Study of The X-ray Coherent Scattering Cross Section of Copper

Khamael Eisaa1, Mohsin Hasan Ali 2

1,2 Physics Department, College of Education for Pure Sciences/ Tikrit University, Iraq
E-mail: muhsin.astro@tu.edu.iq

Abstract:

In this study the coherent scattering function \( f(k) \) has been calculated for x-ray in Copper using the Wave function involving Slater’s roles approximation for the values \( 0 \leq k \leq 1.6 \text{ Å}^{-1} \). The Rayleigh scattering cross section, has been calculated. The Rayleigh scattering cross section was found to be dominate at low energy, where the scattering cross section starting from very small energy and less than 1KeV. Also the increasing of angular distribution for Rayleigh scattering cross section is principle dependent on the value of atomic scattering factor \( f(k) \), and observed Rayleigh scattering decreasing at high energies, while it is more distinct at low energies, for this reason the Rayleigh scattering is very important at low energies, because the scattering angle is large.

Key Words: Coherent Scattering, Atomic Scattering Factor, Differential Cross section of Scattering.

1. Introduction:

There has been more interest in obtaining reliable values of cross section for elements and compounds as well as alloys because of its required in variety of applications in radiography, tomography, space physics, plasma physics etc [1]. Atomic form factor of specimens of various types, from nuclear compounds to biological tissues, have been widely investigated in the past and also recently in different branches of science, since they provide detailed information concerning the electric charge distribution of the specimens [2–7]. By systematically measuring Atomic form factor, information about the electric charge distribution of targets has been extensively extracted from scattering experiments [8, 9]. Atomic Form factor, especially, play an important role in different topics of applied science such as: radiation absorption in shielding and medical diagnostics [10], structural factors of crystals in crystallography and image contrast in Transmission Electron Microscopy [11, 12]. During the last decades, extensive amount of numerical calculations on nonrelativistic atomic form factor and relativistic for atoms and ions have been carried out, mostly by using Hartree-Fock (HF) wave-functions. Such numerical calculations can be found in several tables [13-15]. Simultaneously, there has been many attempts toward analytical evaluations of atomic form factor.
2. Theory:
   a- The Atomic Form Factor $F(k, Z)$:
The atomic form factor $f(k, Z)$ defined as the amplitude of electron oscillation when interact with incident radiation, the electron in turn oscillates with the same frequency of the incoming wave train and since an accelerating electric charge emits electromagnetic radiation, scattered photon appears to emerged from the interaction site with the same frequency of the oscillating electron, consequently the scattered amplitude (as function of the scattering angle of electron, is not equals to $Z$ times the free electron amplitude; but its modified by atomic form factor $f(k, Z)$ where $k$ is the momentum transfer parameter measured in units of $1/\AA^0$ defined as [16] :
   
   $$k = \frac{\sin(\theta)}{\lambda}$$

   Where $\lambda$ is the incident wavelength and is $\theta$ the scattering angle. The function $f(k, Z)$ is related to the ratio of the amplitude of scattered wave form to scattered amplitude from free electron and given by [16]:
   
   $$f(k, z) = \frac{d\sigma_{\text{atom}}}{d\Omega} \frac{d\sigma_{\text{Hadamard}}}{d\Omega}$$

   The various methods of photons interactions with matters allows to utilizes the scattered photons or transmitted through material to determine and calculating the information about the material itself. The probabilities of photons interactions with matter are functions for both incident energy and atomic number $Z$ for material; these probabilities are expressed as a parameter calls cross section express in barn unit (1 barn= $10^{-28}$ m$^2$) [17]. The exact solutions of Schrödinger’s many electron equation may be expressed as linear combinations of these determinant wave-functions [18]. So that the single-electron orbital can then be written as a product of a radial function, a spherical harmonic, and a spin function. This is well-known central-field approximation [19]. The orbitals in turn, are written as an expansion in some set of analytic basis functions [20].

   $$\Phi_{nl} = \sum_i c_i \Psi_{nlm}$$

   the basis function $\Psi_{nlm}$ is the standard Slater-type orbitals and is given by:

   $$\Psi_{nlm}(r, \theta, \varphi) = R_{nl}(r) \times Y_{lm}(\theta, \varphi)$$

   And

   $$R_{nl}(r) = N r^{n-1} e^{-\zeta r}$$

   Where: $N$ is the normalization constant and is given as:

   $$N = (2\pi)^{n+1/2}$$

   and is the orbital exponents and is given as:

   $$\zeta = \frac{Z - \sigma}{n}$$

   and $\sigma$ is the shield constant.

