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A study of electron momentum density in Ti_Al system.

Abdul kader A. Hassan , Fareed M. Mohammed , Sameh H. Salih , Shalash A. Mohammed
Department of physics , College of Science , Tikrit University , Tikrit , Iraq
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Corresponding Author:

Name: Fareed M. Mohammed

E-mail: dr_fr_2006@yahoo.com

Tel:

Abstract

We present the electron momentum densities of TiAl , Ti_3Al and $TiAl_3$ alloys in terms of Compton profile. Compton profiles (CP) of Ti and Al metals were calculated by adopting the renormalized free atom (RFA) and free electron models and choosing ($3d^3 – 4s^1$) configuration to Ti and ($3s^2 – 3p^1$) to Al as best electron configurations. The Compton profiles values were obtained by the Superposition model for the three intermetallic alloys. The theoretical results were compared with the experimental values. The present work results of TiAl , Ti_3Al and $TiAl_3$ alloys are in good agreement with the experimental values.

1. Introduction

The Ti_Al system has a special interest because of its properties. Ti_Al alloys have good oxidization resistance, low density, high elastic modulus and high melting degrees [1]. Ti_Al has three basic alloys i.e Ti_Al , Ti_3_Al and Ti_Al_3 . In these required phases both of Ti_Al and Ti_3_Al have been widely investigated, while that Ti_Al_3 alloy were less interested [1,2]. Most of the previous studies on the Ti_Al system included changes in structure, stability, electronic and elastic properties [3]. The binary alloys between metals are of great importance because the electrons of the valence band (d) have a fundamental role in their electronic and physical properties. The studies of the distribution of electron momentum density (EMD) of the Ti_Al system by the use of Compton profile are very rare, so we present this study in a trial to overcome this lack of study on this great future importance. Compton scattering is the interaction of radiation with mater between the incident photons and the target electron of mater, this incident photon will scatter at a certain angle, the scattering interaction is predominate at high energies[4] .

The scattering radiation beam will have broadened, this broadening is called Doppler broadening[5] . The spectrum produced by the broadened line shape is called Compton profile [5]. The Compton profile (Jp_z) is related to momentum density of electrons in the samples through the relation : _

$Jp_z = \iint n(p)\, dp_\emptyset$ ….(1)

Where $dp_\emptyset = dp_x dp_y$ … (2)

and $n(p) = \sum_i |\int \psi_i(\vec{r}) \exp(-ip.\vec{r} d\vec{r})|^2$ …(3)

$n(p) = x^*(p)\, x(p)$ …(4)

$n(p)$ is the ground state EMD. $x(p)$ is the electron wave function in the momentum representation, it is obtained by Fourier transformation of the position space of x(r) wave function.

We have used the fcc lattice of Ti based on Ehrenreich, Philips and Olechna works (1986)[6], they reported a calculation of the directional CPS for Ti (fcc), Ti (bcc) and TiH_2 based on the results of augmented plan wave (APW) band-structure calculations, they believed that the theoretical average CP calculations of Ti (fcc) simulates well the experimentally measured Ti (HCP) CP, because the two structures have the same density[6]. Al is fcc lattice type too. The lattice constants of Ti (fcc) and Al (fcc) are 4.15A° and 4.05A° respectively[7]. In this paper, we compared the results obtained by using RFA model ,free atom and free electron model with the experimental results obtained from the reference [1] and references mentioned there .

2. Theoretical calculations

2.1. Renormalized Free Atom Model (RFA)

This is a theoretical model used for many complex and noncomplex theoretical calculations [8] like the EMD distribution. It gives valid results and agreement with experimental results. This model considers that the atom is not free but is confined to a specific cell within solid. The first who used RFA model was Chodorow [9]. The success and validity of this theoretical model return very well to the Compton works [10-11] ,who showed that RFA model gives fully correct estimates of the interest band structure characteristics and gives a correct explanation of the cohesion in transition metal series . The RFA model was then used for the calculation of cohesive energies for various 3d and 4d transition metals [12]. The calculation begins from the Hartree-Fock wave function (HFWF) where this function is cut off at the radius (R_0) of Wigner_Seitz and then renormalized the new function to unity within this sphere to maintain the neutrality of charge .

