



e-ISSN: 2319-8753 | p-ISSN: 2347-6710

# IJRSET

International Journal of Innovative Research in  
**SCIENCE | ENGINEERING | TECHNOLOGY**

# INTERNATIONAL JOURNAL OF INNOVATIVE RESEARCH

IN SCIENCE | ENGINEERING | TECHNOLOGY

Volume 12, Issue 4, April 2023

**ISSN** INTERNATIONAL  
STANDARD  
SERIAL  
NUMBER  
INDIA

Impact Factor: 8.423

9940 572 462

6381 907 438

[ijirset@gmail.com](mailto:ijirset@gmail.com)

[www.ijirset.com](http://www.ijirset.com)



# Electronic Band Structure and Related Properties of Paramagnetic FCC Technetium

S. B. Madan

Associate Professor, Department of Physics, M.G.Science Institute, Ahmedabad, Gujarat, India.

**ABSTRACT:** Self-consistent all electron, local density calculations are reported for fcc technetium using linear combination of Gaussian orbitals (LCGO) method. We obtain band structure, density of states, charge form factors and Compton profile. Results are compared with other calculations and with experiments wherever these exist.

**KEYWORDS:** Band Structure, Density of States, Compton profile.

## I. INTRODUCTION

This is new addition in a series of papers concerning the electronic structure of cubic 4d transition metals based on the local density approximation in density functional theory and employing the linear combination of Gaussian orbitals (LCGO) method. The electronic structure of fcc technetium is characterized largely from the plot of the first six bands on the line of symmetry and their orientation with respect to Fermi energy  $E_F$ . Papaconstantopoulos et al [1] studied the superconducting properties of Tc and several other metals. In their work the band structure calculations for h.c.p. structure were carried out in the f.c.c. and b.c.c. structure with a lattice constant determined by assuming the same density as for real h.c.p. structure. It is therefore that they believed to have obtained superconducting temperature 0.03K being very low compared with experimental value 7.73K. Ashokamani et al [2] calculated band structure of h.c.p. Tc using three different potentials, Slater exchange ( $V_s$ ), Overhauser's prescription ( $V_H$ ) and Vashista-Singwi formalism ( $V_{vs}$ ) where  $V_s$  included only the exchange part through Slater's formula whereas the other two potentials  $V_H$  and  $V_{vs}$  include exchange as well as correlation as in the case of Lundqvist et al [3]. They used Herman-Skillman [4] wave functions with the atomic configuration  $4d^5 5s^2$  calculating charge density and KKR method for calculating band structure. They stressed on calculating the superconducting temperature  $T_c$  and Fermi surface of Tc. Parsathi Chatterjee [5] carried out band structure and Fermi surface calculations corresponding to the atomic configuration  $4d^5 5s^2$  of the seven outermost valence electrons through the Brillouin zone using the composite-wave variational version of the augmented plane wave (APW) method in conjunction with  $X\alpha$  ( $\alpha = 0.70299$ ) exchange approximation for obtaining the potentials and for density of states (DOS) and the angular-momentum-decomposed DOS were carried out using the accurate Gilat-Raubenheimer method and the Fermi surface and optical properties of technetium were studied via the imaginary part of the interband dielectric constant for bound electrons. Blaha et al [6] calculated electronic structure of hcp metals including Tc using self-consistent full potential linearized augmented plane-wave (LAPW) method. They have calculated energy-band structure, total and partial densities of states as well as electron densities are presented and discussed in context with available experimental and theoretical data. Their results showed that most of the older self-consistent calculations obtained realistic energy band structures, while calculations based on the quantum defects exhibited completely different results.

In the present paper for the first time we study the band structure and some related properties of fcc technetium on the basis of self-consistent Gaussian orbitals method and local density approximation in density functional theory [10], which has been applied successfully to a number of metals [11,20]. In addition to this we use for the first time the exchange correlation potential due to Von Barth-Hedin (VBH) [21]. We have used here VBH potential with parameters given by [22]. The detailed energy-band structure of hexagonal-close-packed technetium, corresponding to the atomic configuration  $4d^5 5s^2$  of its seven outermost valence electrons, has been obtained by [23] throughout the Brillouin zone using the composite-wave variational version of the augmented-plane-wave (APW) method in conjunction with the  $X\alpha$  ( $\alpha = 0.70299$ ) exchange approximation for obtaining the potentials. From the band-structure data the electronic density of states (DOS) and the angular-momentum-decomposed DOS were calculated by the accurate Gilat-Raubenheimer method. The energy band structure and density of states  $N(E)$  of hexagonal technetium were calculated by [24] the self-consistent linear method of associated plane waves. The frequency dependence of its interband optical conductivity  $\sigma(\omega)$  and the real part of complex permittivity  $\epsilon_1(\omega)$  are calculated for two directions of polarization of the light wave electric vector  $E$  with respect to the hexagonal axis of the crystal  $c$  ( $E$  perpendicular to  $c$  and  $E$  parallel



c).Electronic structure of the fragments (number of atoms from 6 to 93) of hexagonal close-packed and face-centered cubic structures of technetium metal was calculated in the approximation of the  $X_{\alpha}$ -discrete variation nonempirical method. The results agree well with band calculations of both occupied and unoccupied electronic states in solid Tc as well as with the experimental data of conversion electron and optical spectroscopy[25].

