Interaction of X-Rays with Matter: Absorption, Scattering, Emission

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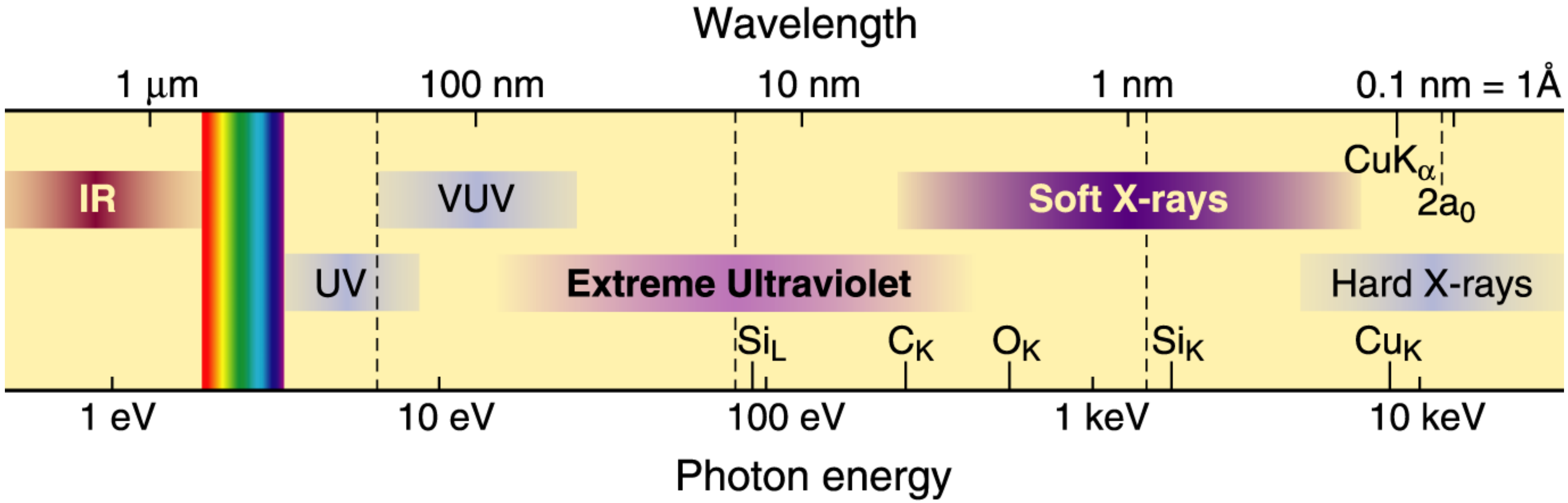
The short wavelength region of the electromagnetic spectrum



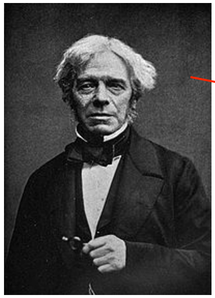
- **See smaller features**
- **Write smaller patterns**
- **Elemental and chemical sensitivity**

$$\boxed{\hbar\omega \cdot \lambda = hc = 1239.842 \text{ eV nm}}$$

$$\boxed{n = 1 - \delta + i\beta \qquad \delta, \beta \ll 1}$$

The equations of light

Michael Faraday



André-Marie Ampère

Charles-Augustin de Coulomb

Carl Friedrich Gauss

Maxwell's Equations

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \cdot \mathbf{B} = 0$$

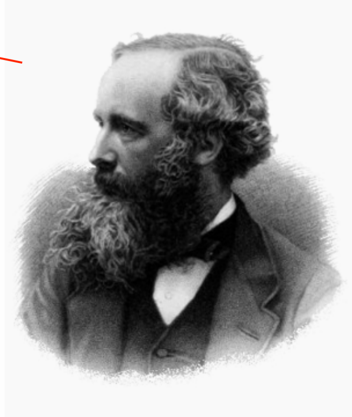
$$\nabla \cdot \mathbf{D} = \rho$$

[written for vacuum, where $\underset{\sim}{\mathbf{D}} = \epsilon_0 \underset{\sim}{\mathbf{E}}$ and $\underset{\sim}{\mathbf{B}} = \mu_0 \underset{\sim}{\mathbf{H}}$]

When combined these lead to the Wave Equation

$$\left(\frac{\partial^2}{\partial t^2} - c^2 \nabla^2\right) \mathbf{E}(\mathbf{r}, t) = -\frac{1}{\epsilon_0} \frac{\partial \mathbf{J}(\mathbf{r}, t)}{\partial t}$$

James Clerk Maxwell

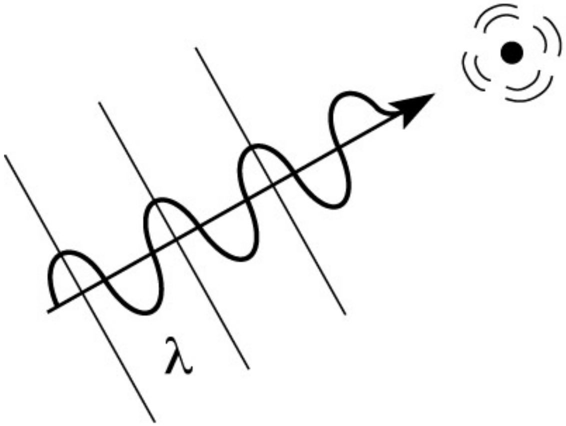


Heinrich Hertz

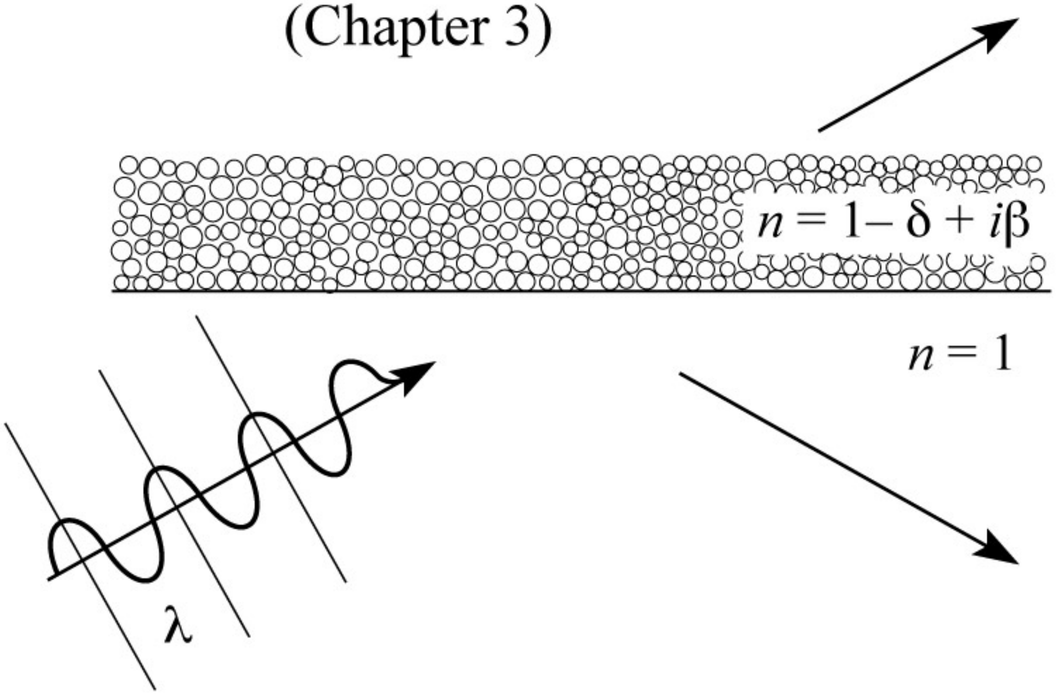
Courtesy of Andrew Aquila (AS&T, UC Berkeley)

Scattering, diffraction and refraction

Single scatterer,
electron or atom,
in vacuum.
(Chapter 2)



Many atoms, each
with many electrons,
constituting a "material".
(Chapter 3)



- How are scattering, refraction, and reflection related?
- How do these differ for amorphous and ordered (crystalline) materials?
- What is the role of forward scattering?

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Maxwell's Equations

↓

Wave Equation

↙ (in vacuum) (Chapter 2)

Radiation by a single electron ("dipole radiation")

Scattering cross-sections

Scattering by a free electron ("Thomson scattering")

Scattering by a single bound electron ("Rayleigh scattering")

Scattering by a multi-electron atom

Atomic "scattering factors", f_0' and f_0''

↘ (in a material) (Chapter 3)

Refractive index with many atoms present

Role of forward scattering

Contributions to refractive index by bound electrons

Refractive index for soft x-rays and EUV

$$n = 1 - \underset{\underset{f_0'}{\downarrow}}{\delta} + i\underset{\underset{f_0''}{\downarrow}}{\beta} \quad (\delta, \beta << 1)$$

Determining f_0' and f_0''; measurements and Kramers-Kronig

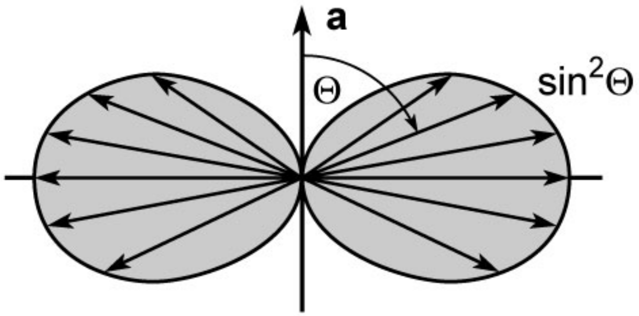
Total external reflection

Reflectivity vs. angle

Brewster's angle

Chapter 2

RADIATION AND SCATTERING AT EUV AND SOFT X-RAY WAVELENGTHS



$$\frac{dP}{d\Omega} = \frac{e^2|\mathbf{a}|^2 \sin^2\Theta}{16\pi^2\epsilon_0 c^3} \qquad (2.34)$$

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2} \qquad (2.44)$$

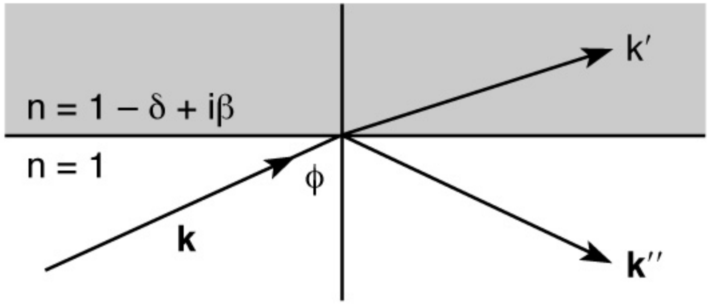
$$\sigma_e = \frac{8\pi}{3} r_e^2 \qquad (2.45)$$

$$\sigma = \frac{8\pi}{3} r_e^2 \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\gamma\omega)^2} \qquad (2.51)$$

$$f(\Delta\mathbf{k}, \omega) = \sum_{s=1}^{Z} \frac{\omega^2 e^{-i\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s}}{\omega^2 - \omega_s^2 + i\gamma\omega} \qquad (2.66)$$

$$f^0(\omega) = \sum_{s=1}^{Z} \frac{\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega} \qquad (2.72)$$

WAVE PROPAGATION AND REFRACTIVE INDEX AT EUV AND SOFT X-RAY WAVELENGTHS



$$n(\omega) = 1 - \frac{n_a r_e \lambda^2}{2\pi}\left(f_1^0 - i f_2^0\right) \qquad (3.9)$$

$$n(\omega) = 1 - \delta + i\beta \qquad (3.12)$$

$$l_{\text{abs}} = \frac{\lambda}{4\pi\beta} \qquad (3.22)$$

$$\sigma_{\text{abs.}} = 2 r_e \lambda f_2^0(\omega) \qquad (3.28)$$

$$\Delta\phi = \left(\frac{2\pi\delta}{\lambda}\right)\Delta r \qquad (3.29)$$

$$\theta_c = \sqrt{2\delta} \qquad (3.41)$$

$$R_{s,\perp} \simeq \frac{\delta^2 + \beta^2}{4} \qquad (3.50)$$

$$\phi_B \simeq \frac{\pi}{4} - \frac{\delta}{2} \qquad (3.60)$$

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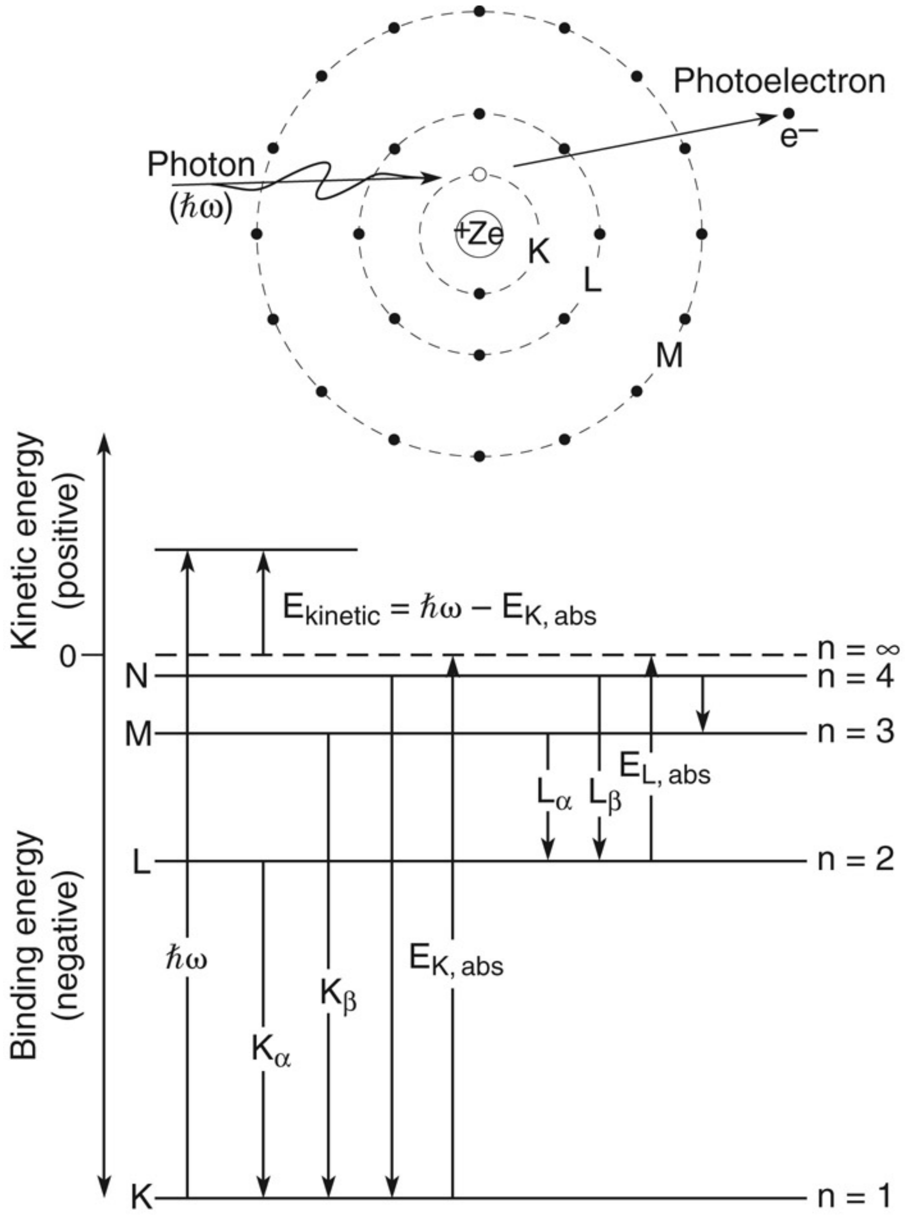
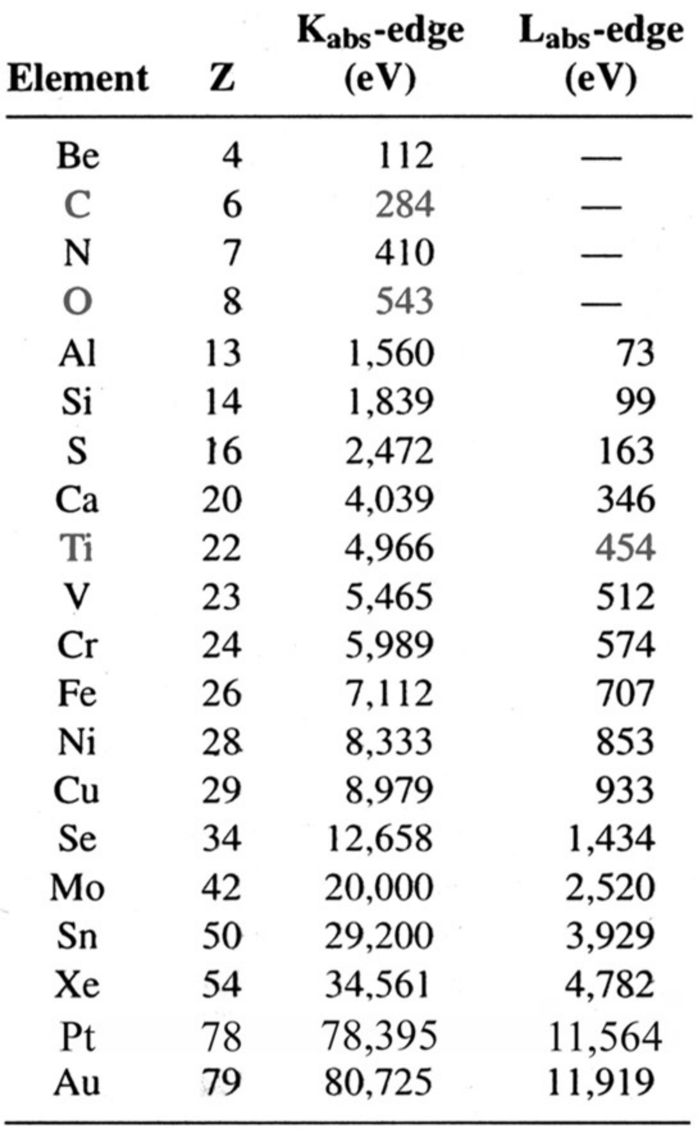
Characteristic absorption edges for almost all elements in this spectral region





Element	Z	K_{abs}-edge (eV)	L_{abs}-edge (eV)
Be	4	112	—
C	6	284	—
N	7	410	—
O	8	543	—
Al	13	1,560	73
Si	14	1,839	99
S	16	2,472	163
Ca	20	4,039	346
Ti	22	4,966	454
V	23	5,465	512
Cr	24	5,989	574
Fe	26	7,112	707
Ni	28	8,333	853
Cu	29	8,979	933
Se	34	12,658	1,434
Mo	42	20,000	2,520
Sn	50	29,200	3,929
Xe	54	34,561	4,782
Pt	78	78,395	11,564
Au	79	80,725	11,919

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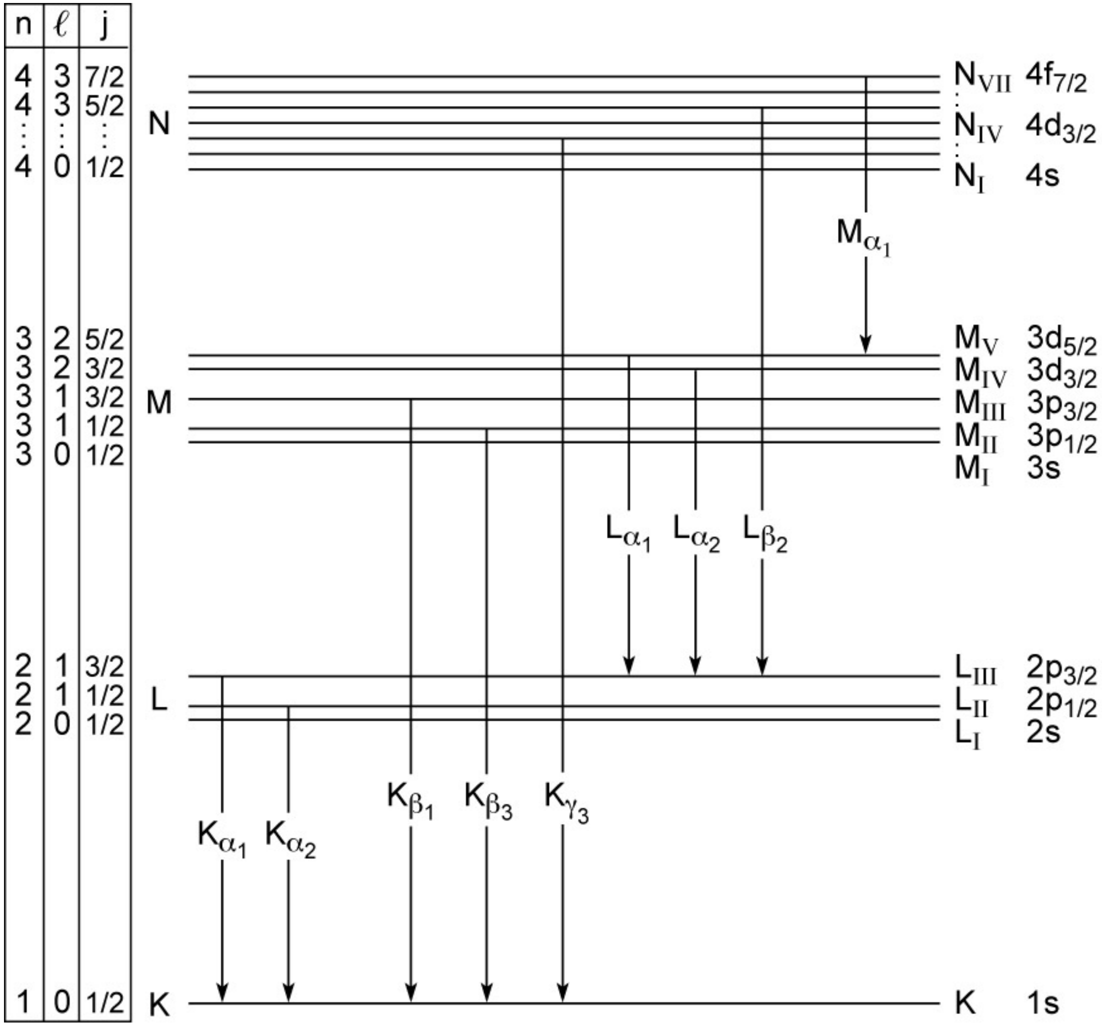
Energy levels, quantum numbers, and allowed transitions for the copper atom



