

**Physics 243A—Surface Physics-
Spectroscopy
Suggested answers to Problem Assignment '**

[3.3] (a) $\Delta E_b(1s, Li^{+1} - Li^0) = -\epsilon_{1s, Li^{+1}} - (-\epsilon_{1s, Li^0})$

Now, using Eq. (47) in "Basic Concepts...", this becomes

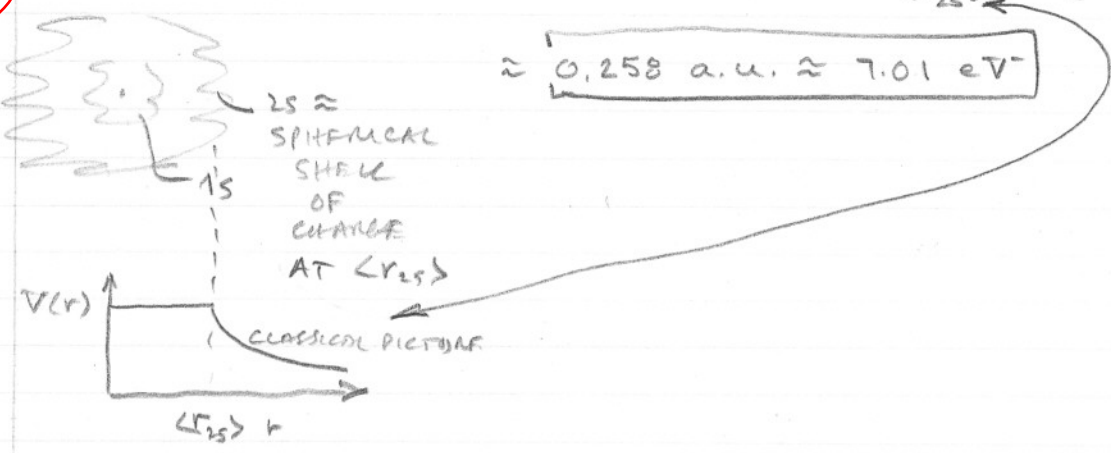
$$\begin{aligned}
 &= -\cancel{\epsilon_{1s, Li^{+1}}^0} - \sum_{j=1}^2 (J_{1s,j} - \delta_{m_s 1s,j} K_{1s,j}) && 1s^2 \text{ ONLY} \\
 &\quad \uparrow \text{UNCHANGED IN COORMANS' PICTURE} \\
 &+ \cancel{\epsilon_{1s, Li^0}^0} + \sum_{j=1}^3 (J_{1s,j} - \delta_{m_s 1s,j} K_{1s,j}) && 1s^2 2s \\
 &\quad \leftarrow \text{EQUAL} \rightarrow \\
 &= -\cancel{J_{1s,1s}} + \cancel{K_{1s,1s}} - \cancel{J_{1s,1s}} \\
 &\quad \quad \quad \uparrow \uparrow \\
 &\quad \quad \quad \text{SELF} \\
 &+ \cancel{J_{1s,1s}} - \cancel{K_{1s,1s}} + J_{1s,1s} + J_{1s,2s} - K_{1s,2s} \\
 &\quad \quad \quad \uparrow \uparrow \quad \quad \quad \uparrow \uparrow \\
 &\quad \quad \quad \text{SELF} \quad \quad \quad \text{SELF}
 \end{aligned}$$

$\Delta E_b(1s, Li^{+1} - Li^0) = J_{1s,2s} - K_{1s,2s}$
IF $\uparrow \uparrow$ ONLY

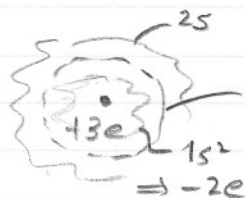
(b) Neglect exchange due to small overlap of 1s + 2s. Then coulomb integral given by

$$\Delta E_b(1s, Li^{+1} - Li^0) \approx J_{1s,2s} \approx \frac{e^2}{\langle r_{2s} \rangle} \approx \frac{e^2}{(3.87 \text{ Bohr})}$$

5



$$(c) E_b(2s, Li^0) = 5.4 \text{ eV}$$



WHAT IS EFFECTIVE CHARGE TO YIELD EXPERIMENTAL E_b ?

FOR H-ATOM:

$$E_b(nl) = - \frac{(13.6 \text{ eV}) Z_{\text{eff}}^2}{n_{\text{eff}}^2}$$

WE WANT $n_{\text{eff}} = 2$, SINCE 2s IS AN "EXCITED STATE" OUTSIDE EFFECTIVE NUCLEUS (YOU COULD ARGUE FOR $n_{\text{eff}} = 1$ ALSO), IN WHICH CASE

$$E_{2s}("1s") = \frac{(13.6) Z_{\text{eff}}^2}{4} = 5.4 \text{ eV}$$

$$\therefore Z_{\text{eff}}^2 = \frac{4(5.4)}{13.6} = 1.588$$

$$Z_{\text{eff}} = 1.26$$

$$= 0.87 \times 1s \text{ CHARGE}$$

\therefore 1s e^- 's HAVE $3.0 - 1.26 = 1.74$ EFFECTIVE SCREENING, WHICH IS SLIGHTLY LESS THAN THEIR ACTUAL CHARGE. (IF YOU USE $n_{\text{eff}} = 1$, YOU'LL GET 1.18 TIMES ACTUAL CHARGE.)



(d) Neglecting trivial nuclear kinetic energy term, the relevant electronic Hamiltonian for this $2-e^-$ system is:

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 - \frac{3e^2}{r_1} - \frac{3e^2}{r_2} + \frac{e^2}{r_{12}}$$

kinetic kinetic e^- -nuc. e^- -nuc. repulsion
 attrac. attrac.

(e) $\Psi_0 (L=0, M_L=0, S=0, M_S=0) = \frac{1}{\sqrt{2}} [\psi_{1s}(\vec{r}_1) \psi_{2s}(\vec{r}_2) + \psi_{2s}(\vec{r}_1) \psi_{1s}(\vec{r}_2)] \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)]$
 $\Psi_1 (L=0, M_L=0, S=1, M_S=1) = \frac{1}{\sqrt{2}} [\psi_{1s}(\vec{r}_1) \psi_{2s}(\vec{r}_2) - \psi_{2s}(\vec{r}_1) \psi_{1s}(\vec{r}_2)] \frac{1}{\sqrt{2}} [\alpha(1)\alpha(2) + \beta(1)\beta(2)]$

First, note that H does not depend on spin, so

that, in either $\langle H \rangle_0$ or $\langle H \rangle_1$, we have separability

$$\langle \Psi_0 | H | \Psi_0 \rangle = \langle \text{space} | \hat{H} | \text{space} \rangle \langle \text{spin} | \text{spin} \rangle$$

