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Theoretical Analysis of the X-ray Mass Absorption Coefficient Produced by the Photoelectric Effect and Comparison of the Accuracy of a Computational Model of NiO and SiC

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ABSTRACT

This study aims to analyze and calculate the mass absorption coefficient of X-rays resulting from the photoelectric effect in nickel oxide and silicon carbide compounds in the energy range of 1-100 keV by using a simple, approximate, and semi-empirical theoretical model with constants that depend on the type of interaction. The effective atomic number was then calculated, and the theoretical model was used to calculate the mass absorption coefficient of the compounds. The results extracted from the application of the theoretical model were compared with the experimental or semi-experimental results extracted from the databases of the programs XCOM and FFAST. To improve the accuracy of the theoretical model, the real atomic number was replaced by the effective atomic number, as the results showed good agreement in the low energy range of the studied model. However, the accuracy of the model decreases at energies higher than 30 keV. The results were improved when using the effective atomic number, especially in the compound where there is a difference in the atomic numbers of its components. Therefore, incorporating the concept of the effective atomic number clearly enhances the accuracy of the theoretical model, making it more realistic in describing mass absorption behaviour. This simple modification to the theoretical model showed a clear improvement in the theoretical results. All calculations and graphical representations were performed using the MATLAB 2020 program.

Keywords: X-ray, absorption coefficient, effective atomic number, XCOM, FFAST, MATLAB.

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1. Introduction

Since Roentgen astonished the world with his discovery of X-rays and their ability to reveal what is hidden from the human eye, understanding their interaction with materials has become the beginning of a scientific revolution. From this point, the concept of the mass absorption coefficient emerged as a factor that determines the fate of rays, whether they are absorbed, scattered, or produced by pairs, depending on their energy and the composition of the material (Iglesias-Juez et al., 2022). This factor is considered the backbone of modern technology, as it is a crucial component in many practical applications used in everyday life. In medicine, bones can be distinguished from soft tissues due to the difference in their absorption coefficient (Abdelmonem, 2025). At airports, security inspection devices analyze the contents of bags by comparing the absorption of materials to rays. Thus, the mass absorption coefficient can be considered the link between abstract physics and solutions that harmonise our lives. From the emergency room to the nuclear control room to industrial production lines, it gives us a reality of the importance of this physical value (Hassan et al., 2021). The interaction of X-rays with materials provides information that contributes to revealing the density of electronic states, the nature of molecular bonds, and other properties of the solid state. Numerous studies in the field of materials surface science have been conducted to elucidate the properties, characteristics, and interactions associated with the surfaces of various materials (Nesterova et al., 2024). The absorption of X-rays by a material, according to specific laws, is a fundamental pillar of applied physics. Many studies have addressed the subject of X-ray absorption, the most prominent of which is the study by Mohammed Sultan Al-Buriahi and Baris T. Tonguc (2020). In their study, the researchers proposed several materials to be used as shielding materials against X-rays and other radiation. These materials are promising and can be used in windows and doors in medical diagnostic laboratories, X-ray rooms, and radiotherapy rooms (Al-Buriahi et al., 2020). In addition to the numerous studies that demonstrate the importance of the processes affecting the interaction of X-rays with matter, accurate calculations are essential for achieving a deeper and more comprehensive understanding of these processes. This enables the independent analysis of each process, followed by comparison with the theoretical model and the experimental or quasi-experimental results issued by the various programs, as indicated in the study by G. Manjula, BR. Roy, S. Jyothsna, AM. Kumar, et al., Materials Today, 2021. In this study, the researchers were able to obtain the highest absorption coefficients for the fine atomic structure region for X-ray absorption, as the results showed a discrepancy between the specified values and the measured values. The results were then compared with the results of the FFAST and WinXCom programs, as there was good agreement with the experimental and theoretical observations (Al-Buriahi et al., 2020). Advances in X-ray science have made it possible to measure the absorption of materials with high accuracy, providing profound insights into the atomic structure of materials and the extent of their density changes. This has opened up many horizons for practical applications across various fields used to test theoretical predictions. These measurements have greatly improved the ability to predict fine structure associated with X-ray absorption (Whitehead & Finke, 2021). Many practical applications also depend on this principle. For example, when using X-rays in imaging, whether in the medical or industrial field, the process relies on the difference in absorption rates when the rays interact with all parts of the material. This difference in the absorption rate makes it possible to determine the internal details of materials (Revenko & Pashkova, 2023). Relative measurements may be sufficient for theoretical calculations when calculating the mass absorption coefficient of X-rays, but measuring attenuation in general, including absorption and scattering, provides a more accurate tool for calculating the absorption coefficient of X-rays (Schweizer et al., 2024). Therefore, the aim of this research paper is to evaluate the theoretical equation and the suitability of its application when calculating the X-ray mass absorption coefficient for the studied targets, while providing a comprehensive explanation of modifying the theoretical equation in support of practical applications based on accurate absorption measurements.