Our computational procedures are briefly described in section II, the band structure in section III, the density of states in section IV, X-ray form factors in section V, Compton profile in section VI, Results and discussions in section VII, and finally conclusion is summarized in section VIII.

## II. COMPUTATIONAL METHOD

**TABLE 1.** Orbital exponents of the Gaussian Basis set for fcc  $T_c$ .

1s	600968.670
2s	88600.264
3s	20540.939
4s	6011.6383
5s	2042.3890
6s	774.55946
7s	320.84393
8s	142.05931
9s	54.025757
10s	24.068560
11s	8.5619192
12s	4.3922094
13s	1.9025018
14s	0.91887545
15s	0.40621293
16s	0.094293551
1p	4763.8664
2p	1153.2828
3p	381.59894
4p	146.32863
5p	61.1119775
6p	27.090821
7p	11.960775
8p	5.4577267
9p	2.3746029
10p	1.0277545
11p	0.39738024
12p	0.08800
1d	188.85753
2d	55.900549
3d	20.995532
4d	8.6920652
5d	3.7865863
6d	1.5703613
7d	0.60884500
8d	0.20775687
1f	0.8

We have used the Linear combination of the Gaussian orbitals (LCGO) method as contained in the BNDPKG programs. The calculations are made based on the local density approximation to the density functional theory. This method does not require any shape approximations to charge densities or potentials. Details of method can be found in [10]. The Bloch wave functions needed in the self-consistent calculations were expanded in a set of independent Gaussian orbitals including in this case sixteen of s symmetry, twelve p, eight d and one f. We employed the basis set for  $T_c$  given by Poirier et al. [26] except that the most diffused s-orbital exponent was deleted, an extra p-orbital exponents [11] was added followed by a single f orbital of exponent 0.8 was added as shown in Table 1. The exchange correlation potential is treated in the manner described in [20]. Relativistic effects are not included. The Hamiltonian and overlap matrices considered in the computations are of dimension 99x99. The equilibrium lattice constant  $a_0 = 7.28$  au of technetium at -0.76 Kbar of pressure was used from [8,9]. In the calculations the iterations leading to self-consistency were continued until the change in the leading Fourier coefficient of potential became  $10^{-4}$  Ry or less. After establishing the self-consistency energy levels and wave functions were evaluated at 505 points in the irreducible wedge (1/48) of the Brillouin zone. The density of states was obtained by employing the linear analytic tetrahedron method [27-30].

## III. BAND STRUCTURE

The calculated energy bands are displayed along certain symmetry directions in Fig.1. The selected energy separations are listed in Table 2. In the fcc lattice  $\Gamma$  and X are convenient points to use for discussing s-d- and d- band band widths. The s-d-band width which is given by the  $X_3-\Gamma_1$  separation is found to be 0.092 Ry. The  $X_3-X_1$  separation measures the d- band width and our value for the quantity is 0.0374Ry. The width of the occupied portion of the s-d-band

$E_F-E(\Gamma_1)$  is found to be 0.491 Ry. Width of the occupied portion of the d- band  $E_F-E(X_1)$  is found to be 0.436 Ry. However there can be minor difference between our band energy values compared with calculations of other authors on account of 1. Use of different exchange-correlation potentials and 2. Inclusion of relativistic effects.





TABLE 2. Selected energy separations (in mRy) of fcc Tc band structure

Method	$\Gamma_{25'}-\Gamma_1$	$X_3-\Gamma_1$	$X_3-X_1$	$E_F-X_1$	$E_F-\Gamma_1$	$W_3-W_F$
LCGO	95	92	37	436	491	121

IV. DENSITY OF STATES

The density of states is shown in Fig. 2. We find a value of the density of states at the Fermi energy  $N(E_F)=16.44$  at  $^{-1}\text{Ry}^{-1}$ . The peaks reported below  $E_F$  are at energy values 0.390 Ry, -0.312 Ry, -0.158 Ry and -0.030 Ry where peak density of states values are 31.0564 at  $^{-1}\text{Ry}^{-1}$ , 17.1594 at  $^{-1}\text{Ry}^{-1}$ , 33.6674 at  $^{-1}\text{Ry}^{-1}$ , 18.4438 at  $^{-1}\text{Ry}^{-1}$  and 20.4702 at  $^{-1}\text{Ry}^{-1}$  respectively. Out of which the first largest peak is obtained at -0.158 Ry and the second largest peak is obtained at 0.390 Ry. Above Fermi energy the first peak is obtained at energy 0.148 Ry and the DOS value being 22.7571 at  $^{-1}\text{Ry}^{-1}$ .

