



Calculation of The Imaginary Part of Atomic Form Factor For X-ray In Nickel

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Abstract

In the present study, we calculated the imaginary part of the x-ray scattering factor of nickel based on the principles of quantum mechanics to find a wave function that describes the electronic state of atoms by approximate methods, observed the study suggested that in both low energy values $\omega \ll \omega_e$, and at high energy values $\omega \gg \omega_e$, the imaginary part is approximately zero, this means that the electrons are intensely connected to the atom, where in the spectrum the photon energies are approximately equal to the electron bonding energy $\omega \sim \omega_e$ we note the study pointed out that the imaginary part of the atomic scattering factor become prominent and the electron becomes highly absorbent, the relative accuracy varies within range (0.03-0.22)%, and there was also a good agreement between the behavior we obtained for the imaginary part of the atomic scattering factor and the behavior that was calculated using other models.

Introduction

The real and the imaginary component of the anomalous scattering of the total atomic scattering factor describe the optical properties of the material. This includes reflection, refraction and absorption of x-rays. The spatial distribution of atomic electrons is important for this research, as in the case of diffraction and total atomic scattering[1]. Where the importance of the subject in the find of optical properties of metals as mentioned in the research board and its applications in laser systems and all optical systems, the attenuation of X-rays in different materials provides a wide range of information about the fundamental properties of matter at the atomic and molecular level. In particular, relative and absolute measurements of the total attenuation factor are used to measure theoretical predictions of photovoltaic absorption using the wave functions of the electron with the specified state[2], Moreover, the dynamics of atomic processes, including Auger transition, and provides information on the density of electronic cases, molecular bonds and other solid state properties[3]. many studies are carried out on this subject ,one of them study for X-ray Extended-Range Technique for Precision Measurement of The X-ray Mass Attenuation Coefficient and Im(F) for Copper Using Synchrotron Radiation, and he find that this technique achieves accuracies of (0.27– 0.5) %

[4]. And the other study for X-ray mass attenuation coefficients and imaginary components of the atomic form factor of zinc over the energy range of 7.2–15.2 keV and with absolute accuracy of (0.044 - 0.197) %, it is Observed that differences between the measured mass attenuation coefficients and various theoretical calculations reach a maximum of about 5% at the absorption edge and up to 2% further than 1keV away from the edge. The measurements call for improvements in the theoretical calculations of mass attenuation coefficients of zinc[5]. The aim of study is to show the evolution the imaginary part of atomic form factor for the nickel .

Theoretical Part

The study will take some of the theoretical bases that show how the imaginary part of the X-ray form factor is calculated in nickel.

1. Time-Dependent Perturbation Theory

Perturbation theory is an important tool for describing real quantum systems, as it turns out to be very difficult to find exact solutions to the Schrodinger equation for Hamiltonians of even moderate complexity, the Hamiltonians to which we know exact solutions, such as the hydrogen atom, the quantum harmonic oscillator and the particle in a box, are too idealized to adequately describe most systems. Using perturbation theory, we can use the known

solutions of these simple Hamiltonians to generate solutions for a range of more complicated systems, Schrodinger equation is treated in the following formula [6].

$$\hat{H}(r)|x, t\rangle = i\hbar \frac{\partial}{\partial t} |x, t\rangle \dots (1)$$

Where $\hat{H}$ the Hamiltonian's effective which represents kinetic and potential energy, $(i\hbar \frac{\partial}{\partial t})$ represents energy, $\hbar$ plank constant, $\frac{\partial}{\partial t}$ is the time variable and $|x, t\rangle$ is the wave function, we found that after separating the variables that:

$$|x, t\rangle = |x\rangle|t\rangle e^{-iEt/\hbar} \dots (2)$$

Studying the approximate theories, we find that by adding small time-dependent variables to the Hamiltonian we can deal with it by the theory of perturbation, theory Time- Dependent perturbation is one of the most appropriate and powerful methods to study the interaction of energy with materials such as electromagnetic radiation, whose effect appears through photons and electrons, these radiations have different frequencies and therefore they are changed with time, so we treat them as time disturbances. As a result of these time disturbances, levels (functions) become unstable, therefore, electrons transport from a higher level to a lower level by spontaneous emission or by a stimulated emission, which is the basis of the theory of laser action [7].

