

Study of Charged States During X-Ray Interference in Crystalline Lattices

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ABSTRACT

The discovery of X-rays at the end of the 19th century led to a real breakthrough in the study of the structure of matter. X-rays, which belong to the group of electromagnetic waves, collide with the atoms of solid matter depending on their wavelength and energy, therefore, their three-dimensional interference occurs in the structure of a crystal lattice. When such radiation is incident on a crystal, a complex pattern of radiation is created which reflects the crystal structure. In this section, the charging of the entire crystal lattice is studied during collision with a specific atom in the crystal lattice.

Keywords- Crystal lattice, X-rays, Interference, Charge of specific atom and crystal lattice.

I. INTRODUCTION

An important characteristic of crystals that distinguishes them from other forms of condensed matter (liquids and amorphous solids) is the spatial periodic structure, the axial periodicity of the structure: the atoms (molecules and ions) that make up the crystal, which Divided into three dimensions by size, the points in three dimensions where the atoms themselves (more precisely, the atoms that vibrate at zero temperature) are called nodes of the crystal lattice. Periodic bars are indicative of axial symmetry.

A primitive space lattice is also called a Brave lattice. In 1848, Brave solved the mathematical problem of volume, such that should be the relationship between the lengths of the sides and the angles of the parallelograms to fill a three-dimensional space (what gap between them of course, this space can be filled by parallelograms of any shape. Anyway, the truth is; that the primary crystal cell may have specific properties of the point lattice (flexibility about certain rotations,

reflections...) that effect the physical properties of the crystal, but not all types of point lattices correspond to it. with the need for change assumptions (for example, sixth-order adjacent blocks can fill gaps without breaking, but this is impossible in fifth-order adjacent blocks). It turns out that there are only seven types of parallelograms with different types of point approximation (seven crystal graphic systems) and some images they can have extra atoms at the center of the volume or at the centers of all the faces and it can be all of these situations. or only at the centers of the upper and lower surfaces [1].

II. THE CHARGE OF A PARTICULAR ATOM IN A CRYSTAL LATTICE

Here, we will explain the charging of a particular atom in the crystal lattice when electromagnetic waves are introduced into the crystal lattice in the framework of classical electrodynamics [1]. Let a wave of

electromagnetic waves impinge freely on an electron in an atom, in figure – 1 we obtain electrical field.

$$E^{(in)}(r, t) = Re\{E_0^{(in)} e^{ikr - i\omega t}\} \quad (1)$$

Creation of electron oscillations (electron motion under a weak field can be considered non-reciprocal, which allows the magnetic wave to pass through the field) Oscillations are started (that is, they move rapidly), so the electron is an electromagnetic wave. Can be studied as The electric field of the waves is the radius of vibration of the charged atom, which is defined by the following formula at the moment t at the point R [2].

$$E^{(rad)} = \frac{1}{c^2 R} [\ddot{d}, e_R], e_R \quad (2)$$

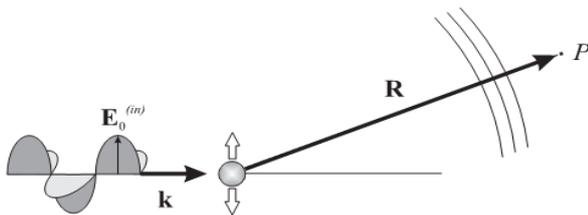


Figure – 1 Electromagnetic wave distribution The point at which electric wave charges accelerate and are charged by (Thomson analysis)

In equation (2), R is the position of the charge from the observer's point $e_R = R/R$ is the unit vector and the second derivative of the dipole moment d is calculated at time $t - R/c$, so in formula (2) \ddot{d} The equation of motion is defined as:

$$\begin{aligned} \ddot{d} &= \frac{e^2}{m} E^{(in)}(\hat{r}, t - R/c) \\ &= \frac{e^2}{m} Re\{E_0^{(in)} e^{ikr'} e^{-i\omega(t - \frac{R}{c})}\} \end{aligned} \quad (3)$$

where \hat{r} is the vector radius of an improbable charged particle (we will place the point at which, in the future, we will use this formula for the radius of several particles, which will see the form $\hat{r} \neq 0$ see figure -1), So then:

$$E^{(rad)} = \frac{e^2}{mc^2 R} Re\{[[E_0^{(in)}, e_R], e_R] e^{ikr'} e^{-i\omega(t - \frac{R}{c})}\} \quad (4)$$

