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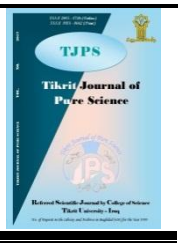

A study of Electronic Structure in W–Cu Alloys by using RFA and FE models

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Abstract

In this paper, Compton profile for Tungsten (W) was computed by employing both the RFA and FE models setting several electronic configurations in subset (5d-6s). same were done for copper (Cu) by chosen (3d-4s) subshells, these Results were compared with recent experimental data, these study are extended to the electronic state in ($W_{0.60}$ $Cu_{0.40}$, $W_{0.72}$ $Cu_{0.28}$) alloys. The superposition are adopted to calculate the total C.P for the two alloys, where the calculated values for W& Cu of the constituent are used, the available measured data on both alloys are in very good agreement with the superposition of Compton profiles of the pure constituent metales .

1.Introduction

Tungsten is a chemical element with symbol **W** and atomic number (Z=74) with a lattice parameter (3.16 A^0) have Body Centered Cubic **(**BCC) crystal structure. While copper have symbol **Cu** and atomic number (Z=29), with a lattice parameter (3.61 A^o) , and have Face Centered Cubic **(**FCC**)** crystal structure and atomic weight **(**63.54**) gm/mol**, density 8.96 **gm/cm^3**. Compton scattering is a technique for obtaining an experimental measure of the momentum distribution of electrons in materials [1] .In Most of the earlier works on W–Cu system is devoted to preparation of W–Cu multilayered films, their properties and electronic structure, etc.[2-5].

It is all well known that the J(pz), the spectrum of inelastical scattering photons by the target's electrons, is an advantageous technique to realize the electronic structural of the target [6]. Theoretically, Compton profile is defined as the one-dimensional projecting of the electron momentum density n(p) along the scattering vector direction, customarily chosen as the z-axis of the Cartesian coordinate system.

The Compton profile **J(pz)** is specified as:

$$J(p_z) = \iint n(\vec{p})\, dp_x\, dp_y \quad (1)$$

Where p_x and p_y are the moment. Ingredients in x& y directions whereas the z is parallel to the resultant of the incident & scattered wave vectors, [7]. And n(**p**) is the ground-state electron momentum density and is given by:

$$n(p) = \frac{1}{(2\pi)^3}\sum_{OCC}|\Psi(r)\exp(-ip.r)dr|^2 \quad (2)$$

Where by Ψ (r) instantiates the electron wave function. The summations indicant is over all the occupied states. Equation (2) is derived within the Impulse Approximation (IA) [8],

2. Computation

A) RFA model:

The renormalized free atom approach was given in details elsewhere by [9]. In the RFA model one begins with the free–Atom wave function, decapitates them at the wigner-seits radius and **equalized** the wave function to one within this Sphere to preserve the charge neutrality.

For the BCC metals, the C.P for 6s electrons, can be inscribed by [10]:

$$J_S(P_z) = 4\pi \sum_{n=zero}^{\infty}|\Psi_{zero}^{c}(K_N)|^2\, G_N(p_z) \quad (3)$$

Where K_N is a reciprocal lattice vector and p_z electron momentum.

the free atom Hartree -Fock wave function was taken from tables of [11].The Compton profile was then computed using equation (3) for appliances statuses choosing various (5d-6s) configuration. The values

of the Compton profile of 5d,3d electrons and other interior electrons were taken than [12] .

B) Free Electron– model**:**

In state of an momentum distribution, eqn. (1) constricts to the form:

As we rewrite eqn.1 for the Compton profile of 6s state

$$J_{6s}(P_z) = 2\pi \int_{pz}^{\infty} dp\, \rho(\vec{p})p \quad (4)$$

and

$$\rho\left(\vec{P}\right) = constant = \frac{z}{\frac{4}{3}\pi p_f^3} \quad (5)$$

Substitution of $\rho(p)$ from eq.(4) to eq.(5) gives

$$J_{6s}(p_z) = \frac{3n}{4\,p_f^3}\left(p_f^2 - p_z^2\right) \quad for\ p_f \le p_r \qquad (6)$$