The new renormalized wave function $R_{nl}(r)$ is given by equation[12,13]: _

$$R_{nl}(r) = \begin{cases} N_{nl} R_{nl}^{atomic(r)} & r \le R_\circ \\ 0 & r > R_\circ \end{cases} \quad \dots (5)$$

$R_{nl}^{atomic(r)}$: _ atomic radial wave function for the state, its used in further computation.

n , l are the quantum number

The Compton profile for (4s) electrons can be defines as [12] :

$$J_{4s}(P_Z) = 4\pi \sum_{n=0}^{\infty} |\Psi_0^c(K_n)|^2 \, G_n(p_z) \dots (6)$$

where K_n is a reciprocal lattice vector.

$p_z$is the projection of electron momentum along the scattering vector direction.

$\Psi_0^c(K_n)$: is the Fourier transform of the RFA wave function$\phi_0^c(r)$.$G_n(p_z)$: auxillary function.

Following Berggren [13] the momentum transform of a Bloch function (for "s" electrons) for the cubic structures is given by:

$$\Psi_{\vec{k}}(\vec{p}) = N\delta\left(P - \vec{k}_1\vec{k}_n\right)\Psi_{\vec{k}}^c(\vec{P}) \quad \dots (7)$$

N: is the total number of atoms.

2.2. Free Electron based model profile (F.E)

We calculated the F.E Compton profile by using the equation: _

$$J_{4s}(p_z) = 2\pi \int_{p_z} dp \, \rho(\vec{p}) p \dots . (8)$$

If we consider the valence electrons in a metal as a non-interacting electron gas, then the momentum density is given by [14]:_

$$\rho(\vec{P}) = \frac{3n}{\pi T} = constant \quad \dots (9)$$

Where : $T = 4p_F^3$ ….(10)

n: _ The number of free electrons per site and p_F is the Fermi momentum.

By substituting eq(9) into (8), we obtain :_

$$J_{4s}(p_z) = \frac{3n}{T}(p_F^2 - p_z^2) \ , \ for \ p_z \le p_F \dots . (11)$$

2.3. Superposition model

The superposition Compton profile for Ti_Al alloys can be obtained from RFA profiles of Ti and Al metals by using equation: _

$$J^{SUP.}(p_z) = CJ^{Ti}(p_z) + DJ^{Al}(p_z) \dots . \ (12)$$

Where C and D represent the fractional atomic concentration of Ti and Al respectively in Ti-Al alloys. The superposition theoretical profile ($J_{RFA}^{sup.}$) is calculated from the RFA profile of Ti and Al metals (J_{RFA}^{Ti} and J_{RFA}^{Al} respectively) by using equation (12) also [1]. For the purpose of comparison we also took the superposition model for free atom and free electron for the Ti _ Al alloys.

Results and Discussion

The eventual Compton profiles after all corrections are given in tables (1), (2) and (3). The calculations are based on the fcc Ti lattice and fcc Al lattice. All values are properly normalized to the number of electrons of the respective free atom Compton profiles in (0-7 a.u.).The RFA Compton profile and experimental values[1] for Ti and Al are given in table (1) .In this table we compared our present work (RFA of Ti and Al metals) with the experimental values[1] for the given metals, we found that our results are in good agreement with the experimental values[1], in considering that the plan wave generalized gradient Compton profile ($J(p_z)_{PW\text{-}GGA}$) values[1] are better than our present work compared with the experimental values[1].

The super position model of present work , free atom, free electron, $J_{PW\text{-}GGA}$[1] and experimental results[1] for the TiAl , Ti_3Al , $TiAl_3$ alloys are given in tables 1, 2 and 3 respectively, we compare the present work , free atom and free electron with the experimental values [1] for the three alloys. Free atom values are taken from reference [15].

