Mustansiriyah Journal of Pure and Applied Sciences, Print ISSN: 2957-9910. Online ISSN: 2957-9929, Vol. 4, No. 1, 2026, Pages 1-7
DOI: 10.47831/mjpas.v4i1.M13

MJPAS

MUSTANSIRIYAH JOURNAL OF PURE AND APPLIED SCIENCES

Journal homepage:
https://mjpas.uomustansiriyah.edu.iq/index.php/mjpas

RESEARCH ARTICLE - PHYSICS

Study and calculation of the mass absorption coefficient for X-rays of zinc oxide and cadmium oxide compounds

Hanaa A. Aziz [1*], Wfaa N. Jasim [2]

[1] Ministry of Higher Education and Scientific Research, Baghdad, Iraq

[2] Department of Physics, College of Education for Girls, University of Kufa, Najaf, Iraq

[*] Corresponding author E-mail: hanaaa.almafarji@student.uokufa.edu.iq

Article Info.

Article history:

Received
1 April 2025

Accepted
16 June 2025

Publishing
30 March 2026

Abstract

In this study, it was calculated the coefficient of mass absorption of X-rays $(\mu/\rho)_E$ resulting from photoelectric absorption in X-ray absorption spectra like an energy function, while determining the effective atomic number (Z_{eff}) for (CdO) and (ZnO) compounds.in the energy range of (1-100 keV) using a theoretical equation, the theoretical results were than compared with the results predicted by using the programs (xcom, ffast) noticeable differences were observed in the values of the theoretical results and the values of the experimental or semi-experimental results from programs (Xcom, Ffast) because the theoretical equation considers the material to be homogeneous and ideal and depends on the absorption resulting from the photoelectric effect, this is in addition to the effect of absorption edges. The equation theoretical followed the same experimentally proven course: with increasing X-ray energy, the mass absorption coefficient of material decreases,.All calculations and graphical representations were performed using MATLAB 2020. The linear correlation coefficient between the theoretical and experimental results was also calculated using one of advanced MATLAB, algorithms were used to demonstrate the degree of agreement between the results MATLAB 2020 theoretical and experimental statistical method using function Cftool.

The official journal published by the College of Education at Mustansiriyah University

Keywords: Absorption; effective atomic number; effective charge; mass absorption; X-ray.

1. Introduction

X-rays are electromagnetic radiation with a short wavelength a high frequency. Roentgen won the first Nobel prize in physics for his discovery of X-rays in 1981. This radiation was described as having the ability to penetrate at high levels and may be absorbed when penetrating a material [1]. From here begin the importance of the concept of the mass absorption coefficient as a factor that determines the fate of the rays, whether they are absorbed or scattered, depending on their energy and the composition of the material through which the X-rays penetrate [2]. There is also a concept no less important than the mass absorption coefficient of X-rays, which plays an effective role in understanding and explaining the mechanism of X-ray absorption by various materials. This concept is represented by the effective atomic number or effective nuclear charge, which is the net charge that the electron is exposed to in the atom, with an explanation of the effects of shielding or protection (s) by other electrons, as it plays a pivotal role in providing explanation for the phenomenon of X-ray absorption through. There is a possibility of X- ray reaction with matter and this possibility increases as the effective atomic number increases [3]. Absorption by materials varies due to the difference between elements according to the periodic table [4]. The effective atomic number is also a basis upon which the design of materials for radiation protection is built, and it also plays a distinct role in improving radiological imaging techniques [5]. Modern studies demonstrate that the effective atomic number enables accurate prediction of material behavior under X-ray exposure, particularly in medical physics and materials science applications [6]. Recent advances in computational modeling have further enhanced our ability to calculate Z_{eff} for complex compounds and mixtures [7]. Therefore, studying and calculating the mass absorption coefficient of x- rays and the effective atomic number of materials aim primarily to evaluate the ability of materials to absorb and understand the physical phenomena associated with absorption, as it has a role in various applications (medical, electronic, protective and industrial). It also helps in studying the chemical properties of materials. One of the methods that highlight its importance and interest researchers, which contribute to understanding and processing X-ray absorption coefficient data, especially for the compounds ZnO and CdO, is the XRD method [8]. It has also been experimentally proven that both compounds have very sensitive structural, electrical and optical properties for thin films and have wide-ranging applications [9].