Absorption edges for copper (Z = 29):

$E_{N_1,\ abs} = 7.7$ eV

$E_{M_3,\ abs} = 75$ eV

$E_{M_1,\ abs} = 123$ eV

$E_{L_3,\ abs} = 933$ eV
$E_{L_2,\ abs} = 952$ eV
$E_{L_1,\ abs} = 1{,}097$ eV

$E_{K,\ abs} = 8{,}979$ eV
(1.381Å)

Cu K_{α_1} = 8,048 eV (1.541Å)	Cu L_{α_1} = 930 eV
Cu K_{α_2} = 8,028 eV (1.544Å)	Cu L_{α_2} = 930 eV
Cu K_{β_1} = 8,905 eV	Cu L_{β_1} = 950 eV

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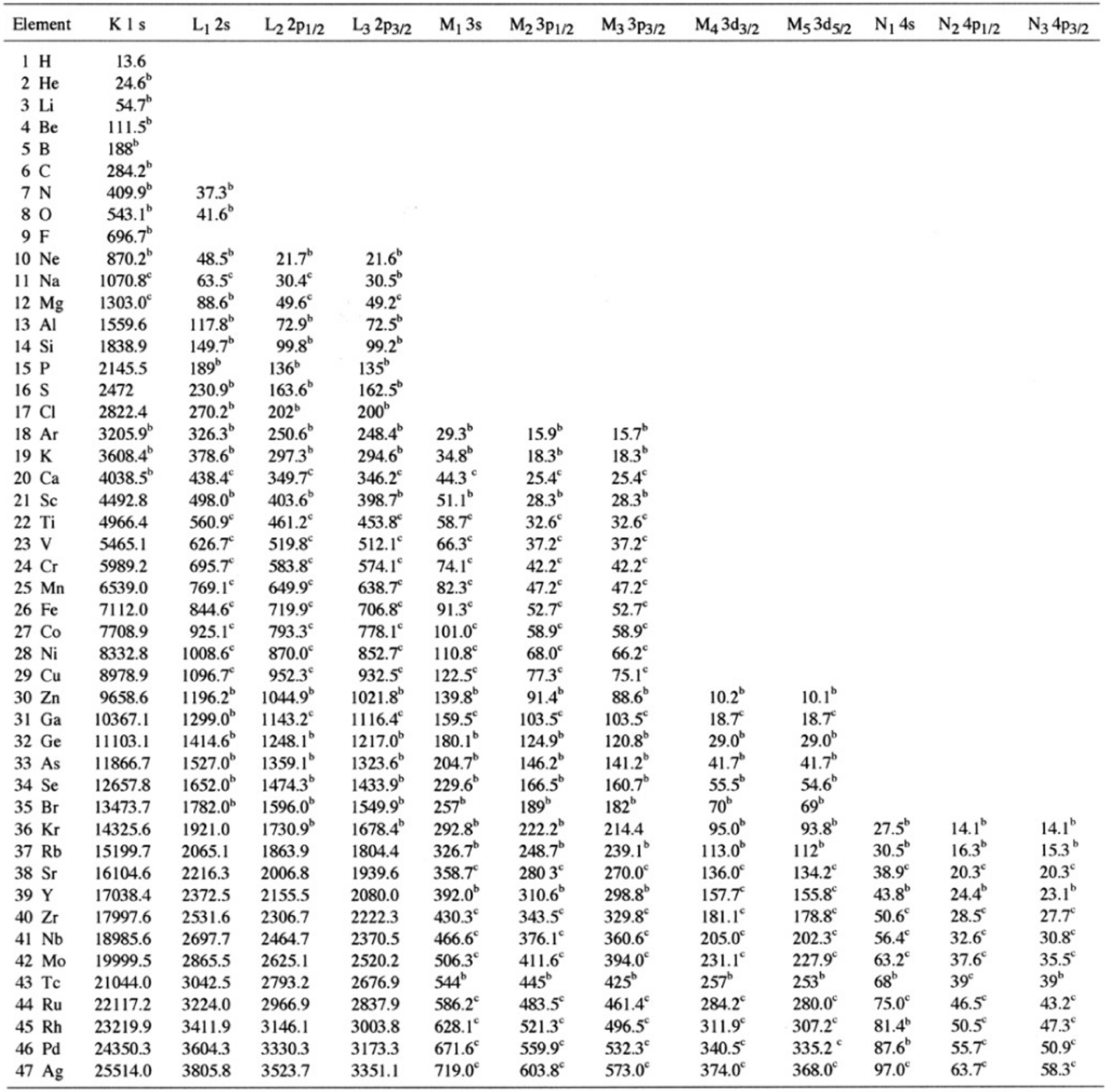
Electron binding energies, in electron volts (eV), for the elements in their natural forms



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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Photon energies, in electron volts, of principal K and L emission lines

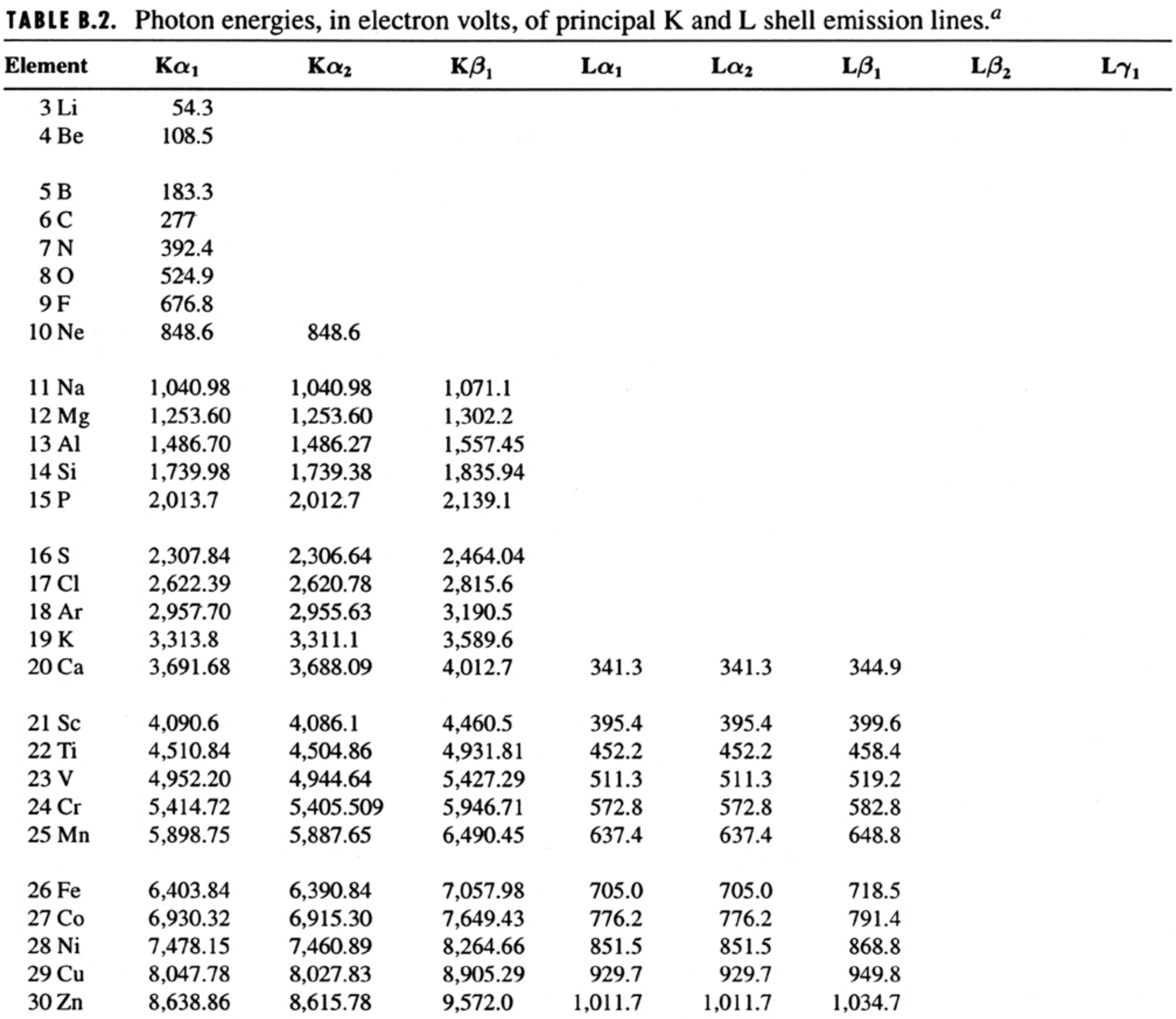
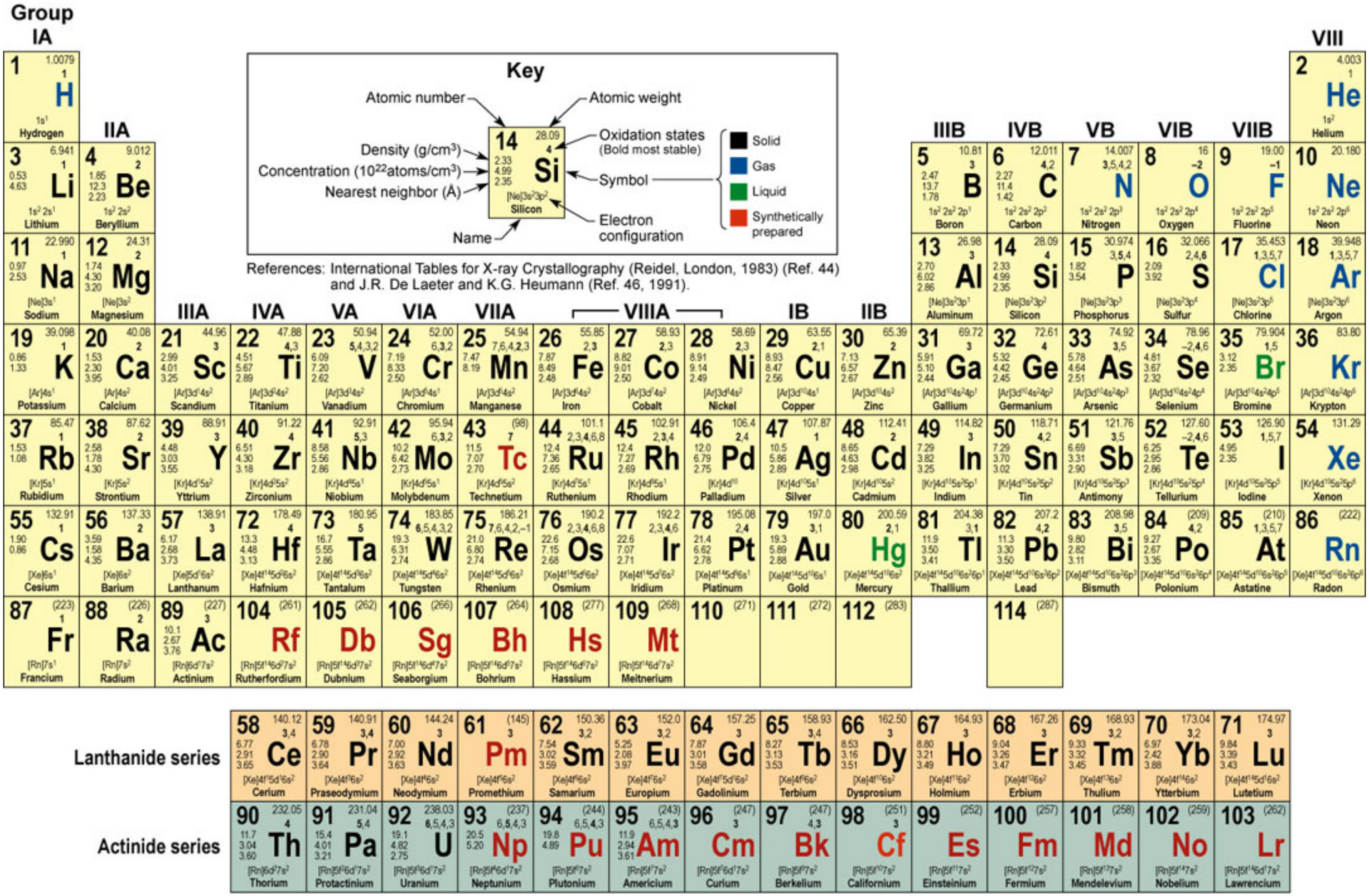


TABLE B.2. Photon energies, in electron volts, of principal K and L shell emission lines.[a]

Element	$K\alpha_1$	$K\alpha_2$	$K\beta_1$	$L\alpha_1$	$L\alpha_2$	$L\beta_1$	$L\beta_2$	$L\gamma_1$
3 Li	54.3							
4 Be	108.5							
5 B	183.3							
6 C	277							
7 N	392.4							
8 O	524.9							
9 F	676.8							
10 Ne	848.6	848.6						
11 Na	1,040.98	1,040.98	1,071.1					
12 Mg	1,253.60	1,253.60	1,302.2					
13 Al	1,486.70	1,486.27	1,557.45					
14 Si	1,739.98	1,739.38	1,835.94					
15 P	2,013.7	2,012.7	2,139.1					
16 S	2,307.84	2,306.64	2,464.04					
17 Cl	2,622.39	2,620.78	2,815.6					
18 Ar	2,957.70	2,955.63	3,190.5					
19 K	3,313.8	3,311.1	3,589.6					
20 Ca	3,691.68	3,688.09	4,012.7	341.3	341.3	344.9		
21 Sc	4,090.6	4,086.1	4,460.5	395.4	395.4	399.6		
22 Ti	4,510.84	4,504.86	4,931.81	452.2	452.2	458.4		
23 V	4,952.20	4,944.64	5,427.29	511.3	511.3	519.2		
24 Cr	5,414.72	5,405.509	5,946.71	572.8	572.8	582.8		
25 Mn	5,898.75	5,887.65	6,490.45	637.4	637.4	648.8		
26 Fe	6,403.84	6,390.84	7,057.98	705.0	705.0	718.5		
27 Co	6,930.32	6,915.30	7,649.43	776.2	776.2	791.4		
28 Ni	7,478.15	7,460.89	8,264.66	851.5	851.5	868.8		
29 Cu	8,047.78	8,027.83	8,905.29	929.7	929.7	949.8		
30 Zn	8,638.86	8,615.78	9,572.0	1,011.7	1,011.7	1,034.7		

Broadly tunable synchrotron radiation is capable of probing the primary resonances of the elements



Atomic number	Atomic weight	Oxidation states	Symbol	Density (g/cm³)	Concentration (10^{22} atoms/cm³)	Nearest neighbor (Å)	Electron configuration	Name
1	1.0079	1	H				$1s^1$	Hydrogen
2	4.003	1	He				$1s^2$	Helium
3	6.941	1	Li	0.53	4.63		$1s^2 2s^1$	Lithium
4	9.012	2	Be	1.85	12.3	2.23	$1s^2 2s^2$	Beryllium
5	10.81	3	B	2.47	13.7	1.78	$1s^2 2s^2 2p^1$	Boron
6	12.011	4,2	C	2.27	11.4	1.42	$1s^2 2s^2 2p^2$	Carbon
7	14.007	3,5,4,2	N				$1s^2 2s^2 2p^3$	Nitrogen
8	16	−2	O				$1s^2 2s^2 2p^4$	Oxygen
9	19.00	−1	F				$1s^2 2s^2 2p^5$	Fluorine
10	20.180		Ne				$1s^2 2s^2 2p^6$	Neon
11	22.990	1	Na	0.97	2.53		$[Ne]3s^1$	Sodium
12	24.31	2	Mg	1.74	4.30	3.20	$[Ne]3s^2$	Magnesium
13	26.98	3	Al	2.70	6.02	2.86	$[Ne]3s^2 3p^1$	Aluminum
14	28.09	4	Si	2.33	4.99	2.35	$[Ne]3s^2 3p^2$	Silicon
15	30.974	3,5,4	P	1.82	3.54		$[Ne]3s^2 3p^3$	Phosphorus
16	32.066	2,4,6	S	2.09	3.92		$[Ne]3s^2 3p^4$	Sulfur
17	35.453	1,3,5,7	Cl				$[Ne]3s^2 3p^5$	Chlorine
18	39.948	1,3,5,7	Ar				$[Ne]3s^2 3p^6$	Argon
19	39.098	1	K	0.86	1.33		$[Ar]4s^1$	Potassium
20	40.08	2	Ca	1.53	2.30	3.95	$[Ar]4s^2$	Calcium
21	44.96	3	Sc	2.99	4.01	3.25	$[Ar]3d^1 4s^2$	Scandium
22	47.88	4,3	Ti	4.51	5.67	2.89	$[Ar]3d^2 4s^2$	Titanium
23	50.94	5,4,3,2	V	6.09	7.20	2.62	$[Ar]3d^3 4s^2$	Vanadium
24	52.00	6,3,2	Cr	7.19	8.33	2.50	$[Ar]3d^5 4s^1$	Chromium
25	54.94	7,6,4,2,3	Mn	7.47	8.19		$[Ar]3d^5 4s^2$	Manganese
26	55.85	2,3	Fe	7.87	8.49	2.48	$[Ar]3d^6 4s^2$	Iron
27	58.93	2,3	Co	8.82	9.01	2.50	$[Ar]3d^7 4s^2$	Cobalt
28	58.69	2,3	Ni	8.91	9.14	2.49	$[Ar]3d^8 4s^2$	Nickel
29	63.55	2,1	Cu	8.93	8.47	2.56	$[Ar]3d^{10} 4s^1$	Copper
30	65.39	2	Zn	7.13	6.57	2.67	$[Ar]3d^{10} 4s^2$	Zinc
31	69.72	3	Ga	5.91	5.10	2.44	$[Ar]3d^{10} 4s^2 4p^1$	Gallium
32	72.61	4	Ge	5.32	4.42	2.45	$[Ar]3d^{10} 4s^2 4p^2$	Germanium
33	74.92	3,5	As	5.78	4.64	2.51	$[Ar]3d^{10} 4s^2 4p^3$	Arsenic
34	78.96	−2,4,6	Se	4.81	3.67	2.32	$[Ar]3d^{10} 4s^2 4p^4$	Selenium
35	79.904	1,5	Br	3.12	2.35		$[Ar]3d^{10} 4s^2 4p^5$	Bromine
36	83.80		Kr				$[Ar]3d^{10} 4s^2 4p^6$	Krypton
37	85.47	1	Rb	1.53	1.08		$[Kr]5s^1$	Rubidium
38	87.62	2	Sr	2.58	1.78	4.30	$[Kr]5s^2$	Strontium
39	88.91	3	Y	4.48	3.03	3.55	$[Kr]4d^1 5s^2$	Yttrium
40	91.22	4	Zr	6.51	4.30	3.18	$[Kr]4d^2 5s^2$	Zirconium
41	92.91	5,3	Nb	8.58	5.56	2.86	$[Kr]4d^4 5s^1$	Niobium
42	95.94	6,3,2	Mo	10.2	6.42	2.73	$[Kr]4d^5 5s^1$	Molybdenum
43	(98)	7	Tc	11.5	7.07	2.70	$[Kr]4d^5 5s^2$	Technetium
44	101.1	2,3,4,6,8	Ru	12.4	7.36	2.65	$[Kr]4d^7 5s^1$	Ruthenium
45	102.91	2,3,4	Rh	12.4	7.27	2.69	$[Kr]4d^8 5s^1$	Rhodium
46	106.4	2,4	Pd	12.0	6.79	2.75	$[Kr]4d^{10}$	Palladium
47	107.87	1	Ag	10.5	5.86	2.89	$[Kr]4d^{10} 5s^1$	Silver
48	112.41	2	Cd	8.65	4.63	2.98	$[Kr]4d^{10} 5s^2$	Cadmium
49	114.82	3	In	7.29	3.82	3.25	$[Kr]4d^{10} 5s^2 5p^1$	Indium
50	118.71	4,2	Sn	7.29	3.70	3.02	$[Kr]4d^{10} 5s^2 5p^2$	Tin
51	121.76	3,5	Sb	6.69	3.31	2.90	$[Kr]4d^{10} 5s^2 5p^3$	Antimony
52	127.60	−2,4,6	Te	6.25	2.95	2.86	$[Kr]4d^{10} 5s^2 5p^4$	Tellurium
53	126.90	1,5,7	I	4.95	2.35		$[Kr]4d^{10} 5s^2 5p^5$	Iodine
54	131.29		Xe				$[Kr]4d^{10} 5s^2 5p^6$	Xenon
55	132.91	1	Cs	1.90	0.86		$[Xe]6s^1$	Cesium
56	137.33	2	Ba	3.59	1.58	4.35	$[Xe]6s^2$	Barium
57	138.91	3	La	6.17	2.68	3.73	$[Xe]5d^1 6s^2$	Lanthanum
72	178.49	4	Hf	13.3	4.48	3.13	$[Xe]4f^{14} 5d^2 6s^2$	Hafnium
73	180.95	5	Ta	16.7	5.55	2.86	$[Xe]4f^{14} 5d^3 6s^2$	Tantalum
74	183.85	6,5,4,3,2	W	19.3	6.31	2.74	$[Xe]4f^{14} 5d^4 6s^2$	Tungsten
75	186.21	7,6,4,2,−1	Re	21.0	6.80	2.74	$[Xe]4f^{14} 5d^5 6s^2$	Rhenium
76	190.2	2,3,4,6,8	Os	22.6	7.15	2.68	$[Xe]4f^{14} 5d^6 6s^2$	Osmium
77	192.2	2,3,4,6	Ir	22.6	7.07	2.71	$[Xe]4f^{14} 5d^7 6s^2$	Iridium
78	195.08	2,4	Pt	21.4	6.62	2.78	$[Xe]4f^{14} 5d^9 6s^1$	Platinum
79	197.0	3,1	Au	19.3	5.89	2.88	$[Xe]4f^{14} 5d^{10} 6s^1$	Gold
80	200.59	2,1	Hg				$[Xe]4f^{14} 5d^{10} 6s^2$	Mercury
81	204.38	3,1	Tl	11.9	3.50	3.41	$[Xe]4f^{14} 5d^{10} 6s^2 6p^1$	Thallium
82	207.2	4,2	Pb	11.3	3.30	3.50	$[Xe]4f^{14} 5d^{10} 6s^2 6p^2$	Lead
83	208.98	3,5	Bi	9.80	2.82	3.11	$[Xe]4f^{14} 5d^{10} 6s^2 6p^3$	Bismuth
84	(209)	4,2	Po	9.27	2.67	3.35	$[Xe]4f^{14} 5d^{10} 6s^2 6p^4$	Polonium
85	(210)	1,3,5,7	At				$[Xe]4f^{14} 5d^{10} 6s^2 6p^5$	Astatine
86	(222)		Rn				$[Xe]4f^{14} 5d^{10} 6s^2 6p^6$	Radon
87	(223)	1	Fr				$[Rn]7s^1$	Francium
88	(226)	2	Ra				$[Rn]7s^2$	Radium
89	(227)	3	Ac	10.1	2.67	3.76	$[Rn]6d^1 7s^2$	Actinium
104	(261)		Rf				$[Rn]5f^{14} 6d^2 7s^2$	Rutherfordium
105	(262)		Db				$[Rn]5f^{14} 6d^3 7s^2$	Dubnium
106	(266)		Sg				$[Rn]5f^{14} 6d^4 7s^2$	Seaborgium
107	(264)		Bh				$[Rn]5f^{14} 6d^5 7s^2$	Bohrium
108	(277)		Hs				$[Rn]5f^{14} 6d^6 7s^2$	Hassium
109	(268)		Mt				$[Rn]5f^{14} 6d^7 7s^2$	Meitnerium
110	(271)							
111	(272)							
112	(283)							
114	(287)							