The first five columns are the same in the three tables. The first column represents the momentum regions (p_z) . the second column represents the best values of RFA for the **Ti ($3d^3$-$4s^1$) configuration** , the third column represents the Ti experimental values[1]. The best values of RFA for **Al ($3s^2$-$3p^1$) configuration** are in the fourth column, and the Al experimental values[1] are in the fifth column. The columns from 6 to 10 in tables 1,2 and 3 represent the superposition model values for the TiAl, Ti_3Al and $TiAl_3$ respectively. The electron configurations **Ti ($3d^3$-$4s^1$)** and **Al ($3s^2$-$3p^1$)** were chosen as the best two electron configurations because they are the closest two configuration to the experimental values[1].

Coming first to the high momentum region ($p_z > 3.5$ a.u.) for the super position model , it can be seen that the RFA , free atom and free electron models smoothly approach the experimental values[1] for the three alloys ,as shown in tables (1) ,(2) and (3) and figs. (1) ,(2) and (3), this is because of the core electron contributions in this region which are clearly described by free atom wave function.

In table (1) we can see that the values of the RFA and free electron models for TiAl alloy are very close to the experimental values[1] in all momentum regions, but the free atom model values are higher than the experimental values[1] in momentum region($0 < p_z < 0.3$)a.u. and smaller than the

experimental values[1] in (0.4 <p_z< 1) a.u. as shown in Fig.(1).

The superposition model for Ti_3Al shows that the RFA model values are very close to the experimental values[1], just slightly higher in the momentum region (0 <p_z< 0.2)a.u. and slightly lower in region (0.5 <p_z< 0.8) as shown in table (2) and Fig.(2) also .

The $TiAl_3$ superposition model shows that the RFA model values are in good agreement with experimental values in all momentum regions , but can a bit be decreased in region (0.4 <p_z< 1) a.u. as shown in table (3) and Fig.(3).

The free electron model calculations for Ti_3Al and $TiAl_3$ are a bit higher than the experimental values[1] at the momentum region (0 <p_z< 0.4)a.u. but a bit less in (0.6 <p_z< 1)a.u. as shown in tables (2) and (3) and Figs.(2) and (3) respectively.

The free atom model values for the three alloys are relatively higher than the experimental values[1] in momentum region (0 <p_z< 0.3)a.u. but it is became relatively lower in region (0.4 <p_z< 1)a.u. as shown in all tables and all Figures .

Figs.(4) , (5) and (6) show the differences (ΔJ) between superposition model (theory) and experimental[1] Compton profiles of TiAl , Ti_3Al and $TiAl_3$ alloys respectively. the Standard deviation applied $\sum_0^{5a.u.}|\Delta J|^2$ was obtained for each case. We calculated the differences(ΔJ) to find the closest electron configurations to the experimental values [1]. We used the following equation to find the differences (ΔJ)[1] :

$$\sum_0^{5a.u.}|\Delta J(p_z)|^2 = \left(\sum_0^{5a.u.}\left(J_{Theo.}(p_z) - J_{exp.}(p_z)\right)\right)^2 \quad (13)$$

Conclusion

In this paper we have presented the electron momentum density (EMD) of Ti , Al elements and their alloys TiAl , Ti_3Al and $TiAl_3$ by using the Compton profile . the calculations of Compton profile are compared with the experimental values[1]. All the theoretical calculations show almost a similar type of agreement with the experiment. The RFA model gives valid results and agreement with experimental results.

Table (1):_ Theoretical results of Compton profile of the TiAl alloy compared with experimental values[1] and with $J(p_z)_{PW\text{-}GGA}$ Superposition model [1] . All quantities are in atomic units. (The Ti cor+RFA for the best electron momentum distribution ($3d^3 – 4s^1$) configuration, and the Al cor+RFA for the best electron momentum distribution ($3s^2 – 3p^1$) configuration).

