

Electronic Configuration and Charge Transfer Study in (CdTe)

Fareed M. Mohammed^{#1}, Fatimah I. Rashid^{#2}, shahad A. Shaaban^{#3}
[#]Department of physics/College of Science/U.O.Tikrit-IRAQ

Abstract

The purpose of this paper is to study theoretically the electronic configuration of (CdTe) using (FA, FE, RFA and superposition) models to the Compton profiles $J(P_z)$ for Cd metal are determined adopting on several theoretical models by choosing different electronic arrangements ($4d^{10-x} 5s^{1+x}$) where ($x=0.1, 0.2, 0.3, \dots, 1$). The obtained theoretical Compton profiles for (CdTe) by applying the superposition model is found to be in best agreement with the available experimental data. Charge transfer for the compound has been evaluated by ionic model for number of arrangement of ($Cd^{+x}(Te^{-x})$). This model support a charge transfer of 0.2 electrons per Cd atom from 4d shell to 5p shell of Te atom.

Keywords

CdTe, Compton profile, Renormalized Free Atom (RFA) model, Free Electron (FE) model, Superposition model, charge transfer.

I. INTRODUCTION

The Compton effect involves of the scattering of electromagnetic waves (photons) by a charged particle in which a part of the momentum and energy of the photons is transferred to the charged particle in an elastic relativistic collision while the photon moves off with a reduced energy and a change of momentum. Compton scattering has emanated as a powerful tool for the realization of the behavior of valence electrons [1]. The Compton profile $J(p_z)$, can also be interpreted in terms of the ground state electron momentum density $\rho(p)$ of the target, i.e [2].

The Compton profile $J(P_z)$ is given as

$$J(P_z) = \iint \rho(p) dp_x dp_y \quad (1)$$

$\rho(p)$ is electron momentum density in ground state and is determined as

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

where $\Psi(r)$ is electronic wave function in the ground state. The equ.(1) have been derived in the impulse approximation (IA)[3].

CdTe is used as an infrared optical substance for optical windows and lenses. Nara et al. [4] have reported onto Compton profiles of CdTe with other tetrahedrally semiconductors namely Sn, GaAs, ZnSe and InSb. In order to gain insight in to the electronic configuration the relative nature of CdTe, in this paper we reports the first ever theoretical Compton

study of the compound. The selection of polycrystalline sample was due to (a) difficulty in getting the wanted size (15mm dia and 3mm thick) single crystals of these materials (b) a comparison of relative nature of bonding in this compound on equal valence electron density scale.

II. THEORETICAL METHOD

A. Renormalized Free Atom model

We have used Berggren's approach to compute Compton profile of elements. we give a few computational details The free atom Hartree Fock (HF) wave function has been taken from tables [5]. It has been truncated at the Wigner Seitz radius and renormalized to one unit to preserve the charge neutrality. The Compton profile $J(P_z)$ for (5s) calculation given by [6]:

$$J_{5s}(P_z) = 4\pi \sum_{n=0}^{\infty} |\Psi_0^c(\vec{k}_n)|^2 G_n(P_z) \quad (3)$$

Where $\Psi_0^c(\vec{k}_n)$ is the Fourier transform of wave function, $G_n(P_z)$ is an auxiliary function and \vec{k}_n lattice vectors.

- -s- electrons shell

The momentum transformation of the Bloch function to the outermost "s" shell electrons is unhybridised of the cubic structure is given by

$$\Psi_k(p) = N \square(P-k, k_n) \Psi_k^c(p) \quad (4)$$

For $k_n=0$

$$\Psi_0^c(0) = (2/\pi)^{1/2} \int_0^{r_0} dr r^2 \phi_0^r(r) \quad (5)$$

For $k_n \neq 0$

$$\Psi_0^c(\vec{k}_n) = (2/\pi)^{1/2} k_n^{-1} \int_0^{r_0} dr r \sin(k_n r) [\phi_0^r(r) - \phi_0^r(r_0)] \quad (6)$$