   the scattered amplitude from an element $dr$ of electron density $\rho(r)$ is given by:

   $$f(k, z) = \rho(r) e^{ikr} dr$$
Thus, the total scattered amplitude is obtained by integration over the whole electron density distribution as:

\[ f(k, z) = \int |\Psi_{nm}|^2 e^{ik.r} r^2 dr \sin \theta d\theta d\varphi \]  

(9)

b- Rayleigh (Coherent) Differential Scattering Cross Section:

In Rayleigh scattering event, a photon scattered off atomic electrons where energies of incident and scattered photons are identical, in this process the recoil energy of absorber atom is negligible and the process occurs at small angle, thus the cross section of Rayleigh depends upon the photon energy \(E\) and atomic number of the absorber \(Z\) [21], and differential cross section is given by [22]:

\[ \frac{d\sigma_{Rayleigh}}{d\Omega} = \frac{d\sigma_{Thomson}}{d\Omega} |f(k, z)|^2 \]  

(10)

where \(d\Omega\) is the solid angle and the term \(\frac{d\sigma_{Thomson}}{d\Omega}\) is defined as the differential cross section of free electron or Thomson cross section [22]:

\[ \frac{d\sigma_{Thomson}}{d\Omega} = \frac{1}{2} r_e^2 (1 + \cos^2 \theta) \]  

(11)

and \(r_e\) is the classical radius of electron \((r_e = 2.817 \times 10^{-15} \text{m})\) and \(f(k, Z)\) is the atomic form factor. So equation (10) can be written as following [23]:

\[ \frac{d\sigma_{Rayleigh}}{d\Omega} = \frac{r_e^2}{2} (1 + \cos^2 \theta) |f(k, z)|^2 \]  

(12)

3. Results and Discussion

The atomic form factor has been calculated for the Copper from eq.(9) the results have been shown in figures (1), from the figure we conclude decreasing as photons energy increases,
The coherent cross section has been calculated for the Copper from eq.(12) the results have been shown in figures (2), from the figure we conclude decreasing as photons energy increases, This means that the Coherent scattering cross section of Rayleigh never dominates the total cross section but at small angles scattering (θ less than 10°)

From the figure (2), we notice that the cross-section of Rayleigh scattering is dominant at low energies, as the cross-section of the scattering starts from very small energy and less than 1KeV. The increase in the angular distribution of the cross-section of Rayleigh scattering depends on the values of the atomic scattering factor f (k, Z), where We notice that Rayleigh scattering at high energies decreases while it is more pronounced at low energies. For this reason, Rayleigh scattering is important at low energies, because the scattering angle is large. This is agreement with [13], and by comparing the results that have been reached with the finding of Hubbell using the Harter-Fock method [13], illustrated in Figure (3), we notice that there is a converging behavior. For the values of the cross section of the scattering, however, the differences between the computed values depend on the method used to find the wave functions. In atomic scattering processes, it is assumed that the atoms are singular and there are no effects of neighboring atoms.
This is contrary to the truth because there are unavoidable interactions such as molecular and chemical effects that are not taken into account [24]. Finding solutions for atomic wave functions for a wide range of elements and energies becomes possible. Through the development of computational techniques, these calculations in turn made it possible to calculate the cross-sections of the photoelectric absorption. As the tables used for the atomic scattering factor differ with the solutions for several elements and the range of important energies, the theoretical models developed do not necessarily give a better agreement with the experimental values. The main differences between the results result from the different theoretical frameworks that were used to calculate the wave function, as each one handles exchange and correlation. The interference that occurs in a different manner therefore results from the diverse application of approximate methods and convergence criteria [25].