In this study we will focus on the effect of small perturbations only, which are added to the non-time dependent primary Hamiltonian. When we deal with the time-dependent Hamiltonian effect, we will not have stable solutions in terms of functions and descriptive values, thus our usual choices which depend on distinct functions (solutions of distinct equations) as the basis of the factorial of any unknown function becomes impractical. [8].

The probability of transition from the primary level $|\varphi_i\rangle$ to the final level $|\varphi_f\rangle$ in the presence of the effective $\hat{H}'$, since the total Hamiltonian $\hat{H}$ consists of two parts: the first non-turbulent Hamiltonian $\hat{H}_0$ (a part of which can be found in complete solution analytically) and the second $\hat{H}'$, which we consider to be too small for $\hat{H}_0$ and is responsible for the disorder and clearly depends on time as follows [8]:

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}'(t), \quad \hat{H}'(t) \ll \hat{H}_0 \dots (3)$$

Where λ is the wave length. Assuming that there is a solution to Schrodinger characteristic equation

$$\hat{H}_0|\varphi_k\rangle = E_k|\varphi_k\rangle \dots (4)$$

Which appears as a time equation in the form:

$$\hat{H}_0|\Psi_0\rangle = i\hbar \frac{\partial}{\partial t} |\Psi_0\rangle \dots (5)$$

Where

$$|\Psi_0\rangle = \sum_k c_k^{(0)} e^{-iE/\hbar} |\varphi_k\rangle \dots (6)$$

Where $c_k^{(0)}$ are coefficients time independent, and the quantity $|c_k^{(0)}|^2$ here expresses the probability of the system being at a stable level k before starting the perturbation, note that the aggregation in equation (6) is done at both separated and related levels, Since the

functions $|\varphi_k\rangle$ are integrated group, therefore, the general solution of Schrodinger's time equation:

$$\hat{H} |\Psi\rangle = i\hbar \frac{\partial}{\partial t} |\Psi\rangle \dots (7)$$

Can be shown as follows:

$$|\Psi\rangle = \sum_k c_k(t) e^{-iE_k t/\hbar} |\varphi_k\rangle, \quad \sum_k |c_k(t)|^2 = 1 \dots (8)$$

Dirac assumed that the coefficients $c_k(t)$ are explicitly dependent on time, if we know that the characteristic functions $|\varphi_k\rangle$ have the properties of orthogonal and calibration and that the function of $|\Psi\rangle$ which has the calibration properties, it is noted that the quantity $|c_k(t)|^2$ express the probability that the system is in the case of (level k) at the specified time t and $c_k(t)$ denotes the probability amplitude, by comparing equations (6) and (8) we note that with the use of the condition $\hat{H}'(t) = 0$ the time coefficient $c_k(t)$ converts to constant $c_k^{(0)}$ this is why we consider it an initial value (initial condition) of coefficient $c_k(t)$ [9].

Here we see a radical shift in the issue, instead of finding special values and functions for Schrodinger's characteristic equation (7), we will look for finding the values of the coefficients $c_k(t)$, to solve this dilemma we substitute equation (8) in equation (7) with the use of equations (3) and (4) to find [10]:

$$i\hbar \sum_k c'_k(t) |\varphi_k\rangle e^{-iE_k t/\hbar} = \sum_k c_k(t) \lambda \hat{H}'(t) |\varphi_k\rangle e^{-iE_k t/\hbar} \dots (9)$$

Where we used the time difference $c'_k(t) = \frac{dc_k(t)}{dt}$ there is using standard multiplication by $\langle\varphi_m|e^{-iE_m t/\hbar}$ from left to both sides of Equation (9) and to integrate the entire space and take into consideration that $\langle\varphi_m|\varphi_k\rangle = \delta_{mk}$ we found that the Equation (9) became in a class of the following differential equations [11]:

$$c'_m(t) = \frac{1}{i\hbar} \sum_k c_k(t) \lambda \hat{H}'_{mk}(t) e^{i\omega_{mk}t} \dots (10)$$

Whereas

$$\hat{H}'_{mk}(t) = \langle\varphi_m|\hat{H}'(t)|\varphi_k\rangle \dots (11)$$

And angular frequency ω_{mk} is :

$$\omega_{mk} = \frac{E_m - E_k}{\hbar} \dots (12)$$

By Solving equations associated with equation (10), we obtain the coefficients and we calculate the probability of system existence in certain condition time.

