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X-RAY ABSORPTION COEFFICIENTS OF THE ELEMENTS (Li TO Bi, U)

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Abstract

The atomic absorption coefficient, μ_a, and the mass absorption coefficient, μ/ρ, have been calculated for the elements Li to Bi and U, based on both photoelectric and scattering effects. Tables include the μ_a and μ/ρ values (i) at 0.01 Å intervals in the wavelength range from 0.1 to 2.89 Å and (ii) at 0.0001 Å intervals in the neighborhood of the K, L_1, L_2, and L_3 absorption edges.

KEYWORDS: Absorption, Atomic absorption coefficient, Mass absorption coefficient, Numerical calculation, Cross section, Relativistic treatment.

INTRODUCTION

Absorption is treated as an intensity loss of primary X-rays passing through matter. The intensity, I_0, of a monochromatic beam decreases exponentially:

$$I = I_0 \exp(-\mu x), \qquad (1)$$

where the linear absorption coefficient, μ (cm^{-1}), represents the average number of absorption and scattering processes which a single photon undergoes through an absorber of thickness x cm.

In this paper we calculate the absorption coefficients. In the X-ray wavelength region, two main processes give rise to continuous absorption: photoelectric absorption and scattering processes.

ABSORPTION EFFECT

When an X-ray incident on an atom has an energy greater than the ionization energy, photon absorption occurs accompanied by the liberation of an atomic electron. In quantum mechanics,1),2) the photoelectric absorption can be described as a time-dependent harmonic perturbation for $| \mathrm{i} > \rightarrow | \mathrm{n} >$, having a transition probability $\varepsilon_n \equiv \varepsilon_i + \hbar\omega$. Then, the quantum system receives energy amounting to $\hbar\omega$ from the potential of a photon and ends up as an excited state. It is considered that in absorption the energy difference between the initial and final states is equal to the energy of the photon. An absorption cross section can be estimated as being the unit-time energy absorbed by the atom in the energy flux of the radiation field. From a consideration of the transition rate, we have

$$\sigma_p = \frac{4\pi^2\hbar}{m^2\omega} (e^2/\hbar c) \, | < \mathrm{n} \, | \, e^{i\mathbf{k}\cdot\mathbf{r}} \, \mathbf{p}\cdot\alpha \, | \, \mathrm{i} > |^2 \, \delta(\varepsilon_n - \varepsilon_i - \hbar\omega), \qquad (2)$$

where $\mathbf{p}$ and $\mathbf{k}$ are the polarization and propagation vectors; α is an operator and δ is the Dirac delta function which can be eliminated by integration over ε. The physical constants are: c is the velocity of light in free space, e the charge of the electron, and m the mass of an electron.

Photoelectric cross-section data for individual electron orbitals of most elements already exist on tape with central-field atomic-structure calculations for the bound-state electron wave functions and the potential.3),4) The basic wave function used in the calculation is the relativistic Dirac-Slater self-consistent-field solution, where the exchange potential is calculated by Slater's $\rho^{1/3}$ method.5)

Scattering by electrons is also important and is associated with the absorption effect. In this case X-ray photon is deflected after mechanical collision with an atom (Thomson scattering) or a loosely bound electron (Compton scattering). Here, the scattering of a photon by an electron is considered using relativistic quantum mechanics.6) When a primary photon of momentum k collides with a free electron of momentum p, the cross section is given by

$$\sigma_s = (2\pi)^2 \frac{p^0 k^0}{|p \cdot k|} S_n S_i \, | < n \, | \, M \, | \, i > |^2 \, \delta(p'+k'-p-k), \tag{3}$$

where k' and p' are momentums of the scattered photon and electron, respectively. The matrix S is called the scattering matrix, and is related to the transition probability. The matrix elements of M are obtained from the S matrix element for the charge-conjugate process. After simplifying Eq. (3) and averaging the spin of an electron and the polarization states, the differential cross section in the rest system of the incident electron can be written as