2. Theoretical background

The mass absorption coefficient $(\mu/\rho)_E$ is defined as the rate at which a substance absorbs X-rays per unit mass. In compounds, it depends mainly on the physical properties of the elements that make up the compounds as shown in Table 1 including the energy of X-rays (E), the atomic number (Z) and the weight fraction of the element in the compound [10].

Table 1. The most important physical and chemical properties of compounds (CdO, ZnO) [11]

The property	CdO	ZnO
Scientific name	Cadmium oxide	Zinc oxide
Density (g/cm^3)	8.15	5.61
Color	Olive green	White
Melting point (C^o)	1500	1975
Boiling point (C^o)	Decomposes upon heating	2360
Crystal structure	FCC- Cubic	Hexagonal
Molecular weight	128.41	81.38

Since the mass absorption coefficient of X-ray in this study depends on the energy of X-ray photons and according to the Beer-Lambert law it is applies only to photoelectric excluding Rayleigh-Thomson scattering, (Compton, reversal), fluorescence Okker electron emission, pair formation, and other nuclear reactions. At low energy levels below 500 keV and for materials with high atomic numbers, photoelectric absorption is dominant [12]. Therefore, the specific was used calculate the X-ray absorption coefficient in compounds [13]:

$$[\mu/\rho]s = \sum_i W_i \, [\mu/\rho]_i \quad (1)$$

Where $[\mu/\rho]s$ refers to the compound the mass absorption coefficient, W_i here it refers to the weight fraction of elements in the compound, $[\mu/\rho]_i$ refers to element the mass absorption coefficient in compound extracted from (2) [14]:

$$\mu/\rho = \rho z^4 / mE^3 \quad (2)$$

The effective charge or effect atomic number, which represents the force felt by the electron from the nucleus, taking into account the effect of shielding by other electrons is extracted according to slater's rule. The importance of Slaters rule lies in understanding the extent to which the nucleus of an atom influences a particular electron. This is a clear way to understand the behavior of electrons within molecules and atoms. It also plays an important role in many chemical and physical applications, especially in atomic physics, as it is used to explain the behavior of metals and non-metals, ionization energy, and other important atomic properties [15] . Accordingly, by knowing the amount of shielding (S), the linear relationship is used to calculate the effective charge or effective atomic number [16]:

$$Z_{eff} = Z - S \quad (3)$$

Z_{eff} refers to the effective atomic number, Z refers to the atomic number and S refers to the amount of shielding. The relationship can also be used to extract the effective atomic number for compounds [17].

$$Z_{eff} = \left(\sum w_i \, z_i^3\right) \quad (4)$$

3. Research methodology

In this study, the X-ray mass absorption coefficient in the range (1-100 keV) resulting from the photoelectric effect of the compounds (ZnO, CdO) and the elements composing the compound were calculated by applying (1) and (2). The X-ray mass absorption coefficient of ZnO and CdO were also extracted using the programs Xcom and Ffast. The shielding factor (S) of the tow compounds was also calculated using Slater's rule to extract the effective atomic number of the studies compounds by applying (3). To obtain theoretical results closer to the practical results, the atomic number in (2) was replaced by effective atomic number. Then, all the results were tabulated and represented graphically, and a comparison was made between all the results extracted by different methods. All calculations were performed using MATLAB 2020. The (Cftool) [18] was used to obtain a fitting model, resulting in an equation with constants that provide optimal results matching those of (1). Therefore, the fitting equation is:

$$\mu/\rho = a * E^{-b} \qquad (4)$$

Where the values of the constants for the compounds were as follows:

- a to ZnO = 7.079×10^4
- a to CdO = 333.3
- b = -3 for both compounds.