Where n is the number of free electrons per site and p_f is the Fermi momentum

3. Results and Discussions

Part 1-(Bcc-W):

The Compton profile For a tungsten W after applying all corrections, is given by in Table 1. Also included here are three computed theoretical profiles values for ($5d^5$-$6s^1$,$5d^{4.9}$-$6s^{1.1}$,$5d^{4.8}$-$6s^{1.2}$) computed by using the renormalized free atom RFA model using the procedure of sec. 2.A. The free atom (FA) values with ($5d^5$-$6s^1$) electron configuration are also consists for comparison, also given here are the Free electron(FE) profile, the experimental value from reference [13]. All calculated and measured values given in this table 1 are obtaineded Before convolution are normalised to 23.8001 being the number of electrons from (0-5) under the free atom area.

Table 1: Our calculated theoretical (unconvoluted) Compton profile of Tungsten (W) compared with experimental value [13]. All values are normalized to 23.8001 electrons.

P_z (a.u.)	$J(p_z)$(e/a.u.)					
			Theory(RFA)			
	Free atom ($5d^5$-$6s^1$)	Free electron ($5d^5$-$6s^1$)	Core+RFA $5d^5$-$6s^1$	Core+RFA $5d^{4.9}$-$6s^{1.1}$	Core+RFA $5d^{4.8}$-$6s^{1.2}$	Expt. [13]
0.0	11.2	8.968	9.153	9.079	9.008	9.21
0.1	10.09	8.936	9.127	9.054	8.985	9.15
0.2	10.01	8.859	9.029	8.965	8.902	9.06
0.3	9.32	8.677	8.796	8.746	8.696	8.93
0.4	8.64	8.449	8.574	8.539	8.501	8.75
0.5	8.17	8.127	8.271	8.253	8.23	8.52
0.6	7.85	7.729	7.78	7.795	7.799	8.28
0.7	7.59	7.242	7.414	7.379	7.344	8.03
0.8	7.34	7.172	7.199	7.166	7.133	7.75
1.0	6.8	6.672	6.699	6.672	6.644	7.06
1.2	6.22	6.161	6.187	6.166	6.144	6.36
1.4	5.65	5.693	5.719	5.703	5.687	5.79
1.6	5.15	5.292	5.317	5.305	5.293	5.29
1.8	4.74	4.955	4.979	4.97	4.961	4.83
2	4.4	4.687	4.709	4.703	4.697	4.44
3	3.49	3.869	3.872	3.872	3.871	3.55
4	2.86	3.188	3.189	3.188	3.188	2.48
5	2.24	2.549	2.549	2.549	2.549	2.24

Part 2-(Fcc-Cu):

The Compton profile For copper Cu after all corrections have been applied is given in Table-2. Also consisted here are three calculated theoretical profiles for ($3d^{9.8}$-$4s^{1.2}$,$3d^{9.7}$-$4s^{1.3}$,$3d^{9.6}$-$4s^{1.4}$) by the renormalized free - atom (RFA) model using the procedure of sec.2.A .

The free atom(FA) theoretical values for ($3d^5$-$4s^1$) are also consisted in order to comparison. Also given here are the Free electron profile, the experimental value of reference [13], all the theoretical and experimental values given in this table-2 are obtained Before convoluting and normalized to an area of 11.69783.

Table 2: Our calculated theoretical (unconvoluted) Compton profile for Copper (Cu) compared with experimental value in reference [13]. All the the value have been normalized to 11.6978 electrons.