V. X-RAY FORM FACTORS

TABLE 3. X-Ray form factors of fcc Tc The X-ray form factors are given by the expression below.

h	k	l	Atom
0	0	0	43.000000
1	1	1	32.473629
2	0	0	30.723803
2	2	0	26.318512
3	1	1	24.158258
2	2	2	23.630541
4	0	0	21.675163
3	3	1	20.644037
4	2	0	20.303638
4	2	2	19.199108
3	3	3	18.490053
5	1	1	18.451567
4	4	0	17.426613
5	3	1	16.859734
4	4	2	16.689970
6	0	0	16.659781
6	2	0	15.992297
5	3	3	15.533835
6	2	2	15.370919
4	4	4	14.797193
5	5	1	14.377026
7	1	1	14.364872
6	4	0	14.240443
6	4	2	13.726809
5	5	3	13.362587
7	3	1	13.356125
8	0	0	12.777864
7	3	3	12.459942
6	4	4	12.357214
8	2	0	12.351137
6	6	0	11.951612
8	2	2	11.948719
5	5	5	11.665424
7	5	1	11.663689
6	6	2	11.571475
8	4	0	11.212173
7	5	3	10.959069
9	1	1	10.956657
8	4	2	10.876019
6	6	4	10.560316

$$\rho(\vec{k}) = \int \rho(\vec{r}) (e^{i\vec{k}\vec{r}}) d^3r \tag{1}$$

Where the integration is over the whole crystal and is normalized so that  $\rho(0)=n_c$  in which  $n_c$  is the number of electrons in the unit cell. The advantage of using LCGO method is that one can obtain  $\rho(\vec{k})$  directly from the band structure calculations in terms of quantities called generalized overlap integrals[10] and without additional labour. We list our calculated X-ray form factors in Table 3. The form factors for the atom are calculated from our starting charge densities, while those for the solid are obtained self-consistently.

VI. COMPTON PROFILE

The experimental innovations such as the use of the energy dispersive detectors and high energy ray sources require careful probe into the study of Compton profile of the heavier solids. Much of the earlier work on the transition metal involved polycrystalline samples, whereas recently measurements have carried out using single crystals. The extensive review of data are given in [31]. We report in this work a computation of the Compton profile and its anisotropy for transition metal technetium. Since the core electrons do not differ appreciably in the solid from those in the free atom, we have calculated total Compton profile of technetium considering core electron contribution of Hartree-Fock[32] and valence electron (5s) contribution as spherically averaged Compton profile from our present calculation. The Compton profile of the valence electrons was computed using expression in [33].

$$J_R(q) = \frac{\Omega}{2\pi^3} \int d^3p \rho(\vec{P}) \delta(q-p.\hat{k}) \tag{2}$$

Where  $\rho(\vec{P})$  is the momentum distribution function,  $\hat{k}$  is a unit vector along  $\vec{k}$ ,  $\Omega$  is the volume of the unit cell

$$q = \frac{\hbar\omega}{|\vec{k}|} - \frac{1}{2} |\vec{k}| \tag{3}$$



and  $\hbar\omega$  is the energy transferred to the electron after a Compton scattering event has occurred. The momentum density requires a summation over all occupied states at  $T=0^0$  K, this can be written as

$$\rho(\vec{P}) = \sum_{n,\vec{k}} \theta(E_F - E_n(\vec{k})) |\Psi_n(k, \vec{P})|^2 \quad (4)$$

Where  $E_F$  is the Fermi energy,  $E_n(\vec{k})$  is the energy of a state,  $\theta$  is the unit step function and  $\Psi_n(k, \vec{P})$  is the momentum-space Bloch function which is related to the position-Space Bloch function by Fourier transformation. The directional profiles were calculated using 505 points in the  $\frac{1}{48}$ th part of Brillouin zone. The Compton profiles  $J_R(q)$  along the [1 0 0], [1 1 0] and [1 1 1] directions together with the spherically averaged profile for each value of  $q$  ranging from 0 to 2.5 a.u. are given in Table 4. Differences of the Compton profile with respect to directions of the momentum transfer are shown in Fig.3 and the spherically averaged profile is plotted in Fig. 4. Apparently there are no experimental results for technetium moreover there are no resulting data available on positron annihilation measurements for showing same qualitative features as Compton profile.