2. Theoretical Background

The X-ray absorption coefficient of compounds depends on several key factors related to the compound's composition and the conditions of interaction between the material and X-rays. These include:

2. 1. The Chemical Composition of the Compound

The absorption coefficient of a compound depends on the elements that comprise it. The higher the atomic numbers of the elements, the greater the efficiency of the compound in absorbing energy.

2. 2. The Mass or Weight Fraction of the Compound

This term originates from mathematics and physics as a basis for analysing ratios. It represents the mass percentage that a particular element contributes to the overall compound, as shown in Table 1. It is used to determine the contribution of each element when calculating the overall properties of the compound, including the X-ray absorption coefficient. The weight fraction directly affects the absorption coefficient, which can be derived for each compound according to the following relationship (Bam et al., 2020; Streltsov et al.).

$$W_i = m_i/M \quad (1)$$

Where: W_i refers to the weight fraction of element i in the compound, m_i refers to the mass of element i in the compound, and M refers to the molar mass of the compound. Therefore, the mass absorption coefficient of compounds can be calculated according to the following relationship (Kasman et al., 2021)

$$[\mu/\rho]_S = \sum W_i (\mu/\rho)_i \quad (2)$$

Where: - $\sum W_i$ refers to the total weight fraction of the elements in the compound.

$[\mu/\rho]_i$ Represents the mass absorption coefficient of the element in the compound. Which is extracted from the application of the theoretical equation:

$$[\mu/\rho]_i = \rho Z^4/mE^3 \quad (3)$$

The effective atomic number can be defined as a convenient quantity for evaluating the interaction of a photon with a substance, as explained by Hine (1952). It can provide a preliminary estimate of the chemical composition of a substance in general. The effective atomic number is large for inorganic compounds and metals, while it is small for organic materials. It is also called the effective charge and can be defined as the number of electrons per unit mass of the absorber. The effective atomic number is symbolised by the symbol Z_{eff}. Its value can be calculated either using a physical law or Slater's rule. It is a suitable parameter for representing the interactions of X-rays and gamma rays. For example, it is used in radiation shielding designs or in calculating the absorbed dose in radiotherapy (Zhou, 2024). Slater was able to calculate the effective nuclear charge (effective atomic number) of electrons in the s, p, d, and f shells (Cheewasukhanont et al., 2022). It is necessary to determine the amount of X-rays absorbed by materials in order to determine the amount of safe dose for individuals, through which the most appropriate materials are chosen for use as radiation shields. In the case of compounds, Slater's rule cannot be applied to extract the effective atomic number. Rather, a more accurate mathematical relationship can be used to calculate the effective atomic number based on the mass fraction of the elements that make up the compound, according to the following relationship (Aldalawi et al., 2021):

$$Z_{eff} = \sum W_i Z^3 \quad (4)$$

Table. 1. shows the most important physical and chemical properties of (NiO, SiC) (Patel, 2023)

Symbol	Density	Molecular weight	Boiling point	Melting point	Crystal structure	Effective atomic number
NiO	6,67	74.69	2800	1955	FCC	25.89
SiC	3.21	40.10	Transcends	2700	FCC	12.57

3. Research Methodology

In this research paper, the mass absorption coefficient of X-rays in the energy range of 1-100 keV was calculated based on photoelectric absorption for the compounds SiC and NiO, as well as the elements that make up the compounds (Si, C, Ni, O). This analysis aims to investigate the absorption behaviour resulting from the photoelectric effect for theoretical purposes and to highlight the influence of atomic number and energy on the absorption capacity of materials. To develop a theoretical model based on photoelectric absorption, the calculations were performed using theoretical equations (2) and (3).

The mass absorption coefficient of the target materials was extracted using standard programs approved by NIST, such as XCOM. XCOM has its roots in the early 1970s, when physicists at the National Institute of Standards and Technology (NIST) developed computational models to calculate the cross sections of photon interactions with matter. It was published as a standalone program in 1987 by Berger & Haberman and later updated. XCOM is a specialized program for calculating the absorption coefficients of X-rays in various materials. Its name reflects the combination of the concept of X-rays and the complex calculations associated with them. It was developed by the NIST Laboratory for Calculating the Absorption Coefficients of X-rays in Various Materials (Berger, 2010), along with the FFAST program.

