List of publications

A: PAPERS IN INTERNATIONAL JOURNALS:

1. Anisotropic superconducting state properties of Nd-Ce-CuO and La-Sr-CuO superconductors.  
   (Dinesh Varshney, R. K. Singh and S. Shah)  

2. Coherence lengths and magnetic penetration depths in Y-Ba-CuO superconductors.  
   (Dinesh Varshney, R. K. Singh and S. Shah)  
   1996, Jour. of Superconductivity. Vol. 9, No. 6, pp. 629-635.

3. Pairing mechanism and transition temperature of Ba-Pb-BiO superconductors.  
   (Dinesh Varshney, R. K. Singh and S. Shah)  

4. Superconductivity in Ba Pb_{1-x}Bi_xO: A coupled charge oscillation with optical-phonon mechanism.  
   (Dinesh Varshney, S. Shah and R. K. Singh)  

   (Dinesh Varshney, S. Shah and R. K. Singh)  

6. Superconductivity and normal state resistivity of Ba_{9.6}K_{0.4}BiO_3: An Optical phonon approach.  
   (Dinesh Varshney, S. Shah and R. K. Singh)  

7. Two component model for optical conductivity in Y-Ba-CuO superconductors.  
   (Dinesh Varshney, S. Shah and R. K. Singh)  

8. Optical-phonon-plasmon pairing mechanism and superconducting state parameters in La-Sr-CuO.  
   (Dinesh Varshney, S. Shah and R. K. Singh)  

B: PAPERS IN INTERNATIONAL PROCEEDINGS:


   1997, Int. Symp. On Intrinsic Josephson Effect and THz Plasma Oscillations in 
   High Tc Superconductors, Japan.

12. Two component model for Optical conductivity in Y-Ba-CuO superconductors. 
   (Dinesh Varshney, S. Shah and R. K. Singh)
   1997, Int. Symp. On Intrinsic Josephson Effect and THz Plasma Oscillations in 
   High Tc Superconductors, Japan.

   1997, VII Asia Pacific Physics Conference Beijing, China.

C: PAPERS IN NATIONAL PROCEEDINGS:

14. Coherence lengths and magnetic penetration depths of Nd-Ce-CuO and La-Sr-CuO 
   superconductors. 
   (Dinesh Varshney, R. K. Singh and S. Shah)

15. Current driven Plasma Instabilities in cuprate superconductors. 
   (Dinesh Varshney, R. K. Singh and S. Shah)

16. Effective interaction potential of Y-Ba-CuO (124) superconductors. 
   (Dinesh Varshney, R. K. Singh and S. Shah)


   (Dinesh Varshney, R. K. Singh and S. Shah)
APPENDIX
RESEARCH PAPERS
Anisotropic Superconducting State Parameters of Nd–Ce–CuO and La–Sr–CuO Systems

Dinesh Varshney, R. K. Singh, and Sanjay Shah

Received 15 November 1995

Major superconducting state parameter of high-$T_c$ electron-doped Nd–Ce–CuO and hole-doped La–Sr–CuO systems have been estimated. The analysis is based on the electronic energy band structure (EEBS) within the local density approximation. Anisotropy of the layered structure is well reflected in the shape of open Fermi surface. Determination of the effective mass of the charge carrier from the Fermi velocity using EEBS and estimates of the anisotropic superconducting state parameters, particularly the magnetic penetration depth $(\lambda_m)$, lead to smaller values than those observed by muon spin relaxation ($\mu$SR) measurements on polycrystalline samples. The coherence length $(\xi)$ and $\xi^* = \lambda_m$ is evaluated and appears to be higher. The temperature dependence of the Ginzburg–Landau parameter $(h)$ and along the plane magnetic penetration depth $(\lambda_p)$ shows the same nature as those revealed from experiments. Furthermore, results on lower and upper critical magnetic field are also presented. The results based on EEBS studies are consistent but do not agree well with experiments. On the other hand, if the Fermi Liquid approach (FLA) parameters are used for this analysis, the results are in better agreement with those reported earlier. The implications of the above investigations are discussed.

KEY WORDS: Anisotropic properties; electronic energy band structure studies; Fermi Liquid approach; superconducting state parameters.

1. INTRODUCTION

The layered-structure cuprate oxides (Nd–Ce–CuO as electron doped and La–Sr–CuO as hole doped) exhibit high transition temperature $T_c$. A large number of experimental and theoretical studies have been devoted, so far, to understand the pairing mechanism as well as the physical properties of these oxides [3]. The normal conducting and superconducting state parameters are of vital importance. Of primary interest are the superconducting state properties such as magnetic penetration depth, coherence length, critical magnetic fields, etc. These properties of high-$T_c$ oxides have been investigated by a range of techniques that include muon spin relaxation ($\mu$SR) measurements, ac and dc magnetic susceptibility, and kinetic inductance measurements. The $\mu$SR measurements give more reliable results with relative ease of interpretation, and experiments are readily performed on polycrystalline samples. Recently, Klauda et al. [4] have reported the magnetic properties of electron-doped cuprates, i.e., Nd$_{1.8}$Ce$_{0.2}$CuO$_4$ in the superconducting state using ac magnetic susceptibility measurements. Critical fields of the polycrystalline Nd$_{1.8}$Ce$_{0.2}$CuO$_4$ samples $(T = 19.5 \text{ K})$ are evaluated as $(H_{c1} = 133 \text{ G})$ and $(H_{c2} = 50 \text{ T})$. Furthermore, Ginzburg–Landau parameter $(\kappa)$, average penetration depth $(\lambda_m)$, and coherence length $(\xi)$ were also estimated from magnetization measurements. $\mu$SR measurements on polycrystalline samples of La$_{1.8}$Sr$_{0.2}$CuO$_4$ superconductors have been performed, and $H_{c1}(0) = 25 \text{ G} \text{ at } T = 0 \text{ K}$ [5] and $2000 \text{ A} \text{ at } T = 10 \text{ K}$ [6]. Li et al. [7] have performed...
magnetization measurements on single crystals of La$_{1-x}$Sr$_x$CuO$_4$ ($0.10 \leq x \leq 0.20$) and found that $\lambda_t(0) = 2500$ A. Furthermore, the temperature dependence of the Ginzburg–Landau parameter $K$ is also reported and obtained by using the variational model as 68.95, at $T = 26.2$ K.

