X-Ray Interaction with Matter: Absorption, Scattering and Diffraction

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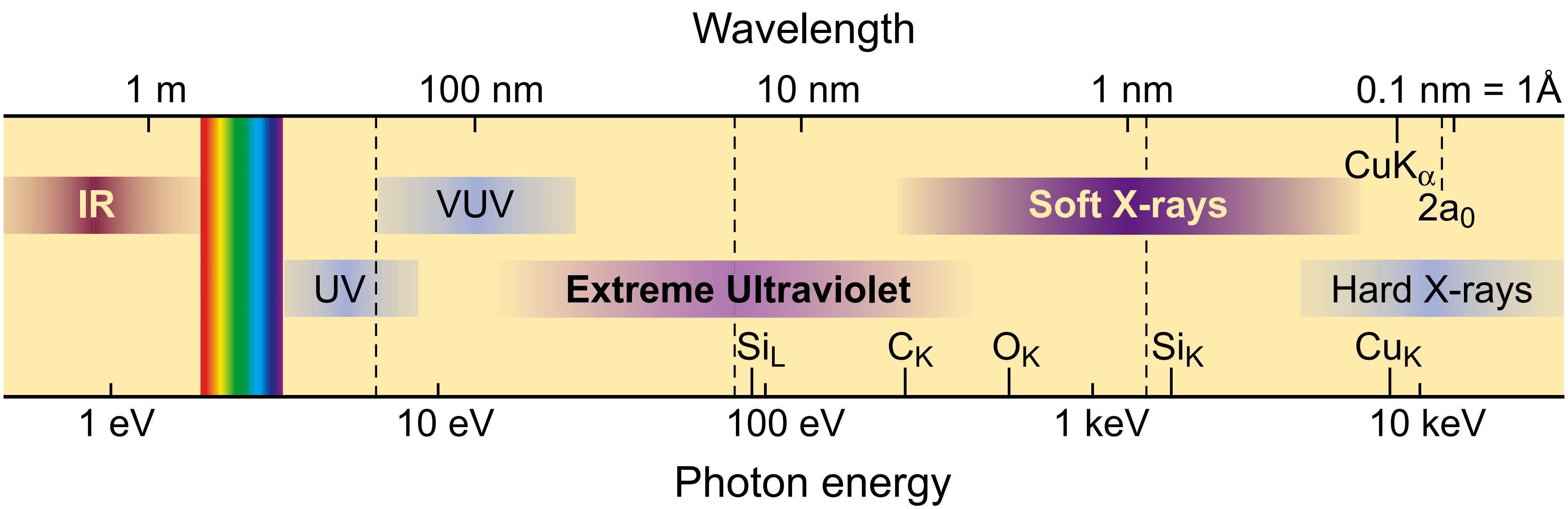
(http://www.coe.berkeley.edu/AST/sxr2009)

The Short Wavelength Region of the Electromagnetic Spectrum



- **See smaller features**
- **Write smaller patterns**
- **Elemental and chemical sensitivity**

Professor David Attwood
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Photon Energy, Wavelength, Power

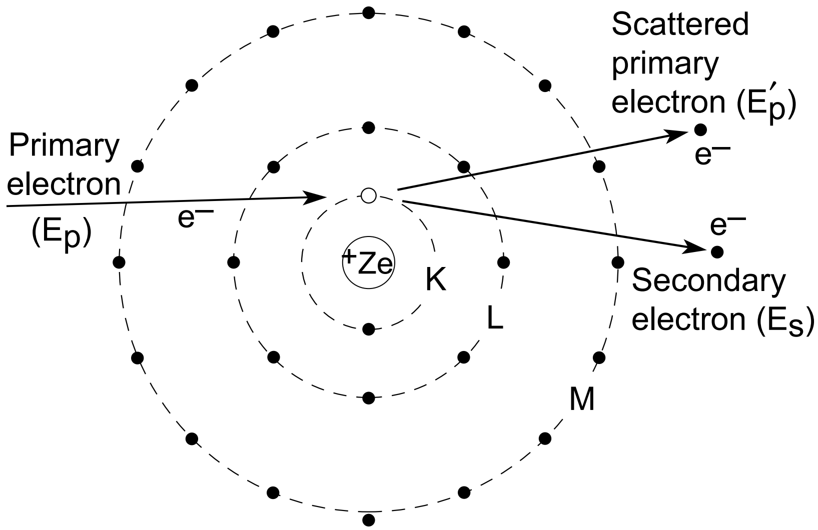
$$\hbar\omega \cdot \lambda = hc = 1239.842 \text{ eV nm} \quad (1.1)$$

$$1 \text{ joule} \Rightarrow 5.034 \times 10^{15} \lambda[\text{nm}] \text{ photons} \quad (1.2a)$$