2. Imaginary Part of Atomic Scattering Factor

When the atoms disperse rays it doesn't make an additional change in the angles of the relative phase usually, this is true, but there are some exceptions in the case of some atoms whose absorption edge is near to the frequency of the falling radiation as it makes an additional change in the corners of the phase, and this is called anomalous dispersion, since the dispersion coefficient is calculated on the assumption that the electrons in the atom can be considered free and this assumption should be modified in the case of abnormal dispersion, the interaction of the falling radiation on the electrons associated with the nucleus as should be considered this interaction is what makes the absorption edge, as the dispersion coefficient

becomes the composite amount of $f + f' + f''$ and the imaginary part f'' is what matters to us as it is the component that enters the change in phase [12].

The interaction of X-rays with atoms can be described by approximation of the atomic dispersion factor f , except for the Compton scattering, which can be written by [13]

$$f = f_0 + f' + f'' \dots (13)$$

Where f_0 is the Thomson Scattering factor, and for forward scattering is equal to the atomic number, ($f' + f''$) the real and imaginary part for correction scattering, which strongly depends on energy near the absorption edge, the method of partial wave analysis was used, which is one of the approximation methods for finding an integrated solution for Schrodinger's equation when the central potential $V(r)$ is large and effective, when the field causing the dispersion is spherically symmetric, the effect of each value of the different angular momentum values will appear independently in dispersion, Therefore, we will deal with falling and scattered waves as an overlap partial waves, in this approximation method, a relationship was obtained between the total cross-section (σ_{total}) of the scatter and the imaginary part of the elastic dispersion in the forward direction of the following relationship [14]:

$$\sigma_{total} = \frac{4\pi}{k} f''(0) \dots (14)$$

Where k is the wave number, similarly to the cross-section of the scattering, the cross-section of absorption (σ_a) is defined by the following relationship [15]

$$\sigma_a = \frac{\omega}{\Phi_0} \dots (15)$$

Where ω is the transitive rate (sec^{-1}) and Φ_0 the falling flow ($\frac{\text{No. of photons}}{\text{cm}^2 \text{ sec}}$), the relationship of the scattering cross section with the mass attenuation coefficient $\frac{\mu}{\rho_a} = \rho \sigma_a$ where ρ is electronic density and ρ_a is mass density.

In the time-dependent perturbation theory of the first order, the transition rate is described by Fermi's Golden Rule [8]

$$W = \frac{2\pi}{\hbar} \underbrace{|M_{fi}|^2}_{\text{matrix element}} \underbrace{\rho(E_f)}_{\text{density of final states}} \dots (16)$$

Where

$$M_{fi} = \langle f | H_{int} | i \rangle \dots (17)$$

Where H_{int} is the Hamilton's effect of the photon interaction system with the electron

$$H = H_e + H_{rad} = \frac{\vec{p}^2}{2m} + H_{rad} \dots (18)$$

Where $\vec{p}$ the electron momentum in the electromagnetic field, $\vec{p} \rightarrow \vec{p} - e\vec{A} = \frac{\hbar}{i} \vec{\nabla} - e\vec{A}$,

and $\vec{A}$ the potential vector, the electric field of the wave is $\vec{E} = \frac{-\partial \vec{A}}{\partial t} = -i\omega \vec{A} = \hat{e}E$, So the

$$H = \frac{\vec{p}^2}{2m} + H_{rad} + \underbrace{\frac{e}{m} \vec{A} \cdot \vec{p}}_{\text{interaction Hamiltonian, } H_{int}} + \frac{e^2 \vec{A}^2}{2m} \dots (19)$$

