

# Theoretical Estimation of Superconducting Transition Temperature in Three oxidic systems

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## ABSTRACT

Lanthanum – Barium , Thallium –Bismuth and Bismuth –Strontium groups with copper oxygen layers are highly interesting oxidic compounds with high super conducting transition temperature  $T_c$  . On the basis of their metallic behaviour, an attempt has been made to evaluate their  $T_c$  , Coherence length ( $\xi$ ) and London Penetration depth ( $\lambda_L$ ) . The results are briefly analysed.

**Key words:** oxidic compounds - Debye temperature- Sommerfeld constant – coherence length – London penetration depth

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## 1. INTRODUCTION

Nearly for four decades from 1900 only about thirty superconductors were known. Then it was found that metals and alloys with A15 structure showed high  $T_c$  values. Further experimental investigation led to the discovery of several super conducting compounds possessing metallic characteristics. The phenomenon of super conductivity in the conventional super conductors has been well explained by BCS theory. However with the discovery of high  $T_c$  superconductors inadequacy of BCS theory was felt. The authors have felt that still the conventional theory of superconductivity along with the modified Mcmillan equation could account for the observed  $T_c$  by assuming proper value to electron-phonon coupling constant  $\lambda_{eph}$  . It is demonstrated by applying it to three systems of oxidic compounds.

## 2. THEORETICAL CONSIDERATIONS

The investigation is based on the following theoretical grounds.

A simple approach to these alloys or compounds is supported by the following argument. They are mostly strong coupling super conductors with large electron-phonon coupling constants ( $\lambda_{eph}$ ). Their electronic properties are well described by the free electron model.  $\lambda$  is a concentration dependent factor. In the superconducting state the electronic specific heat is approximated by  $C_{es} = \gamma T_c \exp(-b T_c / T)$  (1) with a  $\sim 9$  and  $b \sim 1.5$ .

The electronic density of states  $N_\gamma(E_F)$  could be found using independent particle model<sup>1</sup>. In equation(1)  $\gamma$  is the sommerfeld constant. The following compounds are chosen for the present study .

(i) Lanthanum compounds ( $La_{2-x}M_xCuO_4$ ) : In these compounds M atoms can substitute on

the La sites and stands for alkaline earth elements Sr, Ca or Ba. They are superconducting in the range  $0.05 < x < 0.2$  and their  $T_c$  values lying between 20K and 40K. They have a tetragonal structure with the perovskite layers. The stacking is

-CuO<sub>2</sub> -La O - CuO<sub>2</sub> - LaO - LaO - CuO<sub>2</sub>.

(ii) Thallium compounds  $Tl_m Ba_2 Ca_{n-1} Cu_n O_{m+2n+2}$  with  $m = 1$  or  $2$  and  $n = 3$ .

(iii) Bismuth compounds.  $Bi_m Sr_2 Ca_{n-1} Cu_n O_{2m+2n+2}$  with  $m = 2$ .

The thallium and bismuth compounds are tetragonal. The sequence of stacking is

Tl-Ba-Cu-Ca-Cu-Ba-Tl-Tl-Ba-Cu-Ca-Cu-Ba-Tl

For Bismuth compounds it is similar like<sup>2</sup>

-Ca-Cu-Sr-Bi-Bi-Sr-Cu-Ca-Cu-Sr-Bi-Bi-

All these compounds have layered dimensional CuO<sub>2</sub> network with the covalent Cu-O bonds. The superconducting mechanism operates in the Cu-O sheets. It is significant to note that Copper doping in the oxygen deficient systems is the same as increasing oxygen concentration<sup>3</sup> and anharmonic crystalline potentials also may result in superconductivity in the oxygen deficient perovskite. Taking into consideration all these facts the following procedure is adopted in the present investigation.