P_z (a.u.)	$J(p_z)$(e/a.u.)					
			Theory(RFA)			Expt. [13]
	Free atom ($3d^{10}$-$4s^1$)	Free electron ($3d^{10}$-$4s^1$)	Core+RFA $3d^{9.8}$-$4s^{1.2}$	Core+RFA $3d^{9.7}$-$4s^{1.3}$	Core+RFA $3d^{9.6}$-$4s^{1.4}$	
0.0	5.93	5.346	5.192	5.15	5.111	5.12
0.1	5.76	5.323	5.18	5.139	5.101	5.11
0.2	5.37	5.252	5.121	5.083	5.048	5.06
0.3	4.94	5.136	5.014	4.984	4.955	4.97
0.4	4.6	4.967	4.902	4.879	4.855	4.85
0.5	4.38	4.751	4.766	4.75	4.734	4.72
0.6	4.24	4.48	4.527	4.527	4.523	4.56
0.7	4.14	4.158	4.236	4.254	4.266	4.39
0.8	4.05	4.029	4.065	4.047	4.039	4.22
1.0	3.86	3.84	3.875	3.858	3.841	3.89
1.2	3.62	3.611	3.644	3.627	3.611	3.58
1.4	3.36	3.341	3.368	3.353	3.338	3.29
1.6	3.07	3.061	3.083	3.069	3.055	3.01
1.8	2.79	2.784	2.799	2.787	2.774	2.73
2	2.52	2.519	2.528	2.517	2.506	2.46
3	1.47	1.47	1.472	1.466	1.46	1.5
4	0.915	0.915	0.917	0.914	0.911	0.94
5	0.632	0.632	0.634	0.632	0.631	0.66

Part 3-(W-Cu Alloys):

In this work we have studing and computed Cp for two alloys namely $W_{0.60}$-$Cu_{0.40}$ and $W_{0.72}$-$Cu_{0.28}$. the experimental data of the Compton profile for the two constituent metals i.e. Tungsten W and copper Cu of reference [13] were compared with our renormalized free-atom (RFA) calculations for different (3d-4s) and (5d-6s) configurations and our other calculated results, These calculated values were used to obtain the Compton profiles for the two alloys by suitably adding their contributions i.e. by applying the superposition model which was then compared with the measured data on the alloys of [13].

In the superposition model [14], the Compton profile for a given $J(P_Z)_{alloy}$ is given by:

$$J(P_Z)_{alloy} = x\,J^{W}(P_Z) + (1-x)J^{Cu}(P_Z) \qquad (7)$$

Where x is the (fractional) atomic concentration for atoms in the tungsten-copper (w-cu) alloy. $J^{W}(P_Z), J^{Cu}(P_Z)$ are the experimental Compton profiles for tungsten w and copper cu metals.

The calculated Compton profiles values for both the alloys $W_{0.60}$-$Cu_{0.40}$ and $W_{0.72}$-$Cu_{0.28}$ with theirs constituent metals W and Cu from part 1 and 2 are given in Tables 3-a,b.,the results for w ($5d^5 6s^1$) electron configuration and ($3d^{9.6}4s^{1.4}$) for cu configuration.

Now we compare the measured data of ref. [13] on the two alloys of(W-Cu) with our calculated data (the free atom(F.A), free electrons(FE),renormalized free atom(RFA) and superposition model of our work.

In both tables-(3 and 4) at the high momentum region (i.e. p_z above 3.45 a.u.) it is seen that all values are very close to the free atom superposition model, this provides confidence in our data analysis because the superposition model values of ref.[13] are nothing but the yield of experimental values of Compton profile of w and cu, since these values are very close to free atom values in this momentum region hence it is not surprising that for the two alloys they agree very well,in fact this comparison only confirms that the inner electrons do not undergo any drastic change on alloy formation.

For the low momentum region (p_z<3.5 a.u.) it is obvious that the free atom values for both the cases are larger than the experimental values upto 0.4 a.u. but their they become close, the deviations are very obvious and hence we have not considered this model for any analysis of the alloy data. Interestingly, the superposition model of RFA and FE values agree quite well with the experimental values in both the alloys.

Figures- 1, shows the comparison of our calculated data with superposition model of $W_{0.60}$-$Cu_{0.40}$ listed in Table 1 ,it is seen that superposition model values of all cases are approximately equal to experimental values for p_z =(0.1 and 0.15) a.u. between p_z= 0.23 to 1.45 a.u.a the expt.

values are a little bit higher. For p_z=1.65 a.u. the superposition model of alloys is higher but

gets reversed again between p_z= 3.52 to 3.81 a.u whereas at p_z= 4.1 a.u. the values are equal and of p_z=4.51 a.u the superposition model is lightly higher, however the overall natures for the two curve are similar. For the state of $W_{0.72}$-$Cu_{0.28}$, the comparison is seen at Fig.3, It is obvious that in this case the superposition model and the measured values are very close.