The first term of the Hamilton effect of the reaction is the absorption and the second term represents the Thomson scattering, The potential vector $\vec{A}$ can be expressed through the following quantitative relationship [8]

$$\vec{A} = \hat{e} \sqrt{\frac{\hbar}{2\epsilon_0 V \omega}} \left(\underbrace{a_k^+}_{\text{photon creation}} e^{-i\vec{k} \cdot \vec{r}} + \underbrace{a_k}_{\text{annihilation operator}} e^{i\vec{k} \cdot \vec{r}} \right) \dots (20)$$

Where ω is angular frequency, V is potential, ϵ_0 is permittivity of space and $\hbar$ is planck's constant, this relationship to the potential vector represents an expression similar to the general expression of the harmonic oscillator in the three-dimensional coordinates, where a_k^+ and a_k are the effects of creation and annihilation affecting on the wave function of the photon, $|n_k\rangle$ and n_k quantum number of photon with wave vector $\vec{k}$.

For the absorption edge of the atomic shell K, the electrons in the atomic shell K are strongly connected to the nucleus where they can be well described by wave functions similar to hydrogen with a quantitative numbers ($n, l, m = 1, 0, 0$) where

$$|i\rangle = |i\rangle_{\text{photon}} |i\rangle_{\text{electron}} = |1\rangle \Psi_{100}(\vec{r}) \dots (21)$$

The quantitative description of the oscillators can be obtained from the final cases of the photoelectrons $|f_0 + \Delta f\rangle$ and it differs from the flat wave states of free electrons $|f_0\rangle$ resulting from the scattering of the atoms surrounding the material, so the

$$|M_{fi}|^2 = |\langle f_0 + \Delta f | H_{int} | i \rangle|^2 \dots (22)$$

$$|M_{fi}|^2 = \underbrace{|\langle f_0 | H_{int} | i \rangle|^2}_{\sigma_a} + \underbrace{\langle \Delta f | H_{int} | i \rangle \langle f_0 | H_{int} | i \rangle}_{\delta \sigma_a} \dots (23)$$

Any that

$$\delta \sigma_a = \langle \Delta f | H_{int} | i \rangle \langle f_0 | H_{int} | i \rangle \dots (24)$$

Where $|i\rangle$ wave function for electron pulp, the integration $\langle \Delta f | H_{int} | i \rangle$ is prominent for the background scattering of the photoelectron wave function of the original atom when $\vec{r} = 0$.

By equation (15) and Equation (14) the following equations of the imaginary part of the atomic scattering factor were obtained in terms of the energy of the incident photon ω and the electron bond energy in the atom ω_e , where the energy of an electron bond in the atom for each electronic level is $K_{\text{shell}} = 8.332 \text{ KeV}$, $L_{\text{shell}} = 1.031 \text{ KeV}$, $M_{\text{shell}} = 0.858 \text{ KeV}$ [16].

$$f_2 = \left(\frac{\omega_e}{\omega - \omega_e} \right)^2, \omega \leq \frac{1}{2} \omega_e \dots (25)$$

$$f_2 = \left(\frac{\omega_e}{\omega - \omega_e} \right), \omega \cong \omega_e \dots (26)$$

$$f_2 = \left(\frac{\omega_e}{\omega - \omega_e} \right)^{1/2}, \omega \geq 1.5 \omega_e \dots (27)$$

Calculations

To calculate the imaginary part values of the atomic scattering factor, equations (25), (26) and (27) were used by constructing a program using MATLAB programs for different values of incident photon

energy. table (1) shows the imaginary part values of the atomic scattering factor obtained as the falling photon energy changes.

Table (1) The incident photon energies and imaginary part of atomic scattering factor values.