The $G_n(p_n)$ in the equ.(5) give as:

$$G_n(P_z) = \frac{N_n}{4k_n} \{ (P_F^2 - K_n^2) (K_n + P_F - P_z) - \frac{1}{3} [(K_n + P_F)^3 - P_z^3] + K_n [(K_n + P_F)^2 - P_z^2] \} \quad (7)$$

N_n is the lattice reciprocal points number in the n^{th} cell in the reciprocal space the above model doesn't have as we mentioned before hybridization of (d) band is not valid for data on crystal sample, it does how ever give an chance to vary the band electron distribution in (s-d) shell to see the most favorite electron arrangement for a specific metal. For more details see Berggren [7].

B. Free electron model

In the case of an the electron momentum density the equ. (1) reduces to the known form

$$J_{5s}(P_z) = 2\pi \int_{P_z}^{\infty} dp \rho(\vec{p}) p \quad (8)$$

If we consider the electrons of valence in a metal as a non interactive electron gas, the electron momentum density give as following

$$\rho(\vec{p}) = \text{constant} = \frac{n}{\frac{4}{3}\pi p_F^3} \quad (9)$$

The (n) is free electrons number per site, P_F is the fermi momentum replacement $\rho(p)$ from the equation (9) to the equation (8) give as

$$J_{5s}(P_z) = \frac{3n}{4\pi p_F^3} (p_F^2 - p_z^2) \text{ for } P_z \leq P_F \quad (10)$$

Then the Compton profile of the free electron is invert parabola including interruptions of the first derive at $\pm P_F$ cooper [1].

C. Superposition model

The Compton profile of a specific compound $J(P_z)$ is computed by the formula [8].

$$J_s^x(P_z) = J^{Cd/+x}(P_z) + J^{Te/-x}(P_z) \quad (11)$$

$J^{Cd}(P_z)$, $J^{Te}(P_z)$ are the theoretical Compton profiles of Cd and Te metals respectively. The Compton profile $J(P_z)$ values of the formed metals Cd and Te were taken from the available measurements. For the reason of comparison we obtained the Compton profile by employing the free atom values, we also calculate theoretical Compton profiles for Cd and Te.

III. RESULTS AND DISCUSSION

A. Superposition model of CdTe

To calculate the Compton profile $J(P_z)$ for cadmium telluride (CdTe) we applied superposition model, depending on the calculated values of (Cd) element that are obtained by using (RFA, FE and FA) models and for more details see [9]. Theoretical Compton profile values for the telluride element of electronic configuration ($5s^1 5p^5$) are taken directly from tables of (Biggs et al) [10]. All theoretical as well as experimental results of CdTe compound are normalized to an area under curve (39.74833) electrons of free atom. Table (1) contains three theoretical results of $J(P_z)$ for (free atom, free electron & RFA) that calculated through superposition model by using equ. (11) we now compare the various theoretical and experimental profiles in the high momentum region ($P_z > 1.0$ a.u.) it is apparent that theoretical values are close to experimental values. As for the low momentum zone $P_z = (0-0.3$ a.u.) it is apparent that the free atom model and free electron model shows disagreement, on the whole the results are considerably flatter but RFA values are nearby to the experiment. In fig (1) we plot this comparison, when $P_z < 0.5$ a.u. it is seen that the RFA results are lower than (free electron, free atom) results but at ($0.7 \leq P_z \leq 1.2$) a.u the trend is reversed and RFA values are higher than free electron and free atom. For comparison between free atom and free electron it appears that in low momentum zone free atom higher than those results