4. Results and discussion

In Fig. 1 and Table 2, we observe that the mass absorption coeff. of cadmium oxide shows a general decrease as increasing of the X-rays energy. There is a noticeable rise in the mass absorption coefficient at very low energies. However, at higher energy levels, specifically above 40 keV, the mass absorption coefficient becomes very low and then gradually stabilizes due to the weakening of the photoelectric effect. When comparing the curves, we notice that the curve representing the values from (1) ($P.W$) exhibits a greater decrease than the other curves. This decrease between the curve derived from (1) and the other experimental curves arises from interactions between electronic levels of different elements within the compound, at the low-energy range of X-rays, we observe that the mass attenuation coefficient of cadmium oxide is high and sharp in all theoretical and experimental models, with some fluctuations in certain curves. These fluctuations are attributed to potential interactions between absorption mechanisms. In the intermediate range, the mass absorption coefficient begins to decrease gradually, but noticeable differences remain between the values obtained from theoretical and experimental models. However, in the high-energy range, a clear convergence between the models becomes evident. This is due to the weakening of the photoelectric effect in this range, we note a close agreement between the results of (1) after modification by replacing the atomic number alongside the effective atomic number and the experimental data obtained from the Xcom and Ffast programs. This indicates that the equation, expressed in terms of the effective atomic number of cadmium oxide, yields result closer to experimental data. Thus, modifying (1) may align with experimental findings for certain compounds in the intermediate range, the mass absorption coefficient begins to gradually decrease, but the differences remain noticeable between the values of the theoretical and experimental models used. As for the high-energy range, it clearly shows the extent of convergence between the models used, and the reason for this is attributed to the weakening of the photoelectric effect in this range. In the table above, we notice a convergence between the results of (1) after its modification and replacement of its number of atomic with the effective number of atomic and the experimental results extracted from the Xcom and Ffast programs [19]. That is, the equation in terms of the effective atomic number for cadmium oxide yields results closer to the experimental results, meaning that modifying (1) may align with the experimental results for some of the compounds.

Table 2. It shows the values of the mass absorption coeff. of X-rays as an energy function, both theoretically and experimentally, for (ZnO)

Energy (keV)	Absorption coefficient of X-ray by p.w cm^2/g)	Absorption coefficient of X-ray by p.wzeff cm^2/g)	Absorption coefficient of X-ray by XCOM cm^2/g)	Absorption coefficient of X-ray by FFAST cm^2/g)
1	70790.663	53208.843	2146	2014.415
1.5	20975.011	15765.583	4176	4061.1
2	8848.832	6651.105	2040	1979
2.5	4530.602	3405.366	1373.5	1122.3
3	2621.876	1970.697	706.9	690.65
3.5	1651.094	1241.022	516.4	451.971
4	1106.104	831.388	325.9	312.815
5	566.325	425.670	176.9	170.568
6	327.734	246.33	106.8	102.009
8	138.263	103.92	47.74	43.549
10	70.790	53.208	187	184.913
15	20.975	15.765	64.69	65.697
20	8.848	6.651	29.4	31.633
30	2.621	1.970	9.34	10.214
40	1.106	0.831	4.053	3.878
50	0.566	0.425	2.099	2.139
60	0.327	0.246	1.22	1.177
80	0.138	0.103	0.5128	0.530
100	0.070	0.0532	0.2605	0.235