Energy flow in electromagnetic waves is determined by density [3,4].

$$\Sigma = \frac{c}{4\pi} [E, H] = c \frac{E^2}{4\pi} e_{k'} \quad (5)$$

We know that the potential is equal to the absolute value of the electric field and the magnetic field is perpendicular to the direction of propagation of the waves and the direction of the waves (referred to in formula 5 and assumed as such) and the distributed wave $e_{k'}$ (We will introduce the propagation in a single direction and as an exercise we suggest to calculate the magnetic field $[E, H]$ of the presented wave and make sure that the direction of the potential vector matches R , for example $e_{k'} = e_R$. We place the strength of the scattered radiation fields in (4).

$$\overline{R_e A \cdot R_e B} = \frac{1}{2} R_e (A \cdot B^*), \quad (6)$$

Which $A(t) = A_0 e^{-i\omega t}$, $B(t) = B_0 e^{-i\omega t}$ we get the average over the whole period (do not write the sign of the average) the concept of energy flow density :

$$|\Sigma(rad)| = \frac{c}{4\pi} \left(\frac{e^2}{mc^2 R}\right)^2 \frac{1}{2} [[E_0^{(in)}, e_R], e_R]^2 = \frac{c}{8\pi} \frac{E_0^{(in)2}}{R^2} \left(\frac{e^2}{mc^2}\right)^2 [e_0^{(in)}, e_R]^2, \quad (7)$$

which $e_0^{(in)} = E_0^{(in)} / |E_0^{(in)}|$ is the polar vector of the wave.

Multiplying the energy flux density by $R^2 d\Omega$, where $d\Omega$ is the acute angle, we have the energy dissipated per unit time into the angle $d\Omega$ which is:

$$\frac{d\varepsilon}{d\Omega} = E_0^{(in)2} \frac{c}{8\pi} \left(\frac{e^2}{mc^2}\right)^2 [e_0^{(in)}, e_R]^2. \quad (8)$$

The average energy flux density of the imported wave (1) is:

$$|\Sigma(in)| = \frac{c}{8\pi} E_0^{(in)2} \quad (9)$$

Again, we can use equations (5) and (6) and calculate the average energy ratio per unit time at the center of the acute angle of the element distributed in (8). The energy density (absolute value (8)) of the equation is called the differential analysis part. Thomson's analytical formula for unit charge is known as:

$$\frac{d\sigma T}{d\Omega} = \frac{1}{|\Sigma(in)|} \frac{d\varepsilon}{d\Omega} = \left(\frac{e^2}{mc^2}\right)^2 [e_0^{(in)}, e_R]^2 = r_0^2 \sin^2 \vartheta \quad (10)$$

As ϑ is the angle between the polar vector of the wave and $e_0^{(in)}$ observed from the importing system for e_R is the basic constant for $r_0 = \frac{e^2}{mc^2}$ or the classical electron It is known as ray. To describe the non-polarized radiation resulting from equation (10) from all possible directions $e_0^{(in)}$, let's choose the system where the observed point (x, y) is located. (Figure 2). The angle θ with respect to K which is the direction of the incoming wave to the observation point e_R is easily obtained.

$$\cos \vartheta = e_R e_0^{(in)} = (e_R)_x (e_0^{(in)})_x = \sin \theta \cos \alpha$$

Then $\sin^2 \theta$ average price can be obtained by the following equation.

$$\overline{\sin^2 \vartheta} = 1 - \overline{\cos^2 \vartheta} = 1 - \frac{1}{2} \sin^2 \theta = \frac{1}{2} (1 + \cos^2 \theta)$$

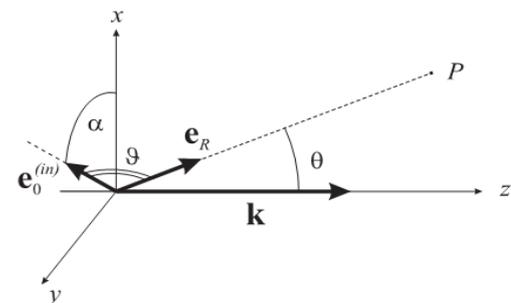


Fig - 2 Thomson's analysis of the phenomenon of polarization. The coordinates of the wave vector and the transmitting wave point K are the (x, y) coordinates of the observer p of the radiation analyzer.