Electronic energy band structure (EEBS) studies have been used as a powerful tool to predict the anisotropic properties of these cuprates. Hamada et al. [8] and Allen et al. [9] have investigated the band structures of Nd–Ce–CuO and La–Sr–CuO systems within the local density functional (LDF) theory and estimates the superconducting as well as normal conducting state parameters. The band calculations proposed a two-dimensional (2D) conduction band with a cylindrical Fermi surface. This conduction is only half filled for La$_2$CuO$_3$, and with doping of Sr$^{2+}$ in place of La$^{3+}$ an appreciable portion of the Fermi surface is destroyed due to the electronic instability, and the hole-like part of the Fermi surface survives. The effective mass of the charge carrier along CuO$_2$ and perpendicular to, $m^v$ and $m^p$, can be easily evaluated from the EEBS Fermi velocities ($v_F$ and $v_p$) of these oxides. It is evident that these oxides possess layered structures with conducting as well as insulating layers and the properties are anisotropic in nature. Recently, Kresin and Wolf [10] have carefully examined the normal conducting and superconducting state properties of lanthanum-based cuprates. Their approach is based on the Fermi liquid description and is valid for any shape of the Fermi curve. The Fermi liquid approach (FLA) facilitates the effect of anisotropy in the respective properties and seems significant in the present analysis.

Motivated by the earlier theoretical and experimental investigations of the normal-conducting and superconducting state parameters of these layered structure cuprates, we thought it pertinent to make a systematic analysis of these properties using EEBS studies as well as FLA and compare them with the magnetization measurements. The purpose of our present studies is not to argue the merits of these two approaches, but to offer a method to test them for predicting the physical parameters associated with the electron- or hole-doped superconductors. In the present analysis, we have explored our efforts to estimate the charge carrier effective mass, the magnetic penetration depth, the coherence length, the critical magnetic fields, and the anisotropic parameters of these properties. Finally, the results obtained are compared with the available experimental data. It is observed that the estimated superconducting state parameters of these oxides from EEBS studies are consistent but do not agree well with the measurements, and are in better agreement when FLA is used. From these two approaches it is proposed that the Fermi liquid picture gives more accurate results and a better estimation of the physical parameters for electron- as well as hole-doped superconductors. The plan of this paper is as follows.

Section 2 gives a brief description of the method used and computational details to derive the anisotropic superconducting state parameters: the magnetic penetration depth, the coherence length, the lower and upper critical magnetic field, the average value of the penetration depth as well as the coherence length, and the temperature derivative of the upper critical magnetic field. The results are presented in Section 3 and compared with the experimental data. Finally, Section 4 gives the conclusions.

2. THEORY AND COMPUTATIONAL DETAILS

In the layered cuprates, it is assumed that the conducting CuO$_2$ layers are sandwiched in between the insulating La$_{1-x}$Sr,O (Nd$_{1-x}$Ce,O) layers [11]. Doping of Sr(Ce) in place of La(Nd) induces the holes (electrons) in the conducting CuO$_2$ layer to form a quasi-two-dimensional system. The energy of a free particle with open Fermi surface is expressed as

$$\epsilon_n = \frac{h^2 k^2}{2m^v} + \frac{h^2}{m^p} \left[1 - \cos(kz_d)\right] - \mu, \quad (1)$$

where $k$ and $k_z$ are the wave vector along and perpendicular to the conducting CuO$_2$ plane. The effective mass of the charge carriers are $m^v$ and $m^p$ in the $k$ and $k_z$ directions. The interplanar separation between two consecutive CuO$_2$ layers is denoted by $d$ and $\mu$ represents the chemical potential.

The electronic group velocity $V(k) = (1/h)[\epsilon \tilde{c}(k)/\epsilon k]$ with the use of Eq. (1) yield the Fermi velocities along the perpendicular to the CuO$_2$ plane as $v_F = \hbar k/m^v$ and $v_p = [\hbar/(m^p-d)] \sin(kz_d)$. This enables one to write $m = \hbar k/v_F$ and $m^p = [\hbar/(v_F d)] \sin(kz_d)$. Here, we restrict ourselves to the case $|k_z|_{\text{max}} = \pi/c$, where $c$ is the lattice parameter in the $k_z$ direction and $d = c/2$. With this approximation, $m^p$ reduces to $\hbar/(v_F d)$.

The estimation of the superconducting parameters essentially depends on the value of the normal state parameters, i.e., the carrier density of the volume surrounded by Fermi surface. For a stack of 2D conducting layers which are well separated by average
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The condition for optimized pairing suggests that the 2D charge carrier density [11] follows: 

\[ n = 2 \eta \rho \]

The London penetration depth of superconductors is expressed as:

\[ \lambda_0 = \left[ \frac{m_e e^2}{4 \pi n e^2} \right]^{1/2} \]

and

\[ \lambda_c = \left[ \frac{m_e e^2}{4 \pi n e^2} \right]^{1/2} \] (2)

where \( n \) is the superconducting charge carrier density in cm\(^{-3}\).

The BCS approach estimates the coherence length of a superconductor and at \( T=0 \) K it is:

\[ \xi(0) = \frac{\hbar v_F}{(1.76 \pi K_B T_c)} \]

and

\[ \xi^*(0) = \frac{\hbar v_F}{(1.76 \pi K_B T_c)} \] (3)

The critical magnetic fields are associated with these two characteristic lengths, and the lower critical magnetic field is expressed as:

\[ H_{c1}(0) = \frac{\phi_0}{4 \pi \lambda_1(0)} \ln \left( \frac{\lambda_1(0)}{\xi(0)} \right) \]

and

\[ H_{c2}(0) = \frac{\phi_0}{2 \pi \xi(0) \xi^*(0)} \] (4)

Similarly, the upper critical magnetic field is evaluated from the expression:

\[ H_{c2}(0) = \frac{\phi_0}{2 \pi \xi(0) \xi^*(0)} \]

where \( \phi_0 \) denotes the magnetic flux quantum, \( 2.08 \times 10^{-7} \) G cm\(^{-2}\).

The temperature dependence of the in-plane magnetic penetration depth can be well fitted from the expression:

\[ H_{c1}(T) = H_{c1}(0) [1 - (T/T_c)^{3/2}] \]

The solid curve in Fig. 1a is for Nd-Ce-CuO with \( H_{c1}(0) = 1.102 \) A. A similar trend is obtained for \( H_{c1}(0) \) of 199 A as shown in Fig. 1b. The temperature dependence of \( H_{c1}(0) \) for both compounds shows the same trend as observed experimentally. The difference in \( H_{c1}(0) \) using EEBS studies and using FLA is attributed to the discrepancies in the Fermi velocity. FLA estimates \( v_F \) as 5.8 \text{ cm sec}^{-1} and EEBS reports it as 2.2 \text{ cm sec}^{-1}. Nevertheless, \( v_F \) from EEBS is higher and makes \( H_{c1}(0) \) shorter. In view of this, it is suggested that FLA estimation of superconducting state parameters is fairly good in the range of the experimental observations.