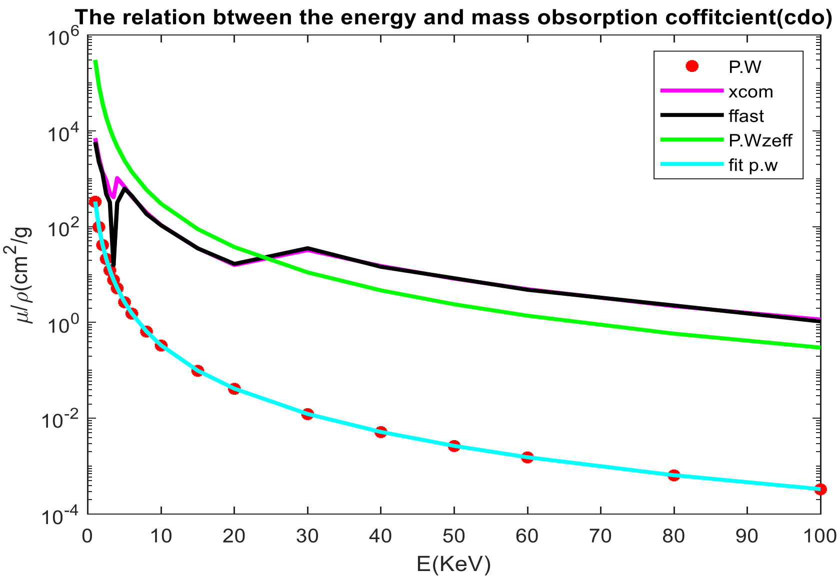

Fig. 1. The mass absorption coeff. of (CdO) as an energy function, theoretically (P.W), P.W.zeff by effective atomic number, fit p.w by fitting P.W and experimentally from the XCOM and FFAST programs

In Fig. 2 and Table 3, at the low-energy range of X-rays, we observe that-the mass absorption coeff. of cadmium oxide is sharp and high in all theoretical and experimental models, with some fluctuations in certain curves. These fluctuations are attributed to potential interactions between absorption mechanisms. In the intermediate range, the mass absorption coefficient begins to decrease gradually, but noticeable differences remain between the values obtained from theoretical and experimental models. However, in the high-energy range, a clear convergence between the models becomes evident. This is due to the weakening of the photoelectric effect in this rang, we note a close agreement between the results of (1) after modification by replacing the number of atomic with the atomic number effective and the experimental results extracted from the Xcom and Ffast programs. This indicates that the equation, expressed in terms of the effective atomic number of CdO, yields result closer to experimental data. Thus, modifying (1) may align with experimental findings for certain compounds.

Table 3. It shows the values of the mass absorption coeff. of X-rays as an energy function, both theoretically and experimentally, for CdO

Energy (keV)	Absorption coefficient of X-ray by p.w (cm^2/g)	Absorption coefficient of X-ray by p.w $zeff$ (cm^2/g)	Absorption coefficient of X-ray by XCOM $cm^2/g)$	Absorption coefficient of X-ray by FFAST $cm^2/g)$
1	330.302	299093.9	7001	5823.34
1.5	97.867	88620.43	2752	2248.204
2	41.287	37386.7	1370	1268
2.5	21.139	19142.0	932.7	476.872
3	12.23	11077.5	495.4	322.101
3.5	7.703	6975.95	410	15.72
4	5.160	4673.34	1031	315.721
5	2.642	2392.75	674.6	620.6
6	1.529	1384.69	419.4	438.109
8	0.645	584.167	195.9	183.088
10	0.330	299.09	107.3	105.963
15	0.097	88.620	35.22	35.138
20	0.041	37.386	15.78	16.686
30	0.012	11.077	32.31	35.405
40	0.005	4.673	15.09	14.483
50	0.002	2.392	8.197	8.377
60	0.0015	1.384	4.936	4.797
80	0.0006	0.584	2.187	2.263
100	0.0003	0.299	1.153	1.050

By comparing the theoretical results with the experimental results issued by the programs (Xcom, Ffast) we notice a significant difference even after modifying the equation by replacing the atomic number with the effective atomic number shown in Table 4. The reason for this noticeable difference is that the theoretical model relies on simplifications that neglect the interactions between the elements of a single compound also, the theoretical model used Tahes into account only the absorption resulting from the photoelectric effect, neglecting the rest of the effects of scattering and absorption edges. That is, it is an approximate model that neglects the small effects of energy and chemical composition. As for the experimental programs, they into account all the physical phenomena a comparing absorption. They even take into account the subtle effects that do not appear in the theoretical equations, by observing the results of both compounds (CdO, ZnO), we note that the CdO compound has properties that make it highly absorbent of X-rays , especially in the low energy range , which can make it the preferred compound in radiation applications that require high shielding efficiency, while the ZnO compound has acceptable performance , which can make it preferred in systems that require a balance between radiation transparency and the minimum level of protection [20]. When comparing the results of both ZnO and CdO at the low energy range, the CdO compound shows higher values for the mass absorption coefficient then ZnO this is attributed to the higher atomic number possessed by Cd. In the range (10-30 keV), ZnO shows a gradual decrease in the mass absorption coefficient with increasing the energy. In the high ranges, the absorption mechanism by Compton scattering is prominent, with the mass absorption coefficient continuing to decrease with increasing energy. However, we note that CdO maintains higher values for the mass absorption coefficient than ZnO, which illustrates the effect of the higher atomic number of CdO. The difference in physical and chemical properties, as shown in Table 4 for the two compounds CdO and ZnO, has a direct and noticeable effect on the values of the mass absorption coefficient of X-rays. For both, the atomic number and high density of the CdO compound play a distinct role in giving it a higher absorption capacity than the ZnO compound, in addition to the absorption edges whose effect is prominent in the medium energy range.