FFAST is a physics-based computer program that serves as a standard reference database developed by the National Institute of Standards and Technology (NIST), last updated in 2005, which contains a detailed table of atomic form factors, absorption cross-section, electro-optical scattering, and mass attenuation coefficients for the range (1-10 eV), the range (-0.4 - 1 MeV), and the atomic range (1-92). Much of the modern theoretical foundation for this data was provided by Cromer, Mann, and Lieberman, while Heky et al. contributed significant experimental data. FFAST is an abbreviation for (Form Factor and Scattering Tables). The program was developed to meet the need for accurate and up-to-date tables of physical parameters related to the interaction of X-rays with materials. This program began in the mid-twentieth century, and with the development of technology, FFAST emerged as an updated tool to obtain higher accuracy and efficiency, using the latest physical theories and practical data to obtain results that meet modern needs. FFAST was developed as an alternative to the XCOM program, but it focuses primarily on diffraction, scattering, and interference. It began in the early 1990s and was developed using new computational methods, including quantum calculations. The program has several functions, including calculating the absorption coefficient of X-rays for single elements, compounds, and mixtures. Further, FFAST provides accurate scientific information about the interaction of matter with X-rays and plays an effective role in the design of X-ray devices, medical imaging, and scientific studies related to radiation. It is widely used in absorption and scattering calculations, as it covers a wide energy range (1 keV - 100 MeV) (Factor, 2009).

The effective atomic number or effective nuclear charge was calculated using a theoretical equation based on the atomic number and mass fraction of the compound. The original atomic number was then replaced by the effective atomic number. The results were then tabulated and represented graphically, and a comparison was made between all the results obtained by different methods. All calculations were performed using MATLAB 2020. As shown in **Figures 1**.