### 3. FORMULAE AND CALCULATION

(i) In Lanthanum compounds the maximum  $T_c$  value is used to calculate the Debye temperature  $\theta_D$ , with the help of McMillan equation<sup>4,5</sup>. This enables an estimation of  $\theta_D$  for different concentrations (i.e. for different  $x$  values) and thereby  $T_c$  values are also calculated. As the electron-phonon coupling constant ( $\lambda_{ep}$ ) plays an important role,  $\lambda_{ep}$  is varied from 3 to 5 whereas the coulomb constant  $\mu^* = 0.8$  for such strong coupling

compounds. The expression for electronic specific heat (eqn. 1) is used for finding the specific heat not only at  $T_c$  but also at temperatures in the vicinity of  $T_c$ , to get an idea of the changing trends.

(ii) In thallium and bismuth compounds for various values of  $n$  and  $m$  using modified Mcmillan equation,  $T_c$  values are evaluated for various  $\lambda_{ep}$  values. Specific heat is calculated at  $T = T_c$ , for each composition.

(iii) The energy gap at the Fermi level in the superconducting state is an important factor which is calculated for all these cases. The basic theory leads to the expression

$$\Delta(T) = \Delta(O) 1.74 [1 - (T/T_c)]^{1/2} \quad (2)$$

where  $\Delta(O) \sim (3.5/2) k_B T$

(iv) The maximum distance upto which the states of pair electrons are correlated to produce superconductivity is brought out by the factor coherence length ( $\xi$ )<sup>7,8</sup>. The best expression is

$$\xi_0 = 2\hbar v_F / \pi \Delta \quad (3)$$

where  $v_F$  is the velocity of electrons at the Fermi surface.

In addition, London penetration depth  $\lambda$  is also calculated for all these compounds. A factor which is normally calculated is the ratio ( $\lambda/\xi$ ), to predict the type of superconductor. However, the authors have calculated the value  $\sqrt{\lambda\xi}$ . All these theoretical calculations lead to some significant and interesting results.

### 4. RESULTS AND DISCUSSION

All the calculated values are given in Tables 1 to 4.

(1) It is an established fact that the high  $T_c$  observed (in oxygen deficient perovskite) is a result of anharmonic crystalline potentials. Moreover the magnetic interaction between<sup>6</sup> the paramagnetic ions and also between these ions and the crystal field also have an influence - This leads to two parts of  $\lambda$  ( $\lambda_{ph}$  electron-phonon and  $\lambda_{sf}$  spin fluctuation). However the

high value of  $\lambda$  chosen by us includes that effect also.

(2) London penetration depth  $\lambda_L$  decreases with temperature.

(3) The ratio  $(\lambda_L/\xi)$  being less than 0.7 indicates the metallic behaviour (not given in Tables)

(4) For a given concentration of Sr,Ca or Ba in Lanthanum compounds  $\gamma$  decreases 11 increase in temperature as one approach  $T_c$ .

(5) Eventhough  $\lambda_L$  and  $\xi$  decrease with temperature for a given concentration, the factor  $(\sqrt{\lambda_L\xi})$  seems to have a have minimum point above and below which it increases steadily.

(6) In thallium and bismuth compounds

specific heat calculated at  $T_c$  shows increase with  $T_c$  value.

(7) However  $\lambda_L$  and  $\xi$  seem to have little variation inspite of change in T values is observed lanthanum series. The change in the concentration of Ca, Cu and O may be responsible for it.

(8) The energy gap also does not show much variation and for the series the values are in the range  $25 \times 10^{-4}$  eV to  $55 \times 10^{-4}$  eV. (However the actual values for each concentration are available with the authors) Inspite of our calculations of  $T_c$  etc. for different values of  $\lambda$ , the values presented in tables corresponded to  $\lambda=5$ . The remaining values are available with the authors.

