s – d occupancy in Iron

Farid M.Mohammed and Yasir K. Mohammed
Departemant of physics. college of education university of tikrit

p.o.box 42

e - mail :- yasirkhalaf @yahoo.com

Abstract

In this paper we have calculated the electronic structure of Fe^{26} by adopting the RFA model and compared with recent available measured data . It is found that $3d^{6.4}4s^{1.6}$ is the best fractional electronic cofiguration for Iron .

1. Introduction

Iron belong to group (2) body center cubic (B.C.C) metal with a = 5.423 a.u [1] and electronic structure mainly accepted for (Fe) atom is $3d^6 4s^2$ [2].First experimantal compton profile for (Fe) reported by Paakkaire et al [3],   includes atomic weight 55.847 g/mol , atomic number 26 , boiling point 3023 c^o , melting point 1808 c^o and density 7.86t g/ml [4] . For the last decade there has been interest in the study of the energy broadening of compton scattering γ-ray or x-ray for probing the behaviour of the slowly moving valance electron in solids this broadened line - shape referred to as the compton profile $J(\vec{P_z})$ which is given as

$$J(\vec{P_z}) = \iint \rho(\vec{P})\, dp_x\, dp_y$$

Where $\rho(\vec{P})$ is the electron momentum density . Provides a useful test of initio electronic structure theory a general review of this topic has been published [5]. In our endeavor to extend the compton scattering of 3d transition metals , we referred to compton profile polycrstalline Fe [6,7,8,9,].Since new measured data where reported for Fe [10]. It was thought to re-establish and hold new study . In this paper we report   the theortical Compton profile results of Iron by using the (RFA) model which is known to be a reasonable compromise between elaborate band structure and simple atomic calculation [11].we have also attempted to interpret the experimental results in terms of this model .

2. RFA model

Chodorow [12] was the first to use this theoretical model.Later it was extended for Cu by Segall [13].

This approach simply considers that the atom is not free but confined to particular cell in the solid . The calculation starts from

Hartree – fock wave function which is truncated at the Winger – Seitz radius (R_o) and re-normalized to unity within this sphere to preserve the charge neutrality, the new wave function $R_{n1}(r)$ is given by :

$$R_{n1}(r) = \begin{cases} N_{n1} \; R_{n1}{}^{atomic}(r) & r \le R_o \\ \\ 0 & r > R_o \end{cases} \qquad (1)$$

Here $R_{n1}{}^{atomic}(r)$ is the atomic radial wave function for the state with quantum number (n) 1 and N_{n1} is defined by

$$N_{n1}{}^{-2} = \int_{0}^{R_o} \left| R_{n1}{}^{atomic}(r) \right|^2 r^2 \, dr \qquad (2)$$

This new function is then used in further computations. In this way the solid is constructed from individual atoms approximately in the same form in which they actually enter the solid before being bound together . As from the successes of this simple model , besides Compton work [14] , has shown that this model gives quantitively correct estimates of important band structure characteristics and also exolanation of cohesion in the transition metal series . Later [15] used the RFA model for the determination of cohesive energies for several 3d and 4d metals even in complicted band theoretical calculation , RFA model is invoked to obtain the one electronic potential [16] .

Berggren has studied overall behaviour of the RFA wave function (4s electron in vanadium) and has followed it to be a good represented of the true crystal wave function at $\overrightarrow{K} = 0$.