TABLE 4. Calculated Compton profile

q(a.u.)	$J_{100}(q)$	$J_{110}(q)$	$J_{111}(q)$	$J_{AVG}(q)$
0.000	2.410201	2.815835	2.695619	2.669027
0.050	2.394227	2.809090	2.698040	2.662002
0.100	2.417540	2.796086	2.686180	2.659669
0.150	2.494278	2.781565	2.643189	2.663901
0.200	2.583851	2.740283	2.613741	2.663049
0.250	2.661435	2.665519	2.583203	2.643185
0.300	2.662604	2.534139	2.506963	2.563855
0.350	2.625180	2.445017	2.450983	2.498027
0.400	2.582206	2.347443	2.456095	2.442457
0.450	2.536159	2.299202	2.439521	2.402986
0.500	2.471786	2.232016	2.395585	2.342583
0.550	2.417886	2.174053	2.350112	2.288992
0.600	2.360231	2.123215	2.283833	2.232236
0.650	2.268641	2.078779	2.199447	2.164054
0.700	2.157753	2.042614	2.133235	2.098814
0.750	2.040869	2.013284	2.090517	2.041026
0.800	1.922978	1.970522	1.979416	1.959225
0.850	1.823294	1.934466	1.879551	1.888582
0.900	1.734871	1.879952	1.801256	1.818264
0.950	1.644040	1.817436	1.752095	1.751092
1.000	1.608887	1.739351	1.695900	1.690903
1.100	1.554765	1.490335	1.497491	1.510584
1.200	1.408588	1.275456	1.296045	1.318788
1.300	1.203147	1.124606	1.143133	1.151811
1.400	1.010412	1.033396	0.966214	1.009554
1.500	0.796982	0.910224	0.820237	0.854730
1.600	0.570195	0.684616	0.633930	0.638891
1.700	0.470268	0.514672	0.513766	0.501752
1.800	0.424803	0.405828	0.412782	0.413038
1.900	0.413015	0.342792	0.381658	0.372850
2.000	0.404529	0.300139	0.361916	0.345850
2.100	0.347739	0.278815	0.313299	0.307375
2.200	0.299420	0.282351	0.273597	0.284977
2.300	0.247263	0.250172	0.238555	0.246354
2.400	0.189874	0.218810	0.210254	0.208342
2.500	0.152082	0.199079	0.190669	0.183489

TABLE 5. Comparison of band values at somepoint of symmetry  $\Gamma$ , X, L, W, and K between present calculation and with Mousse et al. [9] in the case of fcc Tc.

Symmetry point		Band energies in Rydbergs (relative to muffin tin zero)
$\Gamma$	Present work	0.262 0.612 0.612 0.612 0.796 0.796
	Moruzzi et al[9]	0.253 0.607 0.607 0.607 0.800 0.800
X	Present work	0.269 0.358
	Moruzzi et al[9]	0.308 0.345
L	Present work	0.363 0.594 0.594 0.859
	Moruzzi et al[9]	0.348 0.595 0.595 0.861
W	Present work	0.406 0.552 0.552 0.763
	Moruzzi et al[9]	0.419 0.540 0.540 0.768
K	Present work	0.373 0.458 0.704 0.814
	Moruzzi et al[9]	0.379 0.452 0.693 0.819

VII. RESULT AND DISCUSSIONS

The band structure of fcc technetium is shown in Fig.1 along the principal symmetry axis in the Brillouin zone. The density of states  $N(E)$  corresponding to these band structures are shown in Fig.2. However our present calculations of band structure and density of states carried out using lattice constant  $a_0 = 7.28$  au at  $-76$  Kbar of pressure taken from [26] compares well for all the values of bands at different symmetry points relative to muffin tin zero and also compare well for  $N(E)$ ,  $E_F$  and  $N(E_F)$  with Moruzzi, Janak and Williams[9] in their calculated electronic properties of Metals for fcc Tc as shown in Table 5. While as shown in Table 6 the comparative account is presented for the Fermi energy as well as the density of states obtained from previously carried out work employing other band calculation techniques with considering different potentials and the correlation effects. The results by [2], [5] and [6] have hcp consideration of Tc crystal are in good agreement with each other.

While results by [7], [9] where the crystal structure assumed is fcc are in good agreement with the present calculations. Our present result also agree with [2], [5] and [6] in framework of Muffin Tin zero consideration.



TABLE 6. Comparison of available results with present work.

