"EMD of silver(Ag) and it's CopmoundAgCl"

Fareed M.Mohammed[1] , Ahmed W.Maseer [2],Mustafa M.Essa[3]
Department of Physics, College of science ,U.O. Tikreet-Iraq

Abstract

In this paper we study, the electronic momentum density(EMD) of Ag and AgCl compound is using the Comptinprofil technique. We employed different theoretical methods based on {(RFA) ,the Free Electron (FE),free atom(FA)} models to calculate the computational curve shape J(p_z) Of the metal(Ag). The theoretical results were compared with the experimental values [18],where it is found that the best electronic arrangement of the silver in the (RFA) and (FA) models are $4d^6$ $5s^1$. As for the AgCl the super position model used depending on best result found for the metal and compare with experiment volue of [19]

Key word - *RFA model ,FE model, FA model, superposition model, Compton Profile(cp), EMD*

I. INTRODUCTION

It is known that one of the direct ways to probe the ground-state electronic structure of a material is the measurement of compton profile. The compton effect includes the scattering of photons by electrons in which a part of the momentum and energy of the photon is transferred to the charged particle byinelastic relativistic collision while the photon moves off with a reduced energy and a change of momentum [1] Significant developments have taken place in recent years with respect to the electronic composition and properties of substances. There are different types of theoretical and practical methods used to find the electronic structure of materials on a large scale, including spectroscopic and scattering. The technique was first used to study the behavior of plasmids in metals [2]. Comptonprofil is one of the most important methods used to study the behavior of valence electrons in atoms, over the past three decades,this technique used also to distinguishes electrons in crystallization uniformly [3-4] Now, after the use of high-energy sources of radiation as a source of gamma rays, the results of the electronic momentum have become good enough to exploit the technique of Compton absorption as an important tool to study the electronic composition of different materials,the distribution of the electronic momentum of some elements because of the advantages mentioned above, which gives preference than other technigue to study the electronic composition of different crystalline materials[5]

II. THEORY

The computing profile J(p_z) is related to the density of the electronic momentum $n(\vec{p})$ through the relation:

$$(\mathrm{Jpz}) = \iint_{p_y p_x} n(\vec{p})\, dp_x dp_y \ldots\ldots\ldots (1)$$

i)Renormalised free atom (RAF) model

(Berggern et al., 1972) was developed a simple model for computation of the J(p_z) curve of valence electrons using the RFA Model [6], which is valid and appropriate for calculating the spherical J(p_z) for the elements of the first transition series (3d-transition metals) [7] as well as the elements of the second transition series (4d-Transition metals) [8-9]. This method was then used to find a convective curve of string elements (5d-Transition metals) [10] as the theoretical results corresponded well with practical measurements ,also than model used in many complex and non-complex theoretical calculations such as finding the density of the momentum distribution of electrons(EMD)[11], and gives correct results it is well aligned with the results of practical measurements. The (RFA) model assumes that the atom is not free and at the same time connected to a cell in the solid. The chadorow was the first to use this theoretical model in 1939 [12]. Segall then used this model to study the copper element (Cu). The success and validity of the free scale calibration model is evident in the studies and research presented by many scientists in the 1970s. Both Hodges et al. (1972) and Berggern (1972) demonstrated that the RFA model used this model to calculate the binding energy for a set of elements of the first transition series (3d-transition metals) and the second (4d) - Transition metals. [13] used it (Bendick et al., 1985) used it to find the single electron effort even in the calculations of compositions. Complexity [14]

ii)Free electron (FA) –based model profile

The free electron model is a simple model used to study electronic structure and calculation of the computed curve shape of various elements. Most of the results of this model are close to the values of practical measurements. The shape of the curved curve J(p_z)was calculated using the following relationship:

$$J_{4s}(p_z) = 2\pi \int_{p_z}^{\infty} n(\vec{p})\, p\, dp \quad (2)$$

such that$\boldsymbol{n}(\vec{\boldsymbol{p}})$represents the density of the electronic momentum it is found using the relationship:

