Tikrit Journal of Pure Science Vol. 24 (4) 2019

TJPS

Tikrit Journal of Pure Science

ISSN: 1813 – 1662 (Print) --- E-ISSN: 2415 – 1726 (Online)

Journal Homepage: http://tjps.tu.edu.iq/index.php/j

Determination of Relativistic Intensity of X-Ray Diffracted from Aluminum Element.

Muhsin Hasan Ali , Noor Mustafa Fadel

Department of physics , College of Education for Pure Sciences , Tikrit University , Tikrit , Iraq

https://doi.org/10.25130/tjps.v24i4.403

ARTICLE INFO.

Article history:

-Received: 20 / 9 / 2017

-Accepted: 21 / 11 / 2017

-Available online: / / 2019

Keywords: relative intensity, structure factor, atomic scattering factor.

Corresponding Author:

Name: Muhsin Hasan Ali

E-mail:

muhsinhasanali@gmail.com

Tel:

ABSTRACT

In this paper, the relative intensity of X-ray diffracted from Aluminum (Al) was found, and taking into account the influences on the intensity of these rays. There was good agreement between the calculated and measured values, the simple differences between them can be attributed to the fact that all crystals in nature are real and not ideal crystals, on the other hand, the accuracy of atomic positions are must probably effected the calculated results.

1- Introduction

X-ray diffraction is a useful tool to investigate the structure of matter, i.e. the determination of crystal structure. The method is applied, not only to structure determination, but to such diverse problems as stress measurement, chemical analysis, measurement of particle size, and phase equilibrium, to the determination of the ensemble of orientations in a polycrystalline aggregate or the orientation of one crystal [1].

The intensity of x-ray diffraction varies from very weak to strong, in each line of radiation that deviate from crystalline levels with equal d-space, this leads to the important conclusion on the type and method of distribution of atoms in the unit cell. The intensity of the diffraction line is the sum of the x-ray intensity, which is scattered by all the atoms in the unit cell, its value is proportional to the square of structure factor (F), which depends on the coordinates of atomic positions in the unit cell (u, v, w), and atomic form factor (f) [2].

2- Theoretical Part

X-ray intensity is affected by the crystalline levels of a crystallization [1], and here are some factors whom are essential to facilitate the calculations.

1- **Structure factor**
2- **Absorption factor**
3- **Multiplicity factor**
4- **Polarization factor**
5- **Lorentz factor**
6- **Temperature factor**

To calculate the intensity of x-ray diffracted, a brief description of these factors, their effect and what depends on [3],

- The intensity of the reflected ray depends on the nature of the element which the radiation is dispersed. As dispersion occurs the number of electrons around the nucleus, determines the efficiency of the atom to scatter the rays. The efficiency of single atom is called atomic scattering factor (f) [3].
- To derive a formula that express the reflected intensity of the ray it requires the summation of amplitudes of the reflected radiation to be collected by all the atoms in the unit cell, this result is called the structure factor , which depends on the atomic scattering factor and the atoms positions in the unit cell, according to the following equation [4]:

$$F_{hkl} = \sum_{n=1}^{n=N} f_n e^{2\pi i(hu_n+kv_n+lw_n)} \quad (1)$$

Where, F is structure factor, f_n is atomic scattering factor, N number of atom in unit cell, (hkl) Miller indices, (u_n, v_n, w_n) position of atom in unit cell.

- Accompanying the passage of x-rays through the sample the portion of absorption of its energy leading to a reduction in the intensity of the x-ray. This factor is called the absorption factor, which depends on

Bragg angle. At low angles the absorption rate is relatively large, causing a decrease in the intensity of the reflected rays [5].

- **The multiplicity factor:** is an integer that expresses a set of equal levels that have equal intervals and reflect x-rays to a diffraction one line. Each crystalline system has its own value of this factor calculated by knowing the value of Miller indices, the Table (1) shows the values of the multiplicity factor of the face-center cubic (fcc) system[3].

Table (1) value of multiplicity factor (P) [1].