$$\frac{d\sigma_s}{d\Omega} = \frac{1}{2} \frac{e^2}{mc^2} \left(\frac{\omega'}{\omega}\right) \left\{ \frac{\omega}{\omega'} + \frac{\omega'}{\omega} - \sin^2\theta \right\}, \tag{4}$$

where θ is the scattering angle and ω and ω' are the frequencies of the incoming and outgoing photons, respectively. This form is well known as the Klein-Nishina formula.7) Integrating over the angles, the total cross section per electron is calculated from Eq. (4):

$$\sigma_s = \frac{8\pi}{3} \frac{e^4}{m^2c^4} \frac{3}{4} \left[\frac{1+q}{q^2} \left\{ \frac{2(1+q)}{1+2q} - \frac{1}{q} \ln(1+2q) \right\} + \frac{1}{2q} \ln(1+2q) - \frac{1+3q}{(1+2q)^2} \right] \tag{5}$$

where $q = \hbar\omega/mc^2$. Though this equation is independent of the choice of the coordinate system, the binding effect of an electron in an atom is not taken into account. When $\hbar\omega << mc^2$, Eq. (4) represents Thomson scattering, which is elastic. Thus, in the Klein-Nishina formula both Compton scattering and Thomson scattering are already included.

Assuming that other absorption effects are negligible, the total linear absorption coefficient for an atom is given by

$$\mu_a = \sigma_p + Z\sigma_s \qquad (6)$$

in the cm^2 unit, where Z is the atomic number. The mass absorption coefficient of an element is also given by

$$\mu/\rho = \sigma_p/A + Z\sigma_s/A \qquad (7)$$

in the cm^2/g unit, where A is the atomic weight.

ABSORPTION COEFFICIENT

The atomic absorption coefficient, μ_a, and the mass absorption coefficient, μ/ρ, are given for the elements Li to Bi plus U in the MU(A) and MU/RHO rows of Table I, respectively. These values are given as a function of the wavelengths in Å (10^{-10} m) in the range from 0.1 to 2.89 (Å) in intervals of 0.01 Å. The ångström unit can be changed to the *k*eV unit: 1Å = 12.397639 *k*eV. It is noted that the absorption coefficients obtained in the present calculation are slightly smaller than previously reported values.8)

Figure 1 shows the wavelength variation of μ_a and μ/ρ for Fe and Pb atoms. The absorption coefficient increases with increasing wavelength, except in the neighborhood of absorption edges. In order to use the absorption coefficient in an anomalous-scattering study,9) 280 points of μ_a and μ/ρ values were prepared in intervals of 0.0001 Å near the K, L_1, L_2, or L_3 absorption edge (Table II). The wavelength values for the respective absorption edges were taken from Bearden's tables.10) For convenience, all tables are arranged in order of atomic number. Appendix 1 given on page 142 may be useful as an index.

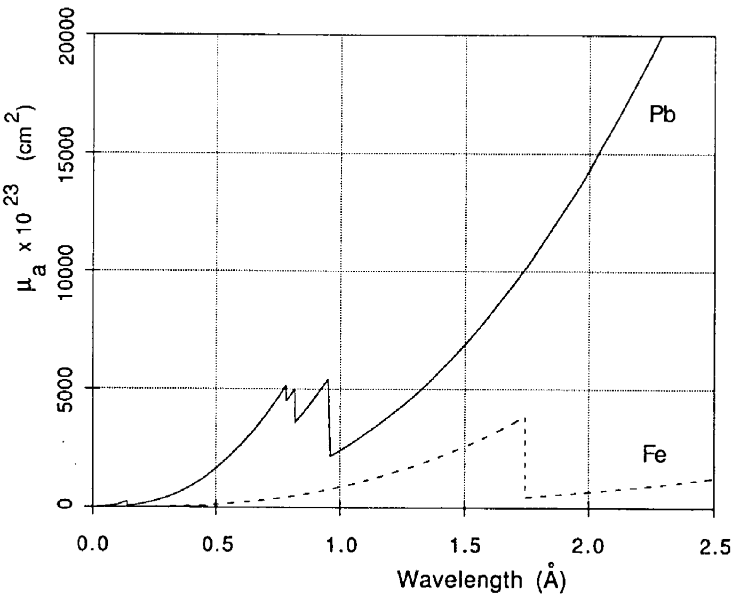

Fig. 1(a), Atomic absorption coefficient μ_a of Fe and Pb as a function of the wavelength.