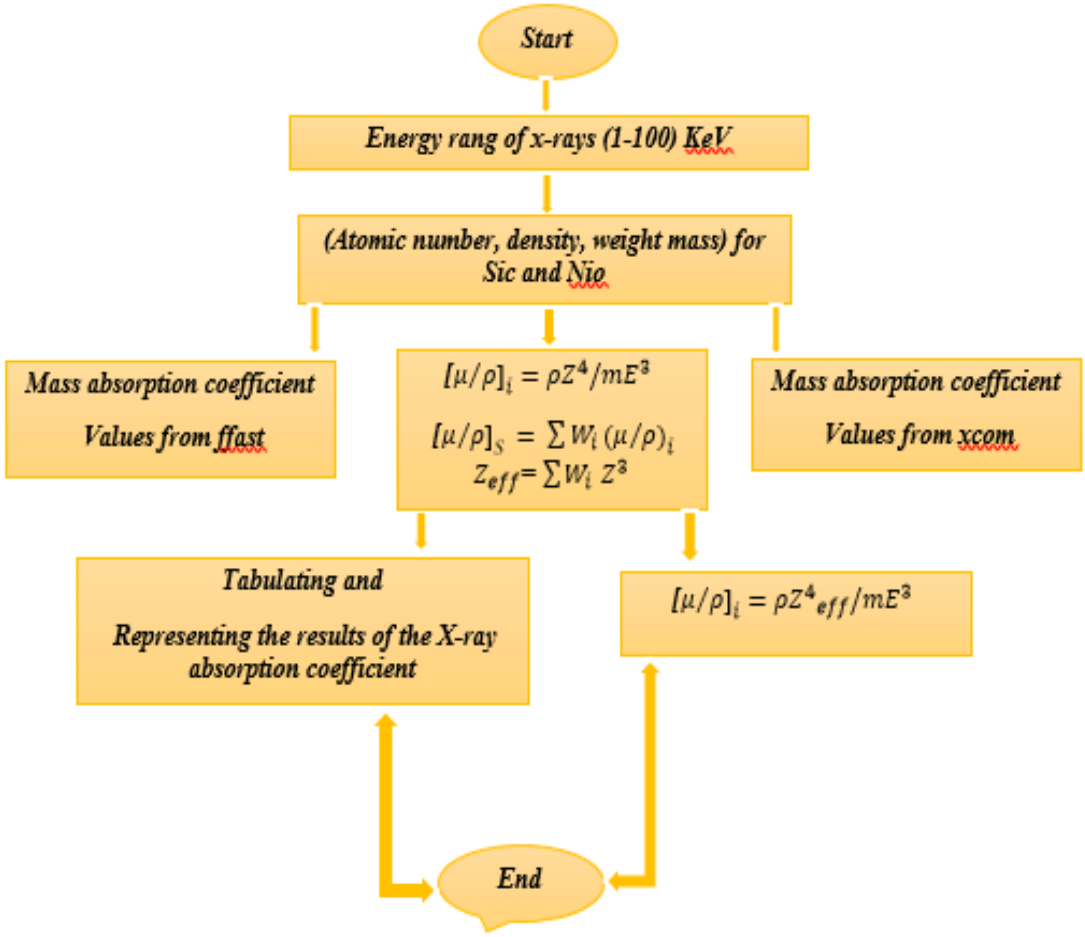

Figure 1. Illustrates the MATLAB algorithm.

4. Results and Discussion

Figures 2 and 3, as well as Tables 2 and 3, show the values of the mass absorption coefficient according to Equation (2) for NiO-Z and SiC-Z, which represent the value of the mass absorption coefficient of X-rays according to the theoretical model studied in terms of the atomic number. The results are compared with data from the XCOM and FFAST programs. From the figure, we note that the mass absorption coefficient is very high in the low range, indicating strong absorption of photons in the low range. As the energy increases, a sharp decrease occurs due to the diminishing influence of the photoelectric effect. At high energies, the absorption coefficient stabilizes at low values, where the dominance of the Compton Effect and pair production becomes apparent. Irregularities are also observed in the absorption edges, which may be attributed to several factors, including the chemical effects resulting from the combination of pure nickel with oxygen and interactions between various physical phenomena. Additionally, the mass absorption coefficient of silicon carbide increases significantly in the low range due to the dominance of the photoelectric effect. In this range we see the conformity of the curve of theoretical equation(2) with the experimental results of the XCOM program.

Then the coefficient begins to decrease significantly, which shows that the results of the equation agree well with the data of *the* XCOM program at medium energies (10-50 keV). At high energies < 50 keV, we notice an increasing and gradual decrease in the values of the mass absorption coefficient, but all the curves are very close in the high-energy range, but we notice that the experimental values of the XCOM program are closest to the results of equation (2). At high energies (<40 keV), we notice that the theoretical values are closer to the experimental values, meaning that in this range the mass absorption coefficient becomes more stable, which reflects that the effects of the electronic structure in this range have begun to decrease. Specifically, compounds that consist of elements with significantly different atomic numbers will have theoretical values that deviate from

the experimental values, whereas compounds that contain elements with similar atomic numbers will have theoretical values that are close to the experimental values. The shielding coefficient of the target compounds (NiO, SiC) was determined by calculating the amount of shielding caused by the inner electrons close to the nucleus on the electrons in the other outer orbits. Based on this calculation, the effective atomic number (effective charge) was measured theoretically according to Equation (4) for the studied compounds. The mass absorption coefficient of the above metals was calculated according to Equation (3), replacing the atomic number (Z) with the effective atomic number (Z_{eff}), which was extracted according to Equation (4). We note the curve of the mass absorption coefficient as a function of energy for nickel oxide. In the low energy range (0-20 keV), its values, according to Equation (2), NiO-Z, are higher than the rest of the curves and tables, indicating greater absorption of X-rays in this range. As for the results of the modified equation in terms of the effective atomic number, NiO-$Z_{eff} for\ the\ compound$, both the results and the curve indicate a sharp decrease in the mass absorption coefficient. This means that when using the effective atomic number instead of the atomic number, the absorption of X-rays by the material decreases. In the medium energy range (20-50 keV), we note that the values extracted from Equation (4) are higher than the experimental values of the XCOM program, and the values of the modified equation (NiO-Z_{eff})are lower than the experimental values of the XCOM program. However, this difference between the curves gradually decreases as the energy increases. In the high energy range (50-100 keV), we note a greater convergence between the curves and the values of the models used, but (NiO-Z_{eff}) remains the lowest of the curves. The reason for the decrease can be explained by the fact that the model used does not accurately reflect the effects of each element. The model also neglects sharp transitions in absorption in the energy range used. In addition, the effective atomic number is an approximation and is not an accurate replacement for the original equation. Therefore, when using it, precise details of X-ray absorption may be lost for some compounds. At low energies (less than 5 keV), oxygen contributes significantly, giving a good approximation to the equation. In Fig. 1 and Table 3, we observe that (SiC) at low energy ranges (0-20 keV) takes a representation similar to nickel oxide, where the curve and values of (SiC-Z) resulting from applying Equation (2) are higher than the rest of the curves, while (SiC-Z_{eff})resulting from modifying Equation (4) are less than XCOM. At medium energies (20-50 keV), we observe convergence in the plots and values between the models used, except for the XCOM program, which remains gradually lower. At high energies (50-100 keV), the curves converge or begin to converge, but (SiC-Z_{eff})remains slightly lower. In addition, the differences at the high range between the studied models become smaller. The reason for this is that silicon carbide shows a different response in absorbing X-rays in a way that affects the computational models. In fact, at low energies, the shielding is more pronounced, leading to a decrease in the effective atomic number and, consequently, a decrease in the absorption coefficient value. The mass is compared to the value calculated according to equation (4). At medium energies, the effect of shielding begins to decrease until the effective atomic number remains less than the normal atomic number. We note that the decrease in the value of the mass absorption coefficient remains less than it was in the case of using the normal atomic number. At high energies, the most important role is in the absorption of the inner electrons, as we note a decrease in the differences between Z and Z_{eff} . At that time, the effect of replacing one of the factors of the theoretical equation (3) is very small in the high-energy range due to the dominance of Compton interactions and pair production in the material.