1, as spin parts orthonormal

$$= \langle \text{space} | \hat{H} | \text{space} \rangle.$$

Now, consider the two sums of $1-e^-$ operators. For $1-e^-$ kinetic and e^- -nuclear attraction. Both of these can be written as a general operator $\hat{O} = \hat{O}(1) + \hat{O}(2)$. Then

$$\begin{aligned} \langle \Psi_{0,1} | \hat{O} | \Psi_{0,1} \rangle &= \frac{1}{2} \langle 1s(1)2s(2) \pm 2s(1)1s(2) | \hat{O}(1) + \hat{O}(2) | 1s(1)2s(2) \pm 2s(1)1s(2) \rangle \\ &= \frac{1}{2} [\langle 1s(1)2s(2) | \hat{O}(1) | 1s(1)2s(2) \rangle \pm \langle 1s(1)2s(2) | \hat{O}(1) | 2s(1)1s(2) \rangle \\ &\quad + \langle 2s(1)1s(2) | \hat{O}(1) | 1s(1)2s(2) \rangle + \langle 2s(1)1s(2) | \hat{O}(1) | 2s(1)1s(2) \rangle \\ &\quad + \langle 1s(1)2s(2) | \hat{O}(2) | 1s(1)2s(2) \rangle \pm \langle 1s(1)2s(2) | \hat{O}(2) | 2s(1)1s(2) \rangle \\ &\quad \pm \langle 2s(1)1s(2) | \hat{O}(2) | 1s(1)2s(2) \rangle + \langle 2s(1)1s(2) | \hat{O}(2) | 2s(1)1s(2) \rangle] \end{aligned}$$

where the orthonormality of $1s, 2s$ has been used. Thus, finally, since labels $1, 2$ can be made the same now:

$$\langle \Psi_{0,1} | \hat{O} | \Psi_{0,1} \rangle = \frac{1}{2} [2 \langle 1s(1) | \hat{O}(1) | 1s(1) \rangle + 2 \langle 2s(1) | \hat{O}(1) | 2s(1) \rangle].$$

This is the same for both $\langle H \rangle_0$ and $\langle H \rangle_1$, so will cancel \therefore no energy difference. Thus, only e^2/r_{12} yields difference.

Finally, treat $e^2/r_{12} = e^2/|\vec{r}_1 - \vec{r}_2|$, which depends on both coordinates so that matrix elements cannot be separated in products of single-coordinate integrals. Then, from 4 terms analogous to those in Eq. (1):

$$\begin{aligned} \langle \psi_{0,1} | e^2/r_{12} | \psi_{0,1} \rangle &= \frac{1}{2} \left[\langle 1s(1)2s(2) | \frac{e^2}{r_{12}} | 1s(1)2s(2) \rangle \pm \langle 1s(1)2s(2) | \frac{e^2}{r_{12}} | 2s(1)1s(2) \rangle \right. \\ &\quad \left. \pm \langle 2s(1)1s(2) | \frac{e^2}{r_{12}} | 1s(1)2s(2) \rangle + \langle 2s(1)1s(2) | \frac{e^2}{r_{12}} | 2s(1)1s(2) \rangle \right] \\ &= \frac{1}{2} [J_{1s,2s} \pm K_{1s,2s} \pm K_{1s,2s} + J_{1s,2s}] \\ &= J_{1s,2s} \pm K_{1s,2s} \end{aligned}$$

Thus, overall

$$\begin{aligned} \langle \psi_0 | \hat{H} | \psi_0 \rangle - \langle \psi_1 | \hat{H} | \psi_1 \rangle &= J_{1s,2s} + K_{1s,2s} - (J_{1s,2s} - K_{1s,2s}) \\ &= \boxed{2 K_{1s,2s}} \end{aligned}$$

which is exactly the $1S - 3S$ spacing predicted by the VanVleck theorem, since the initial $S = 1/2$, so $(2S+1) = \underline{2}$.

(f.) From Equation (140) in "Basic Concepts of XPS":

$$\Delta[E_b(ns)] = (2S+1) K_{ns,n'l} \quad (1)$$

5 For Li $1s^2 2s^2 S'$; $K_{1s-2s} = 0.0285 \text{ a.u.}$
 $= 0.776 \text{ eV}$
 $(1 \text{ a.u.} = 27.21 \text{ eV})$

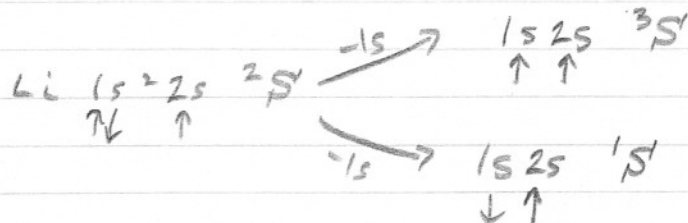
$\begin{matrix} S=0 \\ L=0 \end{matrix} \quad \begin{matrix} \uparrow \\ \uparrow \end{matrix}$
 $\begin{matrix} S=1/2 \\ L=0 \end{matrix} \quad \begin{matrix} \uparrow \\ \downarrow \end{matrix}$

\therefore

$$\Delta[E_b(1s)] = (2(1/2)+1)(0.776)$$

$$\Delta[E_b(1s)] = 1.55 \text{ eV}$$

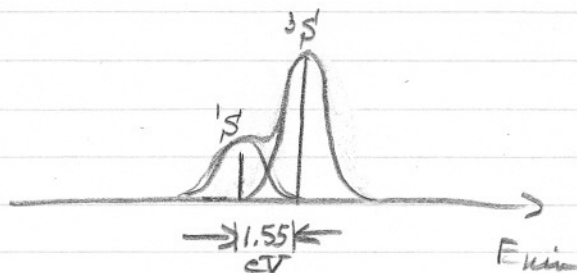
The two final states are:



Overall intensity ratios will be (by Equation (146)) equal to spin multiplicity ratios or

$$\frac{I(3S)}{I(1S)} = \frac{3.0}{1.0}$$

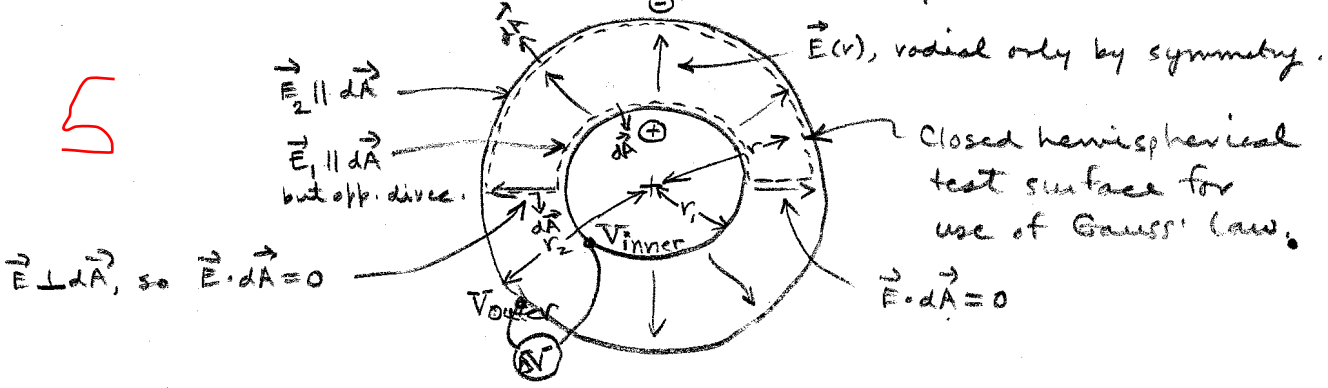
Overall spectrum would thus look like:



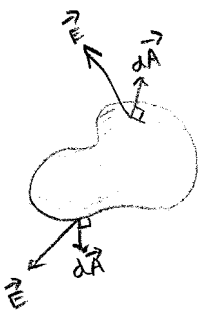
With a FWHM due to instrumental effects ≈ 1.0 eV, such splittings should be observable. The peaks sketched above each have FWHM ≈ 1.0 eV and summing these gives a net spectrum that would clearly show a doublet, or at least a clear peak + shoulder.