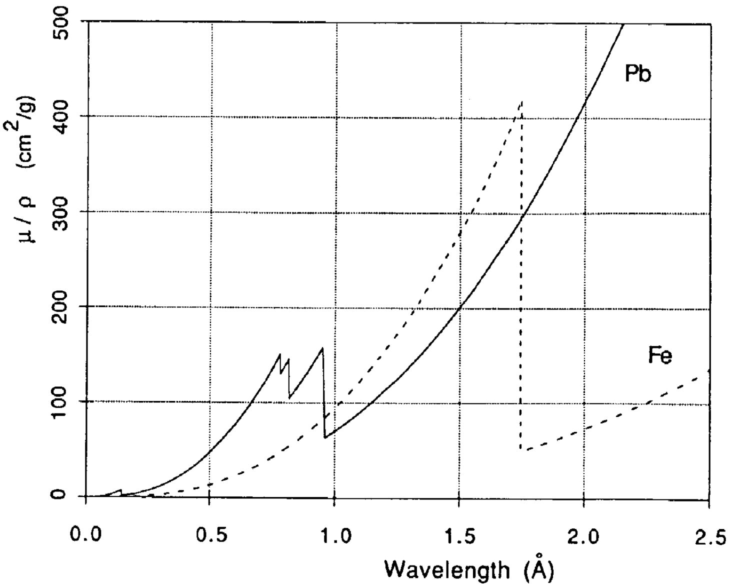

Fig. 1(b), Mass absorption coefficient μ/ρ of Fe and Pb as a function of the wavelength.

LINEAR ABSORPTION COEFFICIENT

Linear absorption coefficient of materials defined by Eq. (1) can be easily calculated by using the μ_a or μ/ρ values given in the tables. Using the atomic absorption coefficient for a crystal, we have

$$\mu = z\,\Sigma(\mu_a)_i/(V \times 10^{-24}), \tag{8}$$

where z is a chemical unit, V is the cell volume in Å unit, and the summation is taken over the constituent elements in the chemical formula. For an example of tetragonal $Tl_2CaBa_2Cu_2O_8$ ($z = 2$, $V = 435$ Å^3) at the wavelength $\lambda = 0.5$ Å, the linear-absorption coefficient is calculated as $\mu = 2\times(2\times1560+44.9+2\times350+2\times192+8\times1.35)\times10^{-23}/(435\times10^{-24}) \cong 196$ (cm^{-1}). In the case of tungsten (cubic W; $z = 2$, $V = 31.4$ Å^3), the calculated μ at $\lambda = 0.5$ Å is: $\mu = 2\times1090\times10^{-23}/(31.4\times10^{-24}) \cong 694$ (cm^{-1}).

Furthermore, the linear-absorption coefficient, μ, can be calculated from μ/ρ as:

$$\mu = d\,\Sigma\,p_i(\mu/\rho)_i, \tag{9}$$

where d is the density (g/cm^3) of the material, p_i is the fractional part (by weight) of the constituent elements of the compound, and the summation is taken over all elements. The μ value of the tungsten having the density of 19.24 g/cm^3 is calculated at $\lambda = 0.5$ Å as $\mu = 19.24 \times 35.7 \cong 687$ (cm^{-1}). The difference in μ values of W between the two equations may appear as the result of an uncertainty in the density.

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References

1) J. J. Sakurai: Modern Quantum Mechanics (The Benjamin/Cummings Publishing Company, Inc, California, U.S.A., 1985).

2) A. I. Akhiezer and V. B. Berestetsky: Quantum Electrodynamics, *Translated by C. M. Volkoff* (Interscience, New York, U.S.A., 1965).

3) D. T. Cromer and D. Liberman: J. Chem. Phys., 53 (1970) 1891-1898.

4) H. Brysk and C. D. Zerby: Phys. Rev., 171 (1968) 292-298.