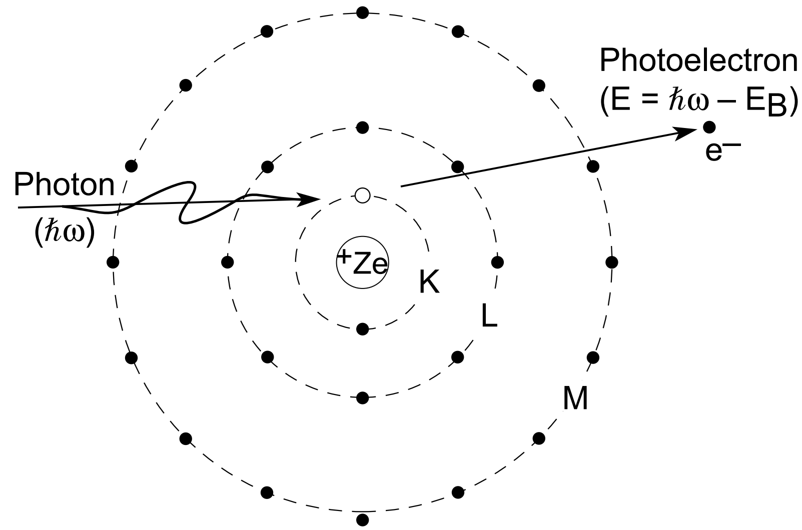
$$1 \text{ watt} \Rightarrow 5.034 \times 10^{15} \lambda[\text{nm}] \frac{\text{photons}}{\text{s}} \quad (1.2b)$$

Basic Ionization and Emission Processes in Isolated Atoms

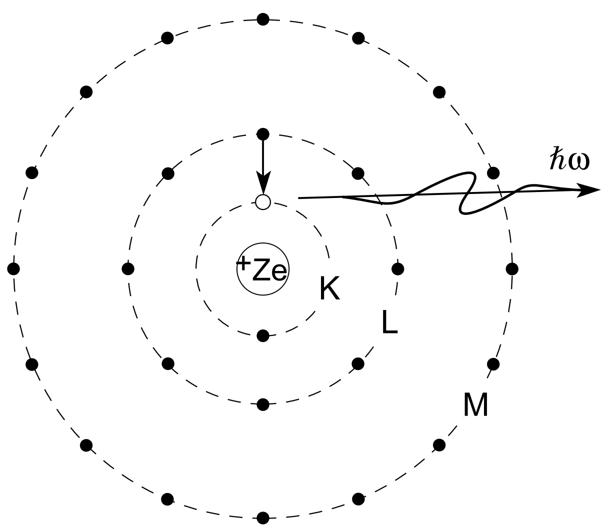
(a) Electron collision induced ionization



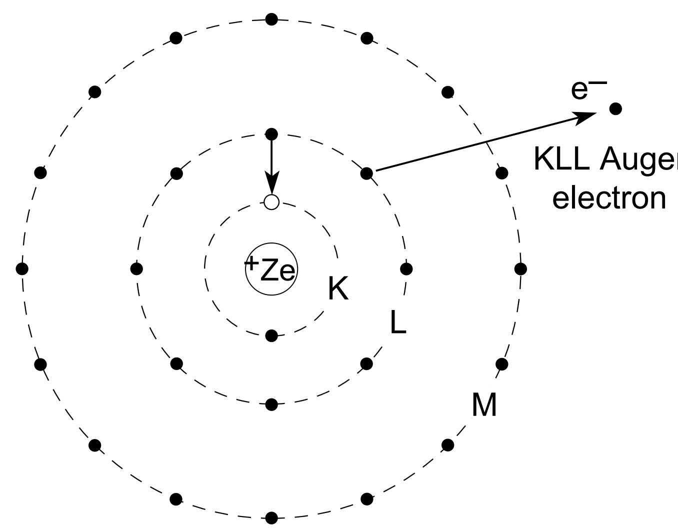
(b) Photoionization



(c) Fluorescent emission of characteristic radiation



(d) Non-radiative Auger process



Electron Binding Energies, in Electron Volts (eV), for the elements in their Natural Forms