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In order to determine the electron configuration and examine any differences in the behavior of the two alloys, we have plotted the differences between a superposition model and experimental values for both the cases. the total square deviation $\sum_{zero}^{5a.u.}|\Delta J|^2$ was obtain for each case, the values obtained are (4.093528, 0.9595944, 0.7103577) for [(free atom ,Free electron, RFA)-(Expt.)] for ($W_{0.60}$-$Cu_{0.40}$) and (4.817486, 1.334751, 0.9862669) for [(free atom, Free electron, RFA)- (Expt.)] for ($W_{0.72}$-$Cu_{0.28}$), these differences are shown in figures-(2,4).

Table 3 : Our calculated theoretical (unconvoluted) Compton profile for the alloy[$W_{0.60}$-$Cu_{0.40}$] compared with experimental value of ref [13].all these values have been normalized to(18.82672) electrons.

P_z (a.u.)	J(p_z)(e/a.u.)					
	W Core+RFA $5d^5$-$6s^1$	Cu Core+RFA $3d^{9.6}$-$4s^{1.4}$	Superposition model $W_{0.60}$-$Cu_{0.40}$			
			Free atom	Free electron	Present work. RFA	Expt. [13]
0.0	9.153	5.111	9.092	7.512	7.529	7.57
0.1	9.127	5.101	8.358	7.483	7.509	7.54
0.2	9.029	5.048	8.154	7.409	7.429	7.46
0.3	8.796	4.955	7.568	7.253	7.252	7.34
0.4	8.574	4.855	7.024	7.049	7.079	7.19
0.5	8.271	4.734	6.654	6.77	6.849	7
0.6	7.78	4.523	6.406	6.423	6.471	6.79
0.7	7.414	4.266	6.21	6.002	6.149	6.58
0.8	7.199	4.039	6.024	5.909	5.929	6.34
1.0	6.699	3.841	5.624	5.534	5.55	5.79
1.2	6.187	3.611	5.18	5.136	5.151	5.25
1.4	5.719	3.338	4.734	4.747	4.762	4.79
1.6	5.317	3.055	4.318	4.395	4.408	4.38
1.8	4.979	2.774	3.96	4.083	4.093	3.99
2	4.709	2.506	3.648	3.816	3.824	3.65
3	3.872	1.46	2.682	2.906	2.904	2.73
4	3.189	0.911	2.082	2.277	2.276	2.08
5	2.549	0.631	1.597	1.78	1.78	1.61

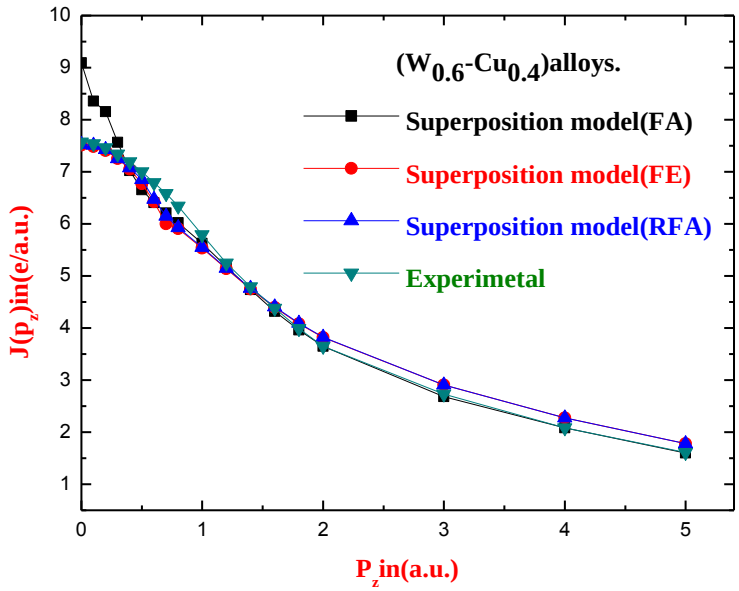

Fig.1 : Comparison of the experimental results in ref [13] Compton profiles of $W_{0.60}$-$Cu_{0.40}$ alloy with thats calculates from superposition model for(FA-FE-RFA)