It is evident that the present high-\( T_c \) oxides have a very short coherence length. The coherence length is estimated from Eq. (3) and is listed in Table I along with the reported data. For both compounds the EEBS studies yield rather low estimated values. On the other hand, if the parameters as suggested by FLA are used, then \( \xi \) is 2.0 A for Nd–Ce–CuO system. This is close to the reported value. Again it is inferred that the discrepancies in the estimated value of \( \xi(0) \) from EEBS and FLA is due to the difference in the Fermi velocities. Nevertheless, FLA gives coherence lengths that are consistent and within the range of observations.
Table I. Superconducting State Parameters of Nd-Ce-CuO and La-Sr-CuO Systems along with the Data Available

<table>
<thead>
<tr>
<th>Sample Composition</th>
<th>Transition temperature</th>
<th>Lattice parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nd2-x,Ce,CuO4</td>
<td>0.15</td>
<td>24 K [1], 19.5 K [4]</td>
</tr>
<tr>
<td>La2-x,Sr,CuO4</td>
<td>0.15</td>
<td>38 K [2], 37 K [5], 35.5 K [7]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sample</th>
<th>$v_F$ (10^9 cm sec^-1)</th>
<th>$v_F^*$ (10^9 cm sec^-1)</th>
<th>$m$ (m_e)</th>
<th>$m^*$ (m_e)</th>
<th>Charge carrier density (10^14 cm^-2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nd2-x,Ce,CuO4</td>
<td>4.9 [8]</td>
<td>0.093 [8]</td>
<td>1.95</td>
<td>20.5</td>
<td>2.74</td>
</tr>
<tr>
<td>La2-x,Sr,CuO4</td>
<td>2.2 [9]</td>
<td>0.41 [9]</td>
<td>3.95</td>
<td>4.25</td>
<td>2.28</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sample</th>
<th>$\lambda_\perp(0)$ Å</th>
<th>$\lambda_\parallel(0)$ Å</th>
<th>$\gamma = \frac{\lambda_\perp(0)}{\lambda_\parallel(0)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nd2-x,Ce,CuO4</td>
<td>1102.14</td>
<td>3575.05</td>
<td>3.24</td>
</tr>
<tr>
<td>La2-x,Sr,CuO4</td>
<td>1799, 2500 [5], 2000 [6], 2545 [7]</td>
<td>1848</td>
<td>1.02</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sample</th>
<th>$\xi(0)$ Å</th>
<th>$\xi^*(0)$ Å</th>
<th>Anisotropic parameter $\gamma = \frac{\xi(0)}{\xi^*(0)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nd2-x,Ce,CuO4</td>
<td>280, 60 [4]</td>
<td>5.30, 30 [4]</td>
<td>52.81</td>
</tr>
<tr>
<td>La2-x,Sr,CuO4</td>
<td>79, 30 [5, 12]</td>
<td>14.62</td>
<td>5.40</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sample</th>
<th>$K = \frac{\lambda_\perp(0)}{\xi(0)}$</th>
<th>Average value of penetration depth $\lambda_\perp = (\lambda_\perp(0)\lambda_\parallel(0))^{1/2}$ Å</th>
<th>Average value of coherence length $\xi = (\xi(0)\xi^*(0))^{1/2}$ Å</th>
</tr>
</thead>
<tbody>
<tr>
<td>La2-x,Sr,CuO4</td>
<td>23, 100 [5, 7]</td>
<td>1823</td>
<td>24</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sample</th>
<th>$H_{c1}(G)$</th>
<th>$H_{c2}^*(G)$</th>
<th>Anisotropic parameter $\gamma = \frac{H_{c1}}{H_{c2}^*}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nd2-x,Ce,CuO4</td>
<td>185.17, 133 [4]</td>
<td>83.8</td>
<td>2.20</td>
</tr>
<tr>
<td>La2-x,Sr,CuO4</td>
<td>158.6, 191.2 [12]</td>
<td>223</td>
<td>0.68</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sample</th>
<th>$H_{c1}(T)$</th>
<th>$H_{c2}^*(T)$</th>
<th>Anisotropic parameter $\gamma = \frac{H_{c1}}{H_{c2}^*}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nd2-x,Ce,CuO4</td>
<td>22, 80 [4]</td>
<td>0.4165</td>
<td>52.81</td>
</tr>
<tr>
<td>La2-x,Sr,CuO4</td>
<td>28, 75 [12]</td>
<td>5.18</td>
<td>5.40</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sample</th>
<th>$-h (T, K)$</th>
<th>$-h^* (T, K)$</th>
<th>Anisotropic parameter $\gamma = \frac{-h}{-h^*}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nd2-x,Ce,CuO4</td>
<td>0.91, 6.1 [4]</td>
<td>0.017</td>
<td>53.52</td>
</tr>
<tr>
<td>La2-x,Sr,CuO4</td>
<td>0.73, 1.75 [12]</td>
<td>0.136</td>
<td>5.36</td>
</tr>
</tbody>
</table>

A number of fundamental parameters of a superconductor, for instance the Ginzburg–Landau parameter ($K=\frac{\lambda_\perp}{\xi}$), the lower and upper critical magnetic field, and the temperature derivative of the upper critical magnetic field can be very well estimated from $\lambda_\perp$ and $\xi$ values. $K$ is deduced as 25 using EEBS and 79 using FLA for La-Sr-CuO superconductors with the reported value of 100 [12].

Thus, the value of $K$ using the Fermi liquid description is rather close to the experimental observations. The temperature dependence of $K$ is plotted in Fig. 2 for Nd1.85Ce0.15CuO4 (10 ≤ $T$ ≤ 23) and La1.85Sr0.15CuO4 (20 ≤ $T$ ≤ 38.0) superconductors, respectively. $K$ is nearly constant at low temperatures, increases near $T_c$, and finally diverges at $T = T_c$. This behavior supports the negligible effect of fluctuation on the magnetism at temperatures below $T_c$ as earlier proposed [7]. The divergence of

are also estimated (see Table I) and consistent with the reported date.
2.0 \text{f} 

Md. Q,Ce CuO,

IB5 015 t

2.0

(T/Tc) \ln

I

K -

Lo:S5Sr5Cu04

Fig. 1. Relative incremental magnetic field penetration depth \([\lambda_1(0), \lambda_2(0)]\) plotted against \((T/T_c)\) for Nd-Ce-CuO and La-Sr-CuO superconductors, respectively.

K near \(T_c\) favors the diamagnetism nature of these cuprates.

From the above analysis, one can, of course, obtain directly the value of upper and lower critical magnetic field from \(\lambda_1\) and \(\lambda_2\) values for polycrystalline samples of Nd–Ce–CuO and La–Sr–CuO superconductors. We thus obtain \(H_{c1}(H_{c2}) = 185.17 (83.80)\) G and \(H_{c2}(H_{c2}) = 22 (0.41)\) T for Nd–Ce–CuO superconductor. Although these estimated values from EEBS are not in good agreement, they fall within the range of observations. The results can be improved using the Fermi liquid description. The temperature derivative of the upper critical field in the \(k\) and \(k\perp\) directions are also estimated and are consistent with the reported data.

4. CONCLUSIONS

In conclusion, we have analyzed the superconducting state parameters using electronic energy band structure and the Fermi liquid description for electron- and hole-doped cuprate superconductors. It is shown that NCCO and LSCO are extreme type II superconductors \((\lambda_1 \gg \lambda_2)\). The Fermi surface is regarded as open. The following points emerged from our simple analysis.