3. Theoretical calculations

The compton profile $J(P_z)$ for pollycrstalline sample is related to spherical average of $\rho(\overrightarrow{p})$ by :

$$J(P_z) = \int\limits_{P_z}^{\infty} dp \; p < \rho(\vec{p}) >$$

to compute $<\rho(\vec{p})>$ the technique developed by Berggern [14] based on RFA model has been used . We start with the free atom wave function , truncate them at Winger-Seitz radius and re- normalized the wave function to one within (W-S) sphere to preserve charge neutrality. $J(P_z)$ due to (4s) electrons of Fe were computed for $(3d^{6+x}4s^{2-x})$.

where (x = 0.1,0.2,0.3,0.4,0.5,0.6,.. ets)

we used the equation :

$$J_{4s}(\vec{P_z}) = 4\pi\sum_{n=0}^{\infty} \left| \psi_o^c(K_n) \right|^2 G_n(P_z)$$

where $\psi oc(\vec{K_n})$: - is the Fourier transfrom of the RFA wave function $Gn(Pz)$ is an auxiliary function depends on Kn , Nn and Pf : Fermi momentum.

In the calculation, free atom Hartree-Fock function were taken from the tables of Clement and Roetti [17] . For x = 0 to x = 1.5 the wave function for $3d^6 4s^2$ was used and for x = 1.6 to 2 the wave function for the $3d^7 4s^1$ were used, for the rest including 3d electronic values were taken from the tables of the Biggs et al [18]. Several combination of 3d 4s configuration were computed . The Winger – Seitzr is 2.67 a.u [2] .

All these theoretical values were finally convoluted with RFA(residual instrumental function) to make them comparable with experimental values which have been de-convolution using the known instrumental function [3] .

4. Results and discussion:

Table (1) shows the different measured and calculated Compton profiles values, all values were normalized to the value (10.65a.u) which

represents the area under the curve for free atom profile.Fig (1) shows some of the curves given in table (1) and it is observed that the momentum region between 0 to 3a.u . the RFA values for $3d^{6.2}4s^{1.8}$ and $3d^{6.4}4s^{1.6}$ are closer to the experiment while beyond 3(a.u) all theoretical values are nearly equal and agree very well with the experiment results . At J(0) the experiment as well as (RFA) $3d^{6.2}4s^{1.8}$ almost the same.

To show the comparison more clearly,Fig (2) the differences between theory and experiment are plotted for the $3d^{6.4}4s^{1.6}$, $3d^{6.3}4s^{1.7}$ and $3d^{6.2}4s^{1.8}$ cases in order to determine the configurtion, the total square deviation $\Sigma(\Delta J)^2$ was obtaind for each case. The values found were 0.05336 , 0.06190 and 0.04195 for the (RFA) $3d^{6.4}4s^{1.6}$, $3d^{6.3}4s^{1.7}$ and $3d^{6.2}4s^{1.8}$.

Same procedures were done but after convoluting the RFA values and found changed in the favoured configuration .

5. Conclusion:

This paper demonstrates the study on (Fe) to investigate its electronic structure , theoretical calculation by applying RFA model and compared with recent measured data of compton profile . It shows that best electron configuration for (Fe) is $3d^{6.2}4s^{1.8}$ before convolution while it turned out to be $3d^{6.4}4s^{1.6}$ after convlution which demonstrates the effect of the convlution on the results.

Table (1)