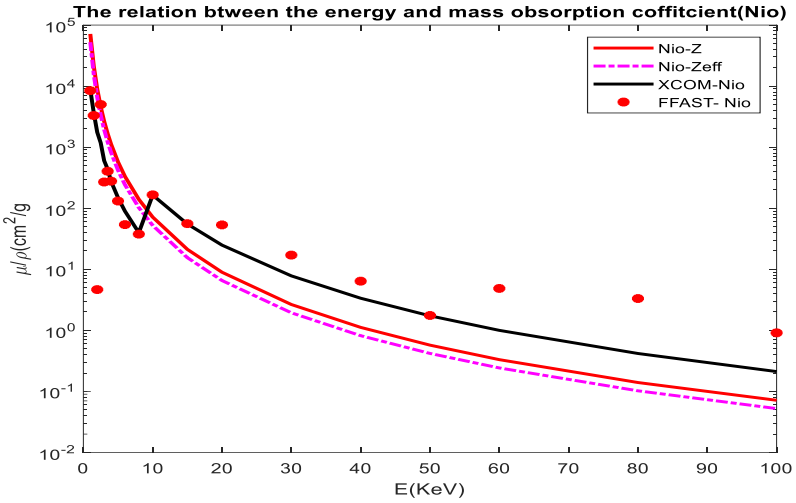

Figure 2. shows the mass absorption coefficient of nickel oxide using various computational and experimental methods.

Table 2. Shows the theoretical and experimental values of the X-ray absorption coefficient as a function of energy for nickel oxide.

Energy (keV)	Absorption coefficient of X-ray by NiO- Z(cm^2/g)	Absorption coefficient of X-ray by NiO- $Zeff$ (cm^2/g)	Absorption coefficient of X-ray by XCOM (cm^2/g)	Absorption coefficient of X-ray by FFAST (cm^2/g)
1	71577.4	52347.8	8723	8428.158
1.5	21208.1	15510.4	3655	3297.925
2	8947.18	6543.4	1755	4.653303
2.5	4580.95	3350.2	1177.9	5005.26
3	2651.01	1938.8	600.8	268.8943
3.5	1669.44	1220.9	437.9	403.5981
4	1118.39	817.93	275	277.6821
5	572.619	418.78	148.70	131.211
6	331.377	242.35	89.5	53.9435
8	139.799	102.24	39.83	37.6931
10	71.5774	52.347	164.2	165.8165
15	21.2081	15.510	55.21	55.933
20	8.94718	6.5434	24.88	53.3352
30	2.65101	1.9388	7.801	17.0735
40	1.11839	0.8179	3.358	6.3902
50	0.57261	0.4187	1.73	1.753
60	0.33137	0.2423	0.9994	4.8594
80	0.13979	0.1022	0.4178	3.3207
100	0.07157	0.0523	0.2113	0.911