of the free electron but between ($0.4 \leq P_z \leq 0.8$) a.u the trend reversed and the values of the free electron are larger than the values of free atom. At ($P_z > 1.2$ a.u.) all values be nearly similar. In the fig (2) we plot the difference between the theoretical and the experimental values for Compton profile of (CdTe). in the low momentum zone ($J_{FA}(p_z) - J_{exp.}(p_z)$) is large than ($J_{FE}(p_z) - J_{exp.}(p_z)$) and ($J_{RFA}(p_z) - J_{exp.}(p_z)$) but are almost the same at $P_z > 1$ a.u. also in the high momentum region ($P_z > 3$), the differences are almost same. In order to determine the best electron arrangement the total square $\sum_0^{7\text{a.u.}} |\Delta J|^2$ was obtained and gives the values (15.06528, 4.029117, 0.2592563) for FA, FE and RFA respectively hence (RFA) gives a better results.

B. Charge transfer

To calculate charge transfer of CdTe compound experimental Compton profile of Cd [11] was used to obtain the valence electrons profile. We supposed that charge transfer from Cd to Te by ionic configuration ($Cd^{+x}(Te^{-x})$ ($0 \leq x \leq 1$) and x is charge transfer. Here, the transfer 0.2 electrons from the valence 4d shell of Cd atom to the 5p shell of Te atom. To estimate the contribution for valence Compton profile for Cd we have subtracted the corresponded inner-core contribution from the experimental Compton profile of the Cd element and then the profile was divided by the number of valence electron. This contribution was added as discussed above that is:

$$J(P_z) \text{ exp. } \{1s^2 \dots 4d^{10}\} - J(P_z) \text{ core } \{1s^2 \dots 4p^6\} = J(P_z) \text{ valence} \quad (12)$$

$$J(P_z) \text{ for one valence electron} = J(P_z) \text{ valence} / 10 \quad (13)$$

IV. TABLE I
GIVEN THE VARIOUS THEORETICAL $J(P_z)$ RESULTS OF COMPOUND (CdTe) WITH EXPERIMENTAL MEASUREMENTS [12]. ALL THE VALUES HAVE BEEN NORMALIZED TO AN AREA OF (39.74833) ELECTRONS.

P_z (a.u)	$J(P_z)$ (e/a.u.)			
	Superposition model for CdTe			Exp.[12]
	Free Atom	Free electron	RFA	
0	18.64	17.049	16.262	16.231±0.034
0.1	18.32	16.983	16.213	16.133
0.2	17.49	16.741	16.018	15.922
0.3	16.37	16.269	15.635	15.567
0.4	15.2	15.544	15.069	15.032
0.5	14.12	14.607	14.344	14.434
0.6	13.21	13.574	13.530	13.785
0.7	12.43	12.527	12.814	13.052
0.8	11.79	11.49	12.159	12.339
1	10.79	10.88	11.093	11.149±0.027
1.2	10	9.9974	10.219	10.133
1.4	9.58	9.2364	9.428	9.321
1.6	8.56	8.5199	8.6674	8.569

1.8	7.84	7.8194	7.9238	7.867
2	7.14	7.1468	7.2216	7.151±0.020
3	4.45	4.4911	4.5216	4.507±0.014
4	3.15	3.1951	3.2029	3.231±0.011
5	2.49	2.528	2.5196	2.560±0.009
6	2.031	2.0668	2.0546	2.055±0.008
7	1.662	1.8517	1.8419	1.663±0.007

relatively in good agreement with the available experimental results of the CdTe compound [12]. The ionic model suggests a transfer of 0.2 electrons from 4d state of Cd atom to 5p state of Te atom on compound formation.

ACKNOWLEDGMENT

The authors would like to thank the dean of college of science and the president of the University of Tikrit for their supports and the department of Physics for putting all the facilities under this our disposal without this work will not be a cheived.