E (KeV)	f'' (e/atom)	E (KeV)	f'' (e/atom)	E (KeV)	f'' (e/atom)
0.0100	1.3739	0.0808	5.3521	1.0976	3.8652
0.0107	1.4066	0.0815	5.0802	1.1848	2.7877
0.0114	1.4406	0.0822	4.8346	1.2720	2.1800
0.0120	1.4758	0.0829	4.6116	1.3592	1.7898
0.0127	1.5123	0.0835	4.4083	1.4464	1.5181
0.0134	1.5502	0.0842	4.2222	1.7164	1.4230
0.0141	1.5896	0.0849	4.0512	1.8080	1.2600
0.0148	1.6304	0.0856	3.8934	1.8996	1.1305
0.0154	1.6729	0.0863	3.7475	1.9913	1.0251
0.0161	1.7170	0.0870	3.6122	2.0829	0.9377
0.0168	1.7629	0.0876	3.4862	2.1745	0.8641
0.0175	1.8107	0.0883	3.3688	2.2662	0.8012
0.0182	1.8604	0.0890	3.2590	2.3578	0.7468
0.0189	1.9122	0.0897	3.1561	2.4495	0.6993
0.0195	1.9662	0.0904	3.0596	2.5411	0.6575
0.0202	2.0225	0.0910	2.9687	2.6327	0.6204
0.0209	2.0813	0.0917	2.8831	2.7244	0.5873
0.0216	2.1427	0.0924	2.8024	2.8160	0.5575
0.0223	2.2068	0.0931	2.7260	2.9076	0.5306
0.0229	2.2739	0.0938	2.6536	2.9993	0.5062
0.0236	2.3440	0.0944	2.5850	3.0909	0.4839
0.0243	2.4175	0.0951	2.5199	3.1825	0.4636
0.0250	2.4945	0.0958	2.4580	3.2742	0.4448
0.0257	2.5752	0.0965	2.3990	3.3658	0.4275
0.0263	2.6598	0.0972	2.3428	3.4575	0.4115
0.0270	2.7488	0.0978	2.2892	3.5491	0.3967
0.0277	2.8422	0.0985	2.2379	3.6407	0.3829
0.0284	2.9406	0.0992	2.1889	3.7324	0.3700
0.0291	3.0441	0.0999	2.1420	3.8240	0.3579
0.0297	3.1531	0.1006	2.0971	3.9156	0.3467
0.0304	3.2682	0.1013	2.0541	4.0073	0.3361
0.0311	3.3896	0.1019	2.0127	4.0989	0.3261
0.0318	3.5179	0.1026	1.9730	4.1905	0.3167
0.0325	3.6537	0.1033	1.9348	4.2822	0.3079
0.0332	3.7975	0.1040	1.8981	4.3738	0.2995
0.0338	3.9500	0.1047	1.8627	4.4655	0.2915
0.0747	10.3260	0.1053	1.8287	4.5571	0.2840
0.0754	9.3595	0.1060	1.7958	4.6487	0.2769
0.0761	8.5585	0.1067	1.7642	4.7404	0.2701
0.0767	7.8838	0.1074	1.7336	4.8320	0.2636
0.0774	7.3077	0.1081	1.7040	4.9236	0.2574
0.0781	6.8100	0.1087	1.6755	9.9992	4.9976
0.0788	6.3758	0.4000	5.4131	11.6660	2.4994
0.0795	5.9937	0.9232	17.0310	13.3320	1.6664
0.0801	5.6547	1.0104	6.3006	14.9980	1.2498

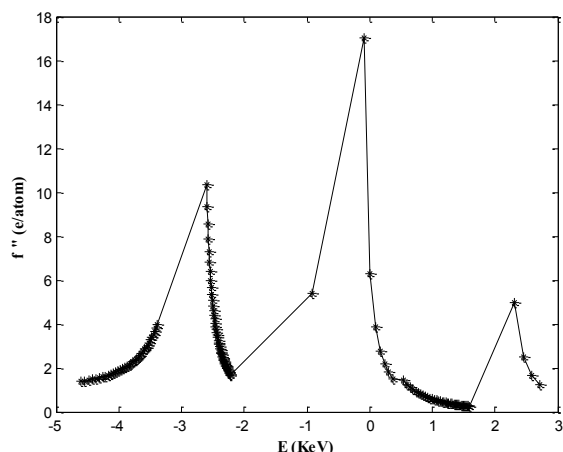


Figure (1) shows the relationship between the imaginary part of the atomic scattering factor and the photon energy logarithm according to the equations (25,26 and 27).