Cubic system	hkl	hhl	0kl	0kk	Hhh	001
	48	42	24	12	8	6

- **Polarization Factor :** The generated radiation is not polarized, but the diffraction of the radiation from the crystalline levels causes partial polarization of the radiation. Which results in a decrease in the intensity of the rays by: $\left(\frac{1+cos^2 2\theta}{2}\right)$ [6].
- **Lorentz Factor :** In addition to the polarization factor, the intensity of the x-ray is affected by another factor called Lorentz factor, which expresses the relative time in which the levels remain in diffraction mode, this factor increases the x-ray intensity that diffracted from the crystalline levels by: $\left(\frac{1}{4sin^2\theta\ cos\theta}\right)$ the factors combine to one factor called the Lorentz-polarization factor, which is equal to: $\left(\frac{1+cos^2 2\theta}{sin^2\theta \cos\theta}\right)$ [6].
- **Temperature Factor:** The ideal image of the crystal is the concentration of atoms in fixed positions within the crystalline structure. This is far from reality. The atoms are usually submitted to vibrate. The amplitude of the atoms increases with increasing temperature leading to a decrease in the x-ray intensity that diffracted from them. The effect of the temperature and absorption factors in opposite directions, and although these two factors do not completely remove each other, their effect on the x-ray intensity is so limited that their negligence will not cause any significant impact on the accuracy of the results [7].

An equation was developed to calculate x-ray intensity [1],

$$I = |F|^2 . P . \left(\frac{1+cos^2 2\theta}{sin^2\theta\ cos\theta}\right) \quad (2)$$

Where, I is the relative intensity, $|F|^2$ structure factor square, P multiplicity factor.

3- Calculations and results

To find the value of the structure factor, the value of the atomic scattering factor must be calculated, where it was found that the scattering factor is given by the following equation [8]:-

$$f(k) = \frac{Z}{(1+4\pi^2k^2{a_0}^2)^2} \quad (3)$$

Where k is the length of the scattering vector, which equal $(\sin\theta)/\lambda$, a_o is the radius of the hydrogen atom.

Calculated values of (f) for (Al) were drawn with various values of $(\sin\theta)/\lambda$, and a curve showing the typical variation of (f) in fig.1. Note that the curve begins at the atomic number of Aluminum, and decreases to very low values for scattering in the backward direction (θ near 90^0) or for very short wavelengths.

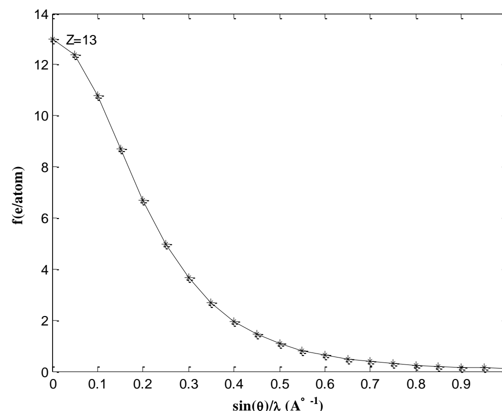

Fig. 1. The atomic scattering factor of Aluminum.

The multiplicity factor of aluminum has a crystalline system of face-center cubic (fcc) type are shown in Table (1), while the positions of the atoms of aluminum are shown in Table (2).

Table (2) atomic positions for each atom within the unit cell [2].

Element	The position of the 1st atom	The position of the 2nd atom	The position of the 3rd atom	The position of the 4th atom
AL	000	$\frac{1}{2}\ \frac{1}{2}\ 0$	$\frac{1}{2}\ 0\ \frac{1}{2}$	$0\ \frac{1}{2}\ \frac{1}{2}$

By adopting mathematical rules and by referring to the laws of simplifying equations containing an exponential function, equation (1) was simplified because it can not be found to have a real value because it contains a complex number as follows:

$$F = \sum_{n=1}^{n=N} f_n[cos2\pi(hu_n + kv_n + lw_n) + isin2\pi\ (hu_n + kv_n + lw_n)] \quad (4)$$

The equations (1) and (4) mean there are two compounds for any amplitude of wave scattering a and b,

$$F = a + ib \quad (5)$$

$$a = \sum_{n=1}^{n=N} f_n[cos2\pi(hu_n + kv_n + lw_n)] \quad (6)$$

$$b = \sum_{n=1}^{n=N} f_n[sin2\pi\ (hu_n + kv_n + lw_n)] \quad (7)$$

$$|F|^2 = (a + ib)(a - ib) = a^2 + b^2 \quad (8)$$

$$|F|^2 = [f_1cos2\pi(hu_1 + kv_1 + lw_1) + f_2cos2\pi(hu_2 + kv_2 + lw_2) + ..]^2 + [f_1sin2\pi(hu_1 + kv_1 + lw_1) + f_2sin2\pi(hu_2 + kv_2 + lw_2) + ..]^2 \quad (9)$$

The equation (9) was used to calculate the structure factor, by substituting the values of the atomic positions and each plane of crystalline produced the values established in the Table (3).