| P_z	$J(P_z)$ a.u Free	$J(P_z)$ a.u Exp	$J(P_z)$ a.u (Core + RFA)		
			$3d^{6.4}4s^{1.6}$	$3d^{6.3}4s^{1.7}$	$3d^{6.2}4s^{1.8}$
0	7.0628	5.17324	5.180293	5.210986	5.24186
.1	6.7752	5.13257	5.152148	5.182845	5.213706
0.2	6.0772	5.10279	5.117597	5.148306	5.179147
0.3	5.2732	5.00878	4.984588	5.015311	5.046092
0.4	4.6832	4.9321	4.884387	4.915129	4.94586
0.5	4.2312	4.77211	4.682451	4.713372	4.74406
0.6	3.9922	4.59421	4.502025	4.533022	4.563772
0.7	3.7776	4.203501	4.164875	4.196707	4.228105
0.8	3.718	4.05491	3.95294	3.984865	4.014133
1	3.5036	3.60101	3.648598	3.637971	3.627386
1.2	3.2072	3.30742	3.333853	3.324212	3.314621
1.4	2.8166	2.83245	2.919027	2.911749	2.904522
1.6	2.4752	2.592056	2.561163	2.554342	2.547573
1.8	2.2936	2.41018	2.363824	2.356793	2.349814
2	2.16954	2.2008	2.225214	2.217288	2.209415
3	1.17486	1.24187	1.187823	1.182759	1.177696
4	0.7994181	0.744939	0.8102163	0.8076541	0.8050908
5	0.580452	0.574738	0.5838681	0.5829254	0.581982
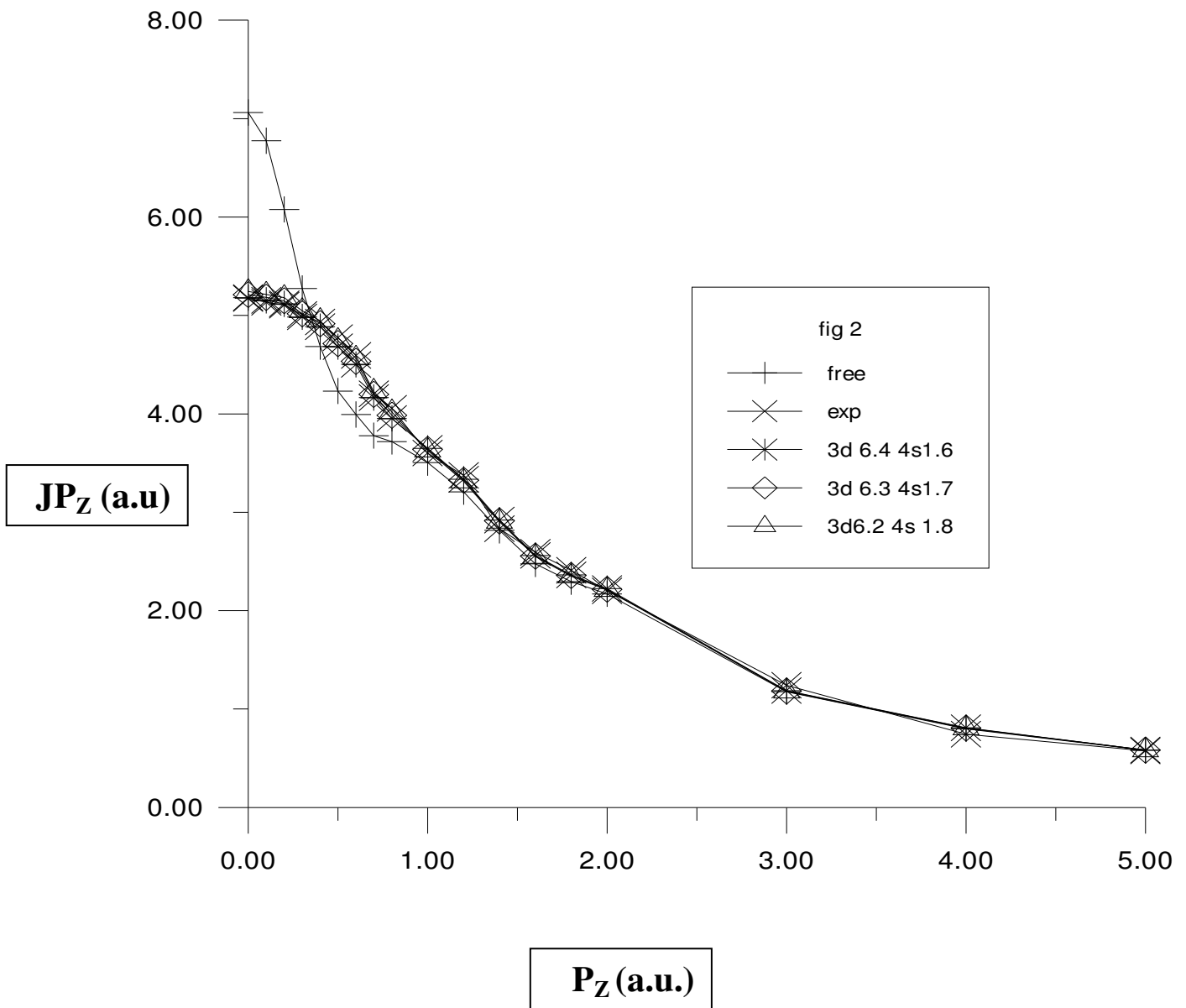
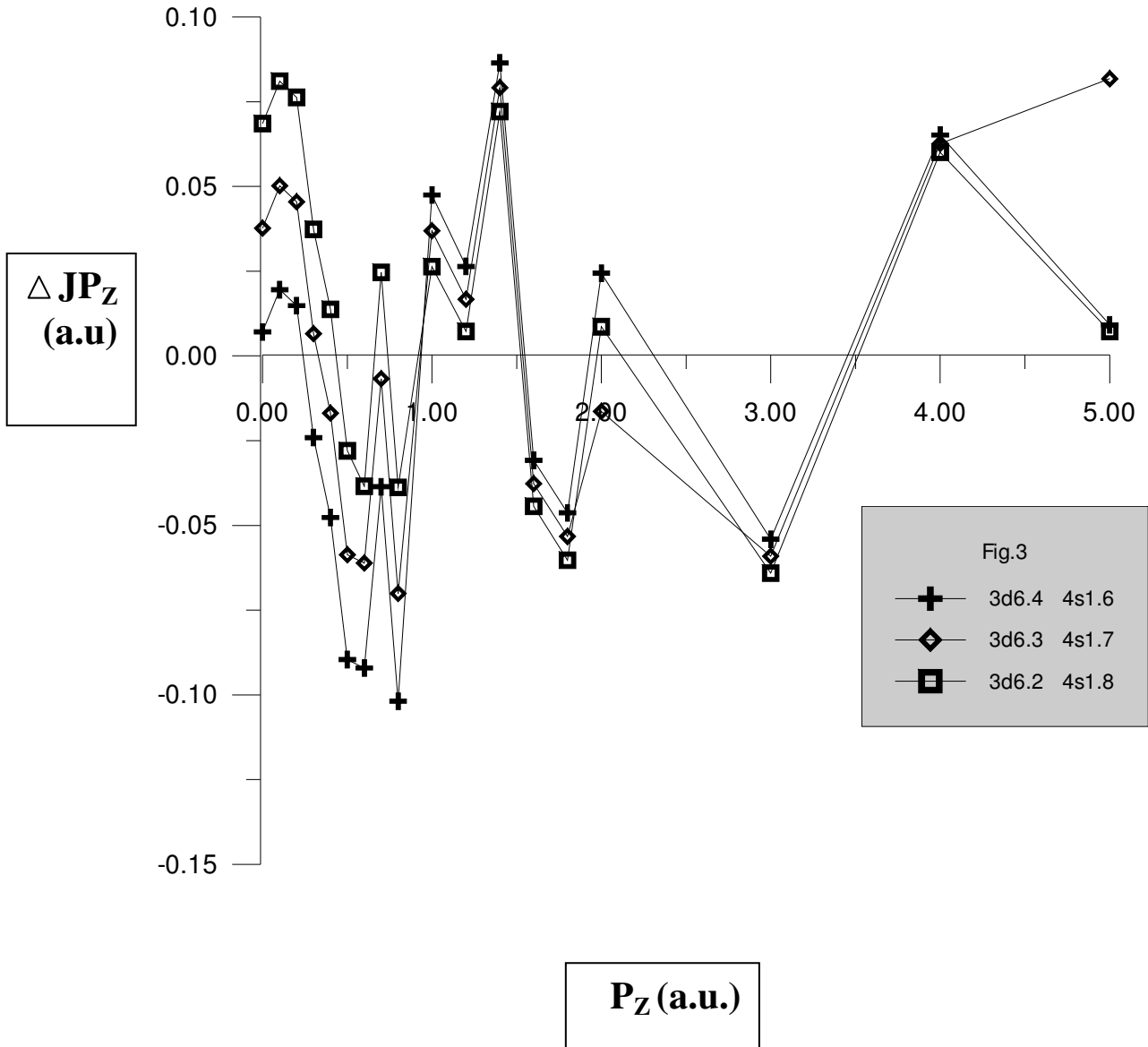Fig (1) shows some of the curves given in table (1)