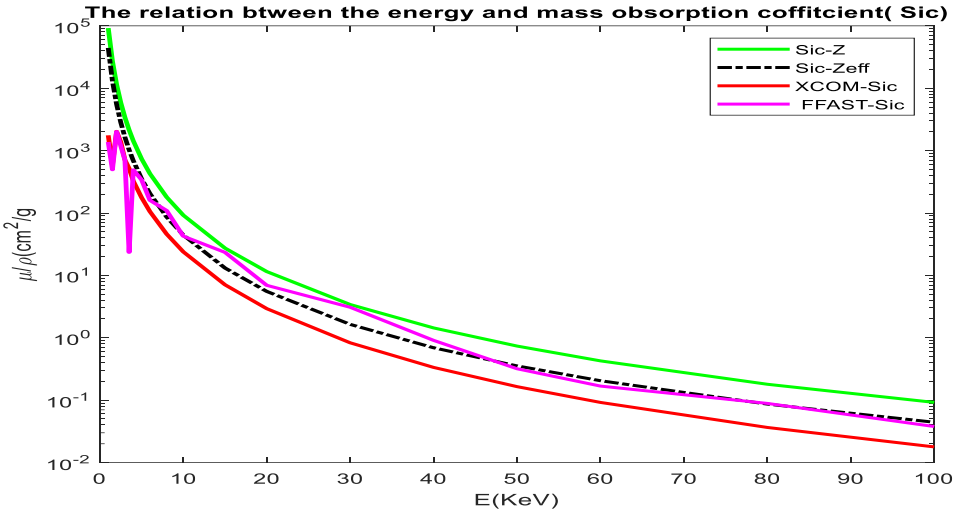

Figure 3. shows the mass absorption coefficient of silicon carbide using various computational and experimental methods

Table 3. Shows the theoretical and experimental values of the X-ray absorption coefficient as a function of energy for silicon carbide.

Energy (keV)	Absorption coefficient of X-ray by SiC-Z(cm^2/g)	Absorption coefficient of X-ray by SiC-$zeff$ (cm^2/g)	Absorption coefficient of X-ray by XCOM (cm^2/g)	Absorption coefficient of X-ray by FFAST (cm^2/g)
1	2295.814	2852.8	1760	1373.385
1.5	680.2412	845.28	583	493.3119
2	286.9767	356.60	2034	2020.3
2.5	146.9321	182.58	1372.5	1191.3
3	85.03015	105.66	711	704.55
3.5	53.54668	66.538	519.15	23.366
4	35.87209	44.575	327.3	491.6185
5	18.36651	22.822	176.4	339.921
6	10.62876	13.207	105.3	159.6442
8	4.484012	5.5719	45.95	109.4068
10	2.295814	2.8528	23.84	42.4616
15	0.680241	0.8452	7.066	23.366
20	0.286976	0.3566	2.929	6.9286
30	0.085030	0.1056	0.8301	3.0826
40	0.035872	0.0445	0.3349	0.9081
50	0.018366	0.0228	0.1647	0.3188
60	0.010628	0.0132	0.09195	0.1681
80	0.004484	0.0055	0.03652	0.0887
100	0.002295	0.0028	0.01781	0.0378

5. Conclusions

When studying and calculating the X-ray mass absorption coefficient for the two compounds in this study within the energy range (1-100 keV), it becomes clear that there is a fundamental discrepancy in using the effective atomic number instead of the real atomic number. When using nickel oxide, which consists of two elements with a difference in atomic number, this difference leads to a small and non-linear interaction, as nickel has a significant effect at the absorption edge energies, i.e., in the low energy

range. In addition, oxygen atoms have a prominent role in the overall absorption of the compound, which makes replacing the real number with the atomic number, i.e., by modifying the equation, very useful to obtain an idea of the average absorption behaviour. However, this idea is less accurate in the high-energy range, especially at the absorption edges of nickel, where sharp discrepancies appear in the values of the mass absorption coefficient, which cannot be represented using the effective atomic number alone.

Therefore, we conclude that modifying the equation is appropriate and useful for obtaining an approximate estimate away from the absorption edges, while using the real atomic number is useful and necessary in cases that require spectral accuracy. As for silicon carbide, which is composed of two relatively light elements, the absorption curve is more consistent and regular in the studied energy range. The absence of absorption edges in the medium and low energy range of X-rays gives a highly accurate prediction when using the effective atomic number to obtain a consistent absorption behaviour. This makes silicon carbide easier to represent both physically and behaviourally in applications that need a general estimate of absorption and do not require a precise interpretation of the spectrum.

Consequently, we conclude that it is preferable to use the true atomic number, as general approximations, and the effective atomic number in precise spectroscopic analyses, particularly for absorption edges for nickel oxide. For silicon carbide, using the effective atomic number from the modified theoretical equation is considered more accurate and appropriate, due to its simple atomic structure and the absence of absorption edges in the compound.

Conflicts of Interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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