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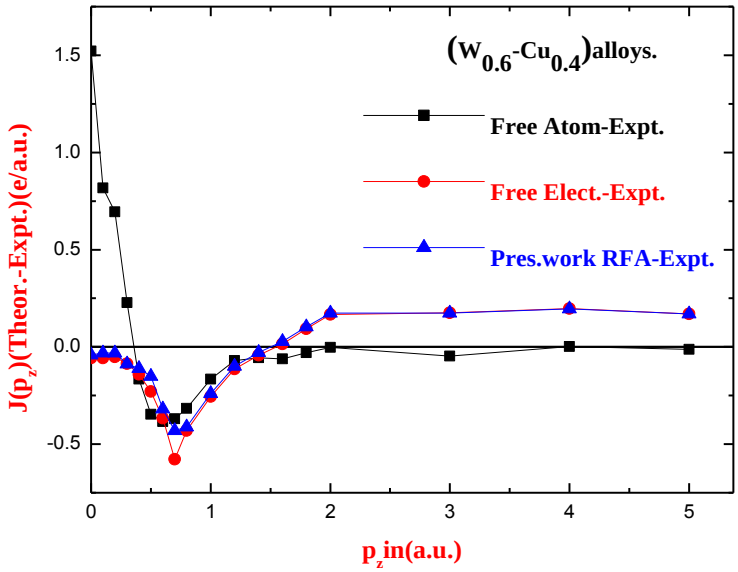

Fig.2: the difference between superposition model (CP-theory) and experimental results [13] Compton profiles of the alloys ($W_{0.60}$-$Cu_{0.40}$)

Table 4: Our calculated theoretical (unconvoluted) Compton profile for the alloy[$W_{0.72}$-$Cu_{0.28}$] compared with experimental value in ref[13]. All These values have been normalized to (20.25207) electrons.

P_z (a.u.)	J(p_z)(e/a.u.)					
	W Core+RFA $5d^5$-$6s^1$	Cu Core+RFA $3d^{9.6}$-$4s^{1.4}$	Superposition model $W_{0.72}$-$Cu_{0.28}$			
			Free atom	Free electron	Present work. RFA	Expt. [13]
0.0	9.153	5.111	9.724	7.938	8.013	8.06
0.1	9.127	5.101	8.878	7.909	7.992	8.02
0.2	9.029	5.048	8.711	7.833	7.906	7.94
0.3	8.796	4.955	8.094	7.67	7.713	7.82
0.4	8.574	4.855	7.509	7.459	7.525	7.66
0.5	8.271	4.734	7.109	7.167	7.273	7.46
0.6	7.78	4.523	6.839	6.806	6.861	7.24
0.7	7.414	4.266	6.624	6.366	6.526	7.01
0.8	7.199	4.039	6.419	6.279	6.308	6.77
1.0	6.699	3.841	5.977	5.867	5.893	6.17
1.2	6.187	3.611	5.492	5.436	5.46	5.58
1.4	5.719	3.338	5.009	5.024	5.047	5.09
1.6	5.317	3.055	4.568	4.658	4.679	4.65
1.8	4.979	2.774	4.194	4.338	4.357	4.24
2	4.709	2.506	3.874	4.072	4.088	3.89
3	3.872	1.46	2.924	3.191	3.193	2.98
4	3.189	0.911	2.315	2.546	2.549	2.31
5	2.549	0.631	1.79	2.008	2.01	1.8