**Table 1**  $La_{2-x}Sr_x CuO_4$  ( $x = 0.2, 0.15, 0.10, 0.05$ )

Mass $10^{-26}$ kg	$T_c$ K	T K	$\gamma(x 10^{-10})$ J/mole/K <sup>2</sup>	$C_{es}(x 10^{-5})$ J/mole/K	$\lambda$ AU	$\xi$ $10^{-6}$ m	$\sqrt{\lambda\xi}$ $10^{-7}$ m
65.601 (x=0.2)	32.27	20	35.044	0.0091	603.65	7.591	6.769
		22	32.227	0.0137	629.49	5.480	5.873
		24	28.534	0.0113	668.98	7.585	7.123
		26	23.784	0.0107	732.76	8.955	8.101
		28	17.807	0.0092	846.85	12.683	10.364
66.027 (x=0.15)	32.84	30	10.402	0.0060	1107.83	26.526	17.142
		20	35.663	0.0090	600.32	7.320	6.629
		22	33.016	0.0104	623.93	6.895	6.559
		24	29.529	0.0112	659.73	7.079	6.834
		26	25.061	0.0107	716.14	8.103	7.618
66.452 (x=0.10)	33.34	28	19.428	0.0099	813.36	10.875	9.405
		30	12.455	0.0071	1015.83	19.723	14.155
		20	36.248	0.0089	597.39	7.133	6.528
		22	33.745	0.0104	619.10	6.617	6.400
		24	30.460	0.0113	651.64	6.751	6.633
66.878 (x=0.05)	33.95	26	26.238	0.0115	702.15	7.460	7.237
		28	20.924	0.0105	786.27	9.560	8.670
		30	10.402	0.0060	1107.83	15.660	13.171
		20	36.865	0.0088	594.25	6.934	6.419
		22	34.518	0.0104	614.12	6.352	6.246
		24	31.444	0.0115	643.43	6.303	6.368
		26	27.485	0.0119	688.09	6.843	6.862
		28	22.520	0.0112	760.32	8.407	7.995
		30	16.356	0.0092	892.19	12.584	10.596

**Table 2**  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ 

Mass $10^{-26}\text{kg}$	$T_C$ K	T K	$\gamma(x 10^{-10})$ J/mole/K <sup>2</sup>	$C_{es}(x 10^{-5})$ J/mole/K	$\lambda$ AU	$\xi$ $10^{-6}$ m	$\sqrt{\lambda\xi}$ $10^{-7}$ m
67.265 (x=0.2)	32.27	20	35.934	0.0093	603.90	7.220	6.603
		22	33.048	0.0106	629.72	6.889	6.586
		24	29.257	0.0113	669.28	7.227	6.955
		26	24.390	0.0110	733.01	8.520	7.903
		28	18.260	0.0094	847.16	12.070	10.112
		30	10.667	0.0062	1108.40	25.247	16.728
67.278 (x=0.15)	32.84	20	36.338	0.0092	600.53	7.058	6.510
		22	33.639	0.0106	624.15	6.632	6.434
		24	30.090	0.0114	659.95	6.820	6.709
		26	25.536	0.0113	716.37	7.804	7.477
		28	19.798	0.0101	813.59	10.471	9.230
		30	12.690	0.0073	1016.22	18.982	13.889
67.291 (x=0.10)	33.34	20	36.706	0.0090	597.52	6.950	6.444
		22	34.172	0.0106	619.28	6.453	6.322
		24	30.845	0.0115	651.82	6.585	6.552
		26	26.569	0.0117	702.31	7.271	7.146
		28	21.189	0.0107	786.45	9.316	8.560
		30	14.522	0.0082	949.96	15.258	12.039
67.304 (x=0.05)	33.95	20	37.095	0.0089	594.38	6.856	6.384
		22	34.737	0.0105	614.22	6.270	6.206
		24	31.642	0.0116	643.56	6.224	6.329
		26	27.665	0.0119	688.26	6.765	6.824
		28	22.659	0.0112	760.49	8.301	7.945
		30	16.460	0.0092	892.29	12.421	10.528