1. The estimated value of \(\lambda_1(0)\) from the Fermi liquid description is in close agreement with the magnetization and \(\mu\)SR experiments in electron- and hole-doped superconductors. This is attributed to the estimated value of the Fermi velocity which is higher.
in EEBS than in FLA. In fact, the effective charge carrier mass is sensitive to the nature of interaction in the Fermi liquid description.

2. The temperature dependence of $\lambda_1$ and $K$ follows the same behavior as observed by measurements. Both $\lambda_1$ and $K$ diverge near $T_c$, showing diamagnetic behavior. The $K$ values suggest that electron- as well as hole-doped cuprates are extreme type II superconductors.

3. Numerical estimates of the critical magnetic field and the slope of the upper critical field are consistent with the experimental findings and favor the open Fermi surface approximation.

4. The anisotropy parameters in the different properties are in agreement and lie in the range 1–54. Normally, the anisotropy in the resistivity ranges from 25 to 300 in these cuprates.

ACKNOWLEDGMENT

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Coherence Lengths and Magnetic Penetration Depths in YBa$_2$Cu$_3$O$_7$ and YBa$_2$Cu$_4$O$_8$ Superconductors

Dinesh Varshney, R. K. Singh, and Sanjay Shah

Received 19 July 1996

The superconducting state parameters of the high-$T_c$ layered structure YBa$_2$Cu$_3$O$_7$ (Y123) and YBa$_2$Cu$_4$O$_8$ (Y124) systems have been evaluated. The two-dimensional (2D) CuO$_2$ planes as well as one-dimensional (1D) CuO chains are the important features of these systems. The anisotropy of the layered structure is well reflected in the shape of open Fermi surface. The carrier effective mass ($m^*$) and the charge carrier density ($n_c$) are deduced from the Fermi velocity and the Hall effect coefficient, respectively, following the electronic energy band structure studies (EEBS) within the local approximation to the density functional theory. Then the anisotropic magnetic penetration depth ($\lambda_L$) as well as the coherence length ($\xi$) are estimated. The analysis yields smaller values of $\lambda_L$ than those revealed from penetration depth measurements in Y124 while the $\lambda_L$ values appear higher in Y123 when compared with the muon spin relaxation ($\mu$SR) and radio frequency surface impedance (RFSI) measurements. The deduced values of coherence lengths and its anisotropy are consistent with the reported data. The temperature dependence of the in-plane magnetic penetration depth and the Ginzburg-Landau parameter predicts that they are of a similar nature as those revealed from experiments. The results on lower and upper critical magnetic fields are also presented. It is found, with a simple analysis of the superconducting state, that the parameters of YBCO (124 and 123) based on EEBS are consistent but are not in good agreement with experiments. Furthermore, the transport parameters ($m^*, n_c$) as obtained from the Fermi Liquid description are used to determine the in-plane magnetic properties. This technique permits a reasonably good agreement with recently published data. The implications of the above analysis are discussed.

KEYWORDS: YBCO systems; electronic energy band structure (EEBS) studies; Fermi-liquid approach (FLA); penetration depths; coherence lengths; critical fields.

1. INTRODUCTION

Following the discovery of high-$T_c$ superconductors (HTSC’s), there have been tremendous worldwide interest and research on the YBa$_2$Cu$_3$O$_{7-\delta}$ superconductors with 2D planes of CuO$_2$ and 1D chains of CuO in a unit cell. Recently, the 80 K superconductor YBa$_2$Cu$_4$O$_8$ (124 phase), a variant of YBa$_2$Cu$_3$O$_7$ (123 phase) with a double chain of CuO, was found as a distinctly ordered phase [1]. In the course of discovery, much attention has been focused on transport parallel as well as perpendicular to the CuO$_2$ planes. As one of the fundamental parameters in superconductivity, the magnetic penetration depth $\lambda_L(T)$ provides information regarding the effective mass ($m^*$) and the density of charge carriers ($n_c$) as well as the possible anisotropy ($\delta$). The electrodynamic response of HTSC’s has been studied by different techniques that includes muon spin relaxation ($\mu$SR), radio frequency surface impedance (RFSI), and inductive and penetration depth measurements. The electrodynamic measurements as RFSI of high-quality single crystals at high frequency will yield
the information regarding the energy gap, the density of states, as well as the nature of pairing, while the μSR measurements are readily performed on polycrystalline samples with relative ease of interpretation.

The magnetic penetration depth and other parameters associated with the magnetic field have been reported in the YBCO (124 phase) system by magnetization measurements [2], where a value of \( \lambda_{\text{mag}}(0) = 2000 \) Å was found and the lower critical magnetic field \( H_{c1}(0) \) was calculated as 130 Oe. The in-plane coherence length \( \xi_{\text{mag}}(0) \approx 14 - 45 \) Å has been reported by Bucher and collaborators [3]. Magnetic measurements have been performed on the Y123 system, such as μSR measurements on polycrystalline samples [4] and radio frequency surface impedance measurements on thin films [5] as well as high-quality single crystals [6,7]. Earlier, Harshman et al. [4] have observed \( \lambda_{\text{mag}}(6k) \approx 1400 \) Å on bulk samples with \( \delta = 0.0 \). Klein et al. [5] have reported the temperature dependence of \( \lambda_{\text{mag}}(T) \) determined from the microwave surface impedance of Y123 thin films and predict the two-energy-gap BCS dependence. Recently, Gasparov et al. [7] have reported \( \lambda_{\text{mag}}(0) = 1400 \) Å from radio frequency surface impedance measurements on high-quality single crystals of Y123. Besides these experimental observations, the overall \( \lambda_{\text{mag}}(T) \) dependence can be described by a two-gap BCS behavior [5] due to the Berezinskii-Kosterlitz-Thouless (BKT) transition of vortex-antivortex pairs with double \( \text{CuO}_2 \) planes [8]. Worthington et al. [9] have measured \( H_{c1}(4.5 \text{ K}) \) as 50 G and derived \( H_{c2}(0) = 140 \) T on single crystals of the Y123 system. Furthermore, they have also reported the temperature derivative of the upper critical magnetic field \( (H_{c2}) \) at \( T \) and derived the coherence length values.