Lanthanide series

Atomic number	Atomic weight	Oxidation states	Symbol	Density (g/cm³)	Concentration (10^{22} atoms/cm³)	Nearest neighbor (Å)	Electron configuration	Name
58	140.12	3,4	Ce	6.77	2.91	3.65	$[Xe]4f^1 5d^1 6s^2$	Cerium
59	140.91	3,4	Pr	6.78	2.90	3.64	$[Xe]4f^3 6s^2$	Praseodymium
60	144.24	3	Nd	7.00	2.92	3.63	$[Xe]4f^4 6s^2$	Neodymium
61	(145)	3	Pm				$[Xe]4f^5 6s^2$	Promethium
62	150.36	3,2	Sm	7.54	3.02	3.59	$[Xe]4f^6 6s^2$	Samarium
63	152.0	3,2	Eu	5.25	2.08	3.97	$[Xe]4f^7 6s^2$	Europium
64	157.25	3	Gd	7.87	3.01	3.58	$[Xe]4f^7 5d^1 6s^2$	Gadolinium
65	158.93	3,4	Tb	8.27	3.13	3.53	$[Xe]4f^9 6s^2$	Terbium
66	162.50	3	Dy	8.53	3.16	3.51	$[Xe]4f^{10} 6s^2$	Dysprosium
67	164.93	3	Ho	8.80	3.21	3.49	$[Xe]4f^{11} 6s^2$	Holmium
68	167.26	3	Er	9.04	3.26	3.47	$[Xe]4f^{12} 6s^2$	Erbium
69	168.93	3,2	Tm	9.33	3.32	3.45	$[Xe]4f^{13} 6s^2$	Thulium
70	173.04	3,2	Yb	6.97	2.42	3.88	$[Xe]4f^{14} 6s^2$	Ytterbium
71	174.97	3	Lu	9.84	3.39	3.43	$[Xe]4f^{14} 5d^1 6s^2$	Lutetium

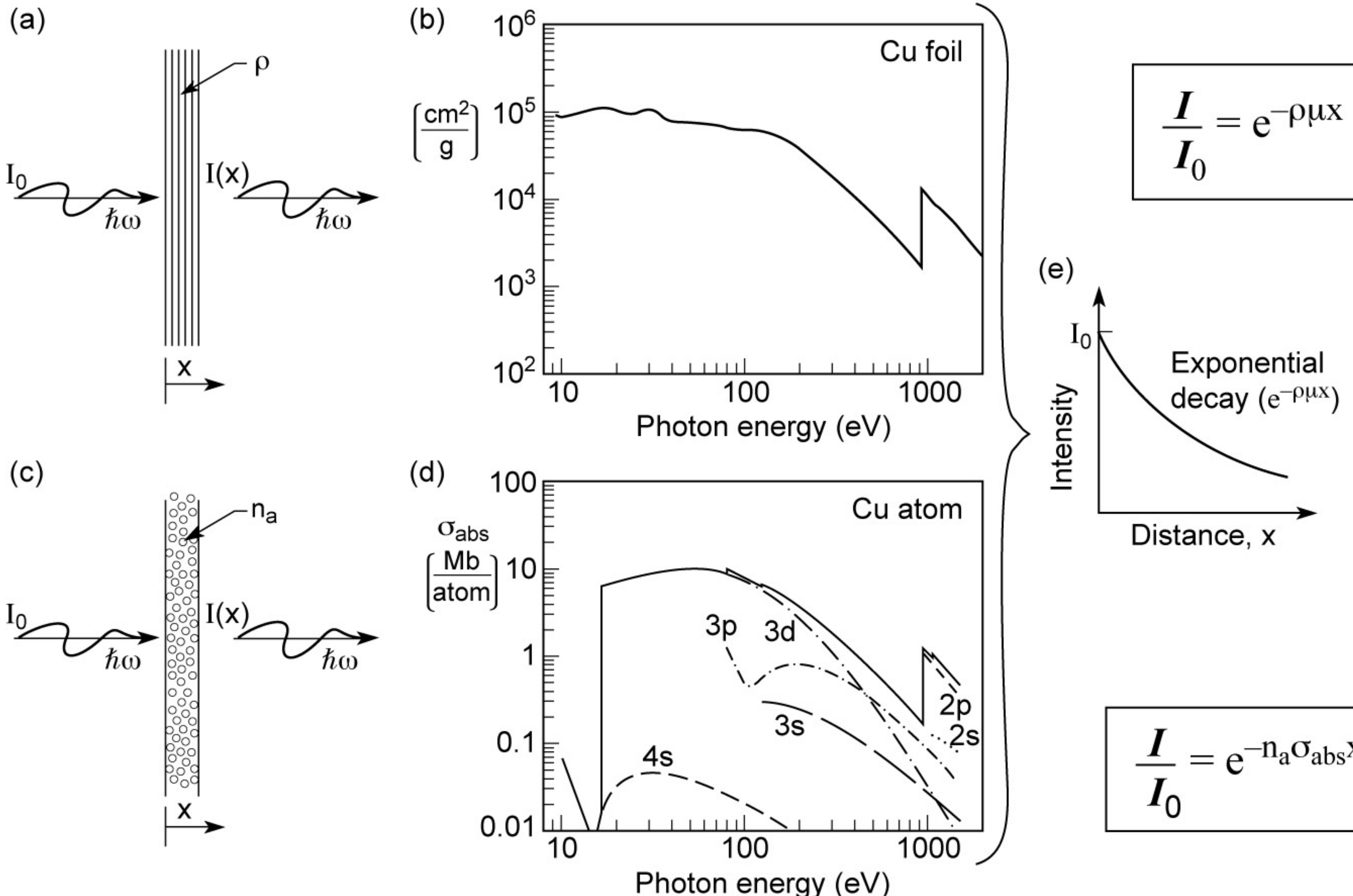
Actinide series

Atomic number	Atomic weight	Oxidation states	Symbol	Density (g/cm³)	Concentration (10^{22} atoms/cm³)	Nearest neighbor (Å)	Electron configuration	Name
90	232.05	4	Th	11.7	3.04	3.60	$[Rn]6d^2 7s^2$	Thorium
91	231.04	5,4	Pa	15.4	4.01	3.21	$[Rn]5f^2 6d^1 7s^2$	Protactinium
92	238.03	6,5,4,3	U	19.1	4.82	2.75	$[Rn]5f^3 6d^1 7s^2$	Uranium
93	(237)	6,5,4,3	Np	20.5	5.20		$[Rn]5f^4 6d^1 7s^2$	Neptunium
94	(244)	6,5,4,3	Pu	19.8	4.89		$[Rn]5f^6 7s^2$	Plutonium
95	(243)	6,5,4,3	Am	11.9	2.94	3.61	$[Rn]5f^7 7s^2$	Americium
96	(247)	3	Cm				$[Rn]5f^7 6d^1 7s^2$	Curium
97	(247)	4,3	Bk				$[Rn]5f^9 7s^2$	Berkelium
98	(251)	3	Cf				$[Rn]5f^{10} 7s^2$	Californium
99	(252)		Es				$[Rn]5f^{11} 7s^2$	Einsteinium
100	(257)		Fm				$[Rn]5f^{12} 7s^2$	Fermium
101	(258)		Md				$[Rn]5f^{13} 7s^2$	Mendelevium
102	(259)		No				$[Rn]5f^{14} 7s^2$	Nobelium
103	(262)		Lr				$[Rn]5f^{14} 6d^1 7s^2$	Lawrencium

References: International Tables for X-ray Crystallography (Reidel, London, 1983) (Ref. 44) and J.R. De Laeter and K.G. Heumann (Ref. 46, 1991).

Periodic_Tb_clr_May2007.ai

Photoabsorbtion by thin foils and isolated atoms



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

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

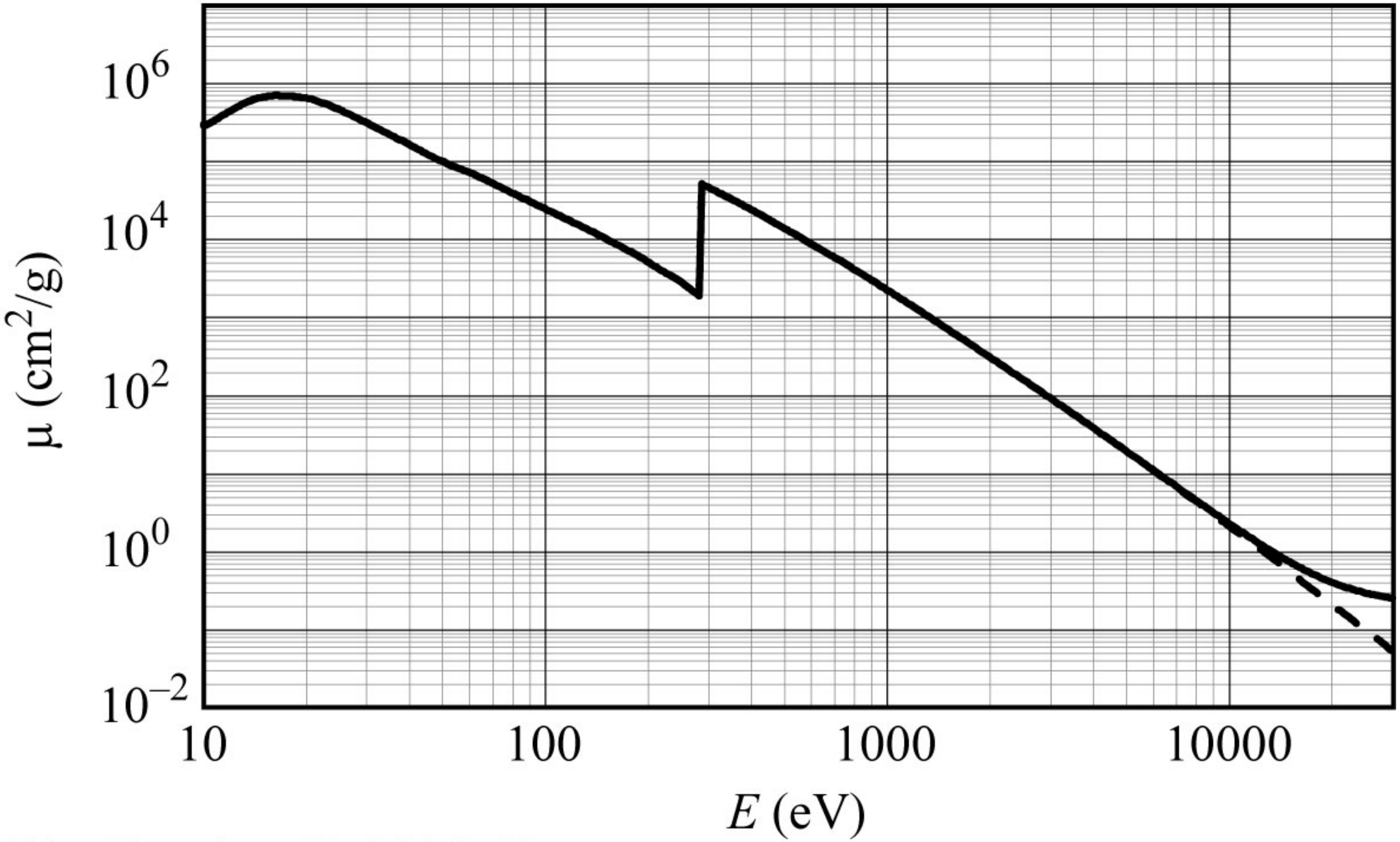
Ch01_F08_Aug05.ai

Absorption coefficients for carbon (Z = 6)

σ_a(barns/atom) = μ(cm^2/g) × 19.95

E(keV)μ(cm^2/g) = f_2^0 × 3503.31

Carbon (C)
Z = 6
Atomic weight = 12.011



Edge Energies: K 284.2 eV

(Henke and Gullikson; www-cxro.LBL.gov)

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Absorption coefficients for silicon (Z = 14)

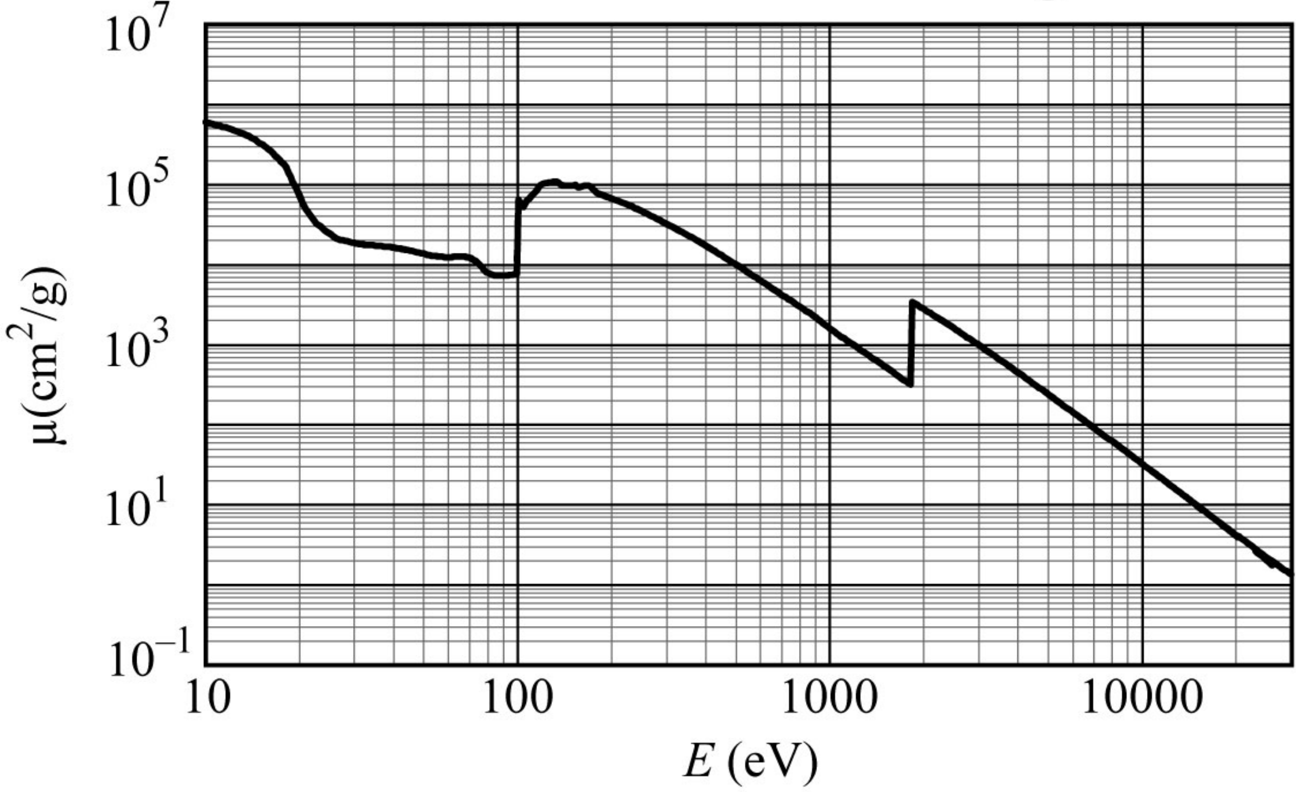
$\sigma_a(\text{barns/atom}) = \mu(\text{cm}^2/\text{g}) \times 46.64$

$E(\text{keV})\mu(\text{cm}^2/\text{g}) = f_2^{\,0} \times 1498.22$

Silicon (Si)

Z = 14

Atomic weight = 28.086



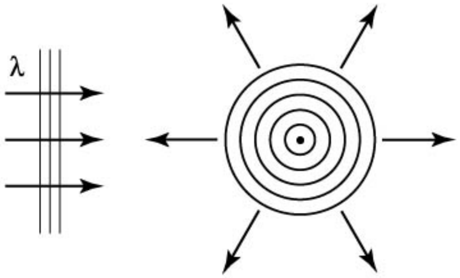
Edge Energies: K 1838.9 eV
L_1 149.7 eV
L_2 99.8 eV
L_3 99.2 eV

(Henke and Gullikson; www-cxro.LBL.gov)

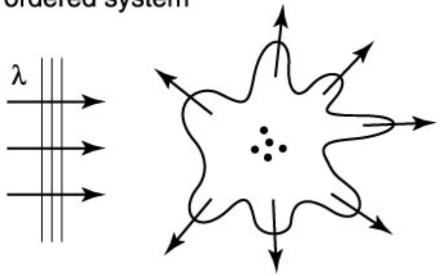
Ch02_ApC_Tb1_F07_leftBot.ai

Scattering, diffraction and refraction

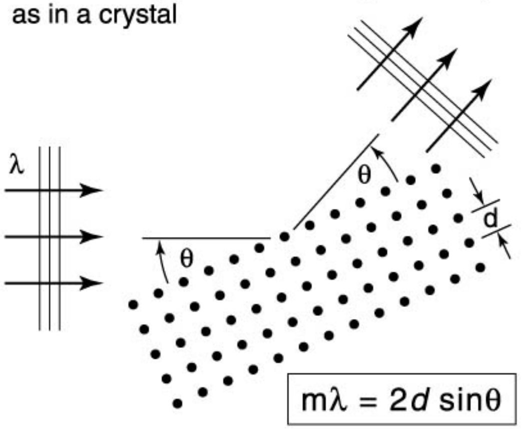
(a) Isotropic scattering from a point object



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

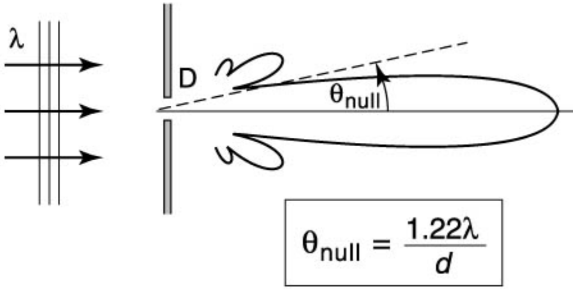


(c) Diffraction by an ordered array of atoms, as in a crystal



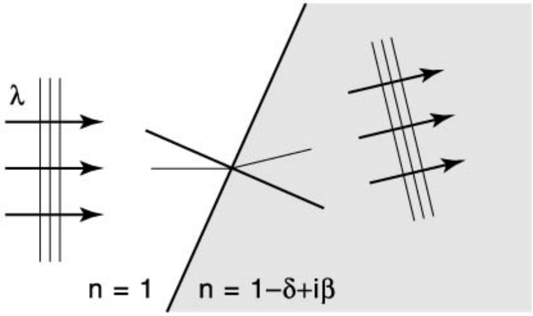
$m\lambda = 2d \sin\theta$

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

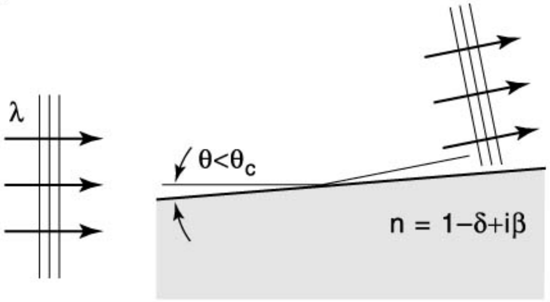


$$\theta_{null} = \frac{1.22\lambda}{d}$$

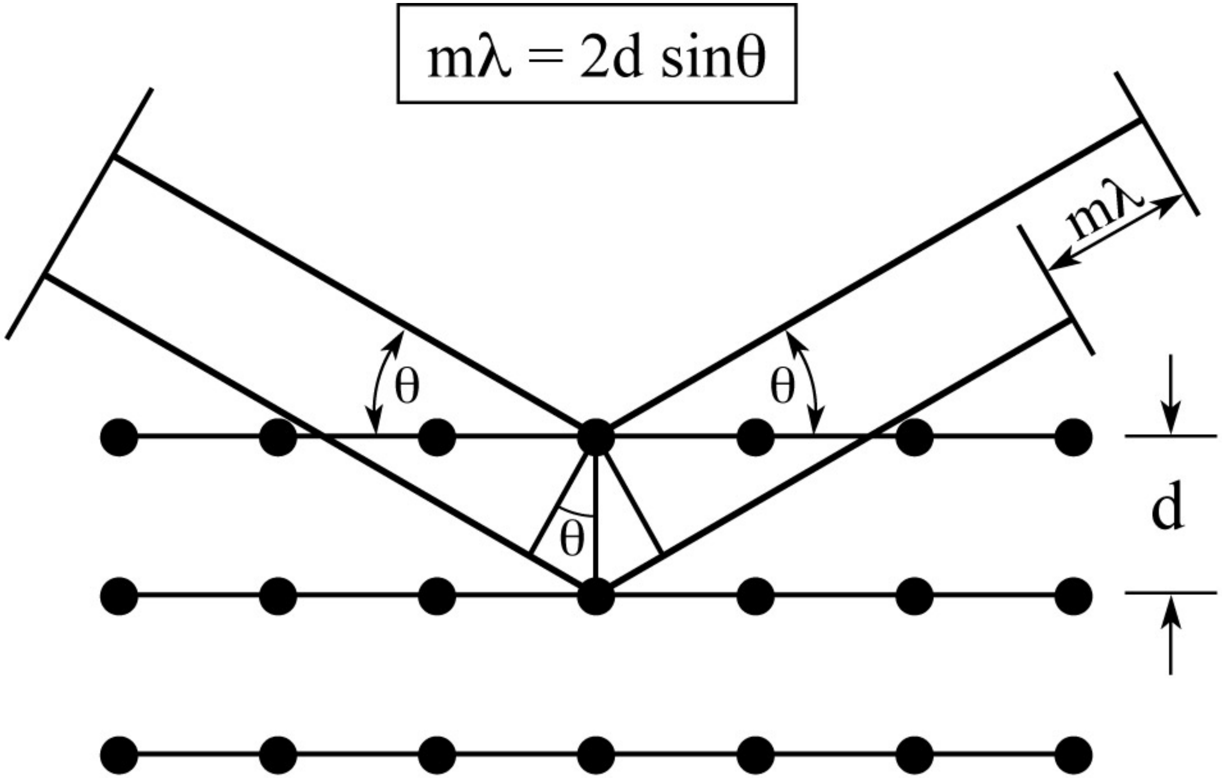
(e) Refraction at an interface



(f) Total external reflection



The derivation of Bragg's law



$$m\lambda = 2d \sin\theta$$

The path difference of radiation "reflecting" off sequential planes must be equal to an interger number of wavelengths.