**Table 3**  $\text{La}_{2-x}\text{Ca}_x\text{CuO}_4$ 

Mass $10^{-26}\text{kg}$	$T_C$ K	T K	$\gamma(x 10^{-10})$ J/mole/ $\text{K}^2$	$C_{es}(x 10^{-5})$ J/mole/K	$\lambda$ AU	$\xi$ $10^{-6}$ m	$\sqrt{\lambda\xi}$ $10^{-7}$ m
64.022 (x=0.2)	32.27	20	34.201	0.0088	603.65	7.972	6.937
		22	31.453	0.0101	629.47	7.543	6.891
		24	27.847	0.0107	668.99	7.969	7.301
		26	23.213	0.0104	732.73	9.469	8.330
		28	17.380	0.0090	846.81	13.318	10.620
		30	10.150	0.0059	1108.08	27.880	17.576
64.842 (x=0.15)	32.84	20	35.022	0.0089	600.53	7.891	6.884
		22	32.421	0.0103	623.96	7.470	6.827
		24	29.000	0.0111	659.75	7.746	7.149
		26	24.611	0.0109	716.15	8.976	8.018
		28	19.081	0.0097	813.33	12.289	9.998
		30	12.227	0.0070	1015.89	23.719	15.523
65.663 (x=0.10)	33.34	20	35.548	0.0085	603.14	7.242	6.609
		22	32.692	0.0105	628.94	6.330	6.310
		24	28.943	0.0112	668.43	6.521	6.602
		26	24.127	0.0109	732.11	7.497	7.409
		28	19.228	0.0099	846.10	9.523	8.976
		30	11.230	0.0065	1107.13	17.818	14.045
65.483 (x=0.05)	33.95	20	35.819	0.0088	597.35	7.300	6.604
		22	33.346	0.0103	619.10	6.783	6.480
		24	30.010	0.0112	651.64	6.864	6.688
		26	25.927	0.0114	702.11	7.635	7.322
		28	20.677	0.0104	786.22	9.786	8.772
		30	14.171	0.0071	949.67	18.048	13.092

**Table 4**  $Tl_mBa_2Ca_{n-1}Cu_nO_{m+2n+2}$  and  $Bi_mSr_2Ca_{n-1}Cu_nO_{m+2n+2}$ 

Tl	Ba	Ca	Cu	O	Mass $10^{-26}$ kg	$T_C$ K	$\gamma(x 10^{-10})$ J/mole/K <sup>2</sup>	$C_{es}(x 10^{-5})$ J/mole/K	$\lambda$ AU	$\xi$ $10^{-6}$ m	$\sqrt{\lambda\xi}$ $10^{-7}$ m
2	2	3	4	12	207.54	140.00	130.379	0.3273	556.64	0.0102	0.238
2	2	2	3	10	163.92	125.00	102.978	0.2585	556.65	0.0183	0.319
1	2	3	4	11	170.94	115.49	107.384	0.2696	556.66	0.0112	0.249
2	2	1	2	10	167.82	113.27	105.425	0.2646	556.65	0.1928	1.036
1	2	2	3	9	148.43	99.44	93.245	0.2341	556.64	0.0281	0.396
2	2	0	1	6	139.99	94.57	87.944	0.2208	556.64	0.3320	1.359
1	2	1	2	7	125.91	85.06	79.100	0.1986	556.65	0.0456	0.504

  

Bi	Sr	Ca	Cu	O	Mass $10^{-26}$ kg	$T_C$ K	$\gamma(x 10^{-10})$ J/mole/K <sup>2</sup>	$C_{es}(x 10^{-5})$ J/mole/K	$\lambda$ AU	$\xi$ $10^{-6}$ m	$\sqrt{\lambda\xi}$ $10^{-7}$ m
2	2	2	3	10	170.022	110	106.542	0.2354	557.33	0.0225	0.354
2	2	1	2	8	147.505	95.43	92.433	0.1771	557.35	0.0344	0.438
2	2	0	1	6	124.988	80.86	78.323	0.1278	557.34	0.0563	0.056

## 5. CONCLUSION

Thus a systematic study of the three oxidic system have revealed some important facts which are useful for theoretical and experimental physicists.

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