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

(T =$4p_F^3$), (n) represents the number of occupancy electrons to the level of Fermi momentum (p_f), putting equation (3) in equation (2) we obtain the equation:

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

Equation (4) represents the final equation used to create a computed form ($J_{4s}(p_z)$)for the various elements[15].

iii)free atom (FA) model:

The value of Compton profiles were taken directly from the tables of (Biggs…et al) [16]

III. RESULTS AND DISCUSSION

In this paper we study the distribution of the electronic momentum of the silver Ag element and compoundAgCl.The results of our calculations were compared with the available measured values to determine the best electronic composition of the silver element.[18]

Table (1) presents the calculated J(p_z), i.e(cp) shape of the silver element by using the{(FA),(RFA),(FE)} models as well as the practical valuesJ(p_z) by [18]

These values represent the closest electronic structures to the practical values adopted.

The closest calculated J(p_z) values to the practical values of the silver element are the electronic structures of:

$(4d^6\ 5s^1)$, $(4d^{5.9}\ 5s^{1.1})$, $(4d^{5.7}4s^{1.3})$

Which were calibrated to the area under curve of the free atom which is (18.88758)electrons of the momentum zone confined between (0→ 0.7 au).Figure (1)shows the results of the theoretical as well asthe measurements given in Table (1). Note that the theoretical results match well with the measurements. It can be seen that the electronic.This arrangement($4d^6\ 5s^1$) . Is the optimal arrangement and the closest to the experimental values.As for the free electron model (FE), the calculations were performed in the electronic order ($4d^6\ 5s^1$)arrangement ($4d^6\ 5s^1$)is found to be close to the measurements. Figure 2 presents the differences between different theoretical and the experimented results of[18]. In order to determine the optimal electronic structure . The summation of the square differences between theory and experiment values was adopted through the relation:

$$\left(\sum_{0}^{7a.u.}\left(J_{Theo.}(p_z) - J_{exp.}(p_z)\right)\right)^2 = \sum_{0}^{7a.u.} |\Delta J(p_z)|^2 \ldots\ldots (5)$$

TABLE 1
Gives all the theoretical Compton profiles J(p_z) values for (Ag) with the experimental values[18]

P_z (a.u.)	J(p_z)(e/a.u.)					
	Free atom	Free electron ($4d^6$-$5s^1$)	Theory(RFA)			Expt. [18]
			Core +RFA $4d^6$-$5s^1$	Core +RFA $4d^{5.9}$-$5s^{1.1}$	Core +RFA $4d^{5.7}$-$5s^{1.3}$	
0.0	8.18	7.443	6.987	6.972	6.945	7.476
0.1	8.01	7.417	6.977	6.963	6.936	7.446
0.2	7.59	7.341	6.942	6.929	6.905	7.365
0.3	7.14	7.208	6.874	6.865	6.846	7.235
0.4	6.79	6.987	6.761	6.754	6.741	7.054
0.5	6.54	6.774	6.69	6.687	6.68	6.843
0.6	6.37	6.455	6.517	6.522	6.526	6.622
0.7	6.22	6.072	6.375	6.367	6.352	6.461
0.8	6.07	5.619	6.234	6.226	6.211	6.126
1.0	5.70	5.735	5.857	5.849	5.833	5.617
1.2	5.24	5.279	5.382	5.375	5.361	5.114
1.4	4.75	4.779	4.853	4.849	4.839	4.632
1.6	4.24	4.274	4.318	4.315	4.31	4.2
1.8	3.77	3.802	3.821	3.82	3.818	3.778
2	3.35	3.377	3.381	3.38	3.38	3.336
3	2.02	2.043	2.054	2.056	2.061	2.029
4	1.5	1.516	1.519	1.523	1.529	1.527
5	1.21	1.222	1.212	1.215	1.221	1.215
6	0.976	0.992	0.98	0.983	0.987	0.984
7	0.781	0.789	0.78	0.782	0.785	0.793