Thus the differential part of the Thomson analysis for the non-polar part is described by the following formula.

$$\frac{d\sigma_T}{d\Omega} = \frac{r_0^2}{2} (1 + \cos^2\theta) \quad (11)$$

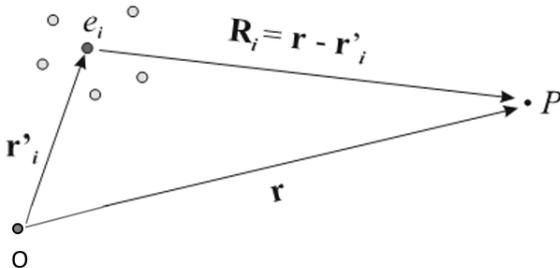


Figure 3: The geometric pattern of system charges on the analysis of electromagnetic waves

Now considering the analysis of the wave (1) system charges such as the electron shell in the atom. Rontgen photons are close to the inner nucleus and constant, in this case the field of the scattered wave at the observation point will be close to the chosen field (4) The formula will be for x-ray diffraction, the distance R_i can be described as follows.

$$R_i = r - r'_i \quad (12)$$

where r is the vector radius of the observer's point, r' will be the vector radius of i am uncharged $|r| \gg |r'_i|$.

$$R_i = \sqrt{(r - r'_i)^2} = \sqrt{r^2 - 2rr'_i + r'^2_i} \approx r \left(1 - \frac{rr'_i}{r^2}\right) = r - e_i r'_i \quad (13)$$

where $e_r = r/r$ is the unit vector towards the observed point, completing the expansion of (4) we get:

$$E_i^{(rad)} = \frac{r_0}{R_i} R_e \{ [E_0^{(in)}, e_i], e_i \} e^{ikr'_i} e^{-i\omega(t - \frac{R_i}{c})} \approx \frac{r_0}{r} R_e \{ [E_0^{(in)}, e_r], e_r \} e^{ikr'_i} e^{-i\omega(t - \frac{r}{c})} \quad (14)$$

If $e_i = \frac{r'_i}{r'_i}$, $K = \left(\frac{\omega}{c}\right) e_r$ is the analyzed wave vector, then this field $E = \sum_{i=1}^Z E_i$ where the Z frames of the wave system are formed and written as follows:

$$E = \frac{r_0}{r} [[E_0^{(in)}, e_r] R_e] \{ e^{-i\omega(t - r/c)} \sum_{i=1}^Z e^{i(k - k')r'_i} \} \quad (15)$$

In this case, the analysis part is easily written as follows:

$$\frac{d\sigma}{d\Omega} = \frac{r_0^2}{2} (1 + \cos^2\theta) \left| \sum_{i=1}^Z e^{iqr'_i} \right|^2 \quad (16)$$

where $q = k - k'$ is the difference of the imported wave vectors, $q = 2k \sin \theta/2$.

What is the frequency of radiation analysis? Charges that depend on the absorbed area at a particular time are therefore simply determined by the $e^{-i\omega t}$ exponential. On the other hand, in a system that has reciprocal atoms performing its motion, the dependence of the electrons in the time-structured system is also present in the vector radiation (optimization of the proposed method in the conditions where the imported

waves frequency ω is unique from others). From this pattern we know that the frequency of coherent waves is conserved and the frequency of composite waves is changeable [5]. To divide the whole analyzed equivalent part (16), which $e^{-i\omega t}$ part is connected to time and the average is $\sum_i e^{iqr'_i}$ sum to time. This pattern is called the analysis of electromagnetic radiation in an atom.

$$\frac{d\sigma_{coh}}{d\Omega} = \frac{r_0^2}{2} (1 + \cos^2\theta) |F(q)|^2 = \frac{d\sigma_T(q)}{d\Omega} |F(q)|^2 \quad (17)$$

It differs from Thomson's analysis by $|F(q)|^2$ which reads as follows:

$$F(q) = \sum_{i=1}^Z e^{iqr'_i} \quad (18)$$

$F(q)$ Its value can be seen as the charge density of an atom in the Fourier series.

$$F(q) = \frac{1}{e} \int \rho(r') e^{iqr'} d^3r'$$

(This is called the nuclear factor). For a wave of large wavelength $\lambda \gg a$ where a is the characteristic size of the analysis of our system (electron shell of an atom), the value of $F(q)$ is attributed to all electrons Z in the system, which is the analysis of coherent waves. differs from Thomson by Z^2 . In the general case, the multiplicative factor $|F(q)|^2$ in formula (17) violates the Thomson analysis symmetry, this symmetry finding will be as large as $\sim ka$ [6,7].