Table 4. The effective atomic number and shielding effectiveness for CdO and ZnO

Compounds	Effective atomic number (Z_{eff})	Shielding effectiveness (S)
CdO	45.92	9.68
ZnO	27.93	2.17

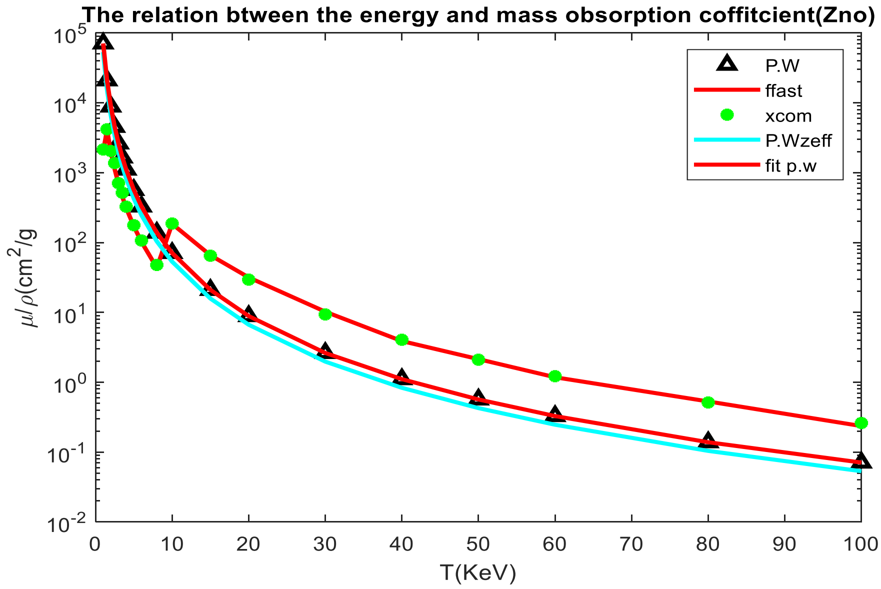

Fig. 2. The mass absorption coefficient Zinc oxide as a function of energy, theoretically (P.W) P.W.zeff by effective atomic number, fit p.w by fitting P.W and experimentally from the XCOM and FFAST

5. Conclusions

The method used in this study is simple, fast and applies at low and medium energy levels, as it relies on the photoelectric absorption of X-rays of the target compounds. However, one of the most important conclusions of this study is that the process of modifying the equation in terms of the effective atomic number in the equations for calculating the mass absorption coefficient of X-rays of the target compounds represents a qualitative shift in describing the relationship between matter and radiation interaction, meaning that it will provide a more accurate representation of the radiation interaction with matter. This substitution is not just a mathematical modification, but rather a transformation in terms of concept that brings theoretical models closer to experimental results and opens up broad horizons for X-rays in terms of application in various fields (medicine, industry and scientific research), thus giving mathematical modern interaction. It can be said that the mass absorption coefficient of CdO is greater than the mass absorption coefficient of ZnO in the energy range where the photoelectric effect dominates, and this difference between them decreases at high energies due to the dominance of Compton scattering. Therefore, we conclude that the atomic number of metals in their oxides has great effect on the mass absorption coefficient, especially at low energies, which makes CdO a higher absorber than ZnO, and with increasing energy this difference decreases.