Berkeley Lab

Element	K 1s	L_1 2s	L_2 $2p_{1/2}$	L_3 $2p_{3/2}$	M_1 3s	M_2 $3p_{1/2}$	M_3 $3p_{3/2}$	M_4 $3d_{3/2}$	M_5 $3d_{5/2}$	N_1 4s	N_2 $4p_{1/2}$	N_3 $4p_{3/2}$
1 H	13.6											
2 He	24.6[b]											
3 Li	54.7[b]											
4 Be	111.5[b]											
5 B	188[b]											
6 C	284.2[b]											
7 N	409.9[b]	37.3[b]										
8 O	543.1[b]	41.6[b]										
9 F	696.7[b]											
10 Ne	870.2[b]	48.5[b]	21.7[b]	21.6[b]								
11 Na	1070.8[c]	63.5[c]	30.4[c]	30.5[b]								
12 Mg	1303.0[c]	88.6[b]	49.6[c]	49.2[c]								
13 Al	1559.6	117.8[b]	72.9[b]	72.5[b]								
14 Si	1838.9	149.7[b]	99.8[b]	99.2[b]								
15 P	2145.5	189[b]	136[b]	135[b]								
16 S	2472	230.9[b]	163.6[b]	162.5[b]								
17 Cl	2822.4	270.2[b]	202[b]	200[b]								
18 Ar	3205.9[b]	326.3[b]	250.6[b]	248.4[b]	29.3[b]	15.9[b]	15.7[b]					
19 K	3608.4[b]	378.6[b]	297.3[b]	294.6[b]	34.8[b]	18.3[b]	18.3[b]					
20 Ca	4038.5[b]	438.4[c]	349.7[c]	346.2[c]	44.3[c]	25.4[c]	25.4[c]					
21 Sc	4492.8	498.0[b]	403.6[b]	398.7[b]	51.1[b]	28.3[b]	28.3[b]					
22 Ti	4966.4	560.9[c]	461.2[c]	453.8[c]	58.7[c]	32.6[c]	32.6[c]					
23 V	5465.1	626.7[c]	519.8[c]	512.1[c]	66.3[c]	37.2[c]	37.2[c]					
24 Cr	5989.2	695.7[c]	583.8[c]	574.1[c]	74.1[c]	42.2[c]	42.2[c]					
25 Mn	6539.0	769.1[c]	649.9[c]	638.7[c]	82.3[c]	47.2[c]	47.2[c]					
26 Fe	7112.0	844.6[c]	719.9[c]	706.8[c]	91.3[c]	52.7[c]	52.7[c]					
27 Co	7708.9	925.1[c]	793.3[c]	778.1[c]	101.0[c]	58.9[c]	58.9[c]					
28 Ni	8332.8	1008.6[c]	870.0[c]	852.7[c]	110.8[c]	68.0[c]	66.2[c]					
29 Cu	8978.9	1096.7[c]	952.3[c]	932.5[c]	122.5[c]	77.3[c]	75.1[c]					
30 Zn	9658.6	1196.2[b]	1044.9[b]	1021.8[b]	139.8[b]	91.4[b]	88.6[b]	10.2[b]	10.1[b]			
31 Ga	10367.1	1299.0[b]	1143.2[c]	1116.4[c]	159.5[c]	103.5[c]	103.5[c]	18.7[c]	18.7[c]			
32 Ge	11103.1	1414.6[b]	1248.1[b]	1217.0[b]	180.1[b]	124.9[b]	120.8[b]	29.0[b]	29.0[b]			
33 As	11866.7	1527.0[b]	1359.1[b]	1323.6[b]	204.7[b]	146.2[b]	141.2[b]	41.7[b]	41.7[b]			
34 Se	12657.8	1652.0[b]	1474.3[b]	1433.9[b]	229.6[b]	166.5[b]	160.7[b]	55.5[b]	54.6[b]			
35 Br	13473.7	1782.0[b]	1596.0[b]	1549.9[b]	257[b]	189[b]	182[b]	70[b]	69[b]			
36 Kr	14325.6	1921.0	1730.9[b]	1678.4[b]	292.8[b]	222.2[b]	214.4	95.0[b]	93.8[b]	27.5[b]	14.1[b]	14.1[b]
37 Rb	15199.7	2065.1	1863.9	1804.4	326.7[b]	248.7[b]	239.1[b]	113.0[b]	112[b]	30.5[b]	16.3[b]	15.3[b]
38 Sr	16104.6	2216.3	2006.8	1939.6	358.7[c]	280.3[c]	270.0[c]	136.0[c]	134.2[c]	38.9[c]	20.3[c]	20.3[c]
39 Y	17038.4	2372.5	2155.5	2080.0	392.0[b]	310.6[b]	298.8[b]	157.7[c]	155.8[c]	43.8[b]	24.4[b]	23.1[b]
40 Zr	17997.6	2531.6	2306.7	2222.3	430.3[c]	343.5[c]	329.8[c]	181.1[c]	178.8[c]	50.6[c]	28.5[c]	27.7[c]
41 Nb	18985.6	2697.7	2464.7	2370.5	466.6[c]	376.1[c]	360.6[c]	205.0[c]	202.3[c]	56.4[c]	32.6[c]	30.8[c]
42 Mo	19999.5	2865.5	2625.1	2520.2	506.3[c]	411.6[c]	394.0[c]	231.1[c]	227.9[c]	63.2[c]	37.6[c]	35.5[c]
43 Tc	21044.0	3042.5	2793.2	2676.9	544[b]	445[b]	425[b]	257[b]	253[b]	68[b]	39[c]	39[b]
44 Ru	22117.2	3224.0	2966.9	2837.9	586.2[c]	483.5[c]	461.4[c]	284.2[c]	280.0[c]	75.0[c]	46.5[c]	43.2[c]
45 Rh	23219.9	3411.9	3146.1	3003.8	628.1[c]	521.3[c]	496.5[c]	311.9[c]	307.2[c]	81.4[b]	50.5[c]	47.3[c]
46 Pd	24350.3	3604.3	3330.3	3173.3	671.6[c]	559.9[c]	532.3[c]	340.5[c]	335.2[c]	87.6[b]	55.7[c]	50.9[c]
47 Ag	25514.0	3805.8	3523.7	3351.1	719.0[c]	603.8[c]	573.0[c]	374.0[c]	368.0[c]	97.0[c]	63.7[c]	58.3[c]