III. INTERFERENCE STRUCTURE IN CRYSTALS

Now consider the situation when atoms are continuously located in space and have a three-dimensional crystal lattice, in this case the vector radiation of charges is shown as follows.

$$r'_i = a_n + r''_s \quad (19)$$

where a_n is the transfer vector of (1), so the r''_s vector of the initial cell is the charge vector, which was present in the initial cell. Simply by heating the positions of the atoms in the angles of the crystal lattice (to simplify this vector we assume an elementary cell and by looking at it we generalize the advanced theory of these cases), then the relation (17) The value of $|F(q)|^2$ takes the following form.

$$|F(q)|^2 = |F_1(q)|^2 \left| \sum_{n=1}^N e^{iq a_n} \right|^2 \quad (20)$$

which $F_1(q)$ is called the uncharged atom factor, the sum of which is a_n radial vector for all atoms of the lattice. In this case, the wave analysis in the crystal and the atom differs by a factor of $\left| \sum_n e^{iq a_n} \right|^2$.

$$d\sigma^{(N)}(q) = \left| \sum_{n=1}^N e^{iq a_n} \right|^2 d\sigma^{(1)}(q) \quad (21)$$

The value of $\left| \sum_{n=1}^N e^{iq a_n} \right|^2$ is the coefficient of interaction of the lawn edge in relation (20), (21), which describes the analysis of Roentgen rays, such as the analysis of neutrons in crystals and some other events were mentioned.

Let's look at the sum of elementary cells $\sum_{n=1}^N e^{iq a_n}$, which $a_n = n_1 a_1 + n_2 a_2 + n_3 a_3$ transition

vector will have three limits, which The sum of the three crystallographic parameters is like this [8].

$$\sum_n e^{iq a_n} = \sum_{n_1=1}^{N_1} e^{i(q \cdot a_1)n_1} \sum_{n_2=1}^{N_2} e^{i(q \cdot a_2)n_2} \sum_{n_3=1}^{N_3} e^{i(q \cdot a_3)n_3}$$

Since the numbers N_1, N_2, N_3 are the axes of the crystallographic directions of the primary cell, each of these three sets forms a geometric sequence:

$$\sum_{n_j=1}^{N_j} e^{i(q \cdot a_j)n_j} = \frac{1 - e^{i(q \cdot a_j)N_j}}{1 - e^{i(q \cdot a_j)}} = \frac{e^{\frac{i(q \cdot a_j)N_j}{2}}}{e^{\frac{i(q \cdot a_j)}{2}}} \frac{e^{-\frac{i(q \cdot a_j)N_j}{2}}}{e^{-\frac{i(q \cdot a_j)}{2}}} = \frac{e^{\frac{i(q \cdot a_j)N_j}{2}} \sin\left(q \cdot \frac{a_j N_j}{2}\right)}{e^{\frac{i(q \cdot a_j)}{2}} \sin\left(q \cdot \frac{a_j}{2}\right)}$$

After taking the square of the absolute value we get:

$$\left| \sum_{n_j=1}^{N_j} e^{i(q \cdot a_j)n_j} \right|^2 = \left(\frac{\sin\left(q \cdot \frac{a_j N_j}{2}\right)}{\sin\left(q \cdot \frac{a_j}{2}\right)} \right)^2$$

This function of $N_j \gg 1$ (exactly $N_j \cdot q \cdot a_j \gg 1$) will represent the series of maximum peaks, which are obtained at zero points.