The abbreviations relative to exchange correlation potentials are as follows:  
 KS(Kohn and Sham); $V_s$ (Slater potential)  
 $V_H$  (Overhauser's prescription)  
 $V_{vs}$  (Vashista and Singwi formula)  
 $V_{xx}$  (Xx exchange potential)  
 VBN-RSK(Von Barth and Hedin, as parametrized by Rajagopal, Singhal, and Kieball)  
 LDA- $J$ (local density approximation as parametrized by Janak [8])

The abbreviations relative to methods are as follows:  
 KKR(Korringa-Kohn-Rostoker)  
 APW(augmented plane wave)  
 ASA(Atomic sphere approximation)  
 LAPW(Linerized augmented plane wave method)  
 LCGO(linear combination of Gaussian orbitals)  
 SC(self consistent);MT( Muffin Tin)  
 MTO(value relative to Muffin Tin zero).  
 Energy differences are in Rydbergs.

	Ref.2	Ref.5	Ref.6	Ref.7	Ref.9	Present work
lattice constant (a.u.)	a = 2.7407 c = 4.3980	a = 5.17958 c = 8.29868	c/a = 1.63	13 or 19 atoms/cluster	a = 7.28	a = 7.28
exchange correlation potential	$V_s$ $V_H$ $V_{vs}$	Xx x = 0.70299	LDA with parametrization of Janak [8]	spherical crystal inside touching sphere and $V_{MT}$ in interstitial	KS	VBN-RSK
method of calculation	KKR-SC	APW-NSC	LAPW-SC	ASA-SC	KKR-SC	LCGO-SC
crystal structure	HCP	HCP	HCP	FCC	FCC	FCC
Fermi energy	$V_s$ (0.803) (MTO) $V_H$ (1.1171) (MTO) $V_{vs}$ (1.055) (MTO)	0.976 (MTO)	0.93 (MTO)	-0.04	-0.057	-0.05483
density of states $N(E_F)$	$V_s$ (1.39) $V_H$ (1.12) $V_{vs}$ (1.235)	-	1.6	states/spin. atom cluster(19 atoms) 5.9 Bulk 7.8	1.22	1.21