P_z (a.u.)	J(p_z)(e/a.u.)								
	Ti		Al		Superposition model TiAl				
	Core+RFA	Expt.[1]	Cor+ RFA	Expt.[1]	Free atom	Free electron	PW-GGA. [1]	Present Work.	Expt.[1]
0.0	5.299	5.359±0.014	3.855	3.871±0.021	12.66	9.448	9.11657	9.154	9.016±0.02
0.1	5.275	5.331	3.841	3.844	12.1	9.400	9.07435	9.116	8.967
0.2	5.168	5.249	3.745	3.766	10.71	9.198	8.9428	8.913	8.82
0.3	4.979	5.119	3.528	3.631	9.13	8.808	8.71701	8.507	8.576
0.4	4.774	4.941	3.259	3.441	7.78	8.301	8.38366	8.032	8.245
0.5	4.513	4.717	2.959	3.204	6.8	7.690	7.94465	7.472	7.83
0.6	4.092	4.456	2.589	2.936	6.14	6.919	7.41285	6.681	7.344
0.7	3.879	4.173	2.225	2.652	5.68	6.169	6.80187	6.104	6.812
0.8	3.722	3.882	1.930	2.368	5.32	5.465	6.1793	5.652	6.272
1.0	3.355	3.320±0.010	1.742	1.876±0.013	4.77	4.942	5.19344	5.097	5.268±0.015
1.2	2.948	2.835	1.603	1.554	4.26	4.417	4.43792	4.551	4.447
1.4	2.542	2.408	1.479	1.361	3.77	3.911	3.83156	4.021	3.813
1.6	2.171	2.064	1.354	1.236	3.3	3.441	3.33669	3.526	3.318
1.8	1.848	1.793	1.229	1.113	2.88	3.015	2.92175	3.078	2.897
2	1.579	1.547±0.006	1.107	1.011±0.009	2.53	2.640	2.92175	2.686	2.535±0.010
3	0.868	0.857±0.005	0.617	0.557±0.007	1.407	1.486	1.39385	1.485	1.405±0.007
4	0.605	0.584±0.004	0.351	0.324±0.005	0.918	0.973	0.9141	0.956	0.937±0.006
5	0.450	0.438±0.003	0.217	0.198±0.003	0.646	0.687	0.64449	0.667	0.662±0.004
6	0.336	0.328±0.002	0.145	3.871±0.021	0.469	0.493	0.46776	0.481	0.486±0.004
7	0.251	0.254±0.002	0.103	3.844	0.346	0.364	0.34502	0.354	0.340±0.003

Table (2) : Theoretical results of Compton profile of the Ti_3Al alloy compared with experimental values[1] and with $J(p_z)_{PW\text{-}GGA}$ Superposition model [1] . All quantities are in atomic units. (The Ti cor+RFA for the best electron momentum distribution ($3d^3 – 4s^1$) configuration, and the Al cor+RFA for the best electron momentum distribution ($3s^2 – 3p^1$) configuration).