[3.4]

(a) For the hemispherical electrostatic analyzer, we can consider an ideal "spherical capacitor" as:



Over the test surface (---) just inside the vacuum between the electrodes, Gauss's law must hold in this form:



$$\oint \vec{E} \cdot d\vec{A} = 0 \quad (\text{since no charge contained within } \vec{A})$$

Or, broken into terms with $\vec{E}_1 = \vec{E}(r_1)$, $\vec{E}_2 = \vec{E}(r_2)$, $\rightarrow 0$, because $\vec{E} \perp d\vec{A}$

$$2\pi r_2^2 E_2 - 2\pi r_1^2 E_1 + \int \vec{E} \cdot d\vec{A} = 0$$

Over flat surface at base of hemispheres

$$\therefore \frac{E_2}{E_1} = \frac{r_1^2}{r_2^2}, \quad E_2 = \frac{r_1^2}{r_2^2} E_1$$

or, since both radii arbitrary, in general

$$\vec{E}(r) = \frac{r_1^2}{r^2} \vec{E}(r_1) \quad (1)$$

But energy difference between two hemispheres is eV (if V in volts, e in coul) and this must equal work between two along a radial line:

$$e\Delta V = e(V_i - V_o) = \int_{r_1}^{r_2} F(r) dr = e \int_{r_1}^{r_2} E(r) dr,$$

$$= e n_1^2 E(r_1) \int_{r_2}^{r_1} \frac{dr}{r^2} = e n_1^2 E(r_1) \left[-\frac{1}{r} \right]_{r_2}^{r_1}$$


$$e \Delta V = e n_1^2 E(r_1) \left[\frac{1}{r_1} - \frac{1}{r_2} \right]$$

$$\text{or } r_1^2 E(r_1) = \frac{\Delta V r_1 r_2}{(r_2 - r_1)}$$

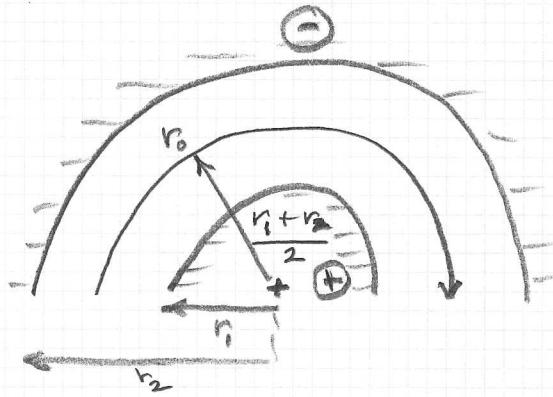
Thus, (1) becomes finally

$$\vec{E}(r) = \frac{\Delta V r_1 r_2}{(r_2 - r_1) r^2} \text{ (in radial direction)}$$

So, it has a $1/r^2$ field (just as Coulomb's law and gravity).



[3.4] (b)



$$\vec{E}(\vec{r}) = \frac{\Delta V r_1 r_2}{(r_2 - r_1) r_0^2} = \frac{\Delta V r_1 r_2}{(r_2 - r_1) (r_1 + r_2)^2} \hat{e}_r$$

$$\vec{F}(\vec{r}) = -e\vec{E}(\vec{r}) = + \frac{m_0 v^2}{r_0} \hat{e}_r \text{ FOR STABLE CIRCULAR TRAJECTORY}$$

↑
NON-RELATIVISTIC

$$\frac{e \Delta V r_1 r_2}{(r_2 - r_1) r_0^2} = \frac{2 E_{kin}}{r_0}$$

$$E_{kin} = \frac{e \Delta V r_1 r_2}{2(r_2 - r_1)(r_1 + r_2)} = \underbrace{\left(\frac{e r_1 r_2}{(r_2 - r_1)^2} \right)}_{\text{CALIBRATION CONSTANT}} \Delta V$$

[4.1] If

$$\frac{SF}{E_0} \approx \frac{SR_{\text{ent}}}{2R_0} + \frac{SR_{\text{det}}}{2R_0} + \alpha_r^2 = 0.170 = 10^{-3}$$

and we require each of the three terms to be equal, then

$$\frac{SR_{\text{ent}}}{2R_0} = \frac{SR_{\text{det}}}{2R_0} = \alpha_r^2 = \frac{10^{-3}}{3}$$

so

$$\begin{aligned} SR_{\text{ent}} = SR_{\text{det}} &= 2(20 \text{ cm}) \frac{10^{-3}}{3} = 1.33 \times 10^{-2} \text{ cm} \\ &= 0.0133 \text{ cm} \\ &= 0.133 \text{ mm} \\ &= \underline{\underline{133 \text{ microns}}} \end{aligned}$$

$$\alpha_r^2 = 0.33 \times 10^{-3} = 3.3 \times 10^{-4} \Rightarrow \alpha_r = 0.0182$$
$$\alpha_r = \underline{\underline{1.04^\circ}}$$

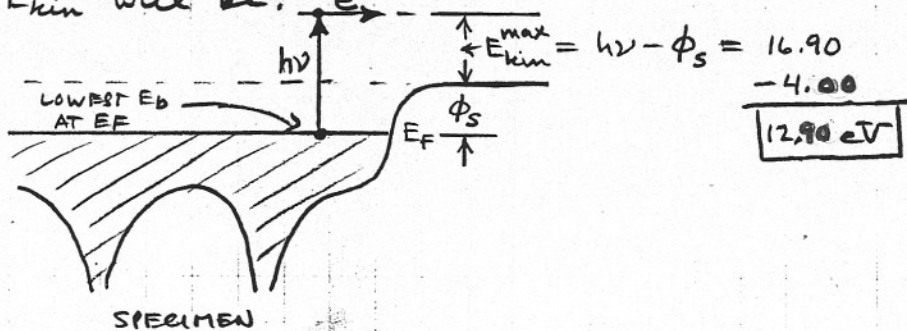


[4.2]

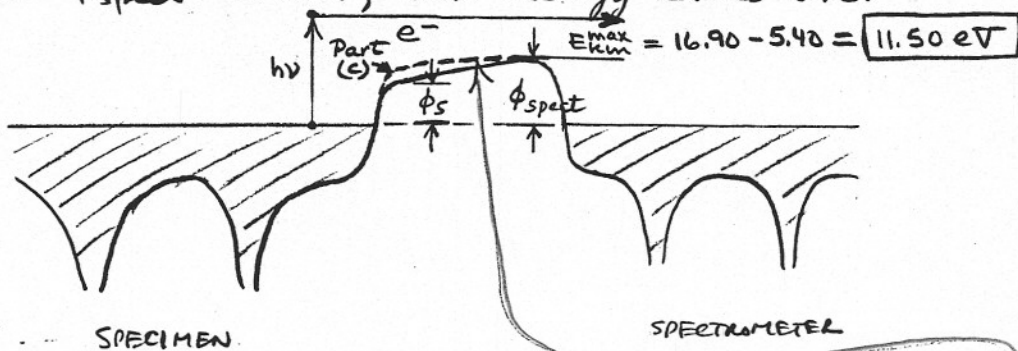
$$\phi_s(\text{Cu (poly)}) = 4.00 \text{ eV}$$

$$h\nu = 16.90 \text{ eV}$$

- (a) Just outside the specimen surface, but before entering the analyzer, the maximum energy E_{kin}^{max} will be:

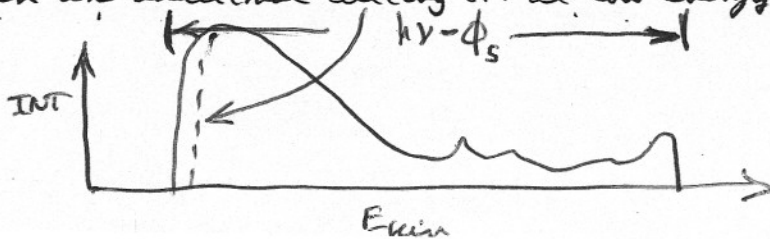


- (b) If $\phi_{spect} = 5.40 \text{ eV}$, then energy levels are:



I.e., there is a retardation by the difference in work functions of $5.40 - 4.00 = 1.40 \text{ eV}$.

- (c) The new specimen work function is now $4.00 + 0.70 = 4.70 \text{ eV}$ and still less than that of the spectrometer (see dashed curve above). Thus, the observed spectra in the spectrometer will still be controlled by the spectrometer ϕ_s and no change will be seen. If $\phi_s > \phi_{spect}$, then an additional cutting off at low energy would occur.



[43] (a) STARTING FROM E.G., EQ. 113 IN "BASIC CONCEPTS...", INTEGRATING
OVER $x+y$ TO GET A_0 , REPLACING Ω BY Ω_0 , AND OMITTING
FACTOR D_0 SINCE ALL WE WANT IS PHOTOELECTRON INTENSITY
EMITTED, WE HAVE

OFTEN MISSED

10

$$dN_k(z) = I_0 \rho(z) \frac{A_0}{\sin\theta} dz \frac{d\sigma_k}{d\Omega} \Omega_0 e^{-z/\Lambda_c \sin\theta}$$

$$= I_0 [Fe]_0 \left\{ 1 - z/z_0 \right\} \frac{A_0}{\sin\theta} dz \frac{d\sigma_k}{d\Omega} \Omega_0 e^{-z/\Lambda_c \sin\theta}$$

OFTEN MISSED

THE TOTAL INTENSITY IS THEN THE INTEGRAL OF THIS FROM
 $z=0$ TO $z=z_0$ (THE POINT AT WHICH $[Fe]_z \rightarrow 0$:

$$N_k = \int dN_k = I_0 [Fe]_0 A_0 \frac{d\sigma_k}{d\Omega} \frac{\Omega_0}{\sin\theta} \int_0^{z_0} \left\{ 1 - z/z_0 \right\} e^{-z/\Lambda_c \sin\theta} dz$$

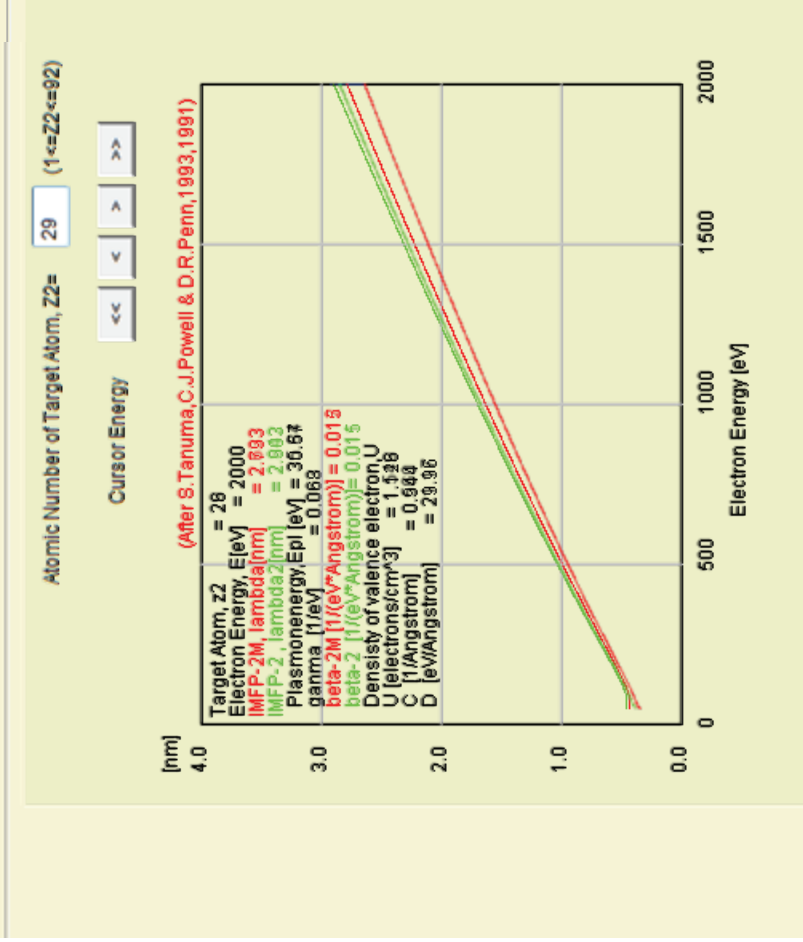
$$= I_0 [Fe]_0 A_0 \frac{d\sigma_k}{d\Omega} \Omega_0 \Lambda_c \left\{ 1 + \frac{\Lambda_c \sin\theta}{z_0} \left(e^{-z_0/\Lambda_c \sin\theta} - 1 \right) \right\}$$

See next page for justification that we can assume a single lambda value for a mixed alloy of Fe and Cu

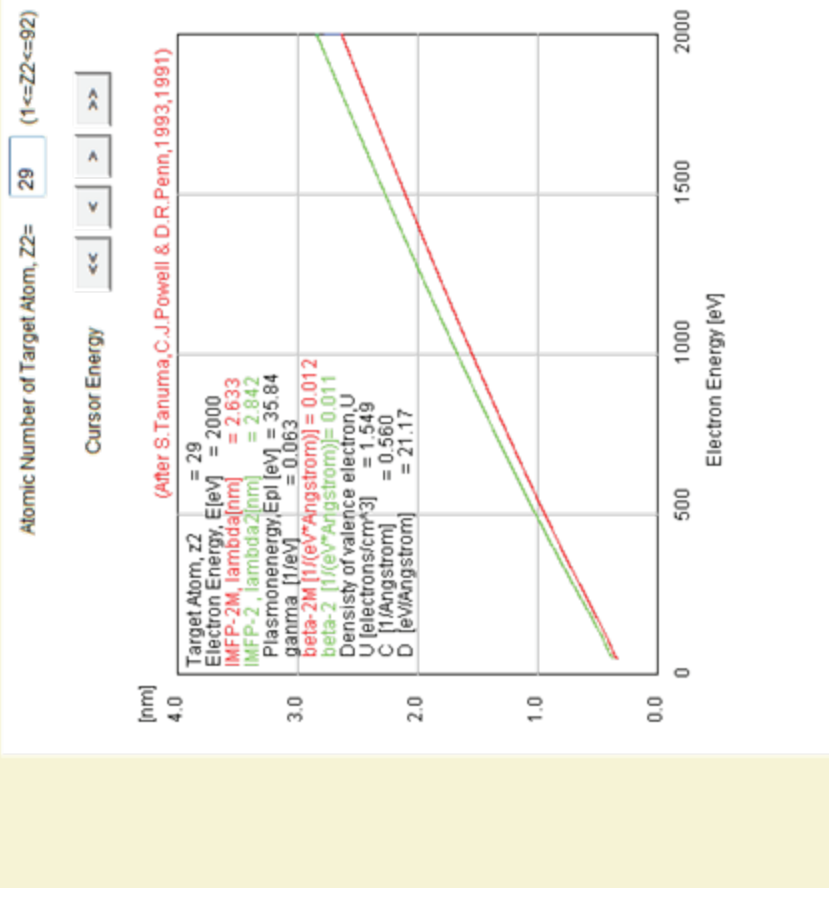


Overlay of Fe and Cu IMFPs from <http://www.ss.teen.setsunan.ac.jp/e-impfp2.html>