Table (3) All details find relative intensity theoretically.

Line No.	hkl	θ	$sin\theta$	k	f(k)	$\|F\|^2$	P	LP	I Cal (theory)	(I/I_0) EXP
1	111	19.23	0.329	0.213	6.16	608	8	15.7	76655	100
2	200	22.36	0.380	0.247	5.06	409	6	11.2	27620	54
3	220	32.56	0.538	0.349	2.67	114	12	4.81	6605.8	46
4	311	39.11	0.630	0.409	1.84	54.3	24	3.37	4397.4	36
5	222	41.21	0.658	0.427	1.65	43.5	8	3.11	1085.6	14
6	400	49.53	0.760	0.494	1.11	20.0	6	2.72	327.71	5
7	331	56.02	0.829	0.538	0.87	12.1	24	2.96	866.30	21
8	420	58.28	0.850	0.552	0.80	10.4	24	3.15	790.70	20
9	422	68.72	0.931	0.605	0.61	5.96	24	4.89	701.29	8

Diffraction files were used for the International Center of Diffraction Database (ICDD) for the Aluminum element in determining the values of each the distance of crystalline plane and Miller indices and relative intensity practically.

There is a good agreement in the sequence of the intensity of the lines in terms of the most strong line down to the weak line in the same order between calculated and measured intensity.

4- Conclusions and Discussion

There is a relative convergence between calculated and measured values and can be recognized to a number of reasons, the calculation of relative intensity was theoretically calculated on the positions of the atoms, since these positions differed from the real positions because they are typical virtual positions, since there is no typical atom in nature.

It is observed that there are almost identical reflections in intensity and others vary in certain proportions. This can be explained by the fact that convergence occurs for the more homogeneous surfaces in the distribution of atoms, it can be said that the study is essential but the theoretical study can avoid all laboratory errors, whether in the measuring devices or in the preparation of the sample, which led to the existence of this difference between the practical and theoretical results [9].

References

[1] Cullity, B.D. (1978). Element of X-Ray diffraction, 2nd edn. Addision-wesley publishing company, Inc, (U.S.A).

[2] د. يحيى نوري الجّمال، (2000)" فيزياء الحالة الصلبة" دار الكتب للطباعة والنشر، جامعة الموصل.

[3] Abd-alrazak, A.H. (2008). Calculations of relative intensity of X-Ray diffracted of (NiAs) compound, *Diala, Jour*, 31.

[4] Jens, A. and Des, M. (2011). Elements of Modern X-ray Physics, 2nd edn. John Wiley and Sons Ltd.

[5] Miao, M.S.; Lukashev, P.; Herwadkar, A. and Lambrech, W. (2005). Crystal structure, electronic structure and magnetism of transition metal nitrides, *Phys. stat.*, **2(7):**2516-2519.

[6] Peiser, H.S.; Rooksby, H.P. and Wilson, A.J.C. (1955), X-Ray diffraction polycrystalline materials, London .Institute of physics.

[7] Xie, Y.; Lu, J.; Yan, P.; Jiang, X. and Qian, Y. (2000). A Safe Low Temperature Route to Nanocrystalline Transition Metal Arsenides, *The chemical Society of Japan*, **29(2):**114.

[8] Ali, M.H. (2017). Calculations of Atomic Scattering Factor For X-ray in Copper, *Tikrit Journal of Pure Science*, **(22):**151-155.

[9] Brennan, S. and Cowan, P.L. (1992). A suite of programs for calculating x-ray absorption, reflection and diffraction performance for a variety of materials at arbitrary wavelengths, *Rev. Science Instrum.*, **63(1):**850–3.

ايجاد الشدة النسبية لحيود الاشعة السينية عن عنصر الالمنيوم

محسن حسن علي ، نور مصطفى فاضل

قسم الفيزياء ، كلية التربية للعلوم الصرفة ، جامعة تكريت ، تكريت ، العراق

الملخص

في هذا البحث تم ايجاد الشدة النسبية للأشعة السينية المُحادة عن الالمنيوم، مع الأخذ بنظر الاعتبار العوامل التي تؤثر على شدة تلك الأشعة، وجد إن هناك تقارب كبير بين نتائج الشدة النسبية المحسوبة نظريا مع القيم العملية، ويمكن أن يُعزى سبب الاختلافات البسيطة بينهما إلى إن جميع البلورات في الطبيعة هي بلورات حقيقية وليست مثالية، من ناحية أُخرى فان دقة تحديد المواقع الذرية تنعكس بشكل مباشر على حساب الشدة النسبية.