P_z (a.u.)	$J(p_z)$(e/a.u.)								
	Ti		Al		Superposition model Ti_3Al				
	Core+RFA	Expt.[1]	Cor+RFA	Expt.[1]	Free atom	Free electron	PW-GGA. [1]	Present Work.	Expt.[1]
0.0	5.299	5.359±0.014	3.855	3.871±0.021	27.68	20.006	19.589	19.751	19.299±0.057
0.1	5.275	5.331	3.841	3.844	26.3	19.916	19.516	19.666	19.214
0.2	5.168	5.249	3.745	3.766	22.99	19.532	19.288	19.250	18.938
0.3	4.979	5.119	3.528	3.631	19.45	18.822	18.894	18.464	18.452
0.4	4.774	4.941	3.259	3.441	16.7	17.957	18.279	17.580	17.754
0.5	4.513	4.717	2.959	3.204	14.88	16.891	17.450	16.499	16.886
0.6	4.092	4.456	2.589	2.936	13.74	15.406	16.458	14.864	15.912
0.7	3.879	4.173	2.225	2.652	12.96	13.983	15.326	13.863	14.881
0.8	3.722	3.882	1.930	2.368	12.28	12.806	14.171	13.097	13.843
1.0	3.355	3.320±0.010	1.742	1.876±0.013	11.07	11.558	12.111	11.807	11.880±0.043
1.2	2.948	2.835	1.603	1.554	9.8	10.246	10.250	10.447	10.149
1.4	2.542	2.408	1.479	1.361	8.55	8.960	8.655	9.105	8.718
1.6	2.171	2.064	1.354	1.236	7.38	7.784	7.404	7.868	7.585
1.8	1.848	1.793	1.229	1.113	6.36	6.741	6.400	6.774	6.646
2	1.579	1.547±0.006	1.107	1.011±0.009	5.53	5.844	5.576	5.844	5.830±0.029
3	0.868	0.857±0.005	0.617	0.557±0.007	3.085	3.287	3.040	3.221	3.226±0.021
4	0.605	0.584±0.004	0.351	0.324±0.005	2.11	2.252	2.095	2.166	2.137±0.017
5	0.450	0.438±0.003	0.217	0.198±0.003	1.54	1.648	1.533	1.568	1.518±0.014
6	0.336	0.328±0.002	0.145	3.871±0.021	1.139	1.213	1.135	1.154	1.125±0.011
7	0.251	0.254±0.002	0.103	3.844	0.848	0.903	0.845	0.856	0.849±0.010

Table (3) : Theoretical results of Compton profile of the $TiAl_3$ alloy compared with experimental values[1] and with $J(p_z)_{PW\text{-}GGA}$ Superposition model [1] . All quantities are in atomic units. (The Ti cor+RFA for the best electron momentum distribution ($3d^3 – 4s^1$) configuration, and the Al cor+RFA for the best electron momentum distribution ($3s^2 – 3p^1$) configuration).

P_z (a.u.)	$J(p_z)$(e/a.u.)								
	Ti		Al		Superposition model $TiAl_3$				
	Core+RFA	Expt.[1]	Cor+RFA	Expt.[1]	Free atom	Free electron	JPW-GGA. [1]	Present Work. RFA	Expt.[1]
0.0	5.299	5.359±0.014	3.855	3.871±0.021	22.96	17.785	16.877	16.864	16.618±0.038
0.1	5.275	5.331	3.841	3.844	22.1	17.685	16.780	16.798	16.466
0.2	5.168	5.249	3.745	3.766	19.85	17.262	16.482	16.403	16.148
0.3	4.979	5.119	3.528	3.631	17.07	16.412	15.973	15.563	15.667
0.4	4.774	4.941	3.259	3.441	14.42	15.246	15.255	14.550	14.96
0.5	4.513	4.717	2.959	3.204	12.32	13.868	15.255	13.389	14.047
0.6	4.092	4.456	2.589	2.936	10.82	12.270	13.192	11.860	13.038
0.7	3.879	4.173	2.225	2.652	9.76	10.692	11.880	10.554	12.01
0.8	3.722	3.882	1.930	2.368	9	9.054	10.545	9.512	10.96
1.0	3.355	3.320±0.010	1.742	1.876±0.013	8.01	8.211	8.662	8.582	8.980±0.028
1.2	2.948	2.835	1.603	1.554	7.24	7.424	7.501	7.758	7.613
1.4	2.542	2.408	1.479	1.361	6.53	6.682	6.670	6.978	6.534
1.6	2.171	2.064	1.354	1.236	5.82	5.979	5.942	6.234	5.811
1.8	1.848	1.793	1.229	1.113	5.16	5.320	5.286	5.536	5.167
2	1.579	1.547±0.006	1.107	1.011±0.009	4.59	4.717	4.695	4.900	4.611±0.019
3	0.868	0.857±0.005	0.617	0.557±0.007	2.543	2.656	2.534	2.720	2.594±0.014
4	0.605	0.584±0.004	0.351	0.324±0.005	1.562	1.640	1.561	1.657	1.582±0.010
5	0.450	0.438±0.003	0.217	0.198±0.003	1.044	1.100	1.044	1.101	1.053±0.008
6	0.336	0.328±0.002	0.145	3.871±0.021	0.737	0.759	0.735	0.772	0.768±0.007
7	0.251	0.254±0.002	0.103	3.844	0.535	0.552	0.534	0.560	0.559±0.005