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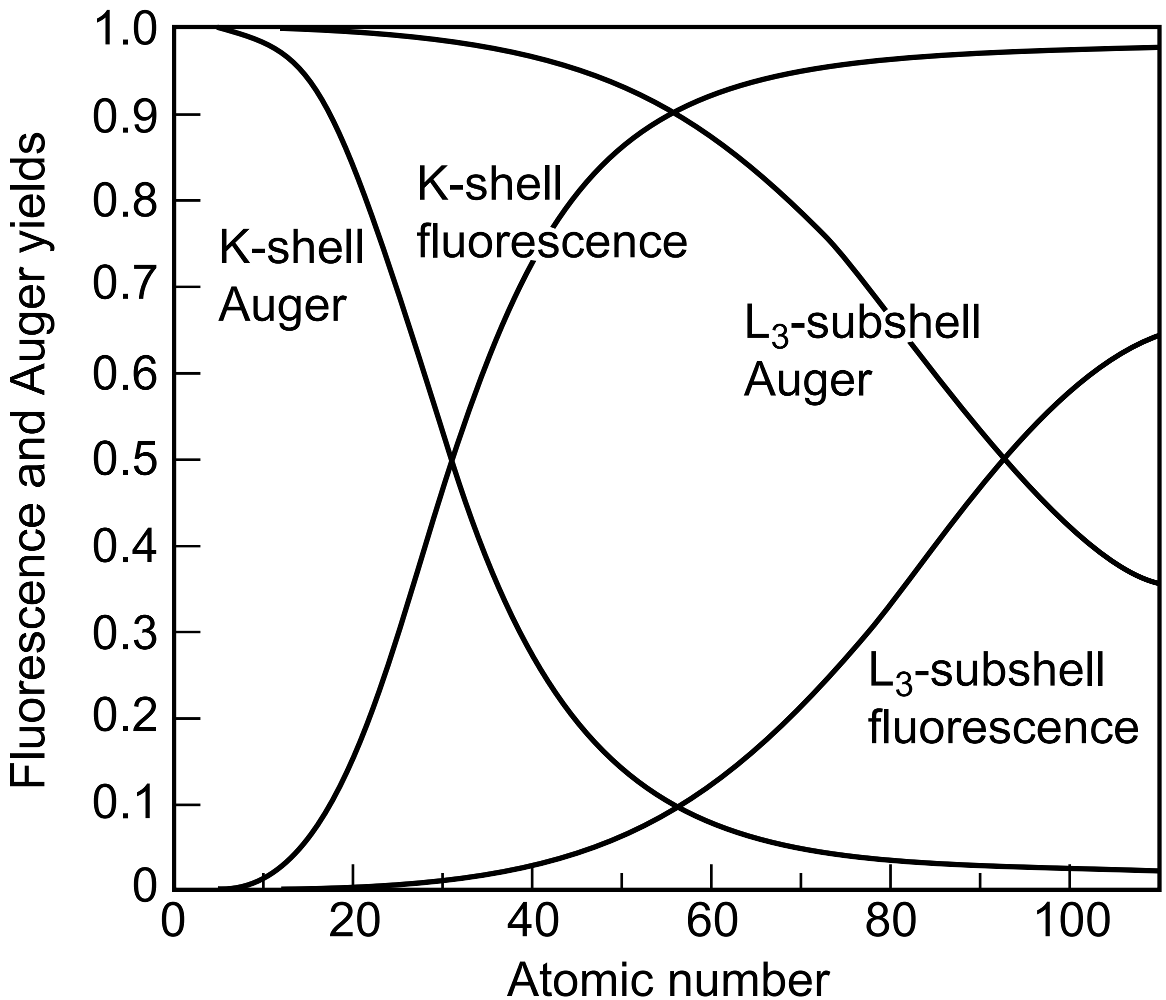
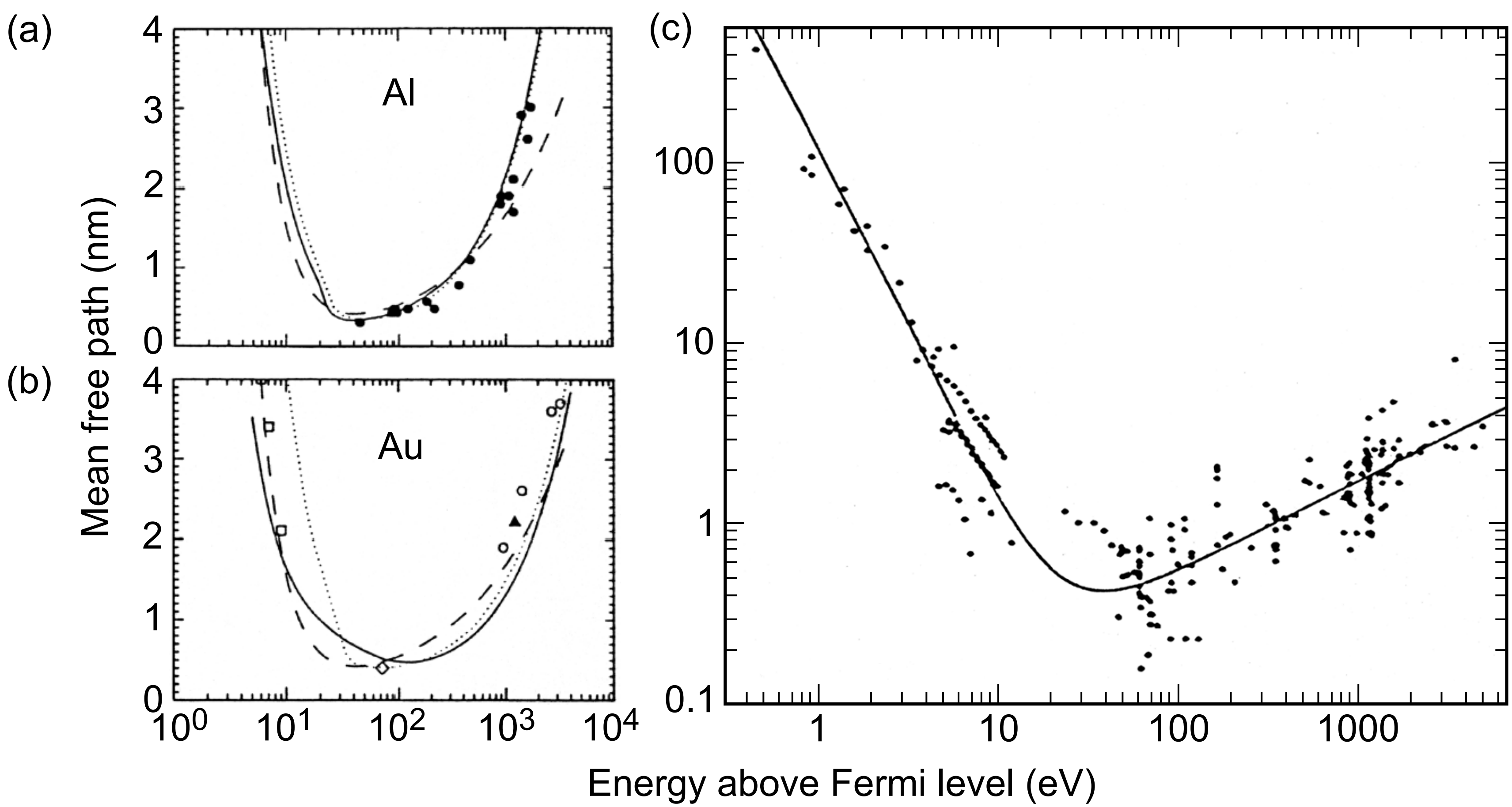
Fluorescence and Auger Emission Yields