Band-structure calculations have been used as a powerful tool to predict the transport properties and hence provides an estimate of the normal and superconducting state parameters of anisotropic cuprates. Massidda et al. [10] have studied the band structures of Y123 and Y124 within the local approximation to the density functional theory and estimated the density of states. Hall coefficients, and Fermi velocity parallel as well as perpendicular to the \( \text{CuO}_2 \) planes. A considerable disparity exists between the transport data on single crystals and polycrystalline samples. The periodic array of Y123 can be conveniently described by the \( \text{CuO}, \text{BaO}, \text{CuO}_2, \text{Y}, \text{CuO}_2, \text{BaO}, \text{CuO}, \ldots \) layers in a quasi 2D systems, with \( T_c = 91 \) K at \( \delta = 0.0 \) [11]. Nevertheless, a unit cell contains metallic and insulating layers. The structure of Y124 is similar to that of the superconductor Y123, but an additional \( \text{CuO} \) chain per formula unit is introduced leading to the formation of 1D \( \text{CuO} \) double chains. The second \( \text{CuO} \) chain is introduced between the \( \text{BaO} \) layers and hence increases the Y-Y distance. No doubt, the presence of single (double) chain and two \( \text{CuO}_2 \) planes makes the YBCO system interesting and complicated. The superconductivity can be induced in the \( \text{CuO} \) chains from the \( \text{CuO}_2 \) planes by the proximity effect and the phonon-mediated charge transfer as noted by Kresin and Wolf [12,13]. They predict that the energy gap of the induced superconducting chain state is much smaller than the energy gap of the planes. It is pointed out here that because of the correlated nature of YBCO materials the application of LDA results can be misleading. Recently, Varshney and Singh [14] have developed an approach based on a free-electron layered electron gas model to elucidate the superconducting transition temperature, the energy gap parameter, and the oxygen isotope effect in lanthanum cuprates with one conducting \( \text{CuO}_2 \) plane in a unit cell. The approach properly uses the transport parameters \( (m^*, n_e) \) as estimated from experimental observations on the specific heat coefficient and structural information. The proposed FELEG model is extended for Y123 superconductors and it is found that the 1D \( \text{CuO} \) chains are metallic and will actively participate in the pairing mechanism. Furthermore, the 2D acoustic plasmons generated in 2D \( \text{CuO}_2 \) plane is of high energy while that of the 1D \( \text{CuO} \) chain is of low energy. Recently, we have investigated the anisotropic magnetic properties of La- and Nd-based cuprate with one conducting \( \text{CuO}_2 \) plane within the open Fermi surface approximation [15]. The simple analysis predicts, on the one hand, that the major superconducting-state magnetic properties when estimated from EEBS will differ from those obtained in experiments; on the other hand, the results show consistency when deduced from the FLA, which rests on realistic physical parameters. We have pointed out that the LDA results are misleading due to the strongly correlated nature of cuprates and the FLA will provide new horizons in the study of HTSC's.

Motivated by earlier experimental observations and theoretical investigations on the superconducting-state magnetic parameters of YBCO (123 and 124) systems, we thought it pertinent to make a systematic analysis of the parameters associated with the magnetic field using LDA as well as FLA and compare them with the available magnetic measurement data. In the present studies we wish to see which approach predicts consistent results for the magnetic parameters.
associated with YBCO superconductors. Furthermore, using the band structure description, we will be able to understand the anisotropic magnetic properties. We first work out the charge density \( n_v \) and the effective charge carrier mass \( m^* \) from the band structure data on the Hall coefficient as well as the Fermi velocity, respectively. Finally, the deduced results on Y123 and Y124 systems are compared with the available experimental observations. It is shown that the obtained results from the LDA lie in the range of observed data but do not agree well, and the in-plane results are in better agreement when the Fermi liquid description is used. The plan of this paper is as follows.

Section 2 gives a brief description of the method used and the computational details in deriving the anisotropic magnetic properties of layered Y123 and Y124 cuprates: the magnetic penetration depth, the coherence length, the lower and upper critical magnetic fields, the average value of the penetration depth as well as the coherence length, and the temperature derivative of the upper critical magnetic field at \( T = T_c \).

The London penetration depth of superconductors is expressed as

\[
\lambda_J(0) = [\frac{(m c^2)}{4\pi \eta_0 e^2}]^{1/2} \tag{2}
\]

and

\[
\xi(0) = \hbar v_F (1.76\pi K_B T_c) \tag{3}
\]

where \( \eta_0 \) is the charge carrier density in cm\(^{-3} \) and \( \epsilon \) denotes the velocity of light.

The BCS approach estimates the coherence length of a superconductor, and at \( T = 0 \) K it is

\[
\xi(0) = \hbar v_F (1.76\pi K_B T_c)
\]

where \( K_B \) is the Boltzmann constant and \( T_c \) is the maximum superconducting transition temperature.

The critical magnetic fields are associated with the two characteristics lengths, i.e., \( \lambda_J \) and \( \xi \). The lower critical magnetic fields are represented as

\[
H_{c1}(0) = \frac{\Phi_0}{4\pi \lambda_J(0)} \ln \left[ \frac{\lambda_J(0)}{\xi(0)} \right]
\]

and

\[
H_{c1}(0) = \frac{\Phi_0}{4\pi \lambda_J(0)} \ln \left[ \frac{\lambda_J(0)}{\xi(0)} \right]
\]

where \( \Phi_0 \) denotes the magnetic flux quantum and is \( 2.068 \times 10^{-15} \) cm\(^2\).

The upper critical magnetic field at \( T = 0 \) K is

\[
H_{c2}(0) = \frac{\Phi_0}{2\pi \xi(0) \xi^2(0)}
\]

and

\[
H_{c2}(0) = \frac{\Phi_0}{2\pi \xi^2(0)}
\]
The temperature derivative of \( H_{c2}(0) \) at \( T = T_c \) is

\[
h'(0) = -\frac{d}{dT}[H_{c2}(0)]T_c
\]

and

\[
h''(0) = -\frac{d}{dT}[H_{c2}(0)]T_c
\]

We have estimated the anisotropic magnetic properties of \( Y_{124} \) and \( Y_{123} \) superconductors. The results obtained are presented and discussed in the following section.

3. RESULTS AND DISCUSSION

In order to estimate the anisotropic properties associated with the magnetic field in the superconducting state for \( YBCO \) \( (124 \) and \( 123 \) \) systems, we have used the band structure parameters \( [10] \) as follows. For \( Y_{124} \), there exists two 2D and two 1D Fermi surface sheets arising from two \( CuO_2 \) planes and two \( CuO \) chain, respectively. Compared to \( Y_{124} \), \( Y_{123} \) shows only one \( CuO \) chain and two \( CuO_2 \) planes. We have used the Hall coefficient of \( YBCO \) \( (124 \) and \( 123 \) \) with \( H || c \) and \( H \perp c \) to estimate the charge carrier density \( (n_v) \) in the respective directions. In fact, \( Y_{124} \) structure is a variant of \( Y_{123} \) in which a second \( CuO \) chain is introduced between the \( BaO \) layers, increasing the \( Y \)-\( Y \) distance from 11.7 Å \( \) (\( Y_{123} \)) to 13.6 Å \( \) [1]. We use the average distance between \( CuO_2 \) planes as 7 Å for \( Y_{124} \) and 6 Å for \( Y_{123} \) systems, respectively. With these the band structure studies will yield the effective mass of the charge carriers \( (m^v \) and \( m^\perp \)) using the Fermi velocity data \( [10] \), within the open Fermi surface approximation. These are listed in Table I.