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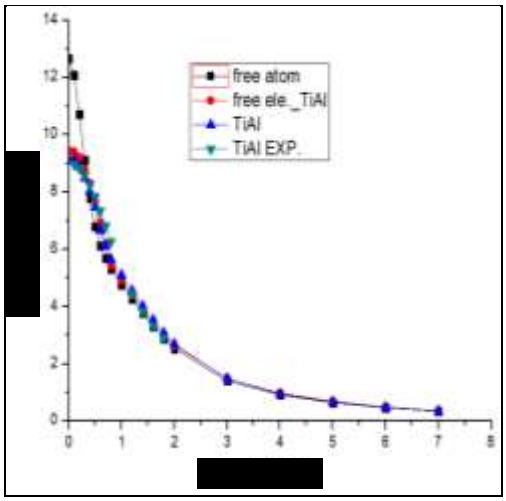

Fig.1: Comparison of experimental [1] Compton profile of TiAl alloy with Calculated values from superposition model

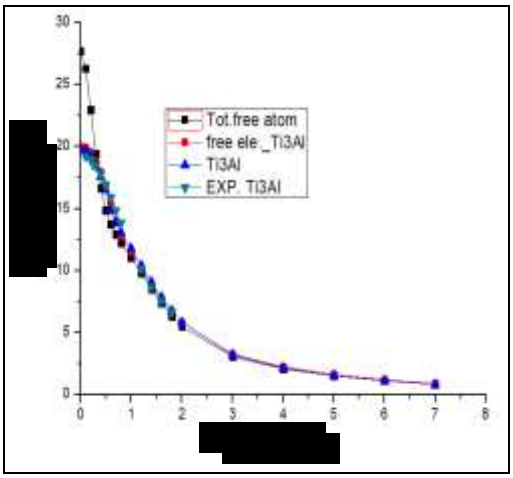

Fig.2: Comparison of experimental[1] Compton profile of Ti_3Al alloy with calculated values from Superposition model

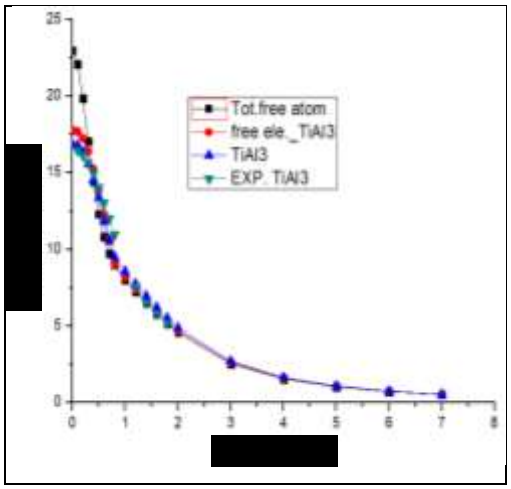

Fig.3: Comparison of experimental [1] Compton profile of $TiAl_3$ alloy with calculated values from Superposition model

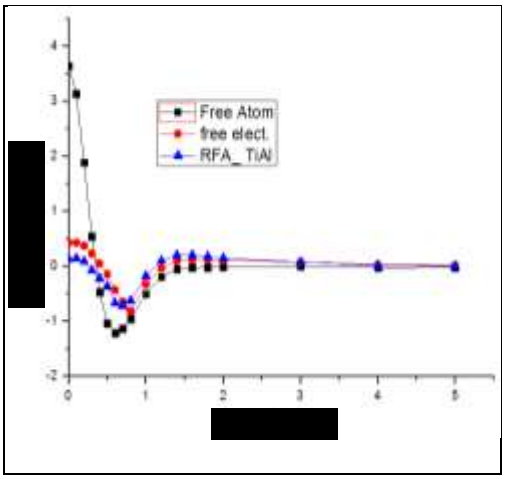

Fig.4: plot of the differences between the super position model (theory) and experimental [1] Compton profiles of TiAl alloys