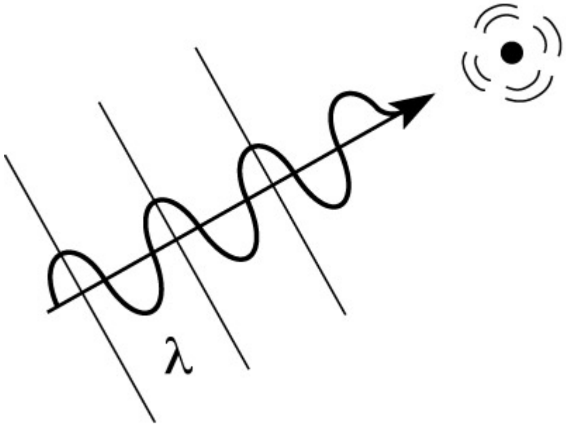
The angle θ is measured from the crystal plane, and the distance between planes is referred to as the "d-spacing".

From A.H. Compton and S.K. Allison, *X-Rays in Theory and Experiment* (D.Van Nostrand, New York, 1926), p.29.
Also see M. Siegbahn, *The Spectroscopy of X-Rays* (Oxford University Press, London, 1925), p.16.

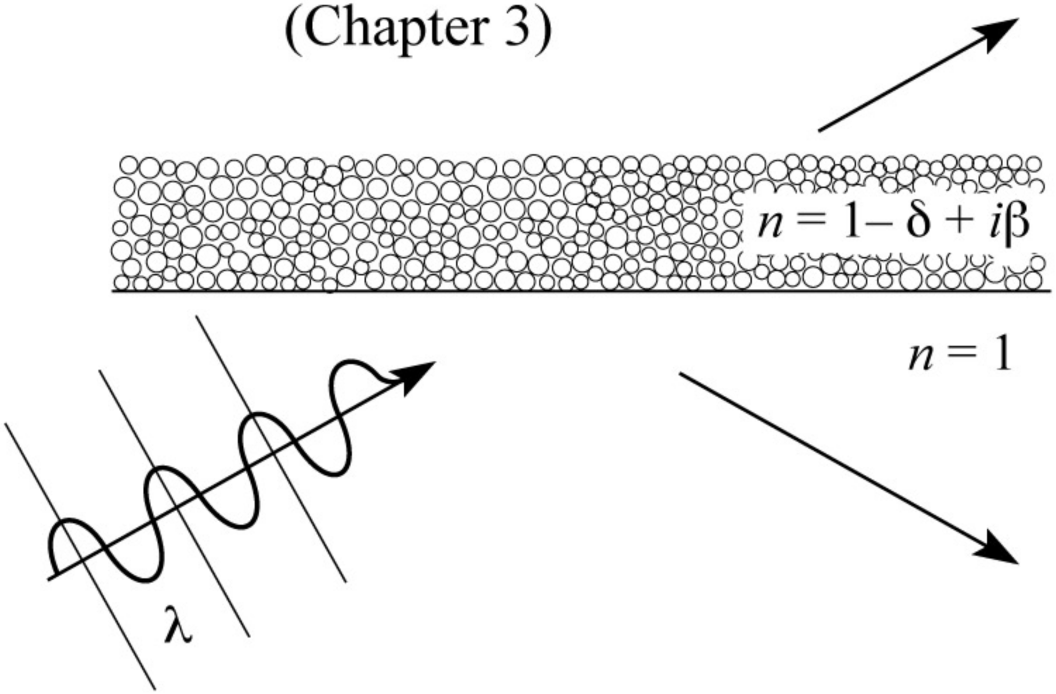
DerivationBraggsLaw.ai

Scattering, diffraction and refraction

Single scatterer,
electron or atom,
in vacuum.
(Chapter 2)



Many atoms, each
with many electrons,
constituting a “material”.
(Chapter 3)



- How are scattering, refraction, and reflection related?
- How do these differ for amorphous and ordered (crystalline) materials?
- What is the role of forward scattering?

Ch02_ScatRefrReflc.ai

Maxwell's Equations

↓

Wave Equation

(in vacuum)
(Chapter 2)

- Radiation by a single electron ("dipole radiation")
- Scattering cross-sections
- Scattering by a free electron ("Thomson scattering")
- Scattering by a single bound electron ("Rayleigh scattering")
- Scattering by a multi-electron atom
- Atomic "scattering factors", f_0' and f_0''

(in a material)
(Chapter 3)

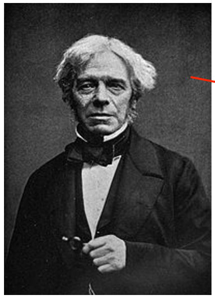
- Refractive index with many atoms present
- Role of forward scattering
- Contributions to refractive index by bound electrons
- Refractive index for soft x-rays and EUV

$$n = 1 - \underset{\substack{\downarrow \\ f_0'}}{\delta} + i\underset{\substack{\downarrow \\ f_0''}}{\beta} \qquad (\delta, \beta \ll 1)$$

- Determining f_0' and f_0''; measurements and Kramers-Kronig
- Total external reflection
- Reflectivity vs. angle
- Brewster's angle

The equations of light

Michael Faraday



André-Marie Ampère

Charles-Augustin de Coulomb

Carl Friedrich Gauss

Maxwell's Equations

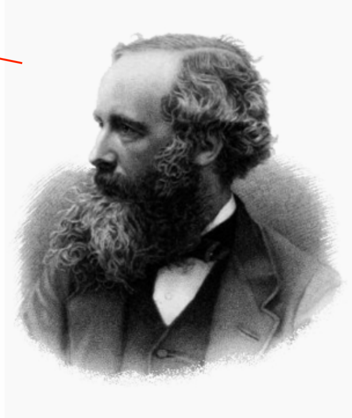
$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{D} = \rho$$

James Clerk Maxwell



[written for vacuum, where $\underset{\sim}{\mathbf{D}} = \epsilon_0 \underset{\sim}{\mathbf{E}}$ and $\underset{\sim}{\mathbf{B}} = \mu_0 \underset{\sim}{\mathbf{H}}$]

When combined these lead to the Wave Equation

$$\left(\frac{\partial^2}{\partial t^2} - c^2\nabla^2\right)\mathbf{E}(\mathbf{r}, t) = -\frac{1}{\epsilon_0}\frac{\partial \mathbf{J}(\mathbf{r}, t)}{\partial t}$$

Heinrich Hertz

Courtesy of Andrew Aquila (AS&T, UC Berkeley)

The time derivative of the current density, ∂J/∂t, drives electromagnetic waves

For electrons the current density is $\mathbf{J} = -en(\mathbf{r}, t)\mathbf{v}(\mathbf{r}, t)$.
Assuming that the electron density $n(\mathbf{r},t)$ varies slowly in time, the question then is what is the velocity **v** and ∂**v**/∂t?

For classically bound electrons with a single resonance at $\omega = \omega_s$ and a decay factor γ, in the presence of a passing electomagnetic wave, the force equation (**F** = m**a**) can be written as

$$m\frac{d^2\mathbf{x}}{dt^2} + m\gamma\frac{d\mathbf{x}}{dt} + m\omega_s^2\mathbf{x} = -e(\mathbf{E} + \underbrace{\mathbf{v}\times\mathbf{B}}_{\simeq 0}) \qquad (2.48)$$

with an acceleration term (m**a**), a damping term, a restoring force term, and the Lorentz force exerted by the fields. For an incident electric field

$$\mathbf{E} = \mathbf{E}_i e^{-i\omega t}$$

the harmonic motion will be driven at the same frequency, ω, so that

$$\mathbf{x} = \frac{1}{\omega^2 - \omega_s^2 + i\gamma\omega}\frac{e\mathbf{E}}{m} \qquad (2.49)$$

By taking the time derivative twice, $\partial^2/\partial t^2$ to get v and then ∂**v**/∂t

$$\mathbf{a} = \frac{\partial\mathbf{v}}{\partial \mathrm{t}} = \frac{-\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega}\frac{e\mathbf{E}}{m} \qquad (2.50)$$

as needed for ∂**J**/∂t.

03_Slide2_Spring2009.ai

The wave equation in vacuum, with a density n of bound electrons of resonant frequency ω_s

$$\left(\frac{\partial^2}{\partial t^2} - c^2\nabla^2\right)\mathbf{E}(\mathbf{r},t) = -\frac{1}{\epsilon_0}\frac{\partial}{\partial t}[-en(\mathbf{r},t)\mathbf{v}(\mathbf{r},t)]$$

$$\left(\frac{\partial^2}{\partial t^2} - c^2\nabla^2\right)\mathbf{E}(\mathbf{r},t) = -\frac{1}{\epsilon_0}\left[\underbrace{-en(\mathbf{r},t)}_{\substack{\text{slowly}\\ \text{varying in time}}}\left(\frac{1}{\omega^2-\omega_s^2+i\gamma\omega}\right)\frac{e}{m}\frac{\partial^2\mathbf{E}}{\partial t^2}\right]$$

Collecting all terms with **E**

$$\left[\left(1-\frac{e^2}{\epsilon_0 m}\,\frac{n(\mathbf{r},t)}{\omega^2-{\omega_s}^2+i\gamma m}\right)\frac{\partial^2}{\partial t^2}-c^2\nabla^2\right]\mathbf{E}(\mathbf{r},t) = 0$$

Which can be written in standard form for the wave equation as

$$\left[\frac{\partial^2}{\partial t^2}-\frac{c^2}{n^2(\omega)}\nabla^2\right]\mathbf{E}_T(\mathbf{r},t)=0$$

where the refractive index is identified as

$$n(\omega)=1-\frac{1}{2}\frac{e^2 n}{\epsilon_0 m}\frac{1}{\omega^2-\omega_s^2\ +i\gamma\omega}$$

More generally, for a collection of atoms n_a, with Z electrons each at several discrete resonances ω_s, and with g_s electrons ("oscillator strengths") associated with each frequency, one has

$$\boxed{n(\omega)=1-\frac{1}{2}\frac{e^2 n_a}{\epsilon_0 m}\sum_s\frac{g_s}{(\omega^2-\omega_s^2)+i\gamma\omega} = 1-\delta+i\beta}$$

where $\sum_s g_s = Z$

WaveEquation_HerculesTriesteApr2010.ai

Special cases: propagation in vacuum, no electrons

For $n(\mathbf{r},t) = 0$:

$$\left[\frac{\partial^2}{\partial t^2} - c^2\nabla^2\right]\mathbf{E}(\mathbf{r},t) = 0$$

For waves of the form $\mathrm{E} = \mathrm{E}_0\, e^{-i(\omega t - \mathbf{k}\cdot\mathbf{r})}$, $\frac{\partial}{\partial \mathrm{t}} \rightarrow -i\omega$, $\nabla \rightarrow -i\mathbf{k}$

$$[\omega^2 - k^2c^2]\,\mathbf{E}(\mathbf{r},t) = 0$$

For waves of finite amplitude **E** to propagate in vacuum one requires the bracketed quantity to be zero

$$\omega^2 - k^2c^2 = 0$$

$\boxed{\omega = \pm kc}$ (natural modes of the system)

with $\omega = 2\pi f$ and $k = 2\pi/\lambda$

$\boxed{f\lambda = \mathrm{c}}$ (dispersion relation for waves propagating in vacuum)

an "outgoing" wave, plus an "incoming" wave (or left and right propagating waves).

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Special cases: propagation in a material of n_a atoms/unit volume, each with many bound electrons

$$\text{Refractive index } n(\omega) = 1 - \frac{1}{2}\frac{e^2 n_a}{\epsilon_0 m}\sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma}\,,\ \sum_s g_s = Z \qquad (2.73)$$

$$\left[\frac{\partial^2}{\partial t^2} - \frac{c^2}{n^2(\omega)}\nabla^2\right]\mathbf{E}_{\mathrm{T}}(\mathbf{r}, t) = 0$$

$$\omega^2 - \frac{k^2c^2}{n^2(\omega)} = 0$$

$$\omega = \pm\frac{kc}{n(\omega)}$$

$\boxed{f\lambda = c/n(\omega)}$ [dispersion relation in a material of refractive index $n(\omega)$]

The phase velocity of the wave is

$$v_\phi = \omega/k = c/n(\omega)$$

Thus the wave is slowed for $n(\omega) > 1$, as for visible light in glass, where $n \sim 1.5$.
Note the change in sign for $\omega^2 <$ or $> \omega_s^2$ in eq. (3.8)

$$n(\omega) = 1 - \frac{1}{2}\frac{e^2 n_a}{\epsilon_0 m}\sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma\omega} \qquad (3.8)$$

For visible light in glass ω_s is in the ultraviolet.

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Refractive index for x-rays

The refractive index, $n(\omega)$, is complex because EUV/soft x-ray radiation is absorbed appreciably by all atoms. This is reflected in the semi-classical model

$$n(\omega) = 1 - \frac{1}{2}\frac{e^2 n_a}{\epsilon_0 m}\sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma\omega} \tag{3.8}$$

where again $\sum_s g_s = Z$ (2.73), or by its quantum mechanical equivalent $\sum_{k,n} g_{kn} = Z$. (2.74)

The convention is to express scattering and refractive index in terms of a complex scattering factor, $f^0(\omega)$ specific to each element

$$f^0(\omega) = f_1^0(\omega) - i f_2^0(\omega) = \sum_s \frac{g_s\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega}$$

where the scattering factor arises from consideration of the scattered electric field due to an atom, relative to that of a free electron. Introducing the classical electron radius

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2} \tag{2.44}$$

The refractive index can be written as

$$\boxed{n(\omega) = 1 - \frac{n_a r_e \lambda^2}{2\pi}\left[f_1^0(\omega) - i f_2^0(\omega)\right]} \tag{3.9}$$

or in simpler notation

$$\boxed{n(\omega) = 1 - \delta + i\beta} \tag{3.12}$$

RefractiveIndex_Jan20162.ai

A numerical example: Propagation of x-rays in a material with $\omega^2 >> \omega_s^2$

Refractive index $$n(\omega) = 1 - \frac{1}{2}\frac{e^2 n_a}{\epsilon_0 m}\sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma\omega} \quad , \quad \sum_s g_s = Z \tag{2.73}$$

For x-rays in carbon, with $\hbar\omega = 1$ keV and binding energy $\hbar\omega_s = 284$ eV, such that $\omega^2 >> \omega_s^2 >> \gamma\omega$, $n_a = 11.4 \times 10^{22}$ atoms/cm^3 (see Table B.1, pg. 420 and data within the periodic chart at book's inside back cover), and (all electrons acting as essentially free), then

$$n(\omega) \simeq 1 - \frac{1}{2}\frac{e^2 n_a \hbar^2}{\epsilon_0 m(\hbar\omega)^2} \cdot \frac{Z}{1 - (\hbar\omega_s/\hbar\omega)^2}$$

$$n(\omega) \simeq 1 - \underbrace{0.000507}_{\delta}$$

This compares well (1.6% difference) with standard values at the website www.cxro.LBL.gov (click "x-ray interactions with matter", then "x-ray properties of the elements"), which gives $\delta = 4.86 \times 10^{-4}$ for a density of 2.20 g/cc, corresponding to $n_a = 11.0$ atoms/cm^3. Values of n_a and ρ vary widely for carbon, depending on preparation: thin carbon film, graphite as in a pencil, diamond, etc. We have neglected the absorptive term, γ. The web site corrected for 11.4 atoms/cm^3, gives $n(\omega) = 1 - 0.000499 + i0.0000499$. Similarity of the numbers is coincidental.

03_Slide7_Spring2009.ai

Quantum mechanical model of refractive index

A shortcoming of the semi-classical model, among others, is that it gives the proper form of scattering cross-sections and refractive index, but does not provide a basis for calculating oscillator strengths. In the quantum mechanical description these oscillator strengths arise naturally as non-integer *transition probabilities*, g_{kn}, between stationary states ψ_k and ψ_n of the atom, leading to an expression similar to Eq. (2.73) when summed over final states n from an initial state k:

$$\boxed{n(\omega) = 1 - \frac{1}{2}\frac{e^2 n_a}{\epsilon_0 m}\sum_{k,n}\frac{g_{kn}}{(\omega^2 - \omega_{kn}{}^2) + i\gamma\omega}}$$

Where

$$\sum_{k,n} g_{kn} = Z \qquad (2.74)$$

That is, the sum of oscillator strengths equals the total number of electrons per atom. Equation (2.74) is known as the Thomas-Reiche-Kuhn summation rule.*

These factors are generally not calculable for many electron atoms. The refractive index is typically written in simplified form as

$$\boxed{n(\omega) = 1 - \delta + i\beta}$$

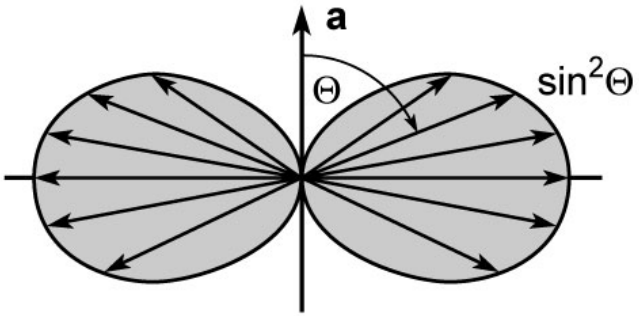
where δ and β are much less than one. Values of δ and β are generally based on measurements and Kramers-Krönig relations.

*For further reading see Liboff, p.769; R.W. James, pp.142-143; and A. Corney, p.108.