The calculations of magnetic penetration depth \( \lambda_v(0) \) in the \( K \) and \( K \perp \) directions were performed from Eq. (2). The estimated values of \( \lambda_v(0)[\lambda^v_c(0)] \) for \( Y_{123} \) superconductors are 1500 [3800] Å, respectively. It is inferred that the deduced values are slightly high when compared with the experimental observations for the model parameters as depicted from EEBS studies. The temperature dependence of the in-plane magnetic penetration depth can be well fitted in the expression \( \lambda_v(T) = \lambda_v(0)[1 - (T/T_c)^2]^{-1.2} \). The solid curve in Fig. 1a is for \( Y_{124} \) with \( \lambda_v(0) = 1268 \) Å and that for \( Y_{23} \) with \( \lambda_v(0) = 1500 \) Å is shown in Fig. 1b. The temperature dependence of \( \lambda_v(T) \) shows the same trend as earlier observed experimentally. It is noticed that \( \lambda_v(T) \) is nearly constant with the temperature below the superconducting transition temperature. Furthermore, it diverges at \( T_c \) and a steep increase infers diamagnetic behavior. The high-\( T_c \) oxides have a very short coherence length and is estimated from Eq. (3) \( \) (see Table I) along with the experimental data \( [16] \). Using the band structure parameters, the deduced value of the anisotropic coherence length are consistent with the reported data.

The average value of \( \lambda_L \) and \( \xi \) are also estimated (see Table I).

Earlier, Kresin and Wolf \( [12,13] \) have evaluated many of the material parameters of \( YBCO \) based on experimental observations within the Fermi liquid description in the reciprocal space. Such a technique is of vital importance as the structural information of the system and the specific heat measurements can be performed well on high-quality single crystals and the data yielded for any theoretical description are more reliable. Recently, we have found that the estimation of superconducting state parameters in \( YBCO \) superconductors essentially depends on the normal state transport parameters, i.e., the carrier density of the volume surrounded by the Fermi surface as well as the effective mass of the charge carriers \( [14] \). For \( YBCO \) superconductors, a stack of 2D conducting planes which are well separated by an average distance \( d \), the condition for optimized pairing suggests that the 2D charge density in the planes will follow \( n_L d^2 = 1 \) and for 1D chains \( n_v d' = 1 \) with \( d' \) as the average distance between the 1D chains. Thus the volume concentration of the charge carriers in \( Y_{123} \) will lead to \( n_v = (n_L n_v/3) \). The Fermi wave vector for the 2D plane is \( K_{FL} = (2\pi n_L)^{1/2} \) and for 1D chain, \( K_{FL} = \pi n_v/2 \). Furthermore, the effective mass of the charge carriers can be well estimated from the electronic specific heat coefficient \( (\gamma) \) value, and for 2D planes \( m_L = 3\hbar^2 \pi \gamma d/K^2 \) and for 1D chains \( \gamma = 12\hbar^2 \pi \gamma d^2 d' \) are used for the 1D chains, respectively. It is suggested that proper incorporation of the realistic physical parameters based on experimental observations in the Fermi liquid description will lead to a clear picture of the properties in cuprates.

For \( Y_{123} \) superconductors, we have used the structural information to deduce \( n_v = 2.77 	imes 10^{14} \) \( cm^{-2} \) and \( n_L = 2.57 \times 10^{17} \) \( cm^{-3} \) to yield \( n_v = 2.38 \times 10^{21} \) \( cm^{-3} \). Taking \( \gamma = 12.6 \) \( mJ/mol/K^2 \) \( [17] \), the effective mass \( m_L = 6.2 m_e \) and \( m_e = 2.0 m_e \) are deduced. While evaluating the magnetic penetration depth as \( T = 0 K \), we use the reduced mass of layers and chains and the volume charge carrier density to estimate \( \lambda_v(0) = 1336 \) Å, which is in good agreement with the microwave surface resistance measurements on high-quality single crystals \( [7] \). Besides the penetration depth value, the coherence length value (28 Å)
Table I. Superconducting state parameter of YBa$_2$Cu$_4$O$_8$ and YBa$_2$Cu$_3$O$_7$ systems along with the data available.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Transition temperature ($^\circ$K)</th>
<th>Average distance between CuO$_2$ planes ($\text{\AA}$)</th>
<th>Average distance between CuO chains ($\text{\AA}$)</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Transition velocity ($V_p$)</th>
<th>Effective mass ($m^*$)</th>
<th>Charge carrier density ($n^*$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>($10^3$ cm sec$^{-1}$)</td>
<td>($m_r$)</td>
<td>($10^{21}$ cm$^{-3}$)</td>
</tr>
<tr>
<td>YBa$_2$Cu$_4$O$_8$</td>
<td>2.7 [10]</td>
<td>1.41</td>
</tr>
<tr>
<td>YBa$_2$Cu$_3$O$_7$</td>
<td>1.5 [10]</td>
<td>2.83</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Penetration depth</th>
<th>Anisotropic parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_{z}(0)$</td>
<td>$\gamma = \lambda_{z}(0)$</td>
</tr>
<tr>
<td>($\text{\AA}$)</td>
<td>($\text{\AA}$)</td>
</tr>
<tr>
<td>YBa$_2$Cu$_3$O$_7$</td>
<td>1500, 1400 [4, 6, 7]</td>
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</table>

<table>
<thead>
<tr>
<th>Coherence length</th>
<th>Anisotropic parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\xi (0)$</td>
<td>$\gamma = \xi (0)$</td>
</tr>
<tr>
<td>($\text{\AA}$)</td>
<td>($\text{\AA}$)</td>
</tr>
<tr>
<td>YBa$_2$Cu$_4$O$_8$</td>
<td>46.41-45 [3]</td>
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</table>

<table>
<thead>
<tr>
<th>Average value of penetration depth</th>
<th>Average value of coherence length</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_{z} = [\xi (0)\lambda_{z}(0)]^{1/2}$</td>
<td>$\xi = [\xi (0)\xi (0)]^{1/2}$</td>
</tr>
<tr>
<td>($\text{\AA}$)</td>
<td>($\text{\AA}$)</td>
</tr>
<tr>
<td>YBa$_2$Cu$_4$O$_8$</td>
<td>1426.13</td>
</tr>
<tr>
<td>YBa$_2$Cu$_3$O$_7$</td>
<td>2386.46</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Lower critical magnetic field</th>
<th>Anisotropic parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_{c1}(0)$</td>
<td>$\gamma = H_{c1}(0)$</td>
</tr>
<tr>
<td>($\text{T}$)</td>
<td>($\text{T}$)</td>
</tr>
<tr>
<td>YBa$_2$Cu$_3$O$_7$</td>
<td>306</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Upper critical magnetic field</th>
<th>Anisotropic parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_{c2}(0)$</td>
<td>$\gamma = H_{c2}(0)$</td>
</tr>
<tr>
<td>($\text{T}$)</td>
<td>($\text{T}$)</td>
</tr>
<tr>
<td>YBa$_2$Cu$_4$O$_8$</td>
<td>69.43</td>
</tr>
<tr>
<td>YBa$_2$Cu$_3$O$_7$</td>
<td>191, 140 [9]</td>
</tr>
</tbody>
</table>