Fig (2) the differences between theory and experiment

REFERENCES

1- Pearson , W.B. (1964). A hand book of Lattice Spacings and Structures of Metals and Alloys, Pergamon press Ltd .

2- Kittle, C. (1996). Introduction to Solid State Physics .

3- Patte, P.,Manninen, S. and Paakkari, T. Deconvolution in Compton Profile Measurement, phil.Mag.30, 1281, (1974).

4- www. Kiv.net .ge (chemistry 2002).

5- Cooper, M.J. (1985), Rep .Prog. phys.48,415.

6- J.W., Taylor , J.A., Duffy, M.J. Cooper,(2001),phys.Rev B,Vol 65.

7- Furness, J.B and McCarthy, I.E. The (e,2e) Experiment as a Probe for Atomic Structure , J. Phys.B6, 204. (1973).

8- Tomak, M. ,Singh, H., sharma, B.K. Manninen, S. (1981), phys. St.Sol. (b) 127, 221.

9- Terasaki, O., Watanabe, D. Fukamachi, T., Hosoya, S. Electron State in TiO Studied by Measurements of Compton Profile Scattering Factors, phys. Lett.A40,357, (1972)

10-www. Rcs. org /suppdata/Cp/b1/chi ", H. siang (1998), phys.rev B75, p.p.314-323.

11-Mohammed,Farid M "Investigation of Electronic Structure of Some Transition-Metals Alloys and Compounds by Compton Scattering Technique" 1988 , Ph.D thesis U.O.Rajasthan,India.

12-Chodorow, M. The Band Structure of Metallic Copper, phys . Rev.55, 675,(1939) .

13-Segall, B. Fermi Surface and Energy Bands of Copper, phys. Rev ., 125-109 , (1962).

14-Berggren, K.F. Renormalised Free Atom Model and the Electron Momentum Distribution in Vanadium, phys . Rev. B.6 . (1972).

15- Gellat, C.D, Ehrenreich, H and Watson, R.E, phys. Rev.15, 4320. (1977).

16- Bendick, R, Prassed, R., Manninen, S., Sharma, B.K., phys. Rev.B32, 7650. (1985)

17 - Clementi , E., and Roetti ., C., 1974, Atomic and Nuclear Data Tables,14, 177. (1977).

18 - Biggs, F., Mendelson, L.B., and Manninen, J.B. Hartree-Fock Compton Profiles for the Elements, Atom.Data and Nuclear tables 16, 201.(1975).

الأشغال الإلكتروني للغلافين (s,d) لعنصر الحديد

أ . م . د . فريد مجيد محمد   والسيد ياسر خلف محمد

جامعة تكريت ـ كلية التربية ـ قسم الفيزياء

ص . ب . ٤٣

البريد الإلكتروني : – yasirkhalaf @ yahoo.Com

الخلاصة

تَمَّ في هذا البحث حساب الترتيب الإلكتروني لعنصر الحديد (Fe) بتبني مثال إعادة المعايرة للذرة الحرة والمقارنة مع آخر البيانات المقاسة والمتوافرة ، وقــد وجــد أن أحـــسن ترتيب إلكتروني للحديد (Fe) هو $3d^{6.4}4s^{1.6}$.