Cu plotted over Fe



Cu alone, slightly lower



(b) INPUTS ARE:

$$I_0 = 10^{12} \text{ ph-sec}^{-1} \text{-cm}^{-2}$$

$$[Fe]_0 = 8.50 \times 10^{22} \text{ cm}^{-3}$$

5

$$A_0 = 2.5 \text{ mm}^2 = (0.1 \times 0.5) \text{ cm}^2 = 0.05 \text{ cm}^2$$

$$\frac{dN_{Fe2p}}{d\Omega} = \frac{G_{Fe2p}}{4\pi} \left[1 + \frac{1}{2} \beta_{Fe2p} \left(\frac{3}{2} \sin^2 \alpha - 1 \right) \right]$$

$$\left(1 \text{ Mb} = 10^{-19} \text{ cm}^2 \right) \quad \left(1 \text{ IF } \alpha = 90^\circ \right)$$

$$= \frac{0.2216 \times 10^{-19} \text{ cm}^2}{4\pi} \left[1 + \frac{1.453}{2} (1/2) \right]$$

$$= 0.0259 \times 10^{-19} \text{ cm}^2 = 2.40 \times 10^{-20} \text{ cm}^2/\text{steradian}$$

Ω_0 (STERADIANS) FOR $\pm 6^\circ$ ACCEPTANCE FROM:

METHOD 2: $r \rightarrow z$ IN SPHER. COORD.

$$\Omega_0 = \int d\Omega = \int_0^{2\pi} \int_0^{6^\circ} \sin \theta d\theta d\phi$$

$$= 2\pi [-\cos \theta]_0^{6^\circ}$$

METHOD 1:



$$\Omega_0 = \frac{A}{r^2} \approx \frac{\pi (r \tan 6^\circ)^2}{r^2} = 0.034 \text{ steradians}$$

$$\approx 2\pi [1 - 0.9945]$$

$$= 0.034$$

$$\Lambda_e @ E_{min} = 1486.6 - E_b(Fe2p) \approx 1497 - \left(\frac{720 + 707}{2} \right)$$

$$\approx 774 \text{ eV}$$

\Rightarrow FROM SEAH + DENCH, SURF. INT. ANAL. 1, 2 (1979):

$$\Lambda_e(\text{nm}) = B_n E^{1/2} = \frac{B_n(\text{elom})}{\text{TABLE 1}} \cdot B_n(Fe) E^{1/2} = (0.054) 0.66 (27.8)$$

$$\frac{\Lambda_e \sin \theta}{z_0} = \frac{10}{10} \sin \theta = \sin \theta$$

FIG. 3
 $\approx R_n(Fe)$

$$= 0.99 \text{ nm} = 9.9 \text{ \AA}$$

$$e^{-z_0/\Lambda_e \sin \theta} = e^{-1/\sin \theta}$$

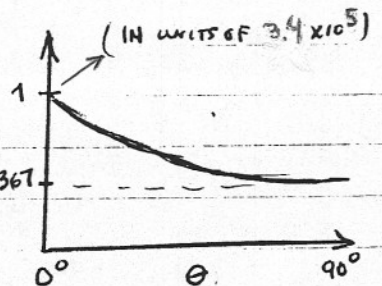
OR TANUNA FIT AL.
CALCULATE 2 11-16 \AA
& OK TOO

SO, INTENSITY FINALLY IS

$$N_{Fe2p} = (10^{12}) (8.5 \times 10^{22}) (0.05) (2.40 \times 10^{-20}) (9.9 \times 10^{-8}) \times$$

$$\left\{ 1 + \sin \theta (e^{-1/\sin \theta} - 1) \right\}$$

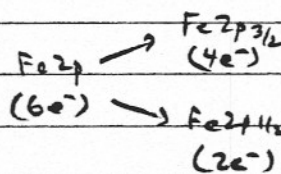
$$N_{Fe2p} = 3.4 \times 10^5 \left\{ 1 + \sin \theta (e^{-1/\sin \theta} - 1) \right\} 0.367$$



FINAL COMMENT--
PHYSICALLY
REASONABLE:

MORE Fe2p
AT MORE SURFACE
SENSITIVE LOW \Rightarrow VALUES.

(d) JUST AS IT BY SPIN OCCUPATION = $2j+1$:



$$N_{Fe_{2p_{3/2}}} = \frac{2}{3} N_{Fe_{2p}}$$
$$N_{Fe_{2p_{1/2}}} = \frac{1}{3} N_{Fe_{2p}}$$

$$\Delta E_{s-o} = 13.1 \text{ eV}$$

YES, SINCE S-O SPLITTING IS 13 eV, IT WOULD BE RESOLVED.

(e) FROM XPS CURVES OF Mn HANDLED OUT (Mn IS JUST BELOW Fe IN ATOMIC NO.), WE EXPECT COHERENT MINIMUM

IN Fe_{3p} AT ABOUT 20 eV ABOVE ITS THRESHOLD OF ≈ 53 eV.

OR AT ≈ 70 eV: ACTUAL CURVE ON NEXT P. SHOWS MINIMUM AT ≈ 80 eV

(f) AGAIN MAKING USE OF Mn CASE, WHICH HAS $3d-3p$

RESONANT PHOTOEMISSION, WE EXPECT Fe_{3d} TO SHOW

RESONANCE AT $h\nu \approx E_b(Fe_{3p}) \approx 53$ eV.