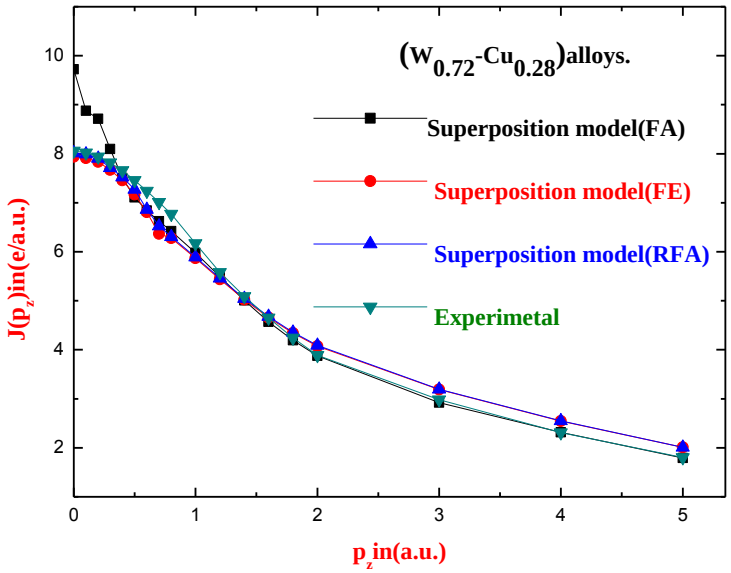

Fig.3 : Comparison of the experimental results in ref [13] C-profiles of multiple - crystalline $W_{0.72}$-$Cu_{0.28}$ with that calculated from superposition pattren for (FA-FE-RFA).

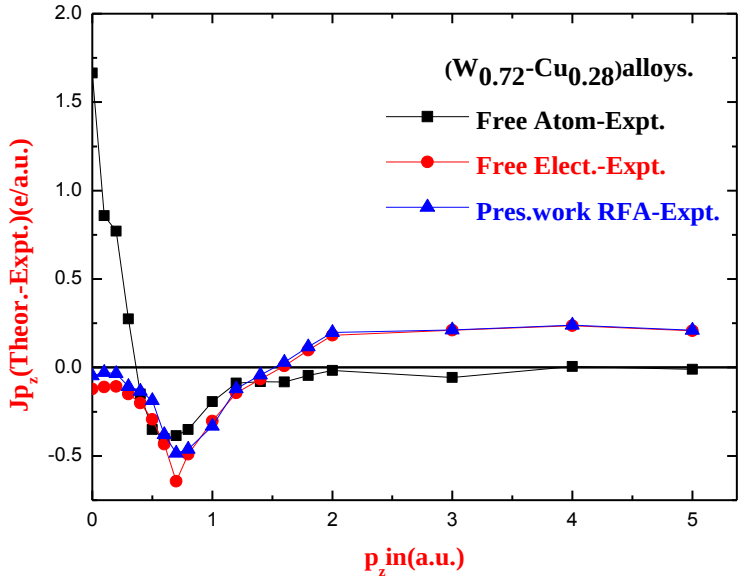

Figure .4: the difference between superposition model and expt.compton profile results [13] for the ($W_{0.72}$-$Cu_{0.28}$) alloy

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دراسة التركيب الالكتروني في سبيكة التنكستن– نحاس باستخدام نموذجي اعادة معايرة الذرة الحرة والالكترون الحر

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الملخص

في هذا البحث تم حساب شكل منحنى كومبتون لعنصر التنكستن (w) باستخدام نموذجي اعادة معايرة الذرة الحرة (RFA) باختيار ترتيبات الكترونيه بصيغة ($5d^{5-x}\,6s^{1+x}$) والالكترون الحر. تمت مقارنة النتائج النظرية بما متوفرة من قيم ونتائج قياسية (عملية).

وتم اعتماد نفس النماذج الحسابية (النظرية) لحساب وايجاد شكل منحنى كومبتون لعنصر النحاس (Cu) وباختيار ترتيبات الكترونية مختلفة للغلافين الثانويين (3d-4s) وقورنت باحدث النتائج العملية المتوفرة.

وتمت ايضا دراسة الحالات الالكترونية للسبيكتين ($W_{0.60}\,Cu_{0.40}$) و($W_{0.72}\,Cu_{0.28}$) باستخدام تقينه استطارة كومبتون، لقد تم استخدام نموذج التركيب الاعظم (superposition) لحساب منحنى كومبتون الكلي للسبيكتين بتوظيف القيم التي حصلنا عليها من الجزئيين الاول والثاني لكل من التنكستن والنحاس وكانت النتائج الحسابية باستخدام التركيب الاعظم متطابقة بشكل جيد جداً مع اخر النتائج العملية التي حصلنا عليها للسبيكتين.

الكلمات المفتاحية: منحني كومبتون ، كثافة الزخم الالكتروني، نموذج اعادة معايرة الذرة الحرة ، نموذج الالكترون الحر، نموذج التراكب الاعظم.