<table>
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<tr>
<th>Temperature derivative of $H_{c2}$</th>
<th>Anisotropic parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-h$ ($\text{T/K}$)</td>
<td>$-h^*$ ($\text{T/K}$)</td>
</tr>
<tr>
<td>YBa$_2$Cu$_4$O$_8$</td>
<td>0.8635</td>
</tr>
<tr>
<td>YBa$_2$Cu$_3$O$_7$</td>
<td>2.098, 1.65 ± 0.23 [19]</td>
</tr>
</tbody>
</table>

appears closer to the earlier suggested value. Similarly for Y124, we use $\gamma = 15 \text{mJ mol}^{-1} \text{K}^{-2}$ [2] to obtain $\lambda_{z}(0) = 184 \text{A}$, which is in agreement with the experimental data. The difference in the two characteristic lengths using band-structure parameters as well as the Fermi-liquid description is attributed to the discrepancies in the transport mass and charge carrier density ratio ($m^*/n^*$). The Fermi-liquid approach estimates $m^*/n^* = 0.63 \times 10^{-24} \text{gm cm}^{-3}$ while the band structure reports it as $0.78 \times 10^{-22} \text{gm cm}^{-3}$. Nevertheless, the higher transport ratio in Y123 from band structure studies makes $\lambda_{z}(0)$ higher as compared to the Fermi-liquid approach. In view of this analysis, we believe that the Fermi-liquid description based on realistic
experimental observations yields reasonably good values of the superconducting-state parameters. Nevertheless, one cannot rule out the band-structure data as it can be useful in several aspects.

The two characteristics lengths, i.e., $\lambda_L$ and $\xi$, will give information regarding the Ginzburg–Landau parameter ($\kappa = \lambda_L / \xi$), the lower and upper critical magnetic fields, and the temperature derivative of the upper critical magnetic field at $T = T_c$. The deduced values of $\kappa$ from band-structure studies are 65.21 and 27.56 for the Y123 and Y124 phases of YBCO superconductors, respectively. The temperature dependence of $\kappa$ is plotted in Figs. 2a and b for Y124 ($60 \leq T \leq 80$) and Y123 ($70 \leq T \leq 90$) superconductors, respectively. It is observed from the figures that $\kappa$ is rather insensitive at low temperatures, increases near $T_c$, and finally diverges at $T = T_c$. Furthermore, the divergence of $\kappa$ near $T_c$ reflects the diamagnetism nature of these systems. Besides these, one can of course obtain directly the lower and upper critical magnetic fields for these systems and these are deduced as $H_{c1}(H_{c2}) = 306 (70) \, G$ and $H_{c2}(H_{c2}(H_{c2}) = 191 (63) \, T$ for Y123 superconductors.

The estimated values from EEBS critical magnetic fields are not in good agreement with the reported data but are in the range of observations. In
the superconducting state too, the magnetic parameters such as the lower critical magnetic field ($H_{c1}$), the upper critical magnetic field ($H_{c2}$), the coherence length ($\xi$), the magnetic penetration depth ($\lambda$), etc. are highly anisotropic. We estimate the anisotropy of the lower critical magnetic field as $\gamma_{H_{c1}} = \frac{H_{c1}}{H_{c2}} = 4.37$ for the Y123 phase, whereas the reported values lie between 6 to 20 [18]. The upper critical magnetic field and the coherence length are $\gamma_{H_{c2}} = \frac{H_{c2}}{\xi} \approx 3.03$ compared with the earlier mentioned value of 5–10 [18]. We estimate the temperature derivative of $H_{c2}$ at $T = T_c$ in the $\Gamma$ and $\Sigma$ directions as 2.098 and 0.702 for Y123 superconductors, and these are consistent with the reported data [19].

4. CONCLUSIONS

In conclusion, we have analyzed the superconducting-state magnetic parameters of $Y$ (124 and 123) superconductors using electronic energy band structure studies as well as the Fermi-liquid approach with an open Fermi surface. The estimated value of $\lambda(0)$ and $\xi(0)$ from the Fermi liquid description are in close agreement with the magnetization measurements. This is attributed to the fact that the Fermi-liquid description takes proper account of structural information and specific heat measurements. No doubt, the transport parameters are sensitive to the nature of the interaction in the Fermi-liquid approach, and we believe that a good quantitative number in the physical properties can be well estimated from this technique and thus provide a better understanding of the subject matter. Although the band structure studies overestimate the transport parameters, it can provide information on the anisotropy in the respective properties that cannot be obtained with the Fermi-liquid picture. The small value of $\xi$ is the key feature of HTSC's. Nevertheless, the small values of $\xi$ in the conventional superconductors ($\xi \approx 10^2$–$10^3$ Å) is a direct consequence of the high transition temperature and the low carrier density. It also reflects the real space pairing nature of these superconductors. The ratio of the characteristic lengths is very large and suggests the extreme type II superconductors. In conclusion, it has been shown that the magnetic properties estimated from the Fermi-liquid picture indeed provide consistent results for all cuprates. It is often found that despite complexities with the structure and correlated nature of the HTSC's, the local approximation to the density functional theory gives meaningful results for anisotropic superconducting-state magnetic properties in YBCO superconductors.

REFERENCES

Pairing mechanism and transition temperature of Ba-Pb-BiO superconductors

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The nature of pairing mechanism in cubic perovskite BaPbBiO, has been investigated by developing a model potential which involves electron-electron, electron-optical phonon as well as electron-plasmon interactions. The interaction potential was used to obtain the pairing parameters as coupling strength and Coulomb repulsive parameter. Coupled oscillations of electronic charge with longitudinal optical phonon describe the superconducting nature of bismuth oxides. Estimated value of coupling strength (λ ~ 0.84) is consistent with a moderate attractive interaction. The screened Coulomb repulsive parameter (µ−0.22) infers the poor screening of charge carriers with low carrier concentration and reflects a small density of states. The superconducting transition temperature (Tc) of BaPb, Bi, O, is evaluated as 15.5 K which is consistent with the earlier reported data. The analysis has led to the conclusion that a weak to moderate coupling exists and the coupling of charge oscillations with longitudinal optical phonon mode could be a reason to the superconductivity in Ba-Pb-BiO superconductors.