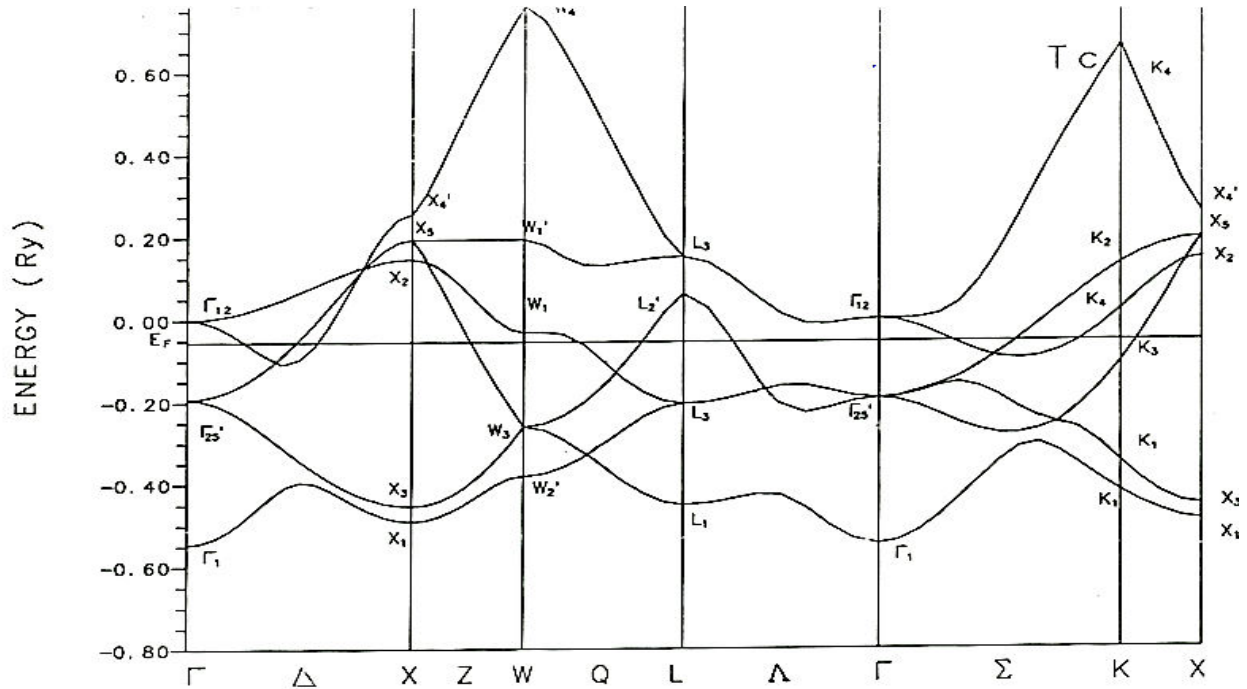


Fig. 1. Band structure of fcc T<sub>c</sub> in paramagnetic phase

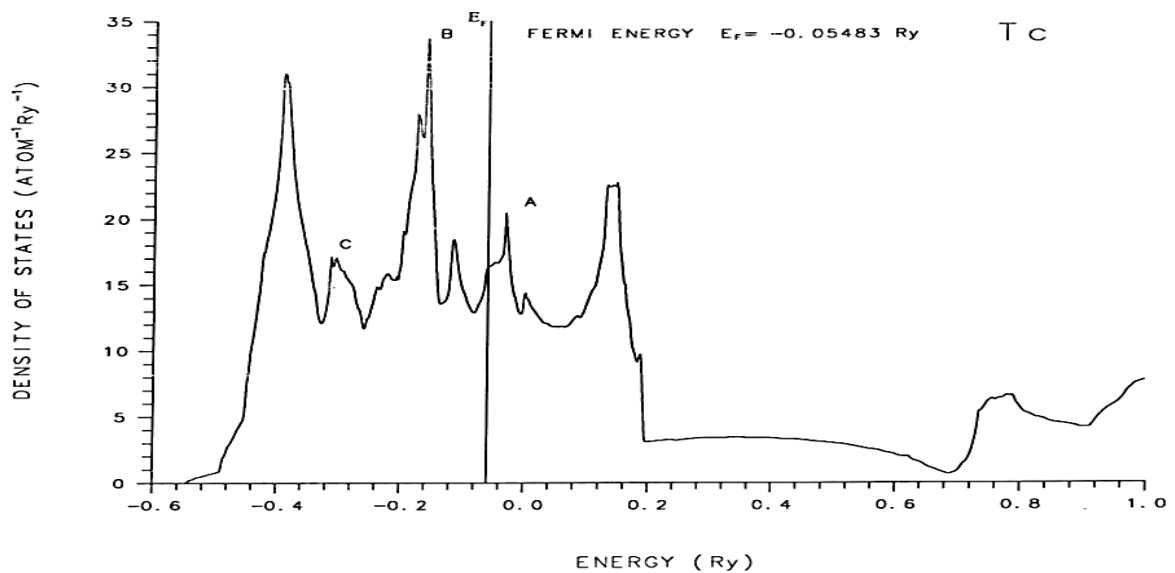


Fig. 2 Density of states in fcc Tc.