References

[1] T. Buzug, "Fundamentals of X-ray physics," in *Computed tomography: From photon statistics to modern cone-beam CT*: Springer, Berlin, Heidelberg, 2008, pp. 15-73.
[2] J. Boogaard and G. M. van Dijk, *Non-destructive testing*. Elsevier, 2012, p. 918.
[3] J. H. Hubbell, "Photon mass attenuation and energy-absorption coefficients," *The International Journal of Applied Radiation and Isotopes,* vol. 33, no. 11, pp. 1269-1290, 1982.
[4] D. Creagh and J. Hubbell, "Problems associated with the measurement of X-ray attenuation coefficients. I. Silicon. Report of the International Union of Crystallography X-ray Attenuation Project," *Acta Crystallographica Section A: Foundations and Advances,* vol. 43, pp. 102-112, 1987.
[5] M. J. Berger *et al.*, "XCOM: Photon cross sections database," *NIST Standard Reference Database,* vol. 8, pp. 3587-3597, 2009.
[6] I. Akkurt, "Effective atomic and electron numbers of some steels at different energies," *Annals of Nuclear Energy,* vol. 36, no. 11-12, pp. 1702-1705, 2009.
[7] E. W. Taylor and P. Cranton, *The handbook of transformative learning: Theory, research, and practice*. John Wiley & Sons, 2012, p. 624.
[8] W. M. Taher, Z. M. Abood, and A. A. Khadayier, “A study of the structural and optical properties of pure copper oxide and doped with zinc at fixed weight percentages,” *Mustansiriyah Journal of Pure and Applied Sciences*, vol. 2, no. 4, pp. 49–58, 2024.
[9] M. A. Abd, A. H. Ali, and A. N. Abd, “Synthesis and investigation of CdO NPs for solar cell applications,” *Mustansiriyah Journal for Sciences and Education*, vol. 20, no. 5, pp. 1–12, 2019.
[10] F. H. Attix, *Introduction to radiological physics and radiation dosimetry*. John Wiley & Sons, 2008, p. 628.
[11] W. M. Haynes, *CRC handbook of chemistry and physics*, 97th ed. CRC Press, Boca Raton, 2016, p. 2670.
[12] V. Streltsov, C. Chantler, R. Ekanayake, and H. Melia, "X-ray absorption," *Laboratory and Computational Physics*, vol. 3, pp. 1-32.
[13] S. Manohara and S. Hanagodimath, "Studies on effective atomic numbers and electron densities of essential amino acids in the energy range 1 keV–100 GeV," *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms,* vol. 258, no. 2, pp. 321-328, 2007.
[14] G. Bunker, *Introduction to XAFS: A Practical Guide to X-ray Absorption Fine Structure Spectroscopy*. Cambridge: Cambridge University Press, 2010.
[15] J. C. Slater, "Atomic shielding constants," *Physical Review*, vol. 36, no. 1, pp. 57–64, 1930.
[16] M. S. A. Abdel Muttalib, *The Splendor of Quantum Chemistry Calculations and Applications: A Brief Practical Introduction*. Hindawi Foundation, 202.
[17] A. A. T. Aldalawi, M. Y. Hadi, and R. A. Hameed, "Calculate effective atomic number, mass and cross-section attenuation coefficients for nonanoic acid by using gamma-ray sources," *NeuroQuantology: An Interdisciplinary Journal of Neuroscience and Quantum Physics*, vol. 19, no. 11, pp. 15–22, 2021.
[18] W. Y. Yang, W. Cao, J. Kim, K. W. Park, H.-H. Park, J. Joung, J.-S. Ro, H. L. Lee, C.-H. Hong, and T. Im, *Applied Numerical Methods Using MATLAB*, Hoboken, NJ, USA: John Wiley & Sons, 2020.
[19] National Institute of Standards and Technology, "X-Ray Form Factor, Attenuation and Scattering Tables." [Online]. Available: https://physics.nist.gov/PhysRefData/FFast/html/form.html
[20] H. E. Salman, *Adsorption Study of the Interaction Between Zinc Oxide Nanoparticles with Albumin and Creatinine*, Ph.D. dissertation, Univ. of Kerbala, Karbala, Iraq, 2019.