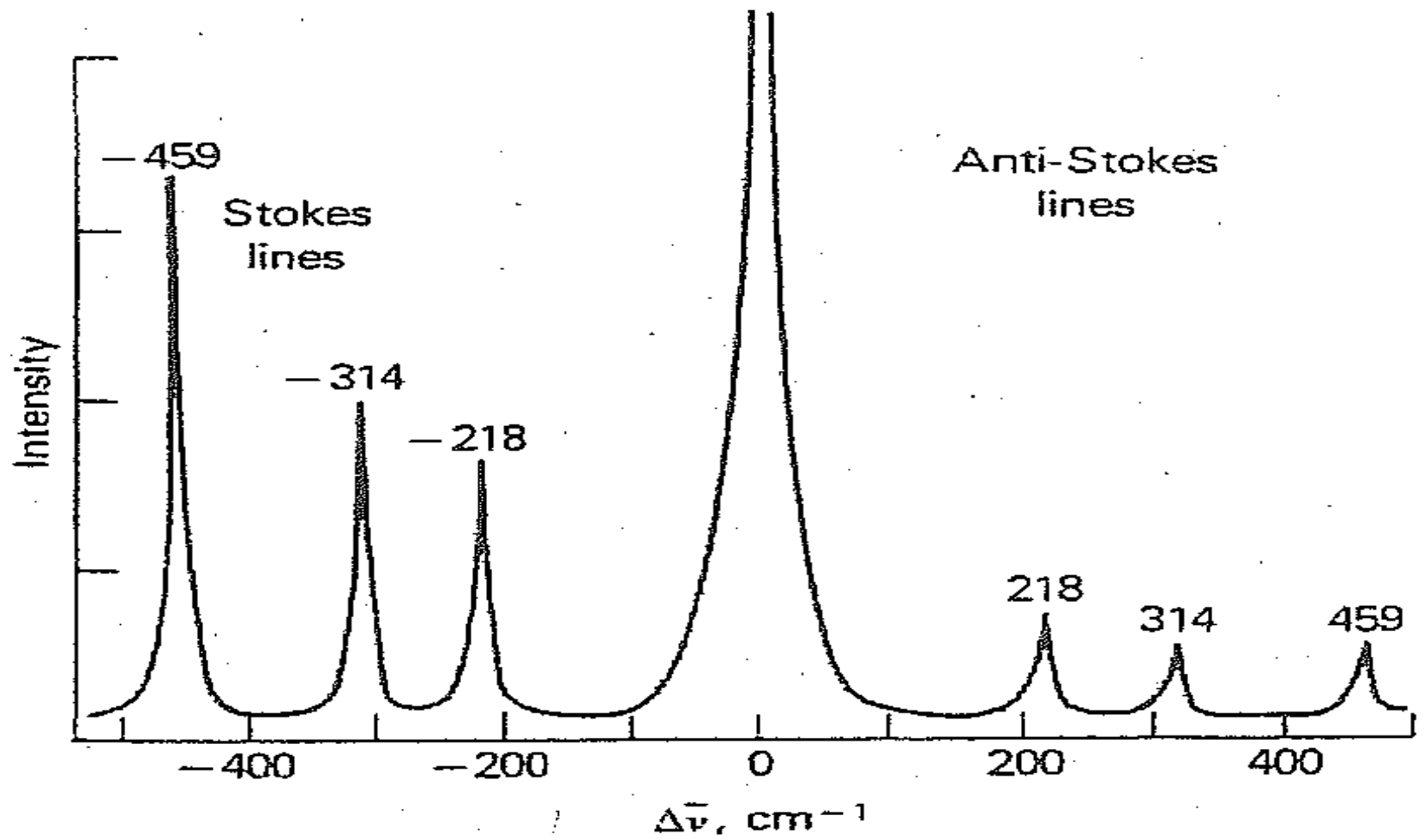
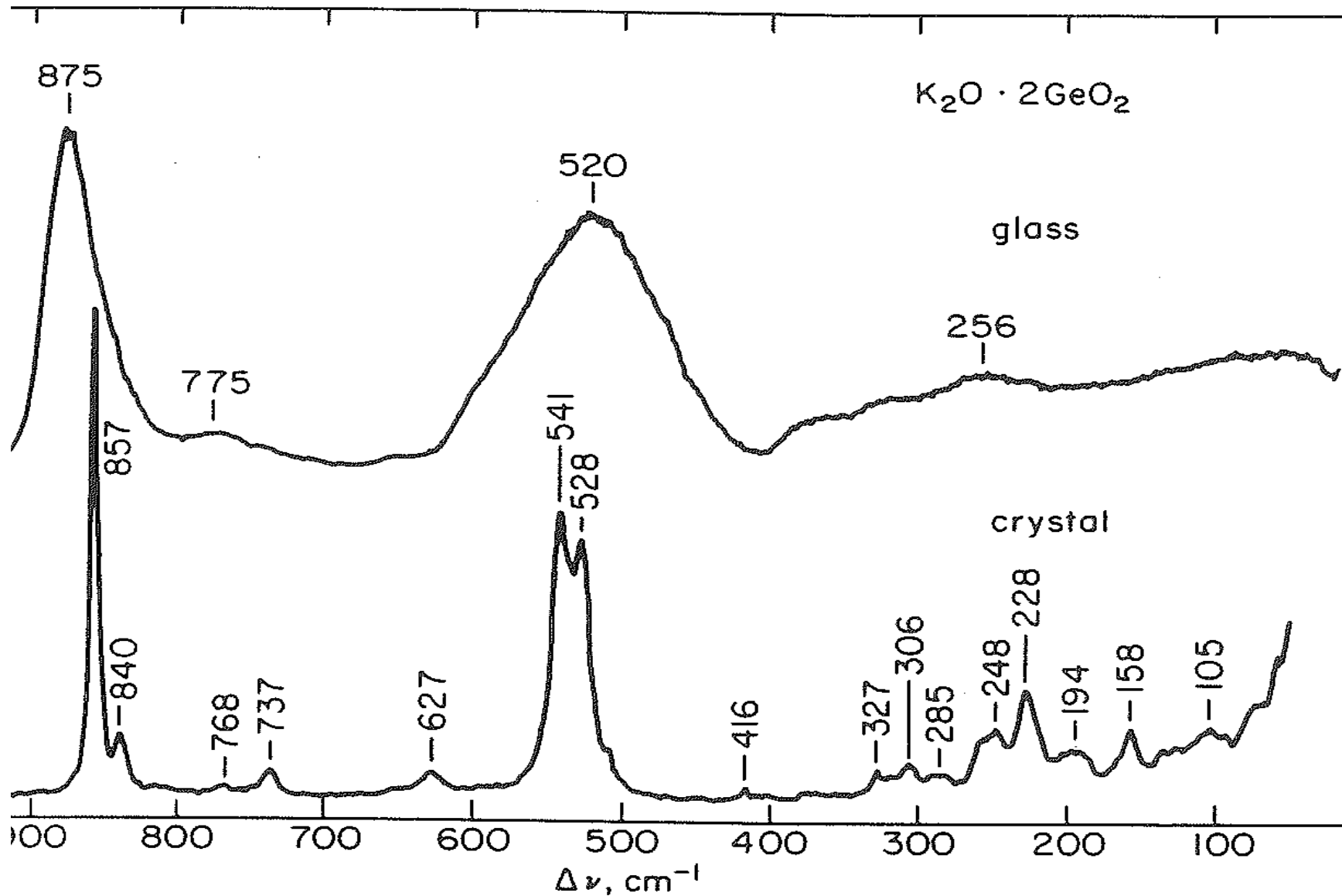


FIGURE 13-1 Raman spectrum for CCl_4 excited by laser



Raman spectra of crystalline and glassy potassium digermanate showing comparison between crystal spectra and glass spectra.