03_Slide8_Spring2009.ai

Chapter 2

RADIATION AND SCATTERING AT EUV AND SOFT X-RAY WAVELENGTHS



$$\frac{dP}{d\Omega} = \frac{e^2|\mathbf{a}|^2 \sin^2\Theta}{16\pi^2\epsilon_0 c^3} \qquad (2.34)$$

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2} \qquad (2.44)$$

$$\sigma_e = \frac{8\pi}{3} r_e^2 \qquad (2.45)$$

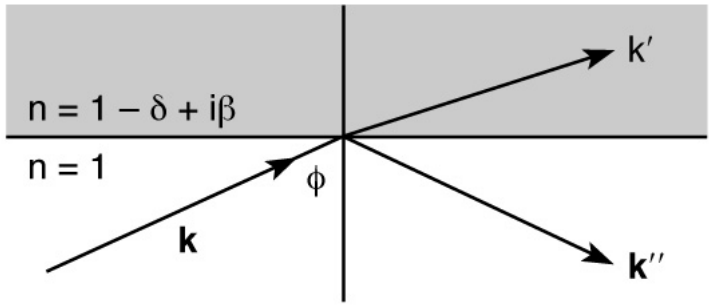
$$\sigma = \frac{8\pi}{3} r_e^2 \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\gamma\omega)^2} \qquad (2.51)$$

$$f(\Delta\mathbf{k}, \omega) = \sum_{s=1}^{Z} \frac{\omega^2 e^{-i\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s}}{\omega^2 - \omega_s^2 + i\gamma\omega} \qquad (2.66)$$

$$f^0(\omega) = \sum_{s=1}^{Z} \frac{\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega} \qquad (2.72)$$

Chapter 3

WAVE PROPAGATION AND REFRACTIVE INDEX AT EUV AND SOFT X-RAY WAVELENGTHS



$$n(\omega) = 1 - \frac{n_a r_e \lambda^2}{2\pi}\left(f_1^0 - i f_2^0\right) \qquad (3.9)$$

$$n(\omega) = 1 - \delta + i\beta \qquad (3.12)$$

$$l_{\text{abs}} = \frac{\lambda}{4\pi\beta} \qquad (3.22)$$

$$\sigma_{\text{abs.}} = 2 r_e \lambda f_2^0(\omega) \qquad (3.28)$$

$$\Delta\phi = \left(\frac{2\pi\delta}{\lambda}\right)\Delta r \qquad (3.29)$$

$$\theta_c = \sqrt{2\delta} \qquad (3.41)$$

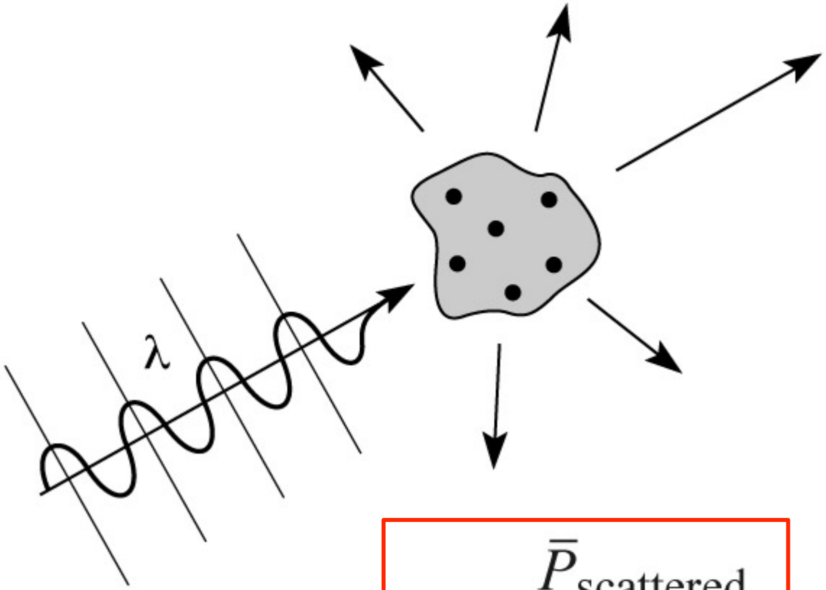
$$R_{s,\perp} \simeq \frac{\delta^2 + \beta^2}{4} \qquad (3.50)$$

$$\phi_B \simeq \frac{\pi}{4} - \frac{\delta}{2} \qquad (3.60)$$

Ch03_F00VG.ai

Scattering cross-sections

Measures the ability of an object to remove particles or photons from a directed beam and send them into new directions



Diminished by both scattering and absorption

$$\boxed{\sigma \equiv \frac{\bar{P}_{\text{scattered}}}{|\bar{\mathbf{S}}|}}$$

$$\left[\text{area} = \frac{(\text{power})}{(\text{power/area})}\right]$$

- Isotropic or anisotropic?
- Energy or wavelength dependent?

Ch02_ScattCrSecs.ai

Scattering by a free electron

Define the cross-section as the average power radiated to all angles, divided by the average incident power per unit area

$$\sigma \equiv \frac{\bar{P}_{\text{scatt.}}}{|\bar{\mathbf{S}}_i|} \tag{2.38}$$

For an incident electromagnetic wave of electric field $\mathbf{E}_i(\mathbf{r},t)$

$$\bar{\mathbf{S}} = \frac{1}{2}\sqrt{\frac{\epsilon_0}{\mu_0}}\,|\mathbf{E}_i|^2\,\mathbf{k}_0 \tag{2.39}$$

For a free electron the incident field causes an oscillatory motion described by Newton's second equation of motion, $\mathbf{F} = m\mathbf{a}$, where $\mathbf{F}$ is the Lorentz force on the electron

$$m\mathbf{a} = -e[\mathbf{E}_i + \cancelto{\text{small}}{\mathbf{v} \times \mathbf{B}_i}] \tag{2.40}$$

Thus the instantaneous acceleration is

$$\mathbf{a}(\mathbf{r},t) = -\frac{e}{m}\mathbf{E}_i(\mathbf{r},t) \tag{2.42}$$

Ch02_ScattFreElctrn1.ai

Power radiated by an accelerated point charge, λ >> a

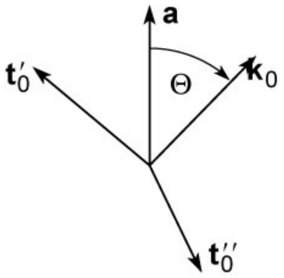
From the wave equation, for an electron with acceleration **a**

$$\mathbf{E}(\mathbf{r},t)=\frac{e\mathbf{a}_T\,(t-r/c)}{4\pi\epsilon_0 c^2 r}\qquad(2.25)\qquad\text{and}\qquad \mathbf{S}(\mathbf{r},t)=\sqrt{\frac{\epsilon_0}{\mu_0}}|\mathbf{E}|^2\mathbf{k}_0\qquad(2.31)$$

one obtains the *instantaneous power per unit area* radiated by an accelerated electron

$$\mathbf{S}(\mathbf{r},t)=\frac{e^2|\mathbf{a}_T|^2}{16\pi^2\epsilon_0 c^3 r^2}\mathbf{k}_0\qquad(2.32)\qquad\left\{\begin{array}{l}\mathbf{k}_0,\ \text{propagation direction}\\ |\mathbf{a}_T|=|\mathbf{a}|\sin\Theta\end{array}\right.$$

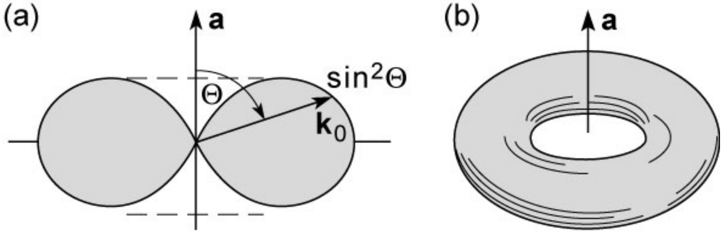
For an angle Θ between the direction of acceleration, **a**, and the observation direction, $\mathbf{k}_0$, the instantaneous power per unit area is



$$\mathbf{S}(\mathbf{r},t)=\frac{e^2|\mathbf{a}|^2\sin^2\Theta}{16\pi^2\epsilon_0 c^3 r^2}\mathbf{k}_0\qquad(2.33)$$

Noting that **S** = (*dP*/*dA*)$\mathbf{k}_0$ and *dA* = $r^2\,d\Omega$, one obtains the power per unit solid angle

$$\boxed{\frac{dP}{d\Omega}=\frac{e^2|\mathbf{a}|^2\sin^2\Theta}{16\pi^2\epsilon_0 c^3}}\qquad(2.34)$$



the well known “donut-shaped” radiation pattern characteristic of a radiator whose size is much smaller than the wavelength (“dipole radiation”).

Ch02_PowrRadiatd_Apr2010.ai

Total power radiated by an accelerated point charge

The total power radiated, P, is determined by integrating $\mathbf{S}$ over the area of a distant sphere:

$$P = \iint_{\text{area}} \mathbf{S} \cdot d\mathbf{A} = \iint_{\substack{\text{solid}\\ \text{angle}}} \mathbf{S} \cdot (r^2\, d\Omega\, \mathbf{k}_0) \qquad (2.35)$$

where for $0 \le \Theta \le \pi$ and $0 \le \phi \le 2\pi$ we have $d\Omega = \sin\Theta\, d\Theta\, d\phi$, thus

$$P = \iint \left[\frac{e^2 |\mathbf{a}|^2 \sin^2\Theta}{16\pi^2 \epsilon_0 c^3 r^2} \mathbf{k}_0 \right] \cdot r^2 \sin\Theta\, d\Theta\, d\phi\, \mathbf{k}_0$$

Thus the *instantaneous power radiated* to all angles by an oscillating electron of acceleration a is

$$\boxed{P = \frac{8\pi}{3} \left(\frac{e^2 |\mathbf{a}|^2}{16\pi^2 \epsilon_0 c^3} \right)} \qquad (2.36)$$

For sinusoidal motion, averaging over a full cycle, $\sin^2\omega t$ or $\cos^2\omega t$, introduces a factor of 1/2

$$\bar{P} = \frac{1}{2} \cdot \frac{8\pi}{3} \left(\frac{e^2 |\mathbf{a}|^2}{16\pi^2 \epsilon_0 c^3} \right)$$

Ch02_TotalPwrRad_Apr2010.ai

Scattering by a free electron (continued)

The average power scattered by an oscillating electron is

$$\bar{P}_{\text{scatt.}} = \frac{1}{2}\,\frac{8\pi}{3}\,\frac{e^2\left(\dfrac{e^2}{m^2}|\mathbf{E}_i|^2\right)}{16\pi^2\epsilon_0 c^3}$$

The scattering cross-section is

$$\sigma = \frac{\bar{P}_{\text{scatt.}}}{|\bar{\mathbf{S}}|} = \frac{\dfrac{4\pi}{3}\left(\dfrac{e^4|\mathbf{E}_i|^2}{16\pi^2\epsilon_0 m^2 c^3}\right)}{\dfrac{1}{2}\sqrt{\dfrac{\epsilon_0}{\mu_0}}\,|\mathbf{E}_i|^2}$$

Introducing the "classical electron radius"

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2} \tag{2.44}$$

One obtains the scttering cross-section for a single free electron

$$\boxed{\sigma_e = \frac{8\pi}{3}r_e^2} \tag{2.45}$$

which we observe is independent of wavelength. This is referred to as the Thomson cross-section (for a free electron), after J.J. Thomson. Numerically $r_e = 2.82 \times 10^{-13}$ cm and $\sigma_e = 6.65 \times 10^{-25}$ cm^2. The differential Thomson scattering cross-section is

Ch02_ScattFreElctrn2_Apr2010.ai

Scattering by a bound electron

For an electromagnetic wave incident upon a bound electron of resonant frequency ω_s, the force equation can be written semi-classically as

$$m\frac{d^2\mathbf{x}}{dt^2}+m\gamma\frac{d\mathbf{x}}{dt}+m\omega_s^2\mathbf{x}=-e(\mathbf{E}_i+\underbrace{\mathbf{v}\times\mathbf{B}_i}_{\simeq 0}) \qquad (2.48)$$

with an acceleration term (m**a**), a damping term, a restoring force term, and the Lorentz force exerted by the fields. For an incident electric field

$$\mathbf{E}=\mathbf{E}_i e^{-i\omega t}$$

the harmonic motion will be driven at the same frequency, ω, so that

$$\mathbf{x}=\frac{1}{\omega^2-\omega_s^2+i\gamma\omega}\frac{e\mathbf{E}_i}{m} \qquad (2.49)$$

$$\mathbf{a}=\frac{-\omega^2}{\omega^2-\omega_s^2+i\gamma\omega}\frac{e\mathbf{E}_i}{m} \qquad (2.50)$$

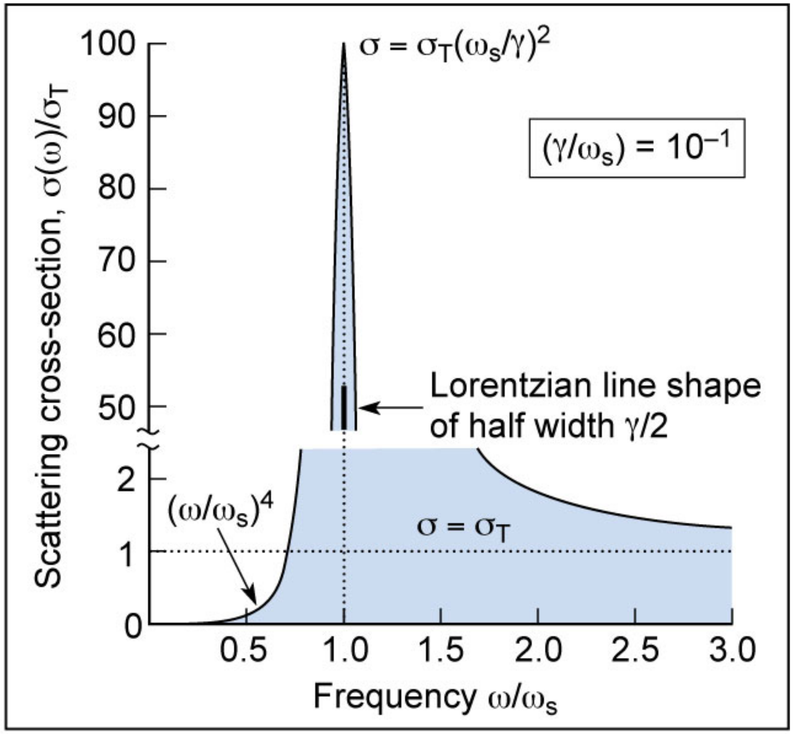
Following the same procedures used earlier, one obtains the scattering cross-section for a bound electron of resonant frequency, ω_s

$$\boxed{\sigma=\frac{8\pi}{3}r_e^2\frac{\omega^4}{(\omega^2-\omega_s^2)^2+(\gamma\omega)^2}} \qquad (2.51)$$

Ch02_ScattBndElctrn_Apr2010.ai

Semi-classical scattering cross-section for a bound electron

$$\boxed{\sigma = \frac{8\pi}{3} r_e^2 \frac{\omega^4}{\left(\omega^2 - \omega_s^2\right)^2 + (\gamma\omega)^2}} \qquad (2.51)$$



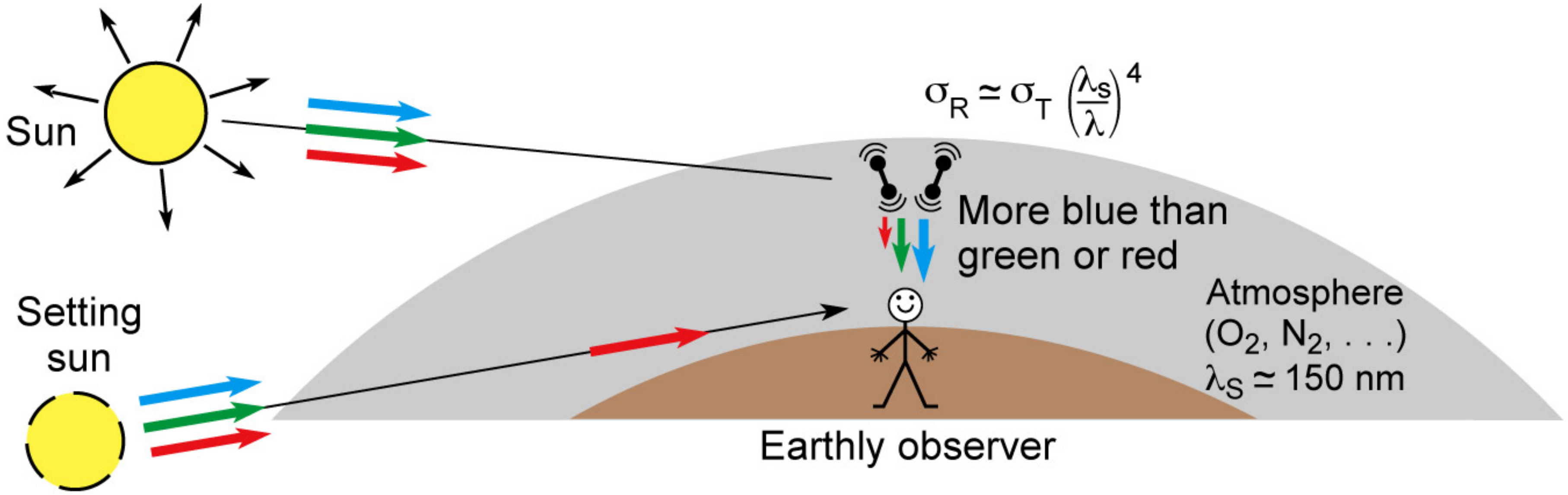
Note that below the resonance, for $\omega^2 << \omega_s^2$

$$\sigma_R = \frac{8\pi}{3} r_e^2 \left(\frac{\omega}{\omega_s}\right)^4 = \frac{8\pi}{3} r_e^2 \left(\frac{\lambda_s}{\lambda}\right)^4 \qquad (2.52)$$

This is the Rayleigh scattering cross-section (1899) for a bound electron, with $\omega/\omega_s << 1$, which displays a very strong λ^{-4} wavelength dependence.

Ch02_SemiClassScatt_Apr2010.ai

The sky appears blue because of the strong wave length dependence of scattering by bound electrons



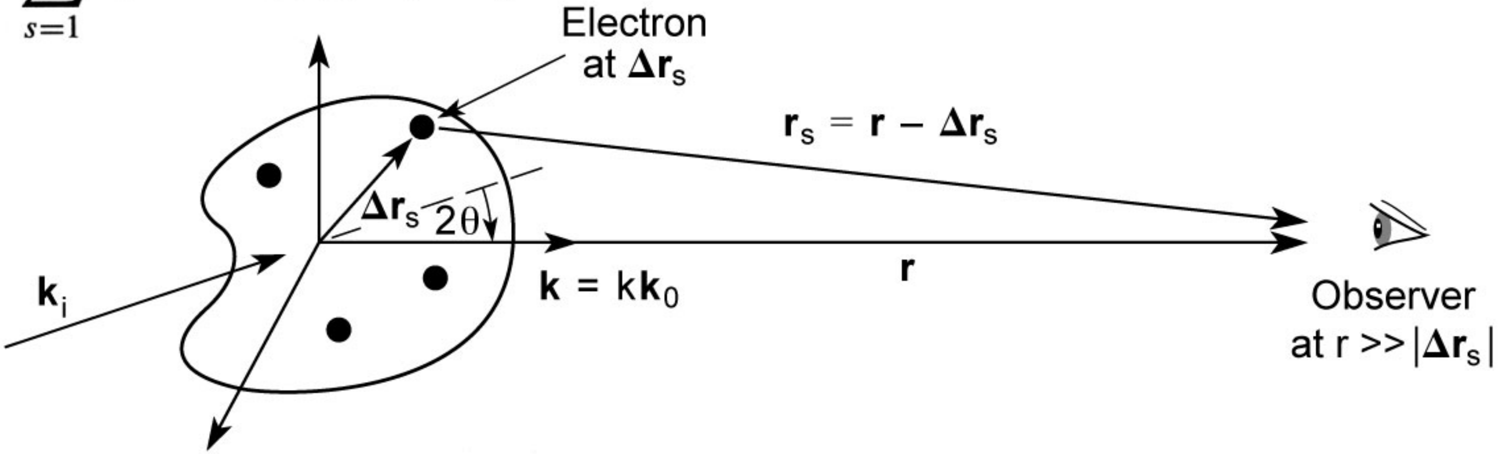
- UV resonances in O_2 and N_2, at 8.6 and 8.2 eV
- Red (1.8 eV, 700 nm), green (2.3 eV, 530 nm), and blue light (3.3 eV, 380 nm)
- Density fluctuations essential
- Long path at sunset, color of clouds
- Photon energy and wavelength effects. Volcanic eruptions

Ch02_F09VG.ai

Scattering by a multi-electron atom

Semi-classical model of an atom with Z electrons and nucleus of charge +Ze at **r** = 0.

$$n(\mathbf{r}, t) = \sum_{s=1}^{Z} \delta[\mathbf{r} - \Delta\mathbf{r}_s(t)] \quad (2.53)$$



For each electron

$$m\frac{d^2\mathbf{x}_s}{dt^2} + m\gamma\frac{d\mathbf{x}_s}{dt} + m\omega_s^2\mathbf{x}_s = -e(\mathbf{E}_i + \underbrace{\mathbf{v}_s \times \mathbf{B}}_{\simeq 0}) \quad (2.58)$$

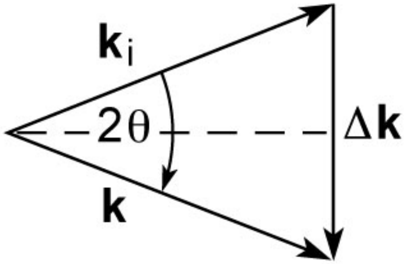
The acceleration has an additional phase term due to the position, $\Delta\mathbf{r}_s$, within the atom:

$$\mathbf{a}_s(t) = \frac{-\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega}\,\frac{e}{m}\,\mathbf{E}_i\, e^{-i(\omega t \boxed{-\mathbf{k}_i\cdot\Delta\mathbf{r}_s)}} \quad (2.61)$$

Ch02_ScattMultiElctrn1_Apr2010.ai

Scattering by a multi-electron atom (continued)

$$E(\mathbf{r},t) = -\frac{r_e}{r}\underbrace{\left[\sum_{s=1}^{Z}\frac{\omega^2 e^{-i\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s}}{\omega^2-\omega_s^2+i\gamma\omega}\right]}_{f(\Delta\mathbf{k},\,\omega)} E_i \sin\Theta\, e^{-i\omega(t-r/c)} \qquad (2.65)$$



$\Delta\mathbf{k} = \mathbf{k} - \mathbf{k}_i$

$|\Delta\mathbf{k}| = 2k_i \sin\theta$

where the quantity $f(\Delta\mathbf{k}, \omega)$ is the complex atomic scattering factor, which tells us the scattered electric field due to a multi-electron atom, relative to that of a single free electron (eq. 2.43). Note the dependence on frequency ω (photon energy $\hbar\omega$), the various resonant frequencies ω_s (resonant energies $\hbar\omega_s$), and the phase terms due to the various positions of electrons within the atom, $\Delta\mathbf{k} \cdot \Delta\mathbf{r}_s$.