(c) KINETIC ENERGY = 774 eV = E_{kin}

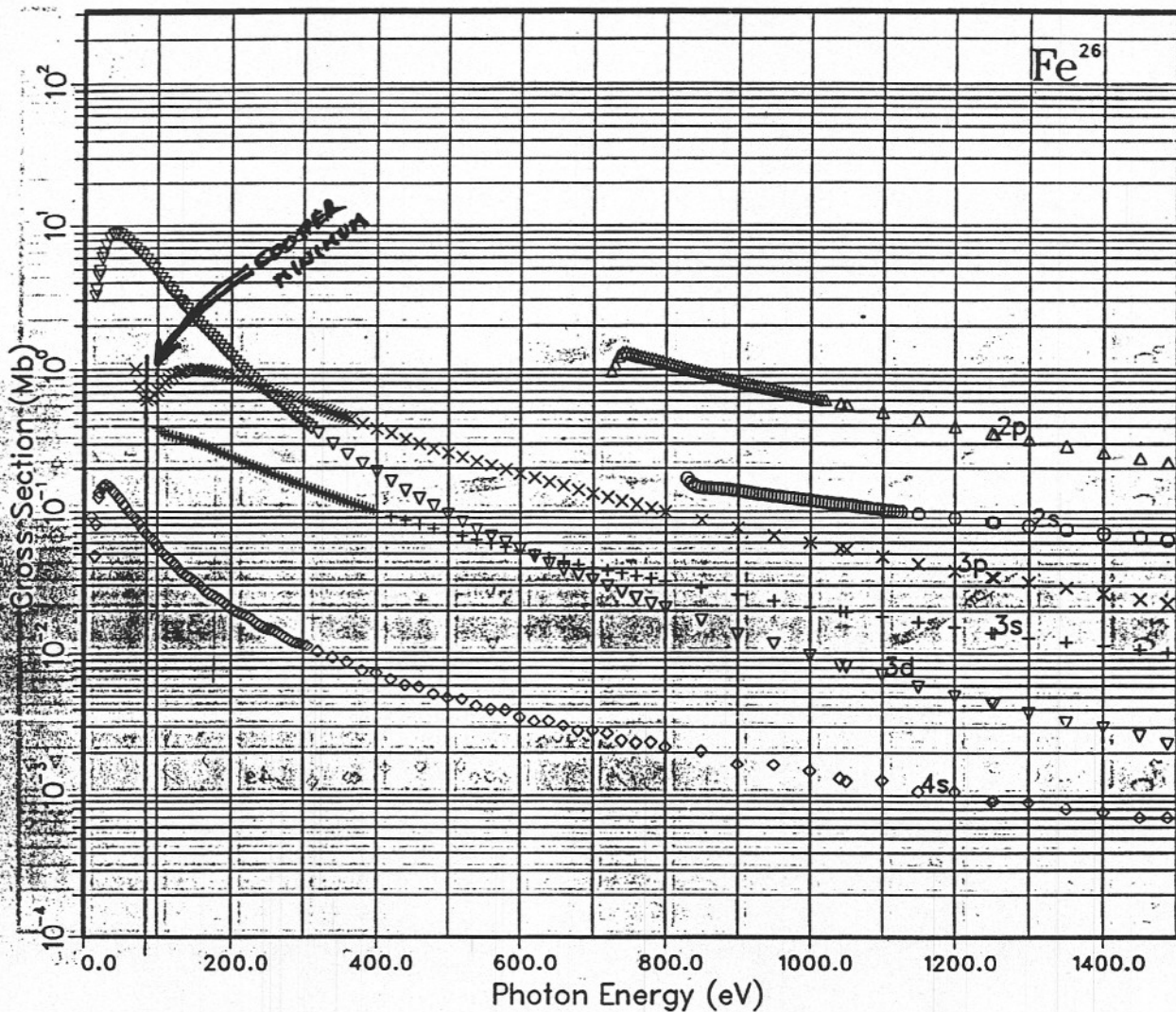
$\Delta E/E_0 = 0.01$. \therefore IF $\Delta E = 1$ eV, $E_0 = 100$ eV.

THUS RETARD VOLTAGE OF -674V WOULD BE NEEDED

OR A "RETARD RATIO" OF $\frac{774}{100} = 7.74$



GRAPH I. Atomic Subshell Photoionization Cross Sections for 0-1500 eV, $1 \leq Z \leq 103$
 See page 6 for Explanation of Graphs

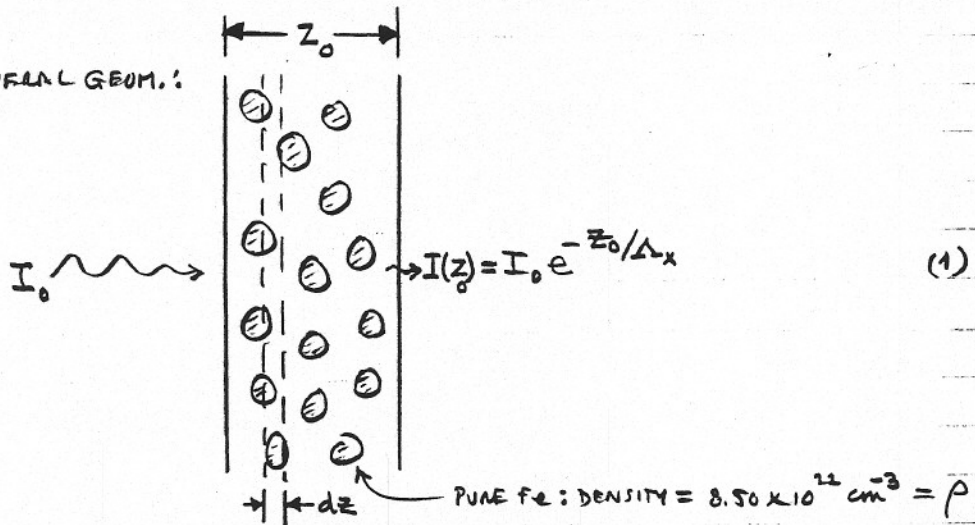


Fe binding energies(eV) are:

1s(2) 7017.74	2s(2) 829.347	2p(6) 722.246
3s(2) 98.9233	3p(6) 66.5706	4s(2) 7.41881
3d(6) 13.1179		

(9) GENERAL GEOM.:

5



WISH TO CALCULATE ATTENUATION LENGTH Δ_x , WHICH IS DOMINATED BY PHOTOELECTRIC EFFECT IN VARIOUS FE SUBSHELLS. SO NEED TOTAL PHOTOELECTRIC CROSS SECTION PER ATOM:

$$G_{TOT} = \sum_{nL} G_{nL} \quad (2)$$

FROM THIS, CAN WRITE FOR DIFFERENTIAL LOSS IN INTENSITY OVER ANY dz :

$$dI = -I(z) \cdot \underbrace{G_{TOT}}_{\substack{\text{PHOTONS} \\ \text{cm}^2 \cdot \text{SEC}}} \cdot \underbrace{\rho}_{\substack{\text{PHOTOE}^- \cdot \text{cm}^2 \\ \text{PHOTON}}} \cdot \underbrace{\left(\frac{\text{NO. ATOMS}}{\text{cm}^3}\right)}$$

$$= -I(z) G_{TOT} \rho dz$$

\therefore

$$\frac{dI}{I(z)} = -G_{TOT} \rho \xrightarrow{\text{INTEGRATE}} I(z) = I_0 e^{-G_{TOT} \rho z} \quad (3)$$

AND COMPARING (1) THEN YIELDS

$$\Delta_x = (G_{TOT} \rho)^{-1} \quad (4)$$

FOR Fe, NOS. ATMS FOR ALLKX @ 1486.6 eV:

(VEH. LINDBAU) TABLE G_{TOT} (MBARN) = $0.06 + 0.22 + 0.01 + 0.02 + 0.00 + 0.00 = 0.310$ MBARNS = $3.10 \times 10^{-19} \text{ cm}^2$