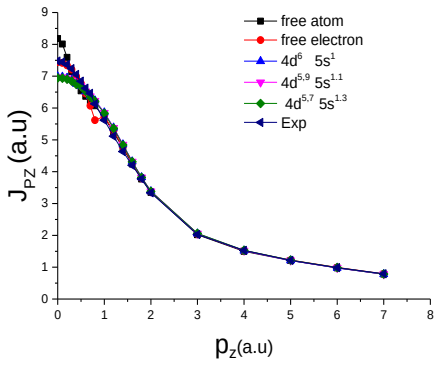

Fig 1. represents various J(p_z) values of the theoretical and practical electronic arrangements of the silver element after calibrating it to an area under the curve of the free atom value

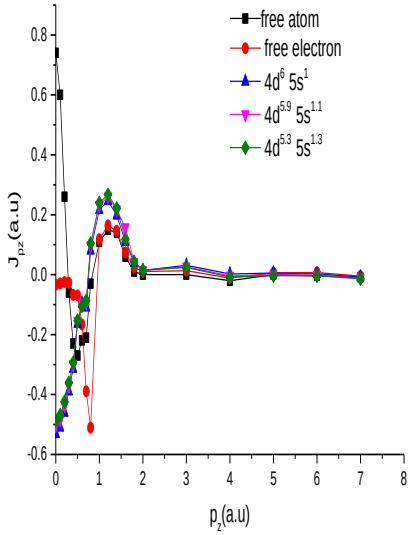

Fig 2. The differences between the calculated and measured J(p_z) of the silver element(Ag).

To compute the J (P_Z) of the silver chloride compound (AgCl) we applied the superposition model based on the calculated values of the silver element (Ag) obtained by using the {free atom(FA) , free electron(FE) and re-calibration of the free atom} models J(p_z) of the chlorine element were taken directly from Biggs tables and others [18]. And all the theoretical and practical results of AgClcalibrated to an area under the curve by (26,69134)electrons free atom electrons. Table (2) contains three theoretical results of the curves of Compton J (PZ) for (free atom, free electron and(RFA) calculated by the overlay model as well as the experimental value of [19]

TABLE II

Theoretical and experiment value [19] for AgCland located in the momentum zone confined between (0-7 a.u.).

P_Z (a.u.)	J(P_Z) (e/a.u.)			
	Superposition model for AgCl			Exp.[19]
	Free Atom	Free electron	RFA	
0	13.26	12.523	12.07	11.537
0.1	13.06	12.469	12.03	11.479
0.2	12.54	12.293	11.894	11.344
0.3	11.91	11.981	11.646	11.136
0.4	11.3	11.499	11.273	10.866
0.5	10.73	10.966	10.882	10.525
0.6	9.68	9.767	9.829	10.116
0.7	9.64	9.494	9.797	9.667
0.8	9.11	8.66	9.279	9.194
1	8.07	8.107	8.228	8.218
1.2	7.12	7.16	7.263	7.307
1.4	6.29	6.32	6.395	6.483
1.6	5.55	5.585	5.629	5.736
1.8	4.93	4.963	4.982	5.084
2	4.4	4.428	4.432	4.591
3	2.745	2.768	2.779	2.856
4	1.929	1.946	1.949	2.013
5	1.539	1.551	1.541	1.549
6	1.2	1.216	1.205	1.19
7	0.939	0.947	0.938	0.94

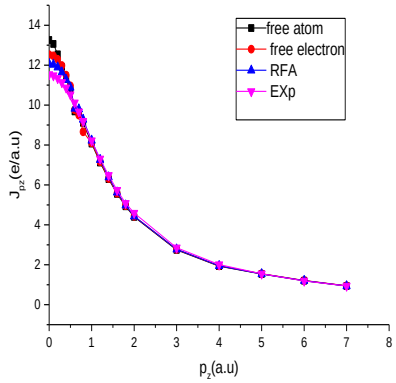

Fig 3. Comparison of different J(p_z) value ofAgCl in the momentum rang between(0-7 a.u.)