Ch02_ScattMultiElctrn2.ai

The atomic scattering factor

$$\boxed{f(\Delta\mathbf{k},\omega)=\sum_{s=1}^{Z}\frac{\omega^2 e^{-i\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s}}{\omega^2-\omega_s^2+i\gamma\omega}} \qquad (2.66)$$

In general the $\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s$ phase terms do not simplify, but in two cases they do. Noting that $|\Delta\mathbf{k}| = 2k_i \sin\theta = 4\pi/\lambda \sin\theta$, and that the radius of the atom is of order the Bohr radius, a_0, the phase factor is then bounded by

$$|\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s| \le \frac{4\pi a_0}{\lambda}\sin\theta \qquad (2.70)$$

The atomic scattering factor $f(\Delta\mathbf{k},\omega)$ simplifies significantly when

$$|\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s| \to 0 \quad \text{for } a_0/\lambda \ll 1 \quad \text{(long wavelength limit)} \qquad (2.71a)$$

$$|\Delta\mathbf{k}\cdot\Delta\mathbf{r}_s| \to 0 \quad \text{for } \theta \ll 1 \quad \text{(forward scattering)} \qquad (2.71b)$$

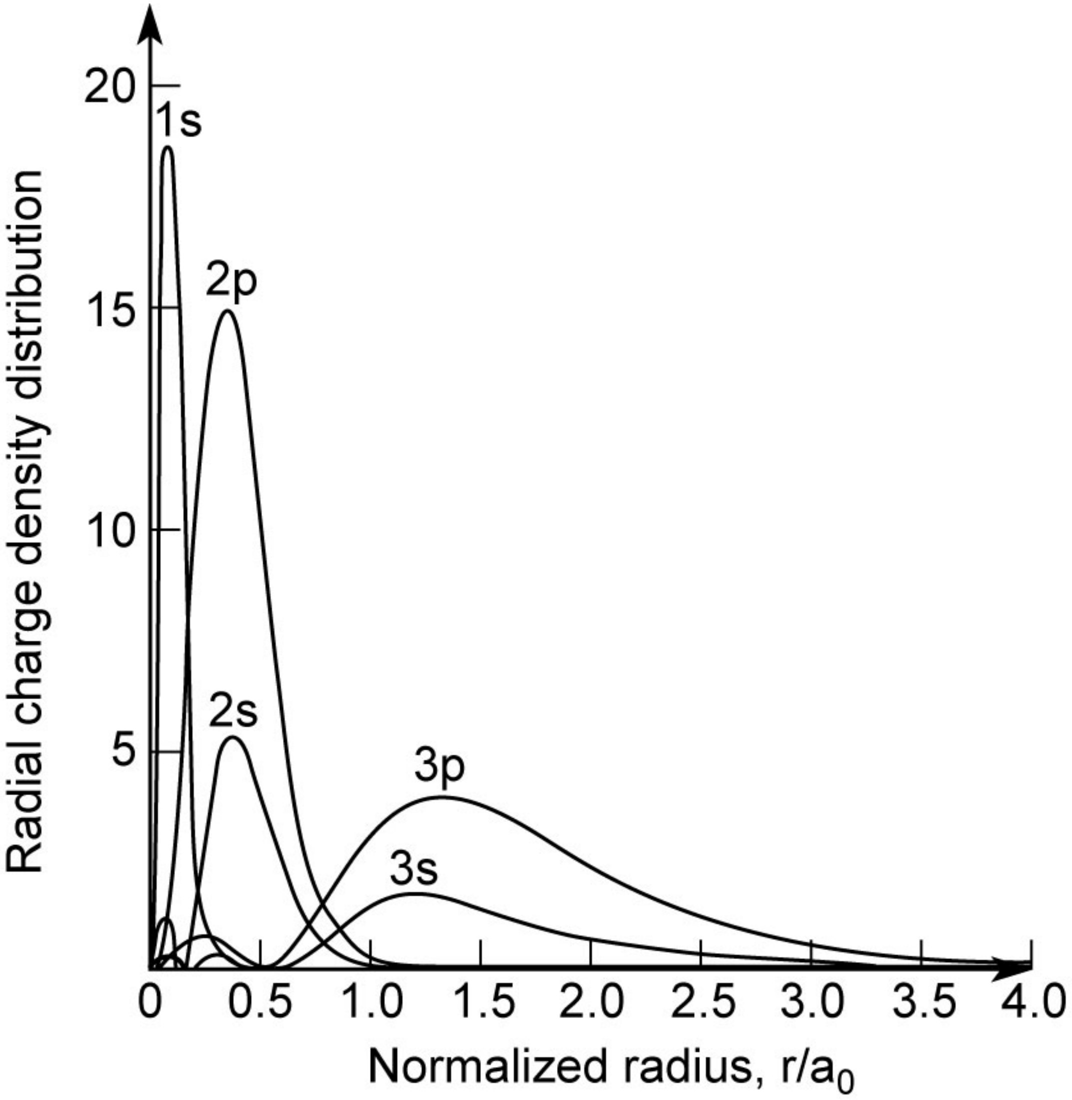
In each of these two cases the atomic scattering factor $f(\Delta\mathbf{k},\omega)$ reduces to

$$\boxed{f^0(\omega)=\sum_{s=1}^{Z}\frac{\omega^2}{\omega^2-\omega_s^2+i\gamma\omega}} \qquad (2.72)$$

where we denote these special cases by the superscript zero.

Ch02_AtomcScatFac_Apr2010.ai

Probabilistic radial charge distribution (e/Å) in the Argon atom



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

Ch01_F12.ai

Refractive index for x-rays

The refractive index, $n(\omega)$, is complex because EUV/soft x-ray radiation is absorbed appreciably by all atoms. This is reflected in the semi-classical model

$$n(\omega) = 1 - \frac{1}{2}\frac{e^2 n_a}{\epsilon_0 m}\sum_s \frac{g_s}{(\omega^2 - \omega_s^2) + i\gamma\omega} \qquad (3.8)$$

where again $\sum_s g_s = Z$ (2.73), or by its quantum mechanical equivalent $\sum_{k,n} g_{kn} = Z$. (2.74)

The convention is to express scattering and refractive index in terms of a complex scattering factor, $f^0(\omega)$ specific to each element

$$f^0(\omega) = f_1^0(\omega) - i f_2^0(\omega) = \sum_s \frac{g_s\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega}$$

where the scattering factor arises from consideration of the scattered electric field due to an atom, relative to that of a free electron. Introducing the classical electron radius

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2} \qquad (2.44)$$

The refractive index can be written as

$$\boxed{n(\omega) = 1 - \frac{n_a r_e \lambda^2}{2\pi}\left[f_1^0(\omega) - i f_2^0(\omega)\right]} \qquad (3.9)$$

or in simpler notation

$$\boxed{n(\omega) = 1 - \delta + i\beta} \qquad (3.12)$$

RefractiveIndex_Jan20162.ai

Complex atomic scattering factors

$$f^0(\omega) = \sum_{s=1}^{Z} \frac{\omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega} = f_1^0(\omega) - i f_2^0(\omega) \qquad \begin{matrix}(2.72)\\(2.79)\end{matrix}$$

which some write as

$$f(\omega) = Z - f_1(\omega) - i f_2(\omega)$$

Ch02_ComplexAtomScatFac.ai

Atomic scattering cross-sections

Comparing the scattered electric field for a multi-electron atom (2.65) with that for the free electron (2.43), the atomic scattering cross-sections are readily determined by the earlier proceedures to be

$$\boxed{\frac{d\sigma(\omega)}{d\Omega} = r_e^2 |f^0(\omega)|^2 \sin^2 \Theta} \tag{2.75}$$

$$\boxed{\sigma(\omega) = \frac{8\pi}{3} r_e^2 |f^0(\omega)|^2} \tag{2.76}$$

where

$$\boxed{f^0(\omega) = \sum_s \frac{g_s \omega^2}{\omega^2 - \omega_s^2 + i\gamma\omega}} \tag{2.77}$$

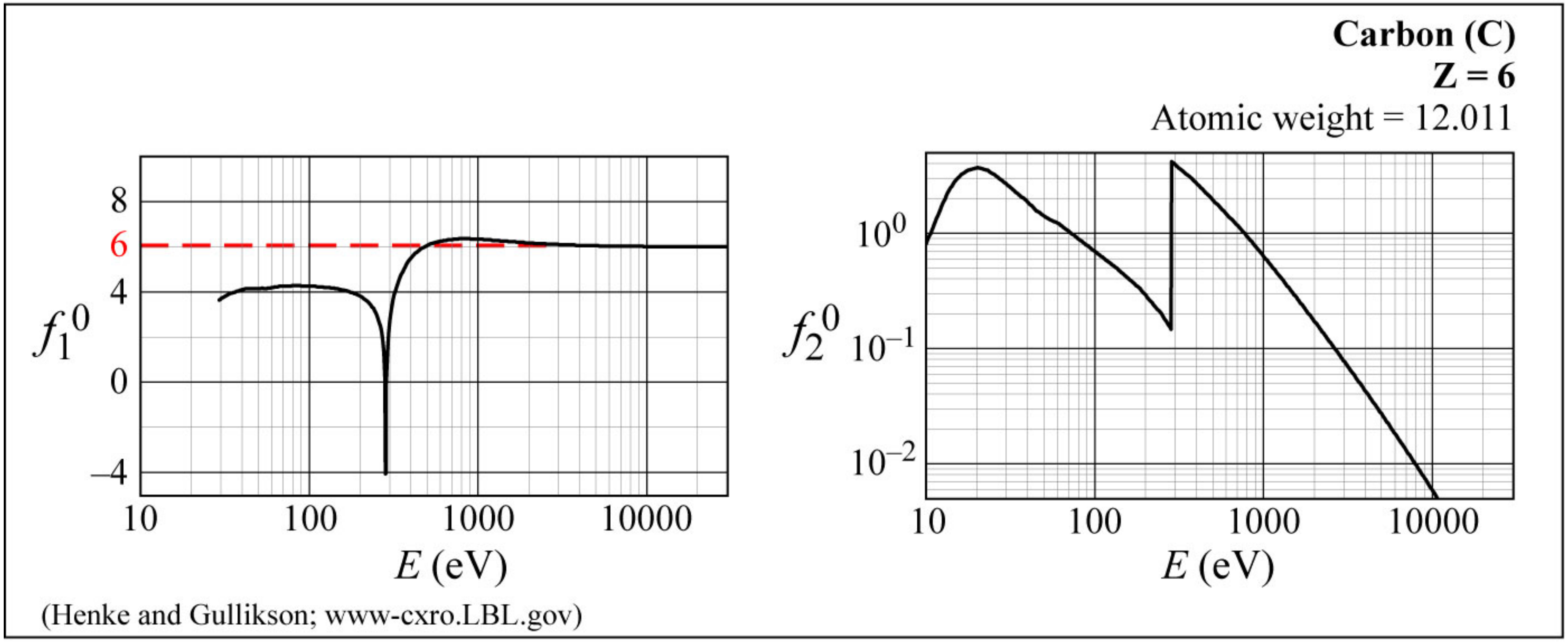
and where the super-script zero refers to the special circumstances of long wavelength ($\lambda >> a_0$) or forward scattering ($\theta << 1$). With the Bohr radius $a_0 = 0.529$ Å, the long wavelength condition is easily satisfied for soft x-rays and EUV. Note too that we have introduced the concept of oscillator strengths, g_s, associated with each resonance, normalized by the condition

$$\sum_s g_s = Z \tag{2.73}$$

Ch02_AtomcScatXSec.ai

Example: complex atomic scattering factor for carbon

$$f^0(\omega) = f_1^0(\omega) - i f_2^0(\omega) \qquad (2.79)$$



(Henke and Gullikson; www-cxro.LBL.gov)

Note that for $\hbar\omega >> \hbar\omega_s$, $f_1^0 \rightarrow Z$. This works here for carbon $f_1^0 \rightarrow 6$, but note that in general this conflicts with the condition $\lambda >> a_0$. For the case of carbon at 4 Å wavelength ($\lambda >> a_0$), and thus $\hbar\omega = 3$ keV ($>> \hbar\omega_s \sim 274$ eV), the atomic scattering cross-section (2.76) becomes

$$\sigma(\omega) \simeq \frac{8\pi}{3} r_e^2 Z^2 = \underline{Z^2 \sigma_e} \qquad (2.78c)$$

that is, all Z electrons are scattering cooperatively (in-phase) - the so-called N^2 effect.

Ch02_Ex_ComplxAtomc_Apr2010.ai

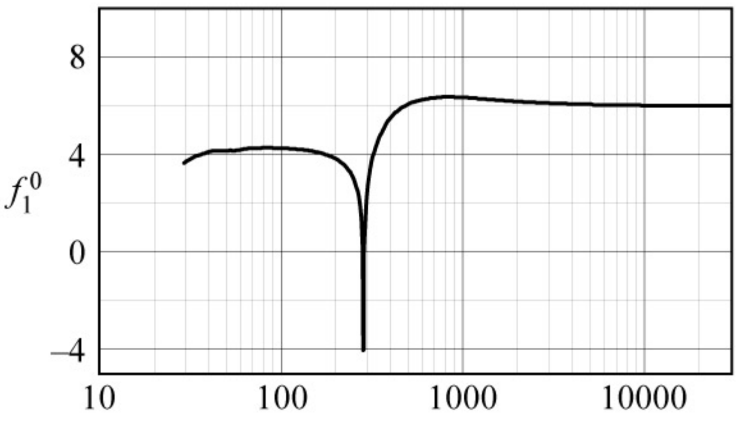
Atomic scattering factors for carbon (Z = 6)

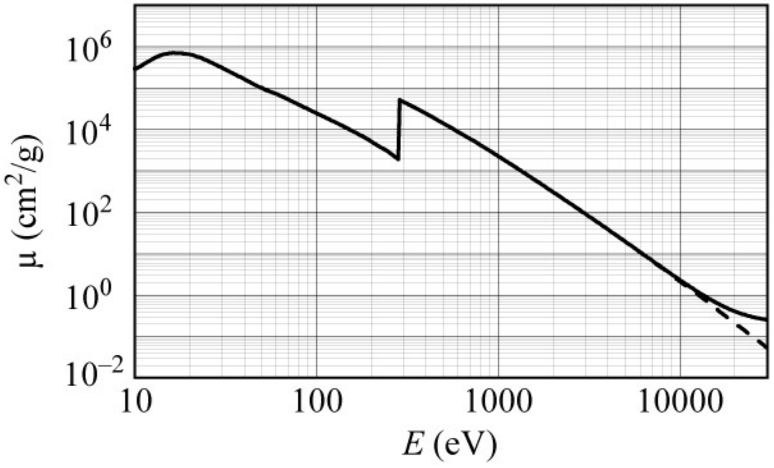
$\sigma_a(\text{barns/atom}) = \mu(\text{cm}^2/\text{g}) \times 19.95$

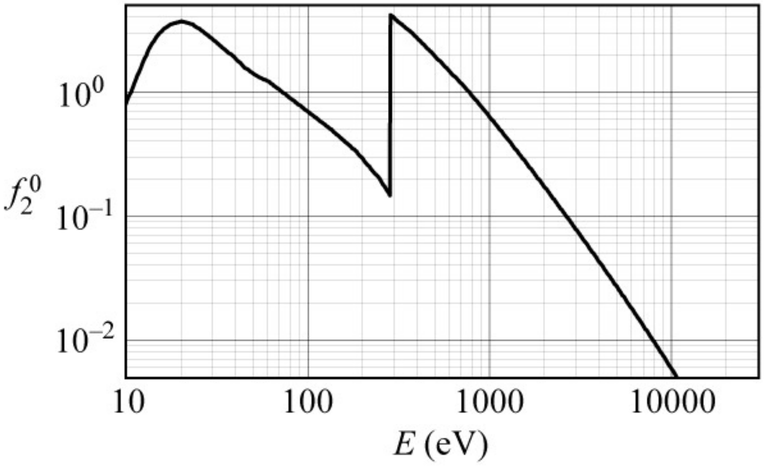
$E(\text{keV})\mu(\text{cm}^2/\text{g}) = f_2^0 \times 3503.31$

Carbon (C)
Z = 6
Atomic weight = 12.011

Energy (eV)	f_1^0	f_2^0	μ (cm^2/g)
30	3.692	2.664E+00	3.111E+05
70	4.249	1.039E+00	5.201E+04
100	4.253	6.960E-01	2.438E+04
300	2.703	3.923E+00	4.581E+04
700	6.316	1.174E+00	5.878E+03
1000	6.332	6.328E–01	2.217E+03
3000	6.097	7.745E–02	9.044E+01
7000	6.025	1.306E–02	6.536E+00
10000	6.013	5.892E–03	2.064E+00
30000	6.000	4.425E–04	5.168E–02





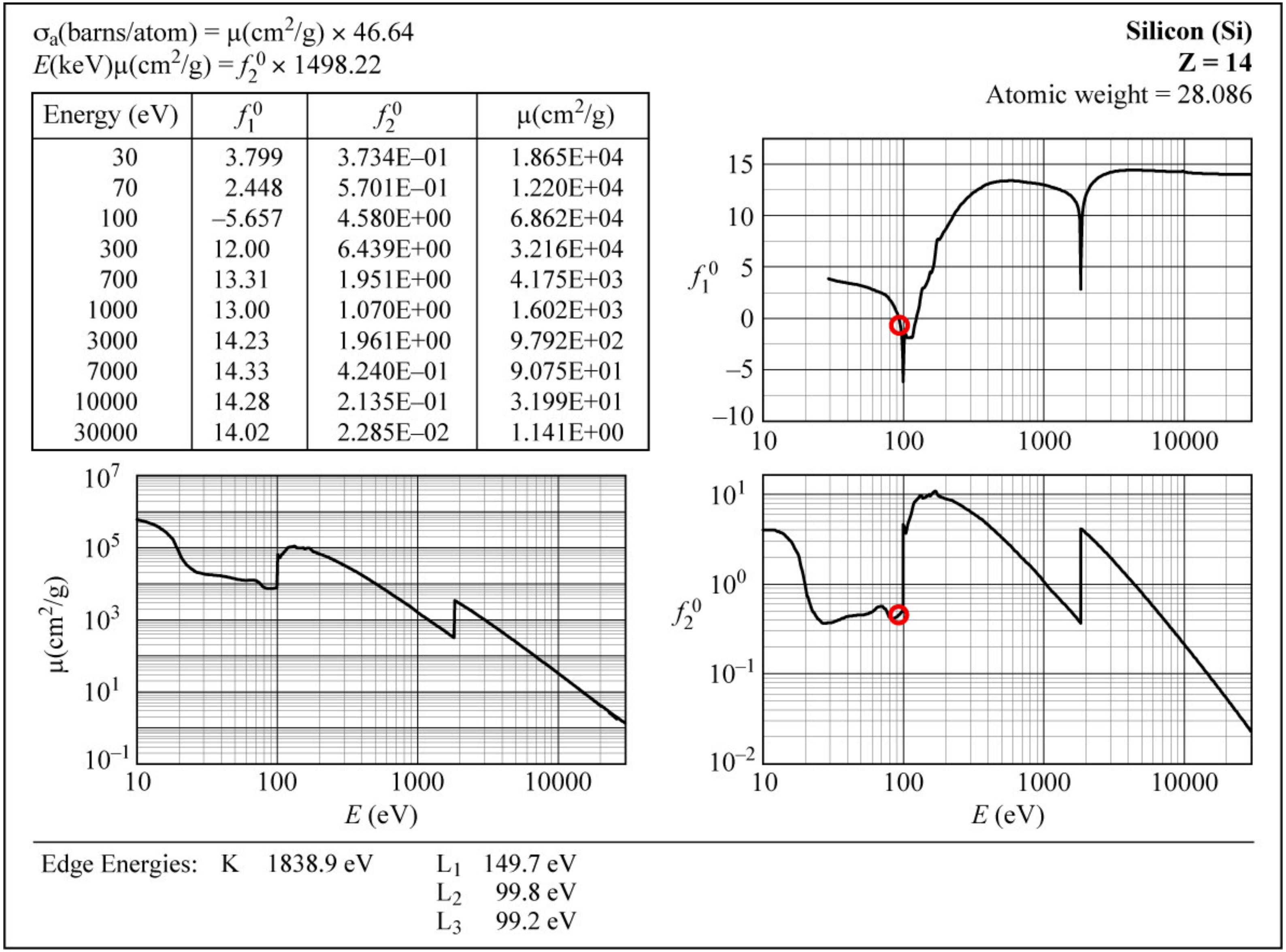


Edge Energies: K 284.2 eV

(Henke and Gullikson; www-cxro.LBL.gov)

Ch02_F13VG.ai

Atomic scattering factors for silicon (Z = 14)



σ_a(barns/atom) = μ(cm^2/g) × 46.64
E(keV)μ(cm^2/g) = f_2^0 × 1498.22

Silicon (Si)
Z = 14
Atomic weight = 28.086

Energy (eV)	f_1^0	f_2^0	μ(cm^2/g)
30	3.799	3.734E–01	1.865E+04
70	2.448	5.701E–01	1.220E+04
100	–5.657	4.580E+00	6.862E+04
300	12.00	6.439E+00	3.216E+04
700	13.31	1.951E+00	4.175E+03
1000	13.00	1.070E+00	1.602E+03
3000	14.23	1.961E+00	9.792E+02
7000	14.33	4.240E–01	9.075E+01
10000	14.28	2.135E–01	3.199E+01
30000	14.02	2.285E–02	1.141E+00