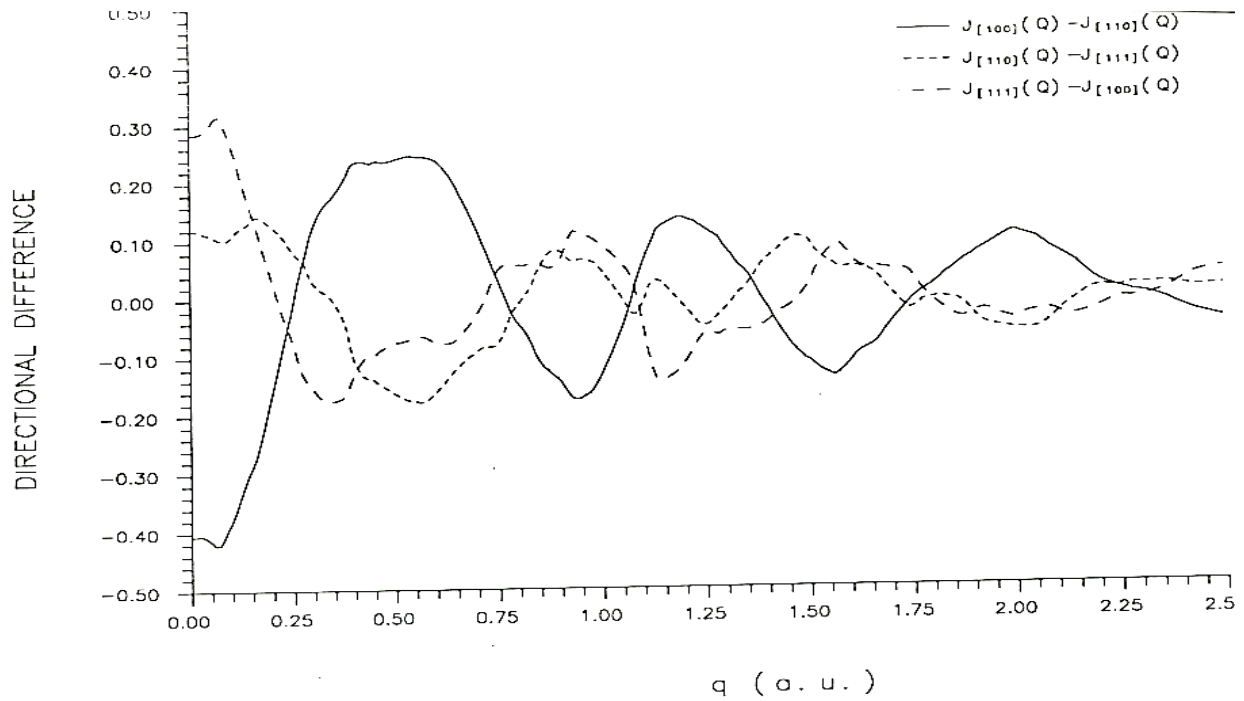


Fig. 3 Anisotropy (compton profile)

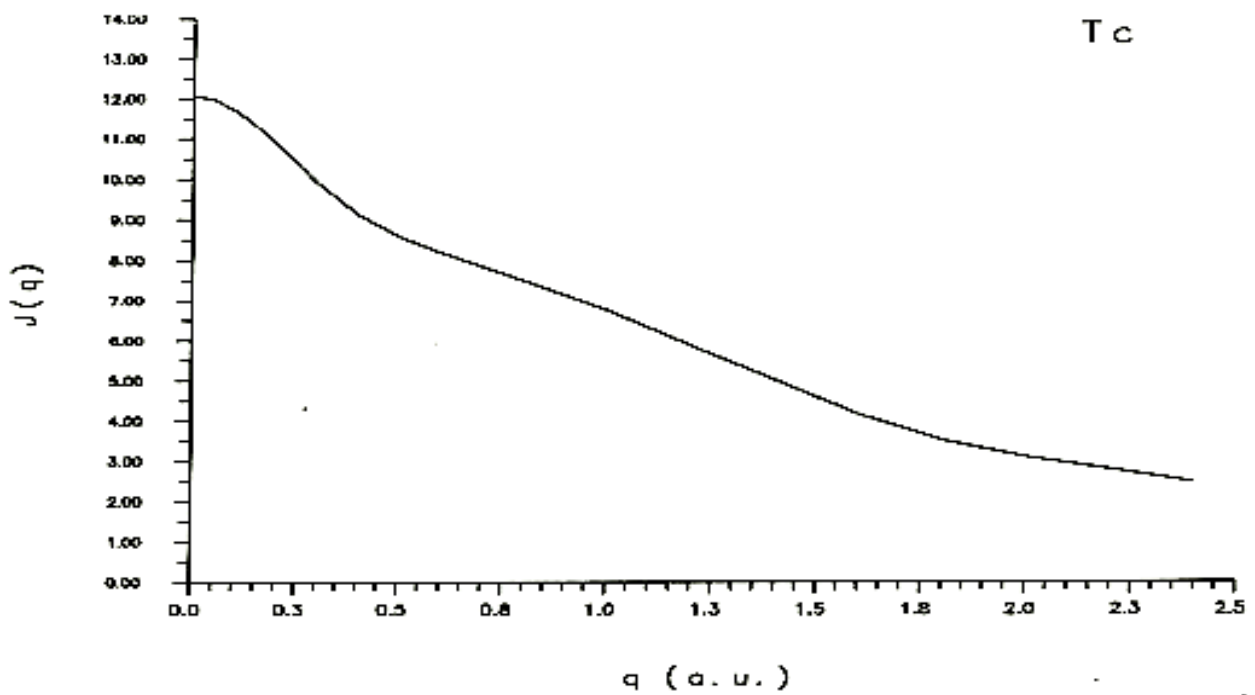


Fig. 4. Total Compton profile



### VIII. CONCLUSION

We have presented band structure, density of states, X ray form factors and Compton profile using Linear combination of Gaussian orbitals successfully. The comparison of band energy values as well as  $E_F$  and  $N(E_F)$  compare well with the values calculated by Moruzzi, Janak and Williams[9] in the muffin-tin approximation by Korringa-Kohn-Rostoker (KKR) method. Though we have not considered any relativistic effect we conclude that LCGO method is very efficient for finding out band structure and related properties of an element like Tc. Study of Fermi surface and optical conductivity could also be made

### ACKNOWLEDGEMENTS

I am thankful to Professor and Head Dr. V. B. Gohel, Department of Physics, Gujarat University, for helping me to understand BNDPKG programs for the computations of band structure.