Fig (1) is important since it tries to identify the behavior of the imaginary part of the atomic scattering factor, especially at the absorption edge.

Results and discussion

The current results of the imaginary part of the atomic scattering factor show the importance of specific values for energy that can be observed in fig (1), where we observe that at low energies when $\omega \ll \omega_c$ as well as at high energies when $\omega \gg \omega_c$, where ω the energy of the incident photon, and ω_c the energy of electron bonding with the atom, the imaginary part is almost zero, this means that the electrons are strongly connected to the atom, while we observe the area where $\omega \sim \omega_c$ is, the imaginary part of the scattering is prominent and the electron becomes highly absorbent.

When comparing the results that have been found in the imaginary part of the atomic scattering factor we found these in agreement with the behavior of the theoretical calculations reached by Chantler [17]. And Practical measurements by Henk [18]. The slight

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difference is due to the method used to solve the wave function, fig (2) explains that.

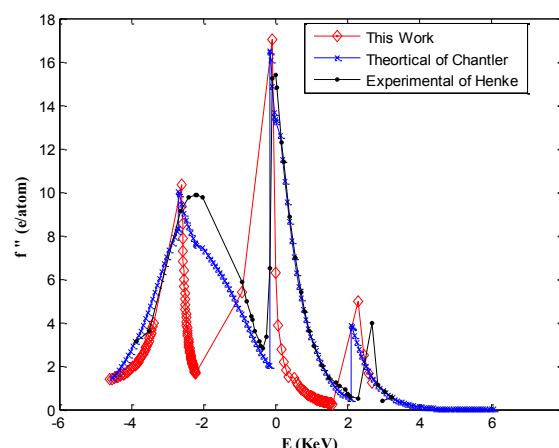


Figure (2) The relationship between the photon energy and the imaginary part of atomic scattering factor for present study and literature review .

Developed models do not give the need for better agreement than experimental values. The main differences between the results produced from the different theoretical bases used to calculate the wave function, each of which addresses the exchange, bonding and interference that occur in a different way, the differences resulted from the varied application of approximate methods and convergence criteria [19] .

Conclusion

In this study we conclude that the imaginary part calculated at low and high energies is close to zero, while at the values close to the absorption edge, the imaginary part is prominently clear, this refers to an interaction between radiation and matter, through this interaction it is possible to study the optical properties of metals, and to identify of the efficiency of the work of optical systems, especially the laser system .

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حساب الجزء الخيالي لعامل التشكل الذري للأشعة السينية في النيكل

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الملخص

في الدراسة الحالية قمنا بحساب المركبة الخيالية لعامل التشتت الذري للأشعة السينية للنيكل بالاعتماد على مبادئ ميكانيك الكم في ايجاد الدالة الموجية التي تصف الحالة الالكترونية للذرات عن طريق الطرق التقريبية، اذ لاحظنا عند القيم المنخفضة للطاقة $\omega_e \ll \omega$ ، وعند القيم العالية للطاقة $\omega_e \gg \omega$ ، ان الجزء الخيالي يساوي صفر تقريباً، وهذا يعني ان الالكترونات تكون مرتبطة بالذرة بشدة، بينما في المنطقة التي تكون فيها قيم طاقة الفوتون مساوية تقريباً الى طاقة ربط الالكترون بالذرة $\omega_e \sim \omega$ نلاحظ ان الجزء الخيالي لعامل التشتت الذري يكون بارز ويصبح الإلكترون ذو امتصاص عالي، ان الدقة النسبية تتراوح ضمن المدى (0.22% - 0.03%)، كذلك تبين ان هنالك توافق جيد بين السلوك الذي توصلنا اليه للجزء الخيالي لعامل التشتت الذري مع السلوك الذي حسب باستخدام نماذج اخرى.