Edge Energies: K 1838.9 eV
L_1 149.7 eV
L_2 99.8 eV
L_3 99.2 eV

(Henke and Gullikson; www-cxro.LBL.gov)

Ch02ApC_Tb1F07_Sept05.ai

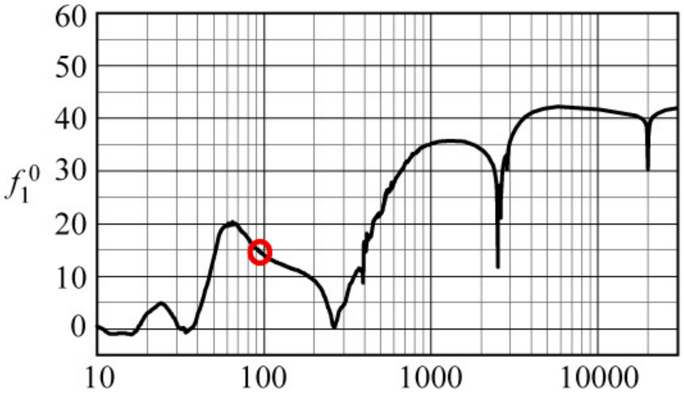
Atomic scattering factors for molybdenum (Z = 42)

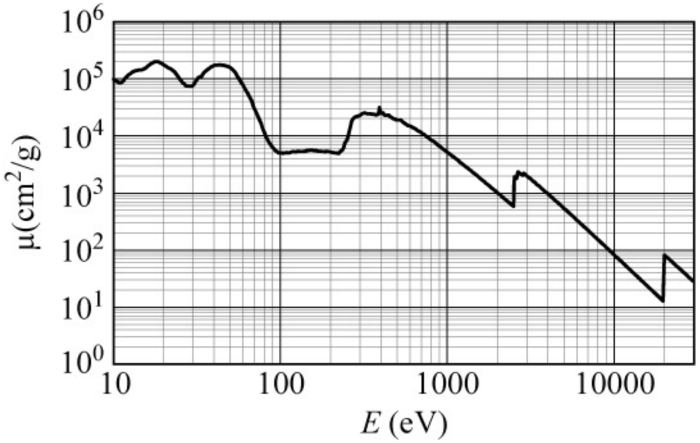
$\sigma_a(\text{barns/atom}) = \mu(\text{cm}^2/\text{g}) \times 159.31$

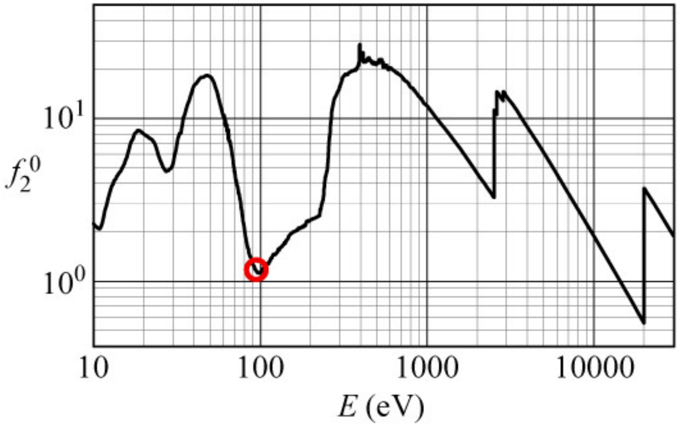
$E(\text{keV})\mu(\text{cm}^2/\text{g}) = f_2^0 \times 438.59$

Molybdenum (Mo)
Z = 42
Atomic weight = 95.940

Energy (eV)	f_1^0	f_2^0	$\mu(\text{cm}^2/\text{g})$
30	1.071	5.292E+00	7.736E+04
70	19.38	4.732E+00	2.965E+04
100	14.02	1.124E+00	4.931E+03
300	4.609	1.568E+01	2.292E+04
700	31.41	1.819E+01	1.140E+04
1000	35.15	1.188E+01	5.210E+03
3000	35.88	1.366E+01	1.997E+03
7000	42.11	3.493E+00	2.189E+02
10000	41.67	1.881E+00	8.248E+01
30000	42.04	1.894E+00	2.769E+01







Edge Energies:

K 19999.5 eV	L_1	2865.5 eV	M_1	506.3 eV	N_1	63.2 eV
	L_2	2625.1 eV	M_2	411.6 eV	N_2	37.6 eV
	L_3	2520.2 eV	M_3	394.0 eV	N_3	35.5 eV
			M_4	231.1 eV		
			M_5	227.9 eV		

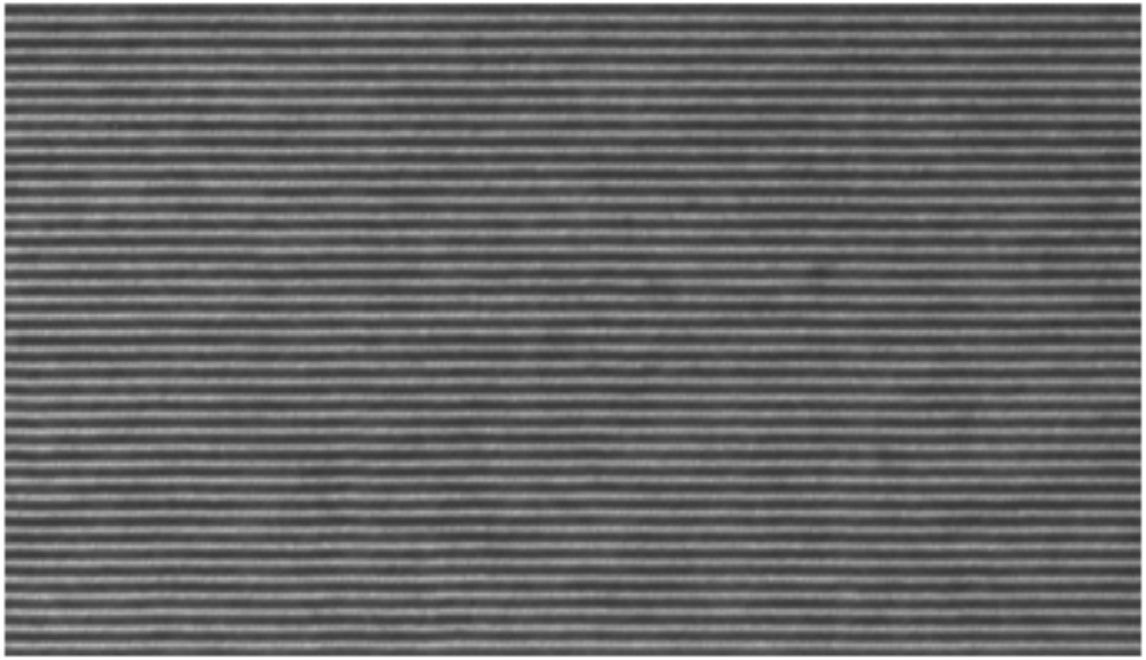
(Henke and Gullikson; www-cxro.LBL.gov)

Ch02ApC_Tb1F12_June2008.ai

A High Quality Mo/Si Multilayer Mirror

Small reflections at many interfaces add in phase at the Bragg angle

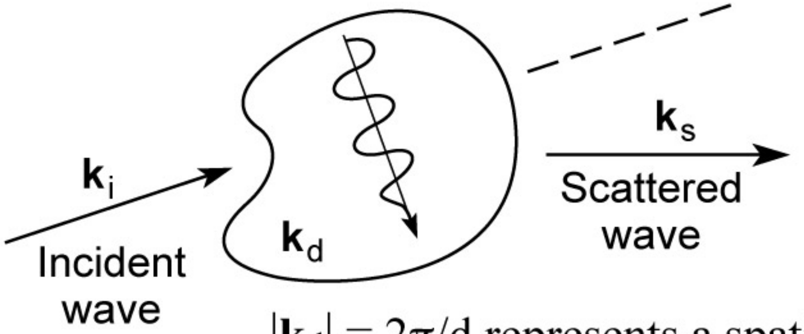
$N = 40$
$d = 6.7$



Courtesy of Saša Bajt (DESY)

Professor David Attwood / UC Berkeley / EXTATIC Lecture 1 / January 12-13, 2016 / Southampton, UK EXTATIC_Attwood1_Jan2016.pptx 23

A general scattering diagram



$$\mathbf{J}(r,t) = -e\, n(r,t)\mathbf{v}(r,t) \qquad (2.10)$$

$$\mathbf{J}_{\text{scatt}} e^{-i(\omega_s t - \mathbf{k}_s \cdot \mathbf{r})} = -e f^0(\omega_i) n_d\, e^{-i(\omega_d t - \mathbf{k}_d \cdot \mathbf{r})} \frac{-e\mathbf{E}_i}{-i\omega_i m} e^{-i(\omega_i t - \mathbf{k}_i \cdot \mathbf{r})}$$

matching exponents

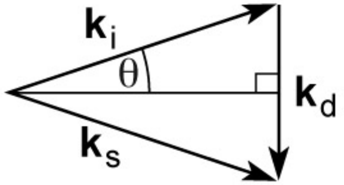
$$\omega_s = \omega_i + \omega_d$$
$$\mathbf{k}_s = \mathbf{k}_i + \mathbf{k}_d$$

$|\mathbf{k}_d| = 2\pi/d$ represents a spatial non-uniformity in the medium, such as atoms of periodicity d, a grating, or a density distribution due to a wave motion.

If the density distribution is stationary

$$\left.\begin{aligned} |\mathbf{k}_i| &= \frac{\omega}{c} = \frac{2\pi}{\lambda} \\ |\mathbf{k}_s| &= \frac{\omega}{c} = \frac{2\pi}{\lambda} \end{aligned}\right\}$$

∴ the scattering diagram is isosceles



$$\mathbf{k}_i + \mathbf{k}_d = \mathbf{k}_s$$

$$\sin\theta = \frac{k_d/2}{k_i}$$

$$\sin\theta = \frac{\lambda}{2d}$$

$$\lambda = 2d \sin\theta \qquad (2.62)$$

(Bragg's Law, 1913)

(Reference: See chapter 4, eqs. 4.1 to 4.6)

Ch02_GenScattDia.ai

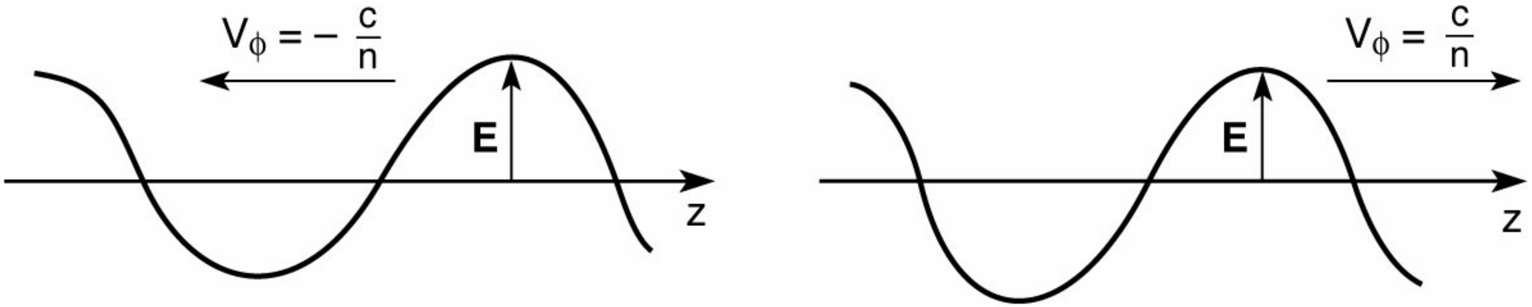
Phase velocity and refractive index

The wave equation can be written as

$$\left(\frac{\partial}{\partial t} - \frac{c}{n(\omega)}\nabla\right)\left(\frac{\partial}{\partial t} + \frac{c}{n(\omega)}\nabla\right)\mathbf{E}_T(\mathbf{r}, t) = 0 \qquad (3.10)$$

The two bracketed operators represent left and right-running waves

$$\left(\frac{\partial}{\partial t} - \frac{c}{n}\frac{\partial}{\partial z}\right)E_x = 0 \qquad\qquad \left(\frac{\partial}{\partial t} + \frac{c}{n}\frac{\partial}{\partial z}\right)E_x = 0$$



Left-running wave

Right-running wave

where the phase velocity, the speed with which crests of fixed phase move, is not equal to c as in vacuum, but rather is

$$\boxed{v_\phi = \frac{c}{n(\omega)}} \qquad (3.11)$$

Ch03_PhasVelo_Refrc1.ai

Phase variation and absorption of propagating waves

For a plane wave $$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 e^{-i(\omega t - \mathbf{k}\cdot\mathbf{r})} \tag{3.14}$$

in a material of refractive index n, the complex dispersion relation is

$$\frac{\omega}{k} = \frac{c}{n} = \frac{c}{1 - \delta + i\beta} \tag{3.15}$$

Solving for k

$$k = \frac{\omega}{c}(1 - \delta + i\beta) \tag{3.16}$$

Substituting this into (3.14), in the propagation direction defined by **k** · **r** = kr

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 e^{-i[\omega t - (\omega/c)(1-\delta+i\beta)r]}$$

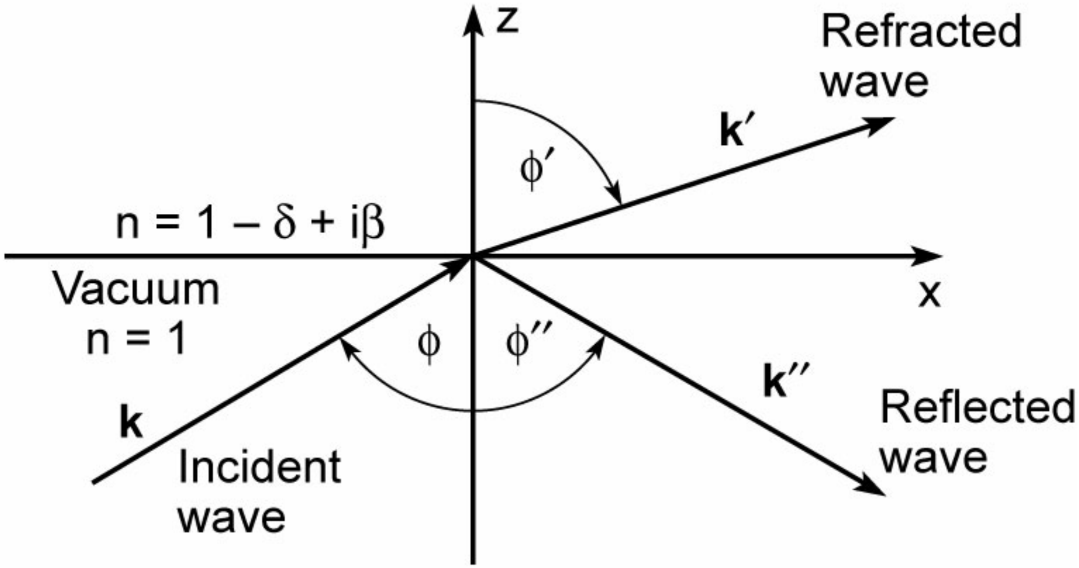
or

$$\mathbf{E}(\mathbf{r}, t) = \underbrace{\mathbf{E}_0 e^{-i\omega(t - r/c)}}_{\text{vacuum propagation}} \underbrace{e^{-i(2\pi\delta/\lambda)r}}_{\phi\text{-shift}} \underbrace{e^{-(2\pi\beta/\lambda)r}}_{\text{decay}} \tag{3.17}$$

where the first exponential factor represents the phase advance had the wave been propagating in vacuum, the second factor (containing 2πδr/λ) represents the modified phase shift due to the medium, and the factor containing 2πβr/λ represents decay of the wave amplitude.

Ch03_PhaseVarAbsrb.ai

Reflection and refraction at an interface



incident wave: $\mathbf{E} = \mathbf{E}_0 e^{-i(\omega t - \mathbf{k}\cdot\mathbf{r})}$ (3.30a)

refracted wave: $\mathbf{E}' = \mathbf{E}_0' e^{-i(\omega t - \mathbf{k}'\cdot\mathbf{r})}$ (3.30b)

reflected wave: $\mathbf{E}'' = \mathbf{E}_0'' e^{-i(\omega t - \mathbf{k}''\cdot\mathbf{r})}$ (3.30c)

(1) All waves have the same frequency, ω, and $|\mathbf{k}| = |\mathbf{k}''| = \dfrac{\omega}{c}$

(2) The refracted wave has phase velocity

$$V_\phi = \frac{\omega'}{k'} = \frac{c}{n} \quad \text{, thus } k' = |\mathbf{k}'| = \frac{\omega}{c}(1 - \delta + i\beta)$$

Ch03_ReflctnRefrctn_Sept05.ai

Boundary conditions at an interface

- **E** and **H** components parallel to the interface must be continuous

$$\mathbf{z}_0 \times (\mathbf{E}_0 + \mathbf{E}_0'') = \mathbf{z}_0 \times \mathbf{E}_0' \qquad (3.32a)$$

$$\mathbf{z}_0 \times (\mathbf{H}_0 + \mathbf{H}_0'') = \mathbf{z}_0 \times \mathbf{H}_0' \qquad (3.32b)$$

- **D** and **B** components perpendicular to the interface must be continuous

$$\mathbf{z}_0 \cdot (\mathbf{D}_0 + \mathbf{D}_0'') = \mathbf{z}_0 \cdot \mathbf{D}_0' \qquad (3.32c)$$

$$\mathbf{z}_0 \cdot (\mathbf{B}_0 + \mathbf{B}_0'') = \mathbf{z}_0 \cdot \mathbf{B}_0' \qquad (3.32d)$$

Ch03_BndryConditns.ai

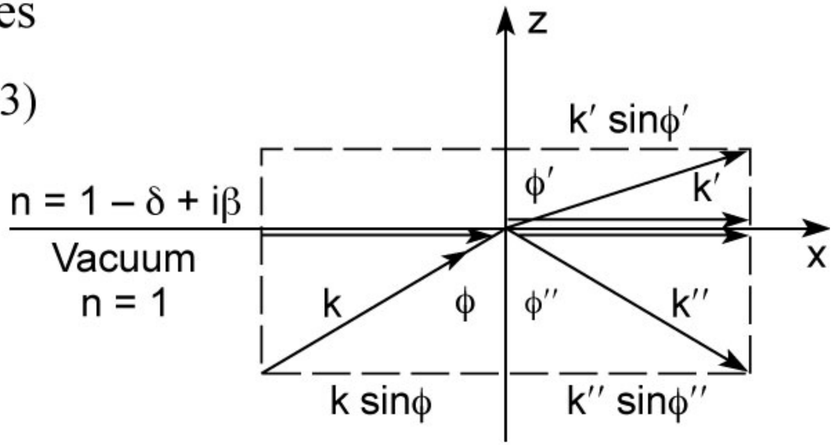
Spatial continuity along the interface

Continuity of parallel field components requires

$$(\mathbf{k}\cdot\mathbf{x}_0=\mathbf{k}'\cdot\mathbf{x}_0=\mathbf{k}''_0\cdot\mathbf{x}_0)\quad \text{at } z=0 \qquad (3.33)$$

$$k_x=k'_x=k''_x \qquad (3.34a)$$

$$k\sin\phi=k'\sin\phi'=k''\sin\phi'' \qquad (3.34b)$$



Conclusions:

Since k = k″ (both in vacuum)

$$\sin\phi=\sin\phi'' \qquad (3.35a)$$

$$\therefore\quad \boxed{\phi=\phi''} \qquad (3.35b)$$

The angle of incidence equals the angle of reflection

$$k\sin\phi=k'\sin\phi' \qquad (3.36)$$

$$k=\frac{\omega}{c}\ \text{and}\ k'=\frac{\omega'}{c/n}=\frac{n\omega}{c}$$

$$\sin\phi=n\sin\phi'$$

$$\boxed{\sin\phi'=\frac{\sin\phi}{n}} \qquad (3.38)$$

Snell’s Law, which describes refractive turning, for complex n.

Ch03_SpatialContin_Apr2010.ai

Total external reflection of soft x-ray and EUV radiation

Snell's law for a refractive index of $n \simeq 1 - \delta$, assuming that $\beta \to 0$

$$\sin\phi' = \frac{\sin\phi}{1-\delta} \qquad (3.39)$$

Consider the limit when $\phi' \to \frac{\pi}{2}$

$$1 = \frac{\sin\phi_c}{1-\delta}$$

$$\sin\phi_c = 1 - \delta \qquad (3.40)$$

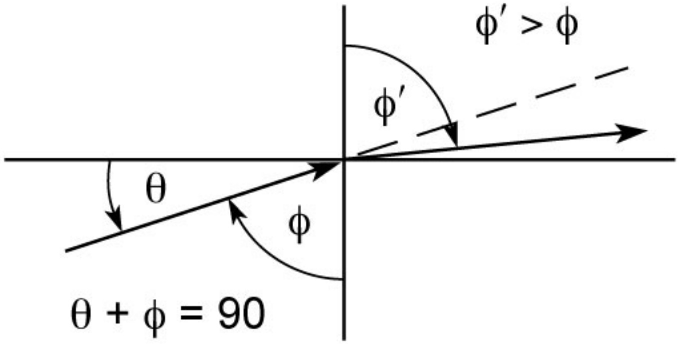
$$\sin(90^\circ - \theta_c) = 1 - \delta$$

$$\cos\theta_c = 1 - \delta$$

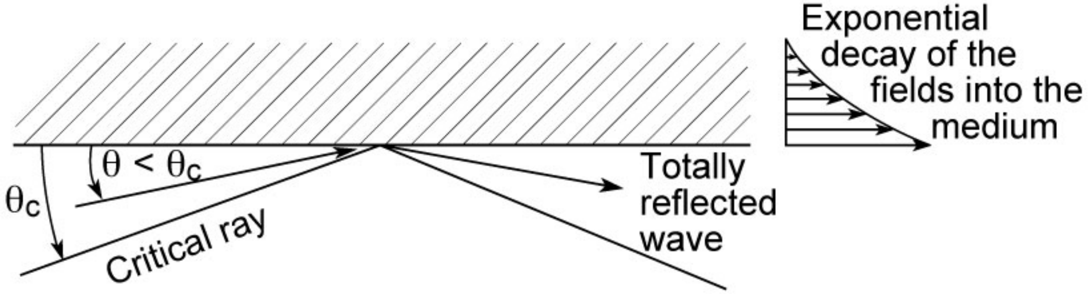
$$1 - \frac{\theta_c^2}{2} + \cdots = 1 - \delta$$

$$\boxed{\theta_c = \sqrt{2\delta}} \qquad (3.41)$$

The critical angle for total external reflection.