4. References
[1] Yakup K., Salih E., Ridvan D. and Yusuf S. 1998. “Measurement of Compton and coherent scattering Differential cross sections” Tr. J. Of Phys. 22: 783-788 Turkey.
[2] Kamal K. Seth et al., Phys. Rev. Lett. 110, 022002 (2013).
[3] Z. Ahmed et al., Phys. Rev. Lett. 108, 102001 (2012).
[4] J. C. Bernauer et al., Phys. Rev. Lett. 105, 242001 (2010).
[5] A. Courtoy, F. Fratini, S. Scopetta, and V. Vento, Phys. Rev. D 78, (2008).
[6] C. T. Chantler, J. Phys. Chem. Ref. Data 29, 597 (2000).
[7] A. Tartari, A. Taibi, C. Bonifazzi, and C. Baraldi, Phys. Med. Biol. 47,163 (2002).
[8] B. W. Batterman, D. R. Chipman, and J. J. DeMarco, Phys. Rev. 122, 68 (1961).
[9] A. Alatas et al., Phys. Rev. B 77, 064301 (2008).
[10] R. Cesareo et al., Phys. Rep. 213, 117 (1992).
[11] C. Giacovazzo et al., Fundamentals of Crystallography (Oxford Science Publications, 1992), chapter 2.
[12] Ewaid, S.H.; Abed, S.A.; Al-Ansari, N. Crop Water Requirements and Irrigation Schedules for Some Major Crops in Southern Iraq. Water 2019, 11, 756.
[13] Ewaid, S.H.; Abed, S.A.; Al-Ansari, N. Water Footprint of Wheat in Iraq. Water 2019, 11, 535.
[14] Ewaid, S.H.; Abed, S.A.; Al-Ansari, N. Assessment of Main Cereal Crop Trade Impacts on Water and Land Security in Iraq. Agronomy 2020, 10, 98.
[15] Salim, M. A. and Abed, S. A. (2019). The first oriental honey buzzard pernis pilorhynchus (Temminck, 1821) in Iraq. Eco. Env. & Cons. 25 (1) : pp. (1926-1929).
[16] Ewaid, S.H.; Abed, S.A.; Al-Ansari, N.; Salih, R.M. Development and Evaluation of a Water Quality Index for the Iraqi Rivers. Hydrology 2020, 7, 67.
[17] D. B. Williams and C. B. Carter, Transmission Electron Microscopy: A textbook for material science (Springer, 2009), chapters 2 and 3.
[18] J. H. Hubbell et al., J. Phys. Chem. Ref. Data 4, 471 (1975).
[19] J. H. Hubbell and I. Øverbs, J. Phys. Chem. Ref. Data 8, 69 (1979).
[20] A. J. C. Wilson and V. Geist, International Tables for Crystallography, Volume C: Mathematical, Physical and Chemical.
[21] Cromer, D.T. and Mann, J.B. 1967 “Compton Scattering Factors for Spherically Symmetric Free Atoms” J. Chem. Phys. 47: 1892-1983.
[22] Hubbell, J.H. and Berger, M.J. 1968 “Attenuation Coefficients, Energy Absorption Coefficients, and Related Quantities”, ed.1 (Springer, Berlin), 167-202.
[23] H. Clark "A first course in Quantum Mechanics" VAN Nostrand, Reinhold Company LTD, New York (1978).
[24] Enge. Wehr. Richards, “introduction to atomic physics”, Addison-Wesley, 1972.
[25] N. H. March, "Self-Consistent Fields in Atoms” first edition, Pergamon Press, New York, 1975.
[26] Ronald G. and William S. 1999. "Theory and Problems of Modern Physics" Schaums Outline Series,2.USA 63.
[27] Kerur. R. ,Thonntaarya S.R and Hamumaiah B.1993. “X-ray attenuation coefficients for various elements” X-ray Spec.22(6):13-15.
[28] Martyn John Key. 1999. "Gas Microstructure X-Ray Detectors and Tomography Multiphase Flow Measurement" UK ,A thesis submitted to the University of Surrey of Doctor .
[29] C.T. Chantler, C.Q. Tran, D. Paterson, Z. Barnea and D.J. Cookson,(2001) "Direct Observation of Scattering Contributions in X-ray Attenuation Measurements, and Evidence for Rayleigh Scattering From Copper Samples rather than Thermal-Diffuse or Bragg–Laue Scattering" Radiation Physics and Chemistry 61, 347–350 .
[30] C.T. Chantler, "Theoretical Form Factor, Attenuation, and Scattering Tabulation for Z=1–92 from E=1–10 eV to E=0.4–1.0 MeV", J. phys. Chem. Ref. vol 24, 1995, pp 71-82.
[31] Ali , W., & R.Annon, M. (2020). Biological Effective of organic solvent extracts of Mirabilis jalapa Leaves in the Non-cumulative for mortality of Immature stages Culex quinquefasciatus Say ( Diptera : Culicidae ). Al-Qadisiyah Journal Of Pure Science, 25(1), Bio 1-6.