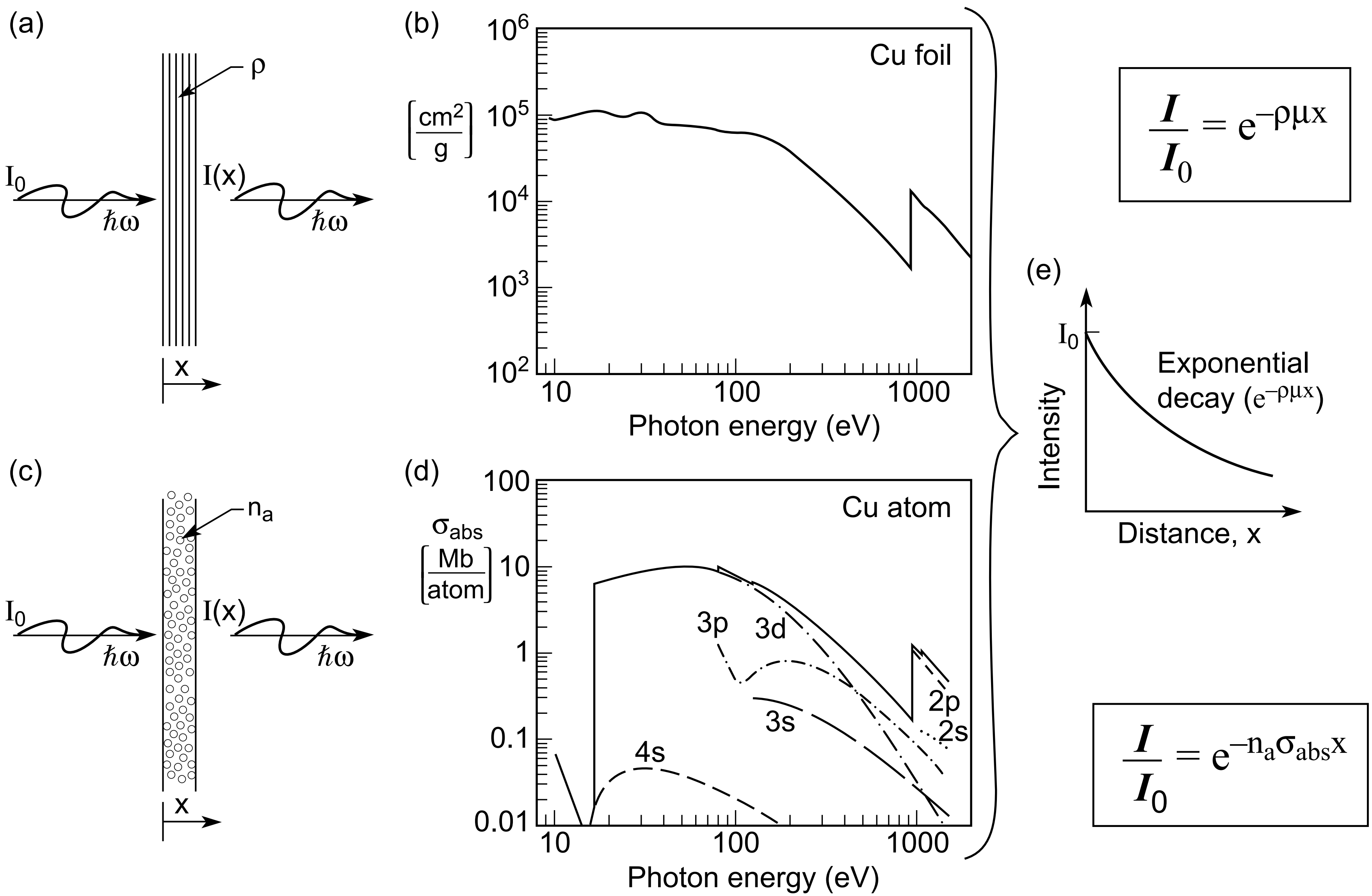
(Courtesy of M. Krause, Oak Ridge)

Electron Mean Free Paths As a Function of Energy



Courtesy of: Penn (a & b), Seah and Dench (c)