### REFERENCES

- [1] D.A.Papaconstantopoulos, L.L. Boyer, B.M. Klein, A.R. Williams, V.L. Moruzzi and J.F. Janak, Phys. Rev. B **15**, 4221 (1977).
- [2] R. Ashokamani and K. Iyakutti and V. Devnathan, Solid state commun. Vol. 30, pp 385-389
- [3] B. I. Lundqvist and S. Lundqvist computational solid state physics, p 19. Plenum Press, New York-London (1972)
- [4] Herman F & Skillman S, Atomic Structure Calculations, Prentice Hall New Jersey 1963
- [5] Parsathi Chatterjee, Phys. Rev. B **27**, 4722 (1982)
- [6] P. Blaha and K. Schwarz and P. H. Dederichs Phys. Rev. B **14**
- [7] G. Zwicknagl, Z. Physik B-condensed matter **40**, 27-31 (1980)
- [8] J. F. Janak, Solid state Commun. , **53** (1978)
- [9] V. L. Moruzzi, J. F. Janak and A.R. Williams, Calculated Electronic Properties of Metals (Pergamon, New York, 1978) P 132
- [10] C. S. Wang and J. Callaway, Comput. Phys. Commun. **14**, 327 (1978)
- [11] G. S. Tripathi, N. E. Brener and J. Callaway, Phys. Rev. B **38** 10454 (1988)
- [12] A. R. Jani, N. E. Brener and J. Callaway, Phys. Rev. B **38** 9425 (1988)
- [13] A. R. Jani, G.S. Tripathi, N. E. Brener and J. Callaway, Phys. Rev. B **40** 1593 (1989)
- [14] D. Bagayoko and J. Callaway, Phys. Rev. B **27** 5419 (1983)
- [15] J. Callaway, Xianwu Zou and D. Bagayoko Phys. Rev. B **27**, 631 (1983)
- [16] D. Bagayoko, A. Zielger and J. Callaway, Phys. Rev. B **27** 7046 (1983)
- [17] J. Callaway and C. S. Wang and Phys. Rev. B **16**, 2095 (1977)
- [18] C. S. Wang and J. Callaway Phys. Rev. B **15**, 298 (1977)
- [19] D. G. Lorent, C. S. Wang and J. Callaway Phys. Rev. B **17**, 455 (1978)
- [20] P. Blaha and J. Callaway Phys. Rev. B **12**, 7664 (1985)
- [21] U. Von Barth and L. Hedin, J. Phys. C, **5**, 1629 (1972)
- [22] A.K. Rajgopal, S.P. Singhal and J. Kimball (Unpublished) as quoted by A. K. Rajgopal, Advances in Chemistry and Physics. Edited by G. I. Prigogine and S.A. Rice (Wiley, New York, 1979, Vol. **41**, P. 59)
- [23] Parsathi Chatterjee <https://doi.org/10.1103/Phys.Rev.B.27.4722> – Published 15 April 1983
- [24] Antonov, V.N.; Kirillova, M.M.; Krasovskij, E.E.; Ponomov, Yu.S. (AN SSSR, Sverdlovsk (USSR). Inst. Fiziki Metallov) 1988
- [25] Yu. V. Plekhanov, K. E. German & R. Sekine *Radiochemistry* volume **45**, pages 27–242 (2003)
- [26] R. Poirier, R. Kari and I. G. Csizmadia, Physical Science Data Vol. P34. Handbook of the Gaussian Basis Set (Elsevier, New York, 1985), P. 483
- [27] O. Jepsen and O. K. Anderson, Solid state commun. **9**, 1763 (1971)
- [28] G. Lehman and M. Taut, Phys Status Solidi **B54**, 469 (1972)
- [29] J. Rath and A. J. Freeman, Phys. Rev. B **11**, 2109 (1975)
- [30] S. P. Singhal, Phys. Rev. B **12**, 6007 (1975)
- [31] B. Williams, Compton scattering McGraw-Hill, New York, (1977), P. 159
- [32] F. Biggs, L. B. Mendelsohn and J. B. Mann, At. Data Nucl. Data Tables **16**, 229 (1975)
- [33] J. Rath, C. S. Wang, R. A. Tawil and J. Callaway, Phys. Rev. B **8**, 5139 (1973)



Impact Factor: 8.423



# INTERNATIONAL JOURNAL OF INNOVATIVE RESEARCH

IN SCIENCE | ENGINEERING | TECHNOLOGY

 9940 572 462  6381 907 438  [ijirset@gmail.com](mailto:ijirset@gmail.com)



[www.ijirset.com](http://www.ijirset.com)

Scan to save the contact details