$$q \cdot a_j / 2 = \pi m_j, \quad m_j = 0, \pm 1, \pm 2, \dots$$

In fact, we see one of these points in this subject, for example:

$$q \cdot a_j / 2 = \pi m_j + \alpha, \quad |\alpha| \ll 1.$$

$$\begin{aligned} \sin(N_j q \cdot a_j / 2) &= \sin(N_j \pi m_j + N_j \alpha) = \\ \cos(N_j \pi m_j) \sin(N_j \alpha), \sin(q \cdot a_j / 2) &= \sin(\pi m_j + \alpha) = \\ \cos \pi m_j \sin \alpha, \end{aligned}$$

and then

$$\frac{\sin^2\left(q \cdot \frac{a_j N_j}{2}\right)}{\sin^2\left(q \cdot \frac{a_j}{2}\right)} = \frac{\sin^2 N_j \alpha}{\sin^2 \alpha} \approx \frac{\sin^2 N_j \alpha}{\alpha^2}$$

Using the known ratio, we have:

$$\lim_{N \rightarrow \infty} \frac{\sin^2 N \alpha}{N \alpha^2} = \pi \delta(\alpha)$$

we get:

$$\left| \sum_{n_j=1}^{N_j} e^{i(q \cdot a_j)n_j} \right|^2 = \pi N_j \sum_{m_j} \delta\left(q \cdot \frac{a_j}{2} - \pi m_j\right) = 2\pi N_j \sum_{m_j} \delta(q \cdot a_j - 2\pi m_j)$$

Thus, for a crystal with many unit cells, the lattice interference factor will have the form:

$$\left| \sum_{n=1}^N e^{iq a_n} \right|^2 = (2\pi)^3 N_1 N_2 N_3 \sum_{m_1, m_2, m_3} \delta(q \cdot a_1 - 2\pi m_1) \delta(q \cdot a_2 - 2\pi m_2) \delta(q \cdot a_3 - 2\pi m_3) \quad (22)$$

For the differential distribution of (21) the differential maxima in the direction of the equation has the following equation [9].

$$\begin{aligned} q \cdot a_1 &= 2\pi m_1 \\ q \cdot a_2 &= 2\pi m_2 \quad (23) \\ q \cdot a_3 &= 2\pi m_3 \end{aligned}$$

They are as clear as Lavin's principles, but we have recognized this equality when we introduced the concept of reciprocal netting! In these samples, the maximum intensity when observed in the crystal along the K' direction of Rontgen radiation is different from that observed in the k direction, which indicates the orientation vector of the reciprocal lattice [10,11].

$$K - K' = g \quad (24)$$

$$K - g = K' \quad (25)$$

The g vector, which we saw in the previous sections, is perpendicular to some of the atoms in the crystal lattice. It can be seen that the imported angle on the plane (the angle between the imported K direction and the normal to the plane can be seen in Figure 4) follows the theory of interference by crystals and the angle between the vectors and K which is θ is shown (the angle between K and K') is equal to the wavelength of the scattered radiation. Thus $|k'| = |K|$ The angle θ formed between the divided rays is obtained from equation (25):

$$2kg = g^2 \quad (26)$$

$$-2kg \cos \theta + \frac{g^2}{2} = 0, \quad k \cos \theta = \frac{g}{2}. \quad (27)$$

This condition is known as Bragg's principle in the form of mutual symmetry in the Roentgen ray crystal. It is written as follows.

$$2d \cos \theta = m\lambda, \quad (28)$$

where d is the angle between the orientations of two m atoms selected in the reciprocal plane and λ is the wavelength of the radiation. (28) The formula explains that the wavelength of the radiation frequency does not accept the Bragg reflection between two connected planes, which are imported at that angle [12-14].

IV. RESULTS AND DISCUSSION

Regular geometrically shaped bodies are called crystals, which have solid and liquid states in solid crystalline materials such as $C, Si, Ge, Cd, Zn, Mn, As$ etc. When the X -ray beam enters it, at the time of interference, the specific atom of the corresponding crystal becomes charged. This process of charging takes place in the entire crystal lattice. This condition is recognized by Roentgen radiation as the reciprocal plane in the crystal as Bragg's principle and is obtained by the relation $2d \cos \theta = m\lambda$, where d is the ratio of two m atoms chosen in the reciprocal plane. is the angle between the directions and λ is the wavelength of the radiation. This formula makes it clear that the wavelength of the radiation frequency does not accept the Bragg reflection between two connected planes which are incident at that angle.

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