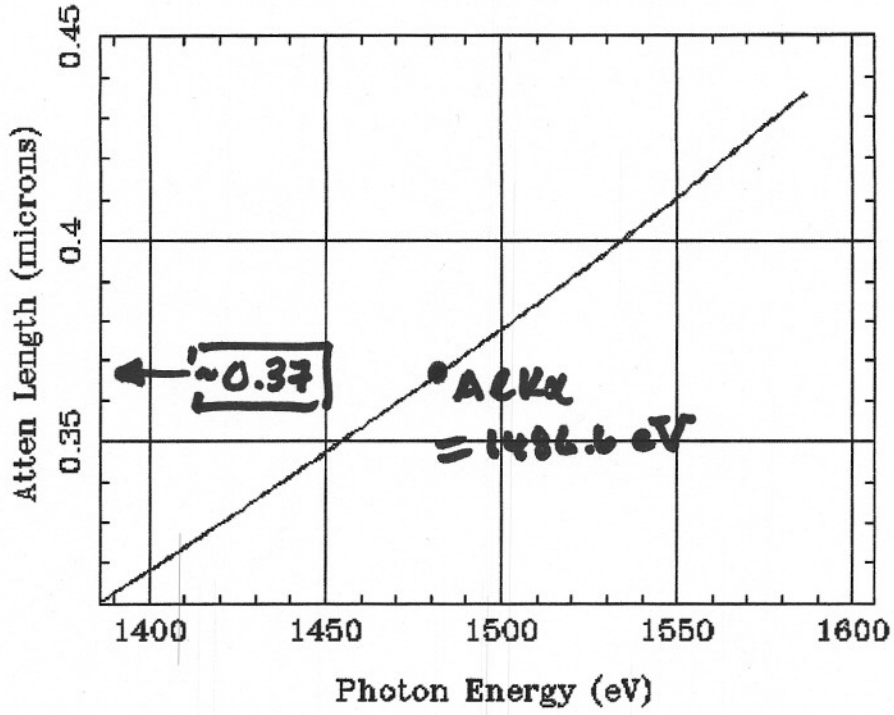
$\hookrightarrow 1 \text{ barn} = 10^{-28} \text{ m}^2 = 10^{-24} \text{ cm}^2$

\therefore WITH ρ FROM ABOVE: $\Delta_x = \left[(3.10 \times 10^{-19} \text{ cm}^2) (8.50 \times 10^{22} \text{ cm}^{-3}) \right]^{-1} = 0.0379 \times 10^{-3} \text{ cm}$
 (NOTE: $\Delta_x > \Delta_E$, AS ASSUMED) $= 3.79 \times 10^{-5} \text{ cm} = 3,790 \text{ \AA} = 0.38 \text{ microns}$

COMPARES VERY WELL WITH RESULT FROM WEBSITE ON NEXT PAGE.

X-Ray Attenuation Length

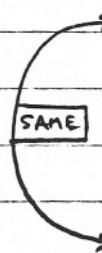
Fe Density=7.874, Angle=90.deg



[411] (a) Peak positions and certain spacings are noted on following figure. Checking E_b tables and Auger charts then gives for assignments:

PEAK	E_b (PHOTOE)	E_{kin} (AUGER)	ASSIGNMENT
a	--	~ 60 eV	(AL LMM Auger of type $L_{2,3}M_{1,2}M_{1,2}$ with $E_{kin} \approx 77 - 10 - 5 = 62$ eV.)
b	--	~ 370 eV	N KLL with 356-377 eV range
c	--	~ 1395 eV	AL KLL with 1301-1392 eV range
d	--	(Series at ~ 17.5 eV spacing below strongest KLL Auger)	(Plasmon losses in AL, which should occur at $tw, \approx 15.5$ eV)
e	~ 870 eV	$\rightarrow \sim 386$ eV	Same origin as b; N KLL.
f	~ 535 eV	---	O 1s photoelectron: very weak
g	---	(Broad peak ~ 19 eV below h)	(Since peaks j and k have same low-energy tail, suggest <u>loss</u> peak of $1-e^-$ type, <u>not</u> plasmon)
h	~ 399 eV	---	N 1s photoelectron, $E_b = 403$ eV
i	--	(Weak peaks ~ 9 eV above h)	(K $\alpha_{3,4}$ x-ray satellites, also seen above j and k.)
j	~ 120 eV	---	AL 2s photoelectron, $E_b = 121$ eV
k	$\sim 73-74$ eV	---	AL 2p " , $E_b = 77$ eV
l	74.0 eV	---	AL 2p, AL metal
m	72.8 eV	---	AL 2p, AL in some AL-N compound, given to be ALN.

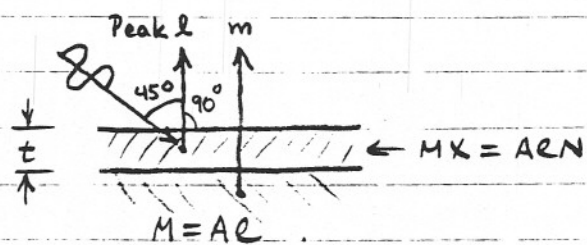
10



COMMON MISTAKE
Cannot be spin-orbit, as this is only ~ 0.4 eV from X-ray Data Booklet.

(b) At such a saturation coverage, we can estimate that the over layer is of some thickness $t \approx$ few atomic layers, and so use a geometry as:

5



Relevant equation is Eqn (119) of Fadley, "Basic Concepts..." or (6) of Fadley, "Angle-Resolved XPS":