REFERENCES

- [1] M.J. Cooper, Rep. Prog. Phys. 48, 415 (1985).
- [2] M.J. Cooper, P.E. Mijnarends, N. Shiotani, N. Sakai, A. Bansil, Oxford Science Publications, New York, 2004.
- [3] I.G. Kaplan, B. Barbiellini, A. Bansil, Phys. Rev. B 68 (2003) 235104.
- [4] H.Nara, T. Kobayasi, and K. Shindo, J. Phys. C: Solid State Phys. 17, 3967 (1984). T. Kobayasi, private communication (2004).
- [5] E.Clementi and C.Roetti, Atomic and Nnclear Data Tables, 14, 177. (1974).
- [6] K.F. Berggren, S. Manninen, and T. Paakkari , Phys. Rev. B552516 (1973).
- [7] K.F. Berggren, Phys.Rev.B6 2156-61,(1972).
- [8] S.Manninen, B.K. Sharma, T. Paakkari, S. Rundqvist, and M.W. Rishardson, (1981) Phys. Stat. Sol. (b)107, 749.
- [9] F.M. Mohammed, F.I. Rashid and Sh.A. Shaaban accepted in Advances in physics theories and applications (IISTE) to be published and appear in, (31 May 2018).
- [10] L.Bigges, L. Mendelsohn, J.B. Mann, At. DataNucl. Data Tables. 1975,16,201.
- [11] Chu-Nan Chang, Loo Kok Ngai, and Bey-Bey Li Vol. 27, No. 6 (1989).
- [12] N.L. Heda, S. Mathur, B. L. Ahuja and B. K.Sharma, Phys. Stat. Sol. (b) 244,No. 3, 1070- 1081 (2007).

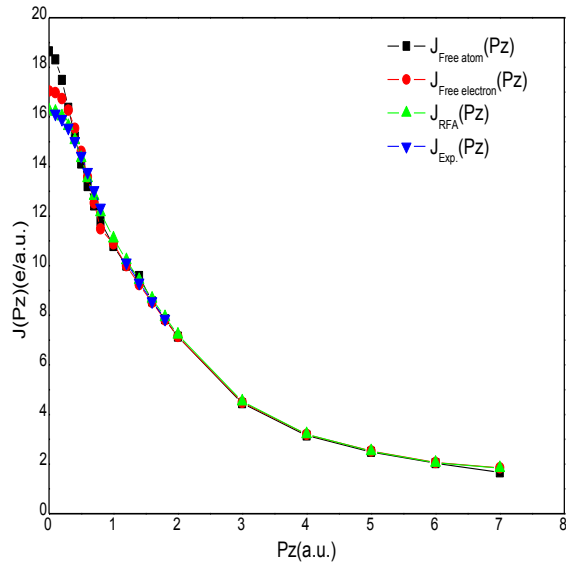


Fig (1): comparison of theoretical results with the recent experimental data [12] for CdTe compound.

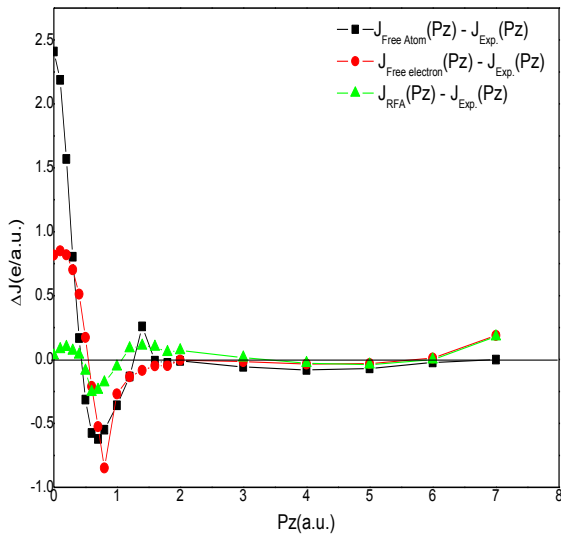


Fig (2) : difference square deflection between theoretical computation and experimental data [12] of CdTe.

V. CONCLUSIONS

The various theoretical Compton profiles are obtained by using different models for the two constituent metals of (CdTe) was compared with recent experimental data, theoretical profile calculated by using superposition model for the CdTe, it was seen that the present RFA work is