5) D. Liberman, J. T. Waber, and D. T. Cromer: Phys. Rev., 137 (1965) A27-A34.

6) J. M. Jauch and F. Rohrlich: The Theory of Photons and Electrons *2nd ed.* (Springer-Verlag, New York, U.S.A., 1980).

7) O. Klein and Y. Nishina: Z. Phys., 52 (1929) 853-868.

8) B. Koch, C. H. MacGillavry, H. J. Millegde, K. Koopmans, G. D. Rieck, and G. E. Bacon: *in* International Tables for X-Ray Crystallography vol. III, *eds*, C. H. MacGillavry and G. D. Rieck (D. Reidel Publishing Company, Dordrecht, Holland, 1968) pp. 157-200.

9) S. Sasaki: KEK Report, 83-22 (1984) 1-136; *2nd ed.*, 88-14 (1989) 1-136.

10) J. A. Bearden: *in* International Tables for X-Ray Crystallography vol. IV, *eds*, J. A. Ibers and W.C. Hamilton (Kynoch Press, Birmingham, England, 1974) pp. 5-43.

Appendix 1. Index for the absorption coefficient tables. Each number shows the page relevant to the element looked up. The atomic number is given in parentheses.

Element	Table I	Table II	Element	Table I	Table II			
		K			*K*	L_1	L_2	L_3
H, He	142							
Li (3)	7		Ru (44)	27	64			
Be (4)	7		Rh (45)	28	64			
B (5)	8		Pd (46)	28	65			
C (6)	8		Ag (47)	29	65	84	103	122
N (7)	9		Cd (48)	29	66	85	104	123
O (8)	9		In (49)	30	66	85	104	123
F (9)	10		Sn (50)	30	67	86	105	124
Ne (10)	10		Sb (51)	31	67	86	105	124
Na (11)	11		Te (52)	31	68	87	106	125
Mg (12)	11	48	I (53)	32	68	87	106	125
Al (13)	12	48	Xe (54)	32	69	88	107	126
Si (14)	12	49	Cs (55)	33	69	88	107	126
P (15)	13	49	Ba (56)	33	70	89	108	127
S (16)	13	50	La (57)	34	70	89	108	127
Cl (17)	14	50	Ce (58)	34	71	90	109	128
Ar (18)	14	51	Pr (59)	35	71	90	109	128
K (19)	15	51	Nd (60)	35	72	91	110	129
Ca (20)	15	52	Pm (61)	36	72	91	110	129
Sc (21)	16	52	Sm (62)	36	73	92	111	130
Ti (22)	16	53	Eu (63)	37	73	92	111	130
V (23)	17	53	Gd (64)	37	74	93	112	131
Cr (24)	17	54	Tb (65)	38	74	93	112	131
Mn (25)	18	54	Dy (66)	38	75	94	113	132
Fe (26)	18	55	Ho (67)	39	75	94	113	132
Co (27)	19	55	Er (68)	39	76	95	114	133
Ni (28)	19	56	Tm (69)	40	76	95	114	133
Cu (29)	20	56	Yb (70)	40	77	96	115	134
Zn (30)	20	57	Lu (71)	41	77	96	115	134
Ga (31)	21	57	Hf (72)	41	78	97	116	135
Ge (32)	21	58	Ta (73)	42	78	97	116	135
As (33)	22	58	W (74)	42	79	98	117	136
Se (34)	22	59	Re (75)	43	79	98	117	136
Br (35)	23	59	Os (76)	43	80	99	118	137
Kr (36)	23	60	Ir (77)	44	80	99	118	137
Rb (37)	24	60	Pt (78)	44	81	100	119	138
Sr (38)	24	61	Au (79)	45	81	100	119	138
Y (39)	25	61	Hg (80)	45	82	101	120	139
Zr (40)	25	62	Tl (81)	46	82	101	120	139
Nb (41)	26	62	Pb (82)	46	83	102	121	140
Mo (42)	26	63	Bi (83)	47	83	102	121	140
Tc (43)	27	63	U (92)	47	84	103	122	141