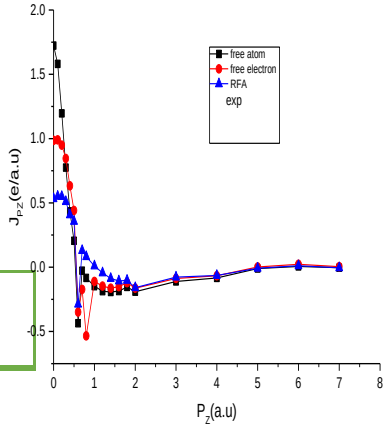

Fig 4.Curves of Difference between theoretical and experiment valuefor the Compton J(P_Z) for AgCl

IV. CONCLUSIONS

It is found that the best electronic configuration results by applying different theoretical models and compared with the a available recent experiment value for Ag is 4d6 5s1 , this result is used for further calculation based on superposition model to find the best match of Compton profile (cp) with also available experiment results of the AgCl compound.

V. REFERENCES

[1] M.J.Cooper, P.E.Mijnarends,N.Shiotani, N.Sakai, and A.Bansil,"X-ray Compton Scattrering" ,Rep. Prog .Phys,48,415(1985)

[2] A.H.Conpton,phys.Rev.21,483(1923).

[3] Raether ,H.,'Springer Tracts in Mdern physics' .38,p,84,Springer VerlagPerlin and New York,(1960)

[4] J. Ritsko , P. Gibbon and S.Schntterly , 'Momentum Transfer Dependance of K Abosorption edge of lithium' ,phys, Rev,P,10,5017,(1974).

[5] W.C. Rontgen ,Uber eineneue Art Von strinhlen' ,Sitz.Wurz.,(1895).Translated and repeinted in H.A.Boorse and L.Motz(eds) the World of the Atom,1.396,New York,(1966)

[6] K.F.Berggren,phys.Rev.B6 2156-61,(1972)

[7] K.F.Berggren,S.Manninen,T.Paakari,O.Aikala and K.Manskka"Compton Scattering(ed)" .B.G.Williams (New York:McGraw Hill) (1977)

[8] B.L.Ahuja,H.Singh,B.K.sharma and Fared M., "Current trend in the physics of material" 151,Ed:M.Yossouff(world scientific pub.co.,Singapore),(1986).

[9] FaridM.Mohammed,ph.D.Thesis submitted to Un. Of Rajasthan,Jaipar,India,(1988)

[10] FaridM.Mohammed,J.Ed.sci.vol 17,Mosul,Iraq,(1944)

[11] M.chodorow,phys.Rev.55,675,(1939)

[12] B.Segall,phys.Rev.125,109,(1962)

[13] C.D.Gelatt,H.Ehrenreich,R.E.Watson,phys.Rev.15,432 0, (1966)

[14] N.Andersson,etal.,"Emission spectra of TiH and TiD Near 938nm",Chmphes.118:10543(2003)

[15] M.J.Cooper,Rep.Prog.Phys.48,415(1985) and referncestherein.AlsoM.J.Cooper , P.E.Mijnarends,N.Shiotani,N.Sakai and A.Bansil,X-ray Compton Scatering (Oxford Unviersitypress,New York,(2004).

[16] Bigges,L.Mendelsohn,L.BandMann,J.B.A*t.DataNucl.DataTables*.**1975,**16,201

[17] P.Chaddah and V.C. Sahni,philMag.B 37,305 (1978)

[18] Journal of The physical S0ciety of Japan Vol.60,No.12,Decemder,1991,pp.4253-4264

[19]] Phys. Stat.Sol.(b)245,No.8,1570-1570 (2008)/Dol10.1002/pssb.200844050