Photoabsorption by Thin Foils and Isolated Atoms



$$\frac{I}{I_0} = e^{-\rho\mu x}$$

$$\frac{I}{I_0} = e^{-n_a \sigma_{abs} x}$$

Atomic Energy Levels and Allowed Transitions in the Bohr Atom

Equate Coulomb Force $Ze^2/4\pi\epsilon_0 r^2$ to the centripetal force mv^2/r:

$$E_n = \frac{mZ^2e^4}{32\pi^2\epsilon_0^2\hbar^2}\,\frac{1}{n^2} \tag{1.4}$$

$$r_n = \frac{4\pi\epsilon_0\hbar^2}{me^2Z}\cdot n^2 \tag{1.5}$$

$$\hbar\omega = E_i - E_f = \underbrace{\frac{me^4}{32\pi^2\epsilon_0\hbar^2}}_{13.6\text{ eV}}\left[\frac{1}{n_\text{f}^2} - \frac{1}{n_\text{i}^2}\right]Z^2 \tag{1.6}$$

$$r_n = \frac{a_0 n^2}{Z} \quad ; \quad a_0 = 0.529\ \text{Å} \tag{1.9}$$

Quantum Mechanics Based on a Probabilistic Wave Function, $\Psi(\mathbf{r}, t)$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{r}, t) + V(\mathbf{r}, t)\Psi(\mathbf{r}, t) = i\hbar\frac{\partial\Psi(\mathbf{r}, t)}{\partial t} \qquad (1.10)$$

$$P(\mathbf{r}, t)d\mathbf{r} = \Psi^*(\mathbf{r}, t)\ \Psi(\mathbf{r}, t)d\mathbf{r} \qquad (1.13)$$

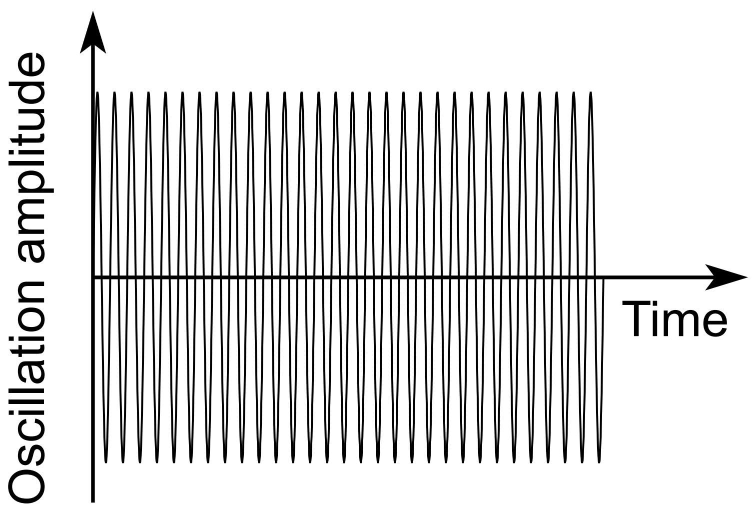
$$\bar{\mathbf{r}} = \iiint \mathbf{r}P(\mathbf{r}, t)d\mathbf{r} = \iiint \Psi^*(\mathbf{r}, t)\mathbf{r}\Psi(\mathbf{r}, t)d\mathbf{r} \qquad (1.15)$$