Fig. 1

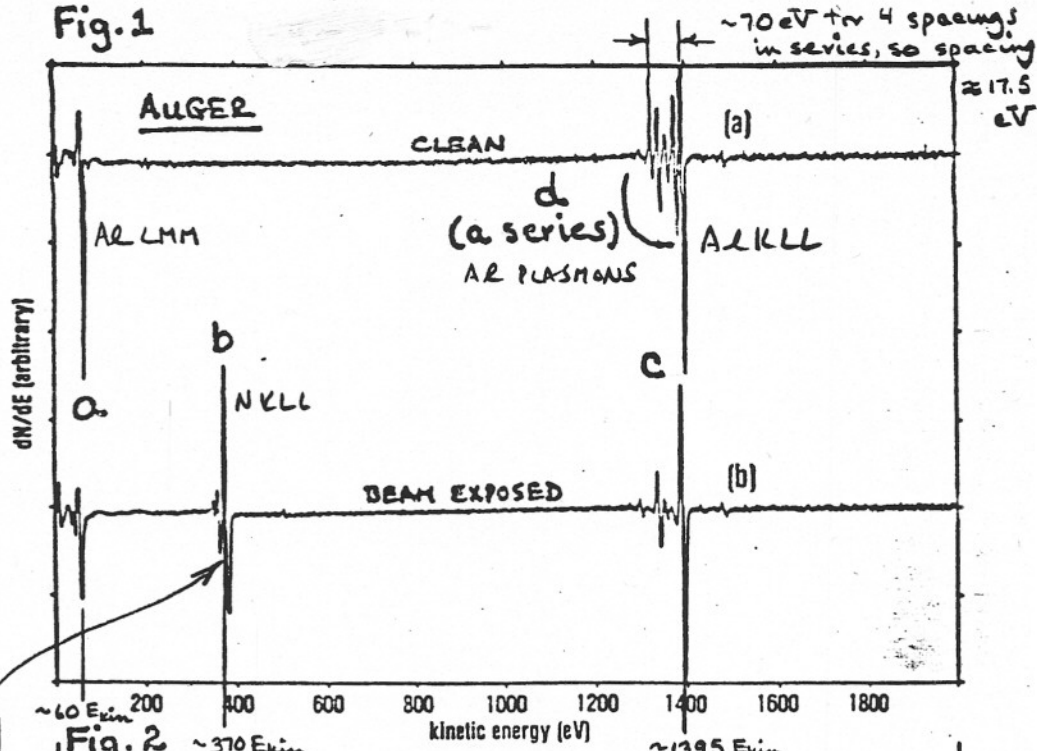


Fig. 2

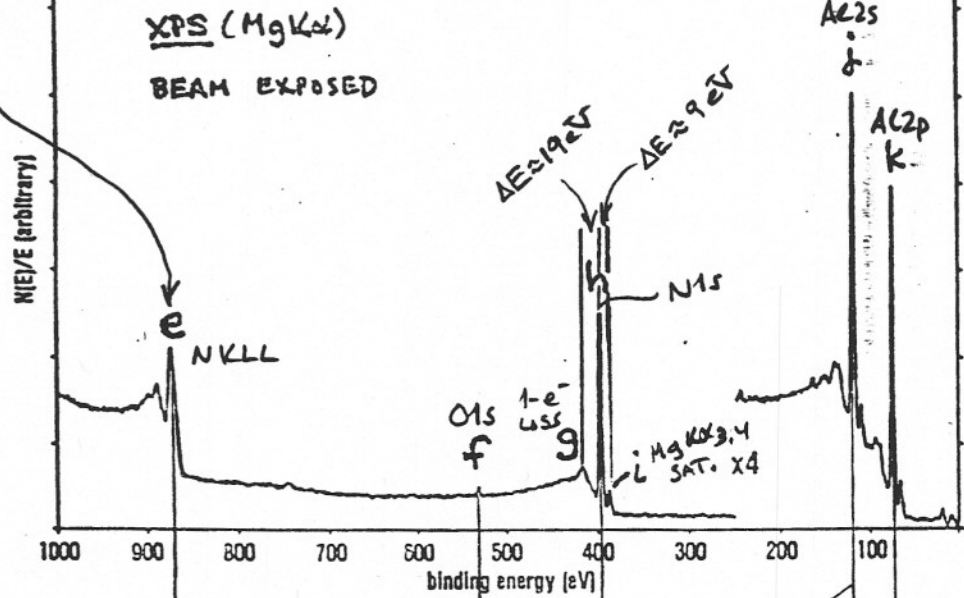
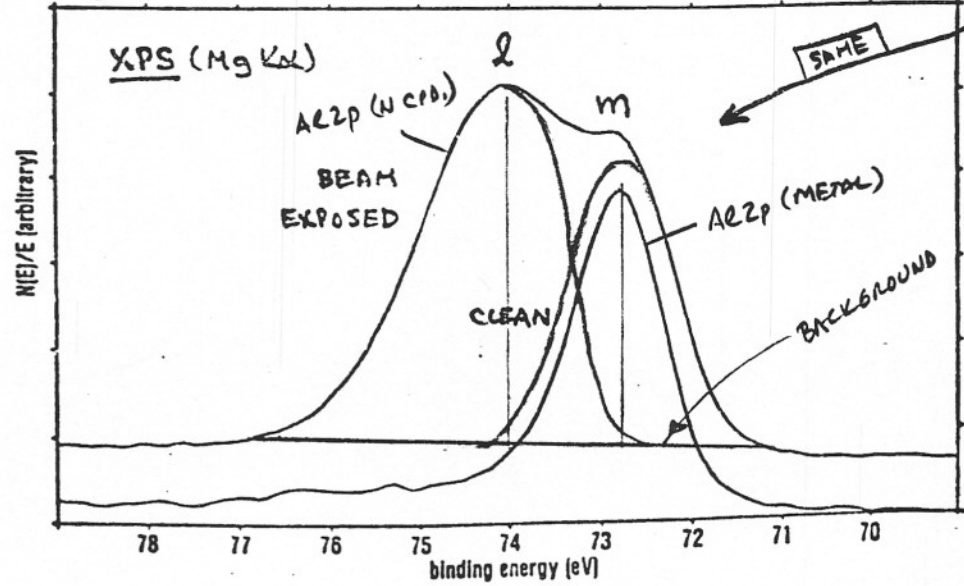


Fig. 3



ARZP(AEN)

$$\frac{N_e(\theta)}{N_m(\theta)} = \frac{\Omega_0(E_e) A_0(E_e) D_0(E_e) p' \left(\frac{dG_e}{dR} \right) \Delta_e'(E_e)}{\Omega_0(E_m) A_0(E_m) D_0(E_m) p \left(\frac{dG_m}{dR} \right) \Delta_e(E_m)}$$

ARZP(metal)

$$\times \left[1 - e^{(-t/\Delta_e' \sin \theta)} \right] e^{t/\Delta_e' \sin \theta}$$

Simplify now by noting that Ω_0, A_0, D_0 factors cancel in ratio, because $E_e \approx E_m$. Also, $p' = \frac{1}{2} p$, as given in problem. Further, $dG_e/dR = dG_m/dR$ because same subshell. Also, $\Delta_e' = \Delta_e$ as given in problem. Finally, $\sin \theta = 1.0$ for $\theta = 90^\circ$. So,

$$\frac{N_e(\theta)}{N_m(\theta)} = \frac{1}{2} \left[1 - e^{(-t/\Delta_e)} \right] e^{t/\Delta_e}$$

(or any other estimation method)

For $E_{kin} \approx 1257 - 74 \approx 1183$ eV, the "Universal Curve" gives $\Delta_e \approx \frac{20-27}{\lambda} \text{ \AA}$. The empirical ratio $N_e/N_m \approx 1.3$ as derived from a hard decomposition of spectrum into two components (see fig. following). So,

$$1.30 = \frac{1}{2} \left[e^{t/\Delta_e} - 1 \right]$$

$$1.80 = \frac{1}{2} e^{t/\Delta_e}$$

$$\ln(3.60) = t/\Delta_e$$

$$t = 1.38 \Delta_e \approx \frac{25 \text{ \AA}}{-32}$$

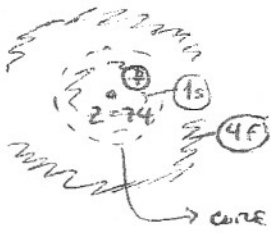
[4.6]

(a) $\rightarrow \bar{W}(Z=74) \rightarrow W^+(1s \text{ hole}) \rightarrow Re(Z=75)$ in influence on outer e^-s

5 $E_b(4f_{7/2}) = 31 \text{ eV} \xrightarrow{Z=74} 40 \text{ eV} \xrightarrow{Z=75} \Delta E_b(4f_{7/2}) \approx 9 \text{ eV}$

(b) $\Delta E_b(4f_{7/2}) = \text{Coulomb integral only} = \int \psi_{4f_{7/2}}^*(1) \psi_{1s}^*(2) \frac{e^2}{r_{12}} \psi_{4f_{7/2}}(1) \psi_{1s}(2) d^3r_1 d^3r_2$

5 Exchange ≈ 0 because overlap between 1s and 4f $7/2 \approx 0$!



\rightarrow core like $Z+1 = 75$