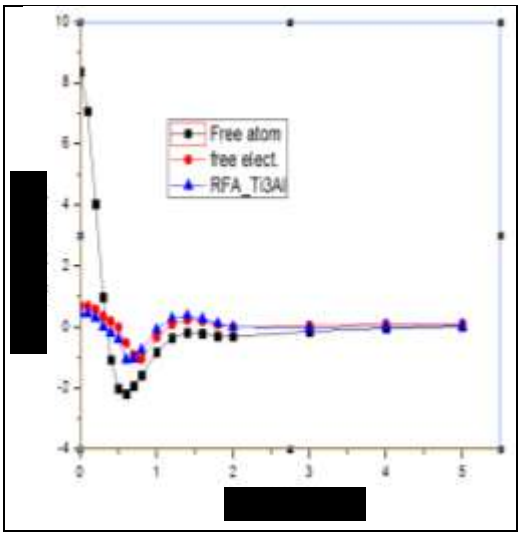

Fig.5: plot of the differences between super position model (theory) and experimental[1] Compton profiles of Ti_3Al alloys

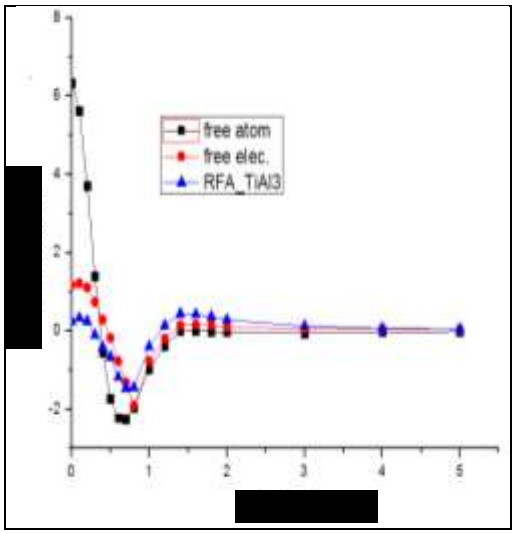

Fig.6: plot of the differences between super position model (theory) and experimental[1] Compton profiles of $TiAl_3$ alloys

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دراسة كثافة الزخم الالكتروني للنظام Ti_Al .

عبدالقادر علي حسن ، فريد مجيد محمد ، سامح حميد صالح ، شلاش عسل محمد

قسم الفيزياء ، كلية العلوم ، جامعة تكريت ، تكريت ، العراق

الملخص

في هذا البحث تم ايجاد كثافة الزخم الالكتروني للسبائك (**$TiAl$, Ti_3Al , $TiAl_3$**) بدلالة شكل منحنى كومبتن. قيم شكل منحنى كومبتن للمعدنين **(Al) , (Ti)** تم ايجادهما بتبني نموذجي اعادة معايرة الذرة الحرة **(RFA)** والالكترون الحر **(FE)** وباختيار **$(3d^3\text{-}4s^1)$** و **$(3s^2\text{-}3p^1)$** كأفضل ترتيبين الكترونيين لكل من التيتانيوم **Ti** والالمنيوم **Al** على التوالي، وبالنسبة للسبائك الثلاثة فان قيم شكل منحنى كومبتن تم الحصول عليها باستخدام نموذج التراكب الاعظم للقيم التي حصلنا عليها باستخدام نموذجي اعادة معايرة الذرة الحرة والالكترون الحر. القيم المحسوبة والمقاسة كانت على تطابق جيد للسبائك الثلاثة.