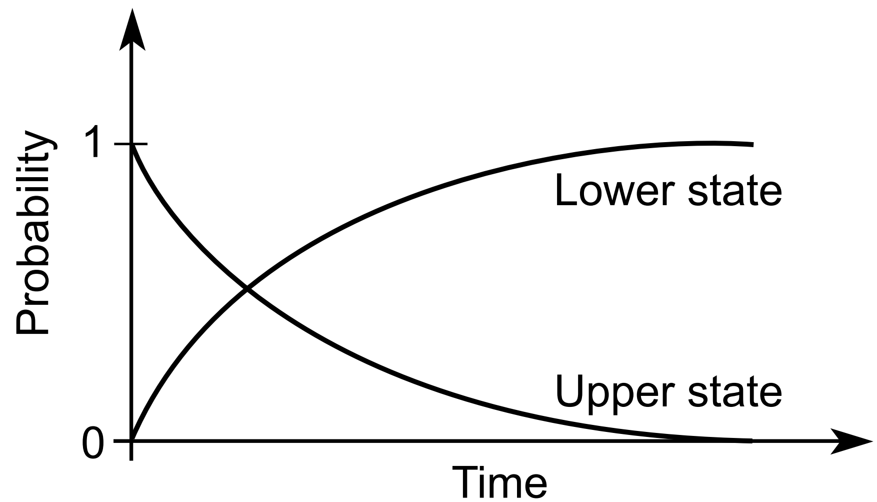
quantum numbers: n, ℓ, m_ℓ, m_s

selection rules for allowed transitions: $\Delta\ell = \pm 1$

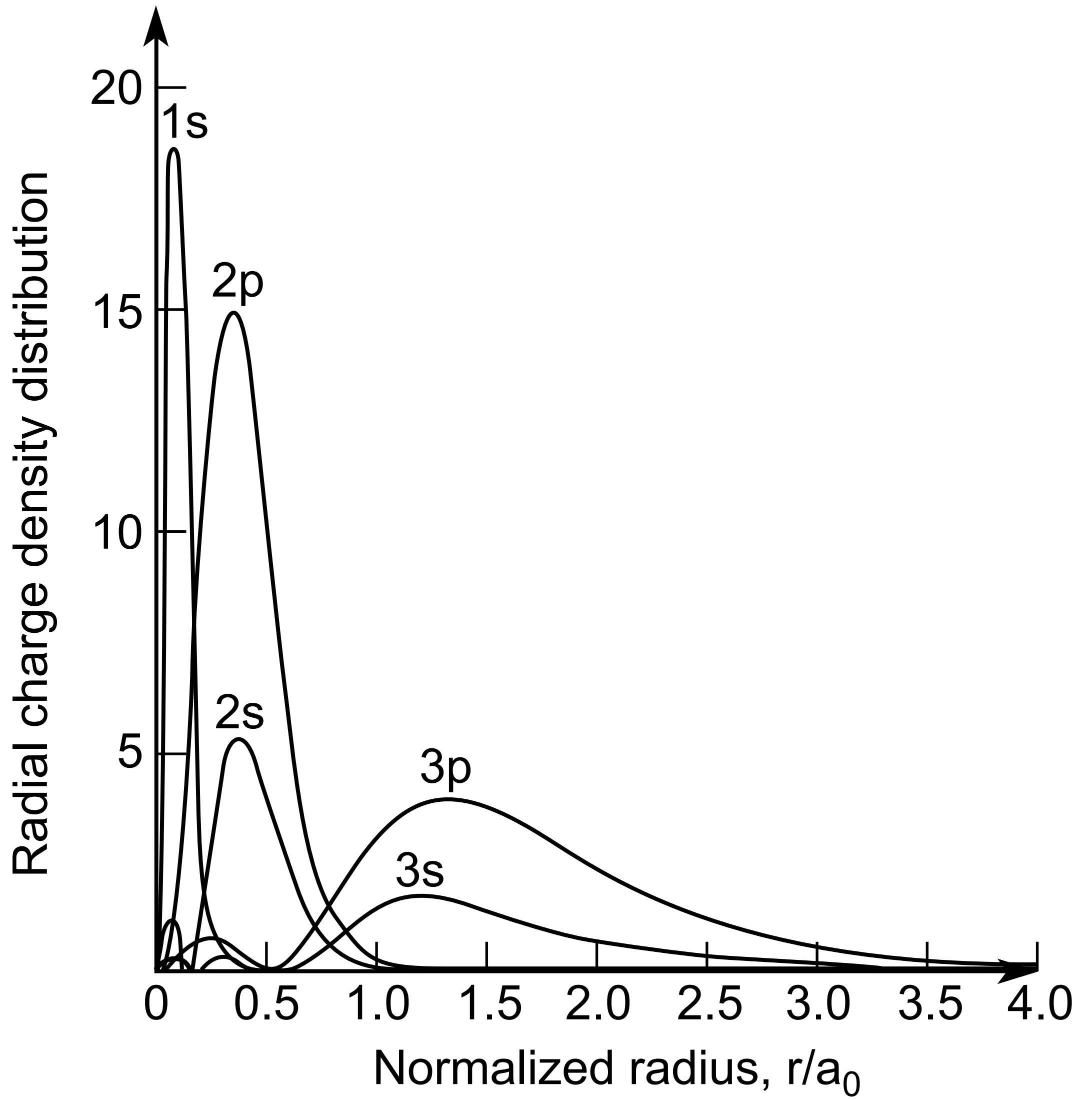
$\Delta j = 0, \pm 1$

Radiative Decay Involves An Atom Oscillating Between Two Stationary States at the Frequency $\omega_{if} = (E_i - E_f) / \hbar$