Glancing incidence ($\theta < \theta_c$) and total external reflection



Ch03_TotalExtrnlRflc1_Apr2010.ai

Total external reflection (continued)

$$\boxed{\theta_c = \sqrt{2\delta}} \qquad (3.41)$$

$$\delta = \frac{n_a r_e \lambda^2 f_1^0(\lambda)}{2\pi}$$

$$\theta_c = \sqrt{2\delta} = \sqrt{\frac{n_a r_e \lambda^2 f_1^0(\lambda)}{\pi}} \qquad (3.42a)$$

The atomic density n_a, varies slowly among the natural elements, thus to first order

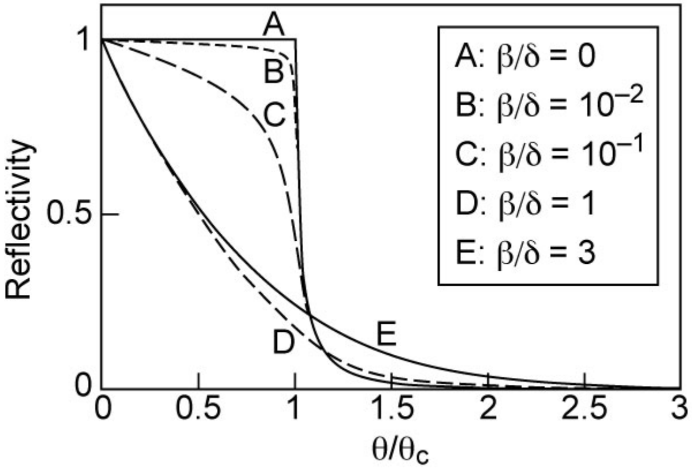
$$\underline{\theta_c \propto \lambda\sqrt{Z}} \qquad (3.42b)$$

where f_1^0 is approximated by Z. Note that f_1^0 is a complicated function of wavelength (photon energy) for each element.

Ch03_TotalExtrnlRflc2_Apr2010.ai

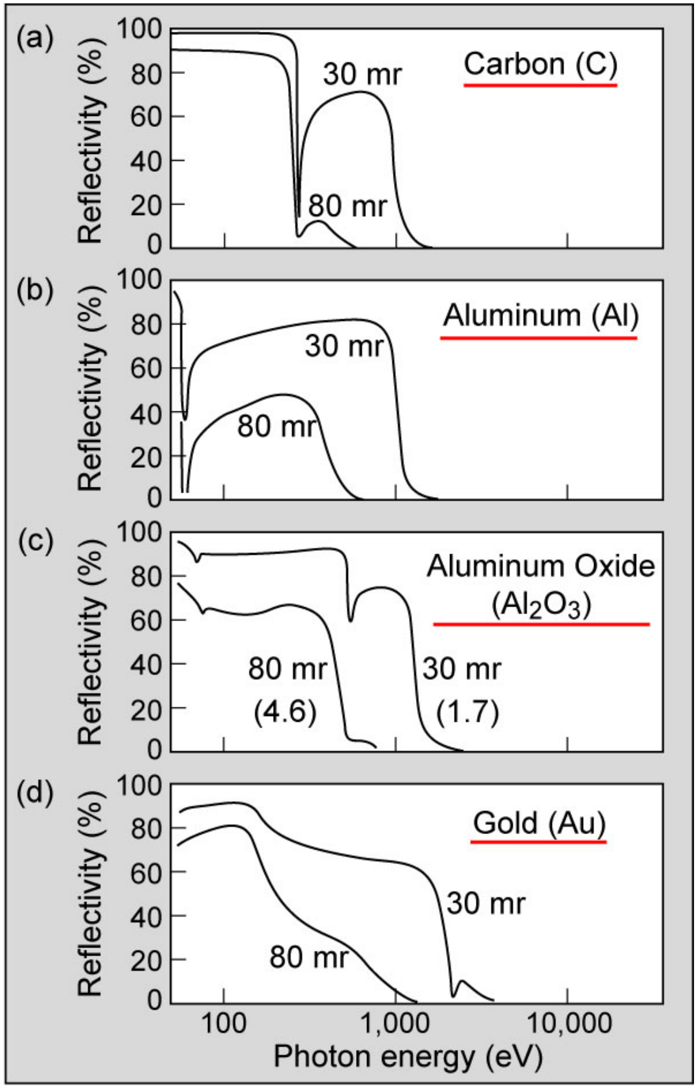
Total external reflection with finite β

Glancing incidence reflection as a function of β/δ



- finite β/δ rounds the sharp angular dependence
- cutoff angle and absorption edges can enhance the sharpness
- note the effects of oxide layers and surface contamination

. . . for real materials

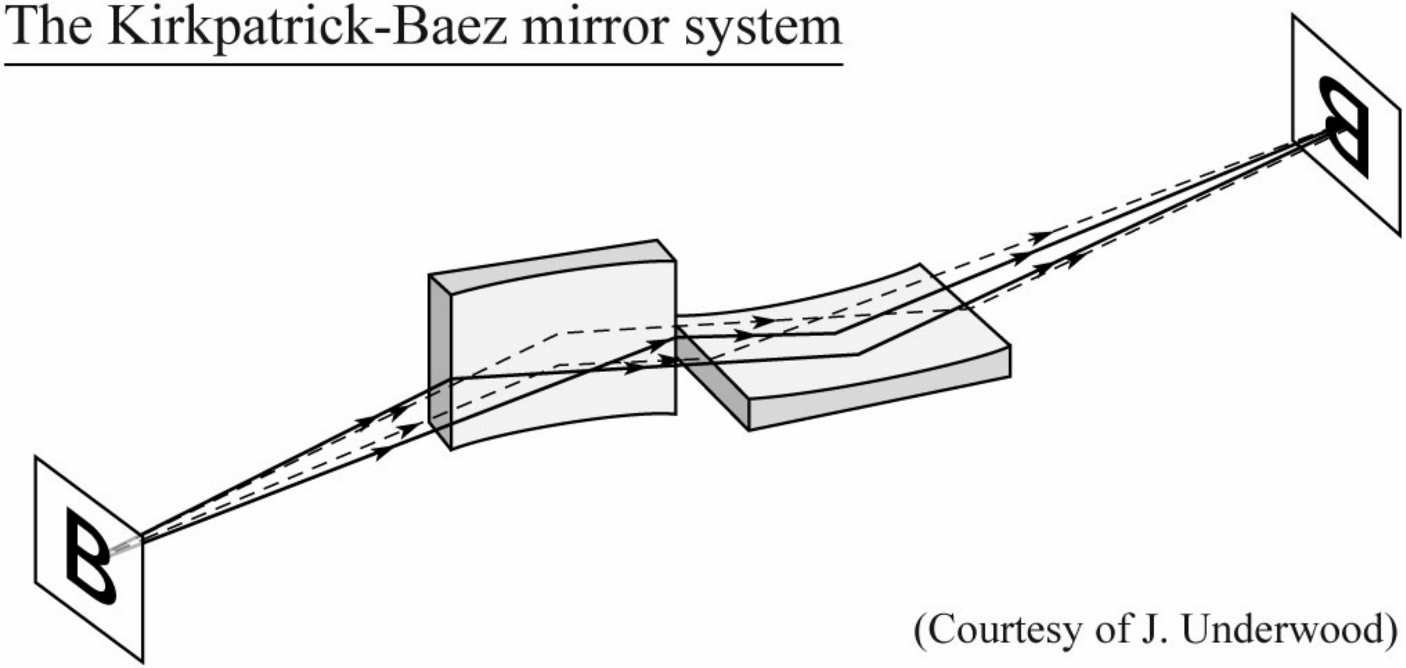


(Henke, Gullikson, Davis)

Ch03_TotalExtrnlRflc3.ai

Focusing with curved, glancing incidence optics

The Kirkpatrick-Baez mirror system



(Courtesy of J. Underwood)

- Two crossed cylinders (or spheres)
- Astigmatism cancels
- Fusion diagnostics
- Common use in synchrotron radiation beamlines
- See hard x-ray microprobe, chapter 4, figure 4.14

Ch03_FocusCurv.ai

Reflection at an interface

E$_0$ perpendicular to the plane of incidence (s-polarization)

tangential electric fields continuous

$$E_0 + E_0'' = E_0' \qquad (3.43)$$

tangential magnetic fields continuous

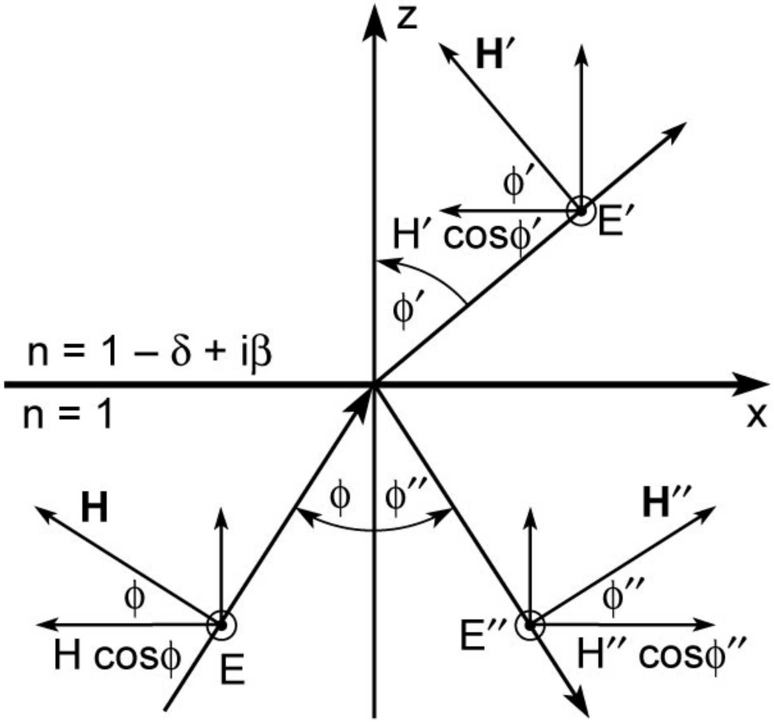
$$H_0 \cos\phi - H_0'' \cos\phi = H_0' \cos\phi' \qquad (3.44)$$

$$\mathbf{H}(\mathbf{r}, t) = n\sqrt{\frac{\epsilon_0}{\mu_0}}\mathbf{k}_0 \times \mathbf{E}(\mathbf{r}, t) \Rightarrow H = n\sqrt{\frac{\epsilon_0}{\mu_0}}E$$

$$\sqrt{\frac{\epsilon_0}{\mu_0}}E_0 \cos\phi - \sqrt{\frac{\epsilon_0}{\mu_0}}E_0'' \cos\phi = n\sqrt{\frac{\epsilon_0}{\mu_0}}E_0' \cos\phi'$$

$$(E_0 - E_0'')\cos\phi = n E_0' \cos\phi' \qquad (3.45)$$

Snell's Law: $\sin\phi' = \dfrac{\sin\phi}{n}$



Three equations in three unknowns
(E$_0'$, E$_0''$, ϕ′) (for given E$_0$ and ϕ)

Ch03_ReflecInterf1.ai

Reflection at an interface (continued)

E_0 perpendicular to the plane of incidence (s-polarization)

$$\frac{E_0'}{E_0} = \frac{2\cos\phi}{\cos\phi + \sqrt{n^2 - \sin^2\phi}} \tag{3.47}$$

$$\frac{E_0''}{E_0} = \frac{\cos\phi - \sqrt{n^2 - \sin^2\phi}}{\cos\phi + \sqrt{n^2 - \sin^2\phi}} \tag{3.46}$$

The reflectivity R is then

$$R = \frac{\bar{I}''}{\bar{I}_0} = \frac{|\bar{\mathbf{S}}''|}{|\bar{\mathbf{S}}|} = \frac{\frac{1}{2}\mathrm{Re}(\mathbf{E}_0'' \times \mathbf{H}_0''^{*})}{\frac{1}{2}\mathrm{Re}(\mathbf{E}_0 \times \mathbf{H}_0^{*})} \tag{3.48}$$

With n = 1 for both incident and reflected waves,

$$R = \frac{|E_0''|^2}{|E_0|^2}$$

Which with Eq. (3.46) becomes, for the case of perpendicular (s) polarization

$$\boxed{R_s = \frac{\left|\cos\phi - \sqrt{n^2 - \sin^2\phi}\right|^2}{\left|\cos\phi + \sqrt{n^2 - \sin^2\phi}\right|^2}} \tag{3.49}$$

Ch03_ReflecInterf2_Apr2010.ai

Normal incidence reflection at an interface

Normal incidence ($\phi = 0$)

$$R_s = \frac{\left|\cos\phi - \sqrt{n^2 - \sin^2\phi}\right|^2}{\left|\cos\phi + \sqrt{n^2 - \sin^2\phi}\right|^2} \qquad (3.49)$$

$$R_{s,\perp} = \frac{|1-n|^2}{|1+n|^2} = \frac{(1-n)(1-n^*)}{(1+n)(1+n^*)}$$

For $n = 1 - \delta + i\beta$

$$R_{s,\perp} = \frac{(\delta - i\beta)(\delta + i\beta)}{(2 - \delta + i\beta)(2 - \delta - i\beta)} = \frac{\delta^2 + \beta^2}{(2-\delta)^2 + \beta^2}$$

Which for $\delta \ll 1$ and $\beta \ll 1$ gives the reflectivity for x-ray and EUV radiation at normal incidence ($\phi = 0$) as

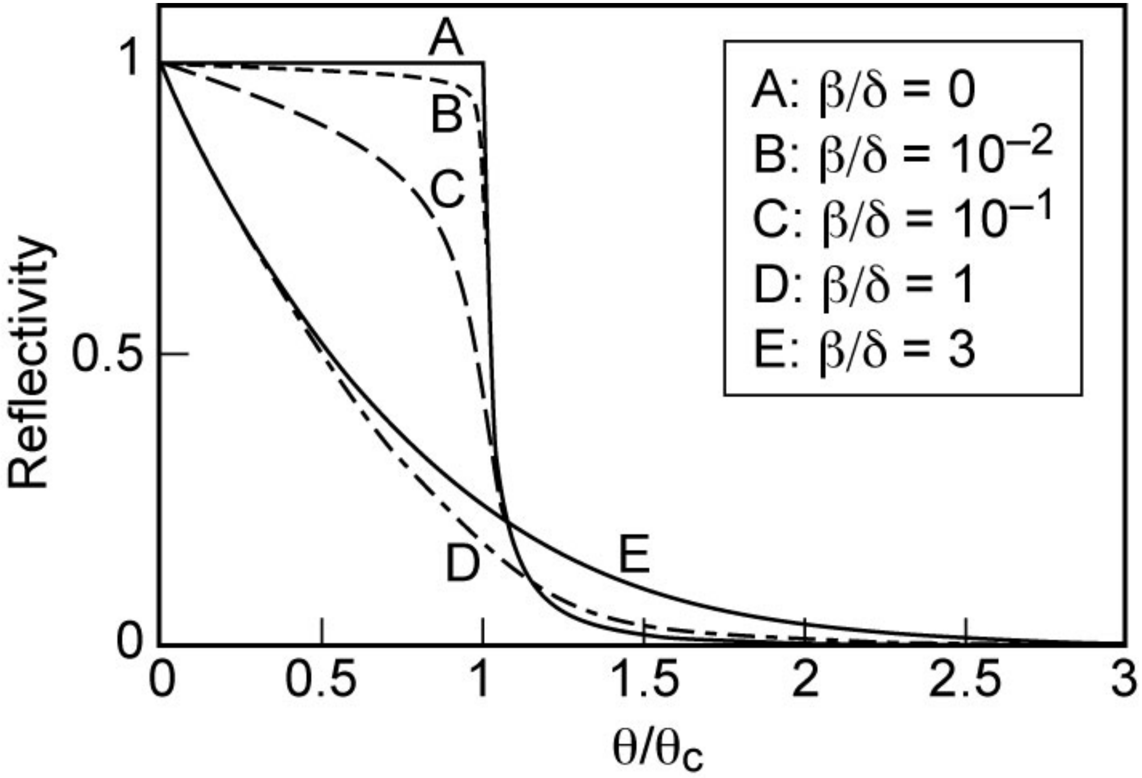
$$\boxed{R_{s,\perp} \simeq \frac{\delta^2 + \beta^2}{4}} \qquad (3.50)$$

Example:

$$\left.\begin{array}{ll} \text{Nickel @ 300 eV (4.13 nm)} & \\ \text{From table C.1, p. 433} & \\ f_1^0 = 17.8 & f_2^0 = 7.70 \\ \delta = 0.0124 & \beta = 0.00538 \end{array}\right\} R_\perp = 4.58 \times 10^{-5}$$

Ch03_NormIncidReflc.ai

Glancing incidence reflection (s-polarization)

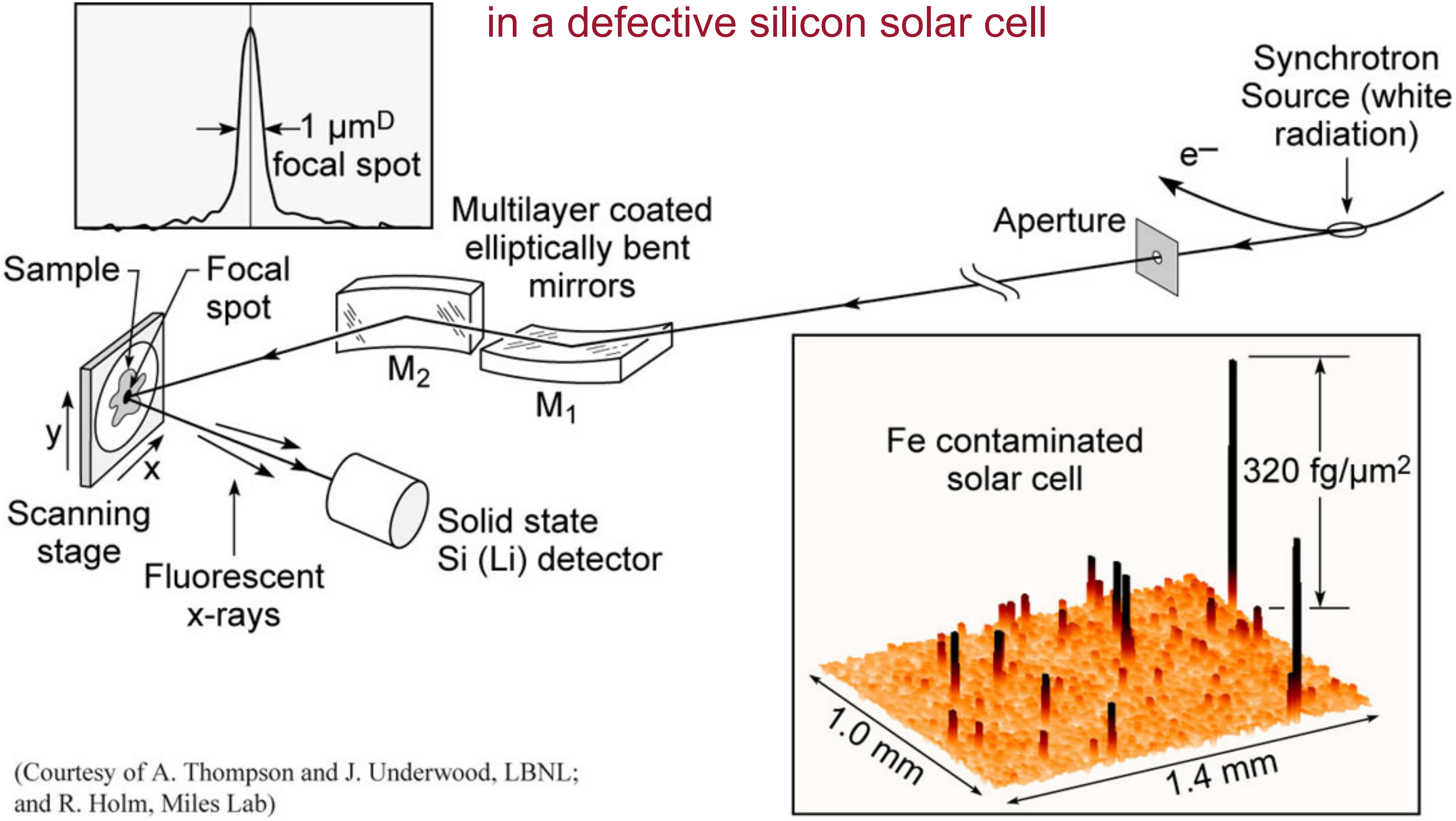


E. Nähring, "Die Totalreflexion der Röntgenstrahlen", Physik. Zeitstr. XXXI, 799 (Sept. 1930).

Ch03_GlancIncidReflc_Right.ai

Application of glancing incidence reflection: the focused x-ray microprobe

Buried, trace amounts of iron
in a defective silicon solar cell



(Courtesy of A. Thompson and J. Underwood, LBNL;
and R. Holm, Miles Lab)

Ch04_F14VG.ai