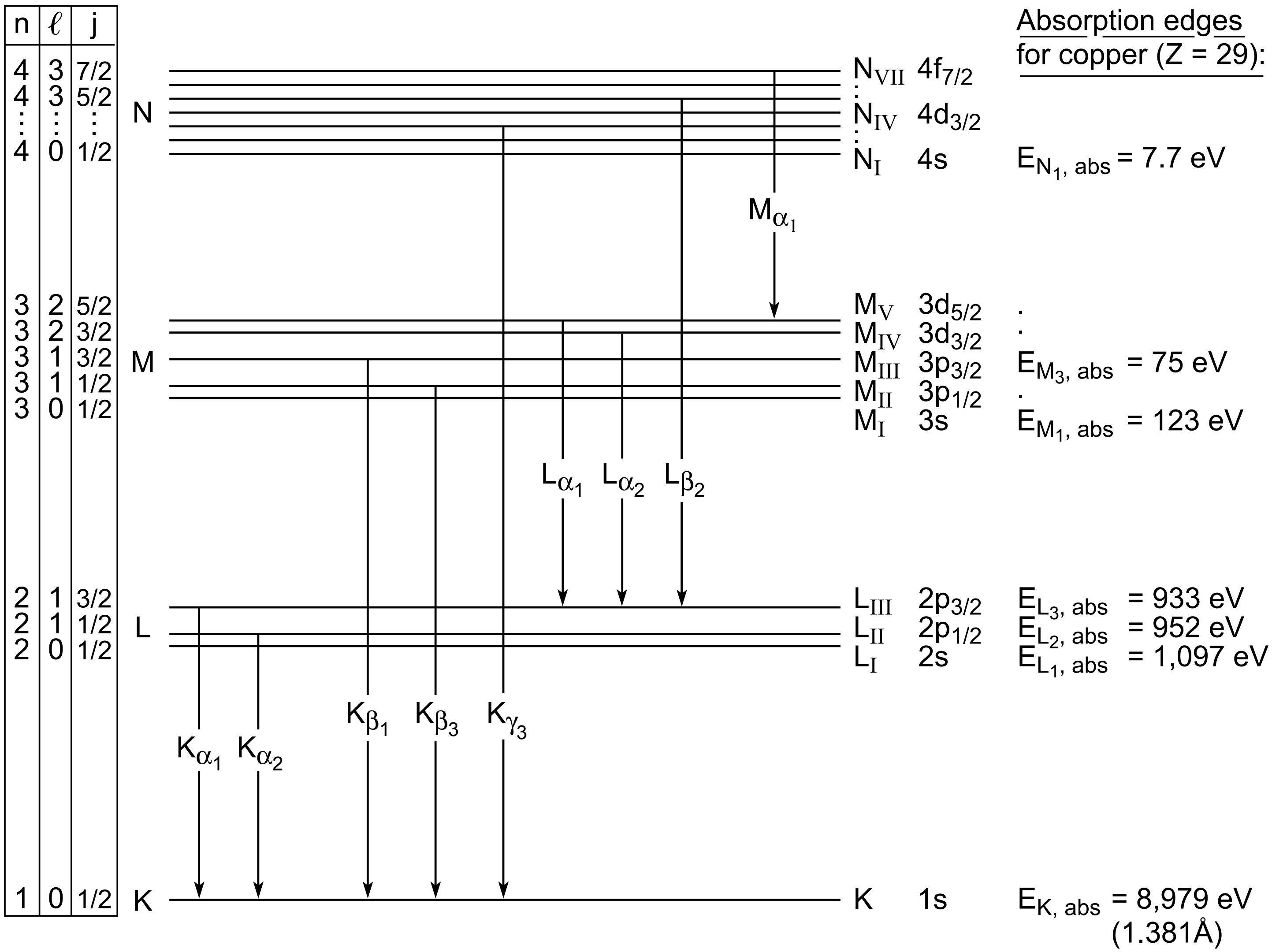


Probabilistic Radial Charge Distribution (e/Å) in the Argon Atom



Courtesy of Eisberg and Resnick, *Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles.*

Energy Levels, Quantum Numbers, and Allowed Transitions for the Copper Atom

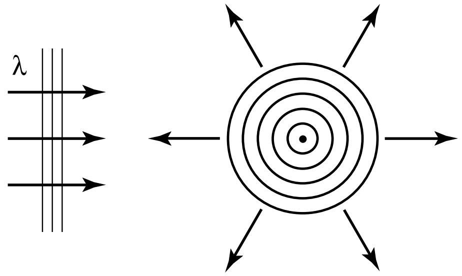


Cu K_{α_1} = 8,048 eV (1.541Å)
Cu K_{α_2} = 8,028 eV (1.544Å)
Cu K_{β_1} = 8,905 eV

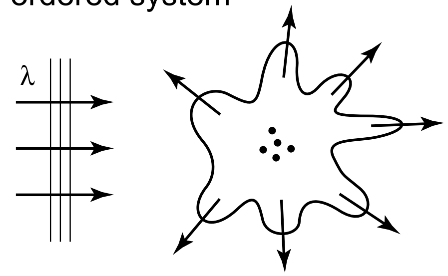
Cu L_{α_1} = 930 eV
Cu L_{α_2} = 930 eV
Cu L_{β_1} = 950 eV

Scattering, Diffraction, and Refraction

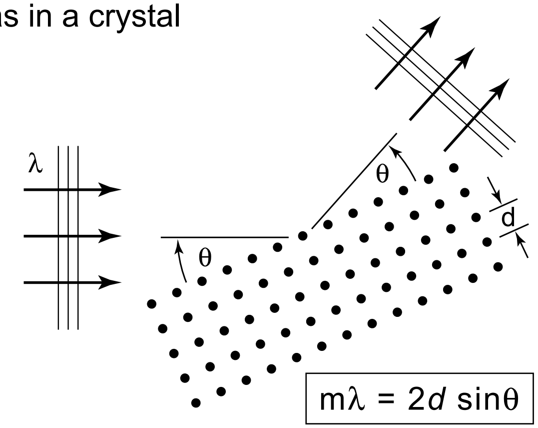
(a) Isotropic scattering from a point object



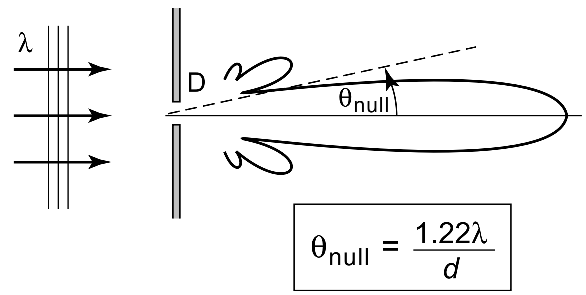
(b) Non-isotropic scattering from a partially ordered system



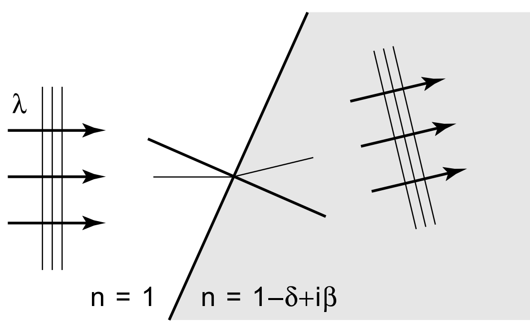
(c) Diffraction by an ordered array of atoms, as in a crystal



(d) Diffraction from a well-defined geometric structure, such as a pinhole



(e) Refraction at an interface



(f) Total external reflection