The occurrence of superconductivity1 in cubic perovskite oxide BaPb, Bi, O, (x=0.25, Tc = 13 K) provides an opportunity to understand the mechanism of pairing as well as the nature of superconducting state. The interest in BiO system is renewed with the recent findings2 of Ba, K, Bi, O, with superconducting transition temperature, Tc=30 K which have similar Tc as those of La based cuprates. The copper oxide based superconductors are highly anisotropic in their physical properties due to the two dimensional (2D) character of the conducting copper oxide (CuO2) planes. On the other hand the non-transition metal compound BaPb, Bi, O (BPBO) is isotropic as the oxygen octahedra form a three-dimensional (3D) network. The parent compound La, Cu, O, is an antiferromagnetic insulator, instead BaBiO, is semiconducting with low density of states at the Fermi level. The high value of Tc besides essential differences in copper and bismuth families have raised serious queries regarding the common pairing mechanism.

The parent compound BaBiO, is semiconducting, the breathing mode is completely softened and the static displacements of the oxygen atoms have been observed from the crystallographic studies3. The chemical substitution of Pb in place of Bi introduces free charge carriers and the BiO lattice is modified. The resistivity and Hall-coefficient measurements4 revealed that the system BaPb, Bi, O, shows a metallic behaviour in the compositional range 0.0 ≤ x ≤ 0.05. The superconducting nature1 is observed for 0.05 ≤ x ≤ 0.35 with a maximum Tc ~ 13 K at x = 0.25, despite of the fact that the charge carrier density9 (n ~ 10^21 cm^-3) and the density of states at the Fermi level10 is 0.1 states/eV unit cell spin) are much smaller than the conventional superconductors with similar Tc’s. The metal to semiconductor transition in BPBO occurs at x = 0.35 and exhibit semiconducting characteristics in the range 0.35 ≤ x ≤ 1.0.

Band structure calculations on BaPb, Bi, O, have been performed by Mattheiss and Hamann11. The Raman study of lattice vibrations together with infrared spectroscopy results12 confirms the presence of LO and TO breathing vibration in Ba-Pb-BiO perovskites. The electron-lattice interaction of Ba-Pb-BiO is studied microscopically by using the realistic electronic bands of BaBiO, reproduced by the tight binding model13. The superconductivity was discussed in the frame work of strong coupling theory of electron-lattice interactions caused by the
longitudinal modes of oxygen stretching/breathing vibration.

The reflectivity measurements have been carried out by Tajima et al.\textsuperscript{10} over a wide energy range and also over the whole compositional range in BaPb\textsubscript{1-x}Bi\textsubscript{x}O\textsubscript{3} superconductors. The phonon structure is observed by far-infrared optical and Raman scattering measurements and the plasma excitations in the visible and near infrared region. The existence of plasmons are well confirmed by Tajima et al.\textsuperscript{11} from the Electron-Energy Loss Spectroscopy (EELS) at the bismuth dopant level (\(x=0.27\)). This suggest the participation of collective excitation besides optical phonons in the pairing mechanism in BaPb\textsubscript{1-x}Bi\textsubscript{x}O\textsubscript{3} superconductors. However, the presence of oxygen isotope effect\textsuperscript{12} (coefficient \(\alpha=0.22\)) and the energy gap ratio \(\left(\beta=2\Delta/K_B T_c=3.5\pm0.5\right)\), now clearly indicate that usual electron-phonon interaction plays an important role. Batlogg et al.\textsuperscript{12} have suggested that anomalous high \(T_c\) in BiO superconductors is not due to conventional strong electron-phonon coupling but the pairing is mediated by electronic excitations which involve the atomic displacements as a result of charge redistribution\textsuperscript{13}. During the recent past plasmon mechanism\textsuperscript{14} emerges as a central theme in the formation of additional pairing mechanism and could lead to high \(T_c\) values in copper oxides. Recently, Varshney and Singh\textsuperscript{15} have made an attempt to study the joint phonon and plasmon mechanism in the lanthanum copper oxides based on Free electron layered electron gas model. The approach facilitates the various interactions, dielectric response function and the 2D acoustic phonon, plasmon modes by properly considering the layered structure. The purpose of the present paper is to study the role of charge oscillations as well as of the breathing phonon mode in the cubic perovskite Ba-Pb-BiO and to see what set of parameters can explain well the experimental measurements about the normal metallic state. Such studies on Ba-BiO systems have wide potential as the \(T_c\) is high and resembles with CuO based superconductors. Earlier, Tachik and Takahashi\textsuperscript{16} have explained the superconductivity in copper oxides, when the pairing interaction is mediated by the charge transfer oscillations associated with LO phonons and suggested the similar mechanism in Ba-Pb-BiO\textsubscript{3} superconductors. In view of the earlier experimental and theoretical findings a model potential is developed including Coulomb, electron-optical phonon and electron-plasmon interactions to look for the pairing mechanism as well as physical parameters in the superconducting state. The approach is used to work out (a) the coupling strength \(\lambda\), (b) the screened Coulomb repulsive parameter \(\mu^*\), (c) the 2D acoustic plasmon energy \(\hbar \Omega_\perp\), and (d) the coupled oscillations of electronic charge associated with longitudinal optical phonon energy \(\hbar \Omega_L\) in Bismuth oxides. Finally, transition temperature for maximum \(T_c\) doping concentration \(x_c\) is evaluated.

**Essential Formalism**

The parent BaPbO\textsubscript{3} compound is regarded as semimetal. The empty Pb(6s) band slightly overlaps with O(2p) band. Chemical substitution of Bi\textsuperscript{3+} in place of Pb\textsuperscript{4+} introduces one electron per one Bi atom in the empty Pb(6s) band which are the active charge earners (electrons) of effective mass \(m^*\) and will participate in the pairing mechanism. Besides these active charge carriers the contraction and expansion of oxygen octahedra around the Bi or Pb atoms will give rise to breathing modes of phonons. The Bi atom has two stable ionic states in the form of Bi\textsuperscript{3+} and Bi\textsuperscript{5+} which allows the valence of Bi atom to fluctuate even in the Pb\textsuperscript{4+} matrices. The dielectric constant of the oxide is given by a sum of ionic and electronic dielectric constants. The model dielectric constant is represented by

\[
\varepsilon(q,\omega)=\varepsilon_{\text{cor}}+P(q,\omega)+P(q,\omega)
\]

where, the first term is the polarizability of ionic core-electrons. In the frequency region of interest, \(\varepsilon_{\text{cor}}\) is assumed to be independent of frequency and is a constant \(=\varepsilon_\infty\). The electronic and ionic polarizabilities are represented by the second and third terms respectively. When an ionic semimetal is doped with the small number of electrons or holes, the crystal becomes metallic and the current carriers also contribute to the dielectric constant. A realistic calculation of \(P(q,\omega)\) requires a many body treatment for the behaviour of charge carriers and is rigorous. The random phase approximation forms of polarizability are widely used to describe the plasmon behaviour to see the coupling effects...
and recently, Mahan and Wu\(^7\) have applied it to the copper oxides. In the long wave length limit \((q \rightarrow 0)\), the electronic polarizability is expressed as

\[
P_e(q, \omega) = D_1 / (\Delta_2^2 - \omega^2) = D_2 \omega_2^2
\]

where \(D_1 = \Omega_p^2\) \(\ldots\) \(2\)

and \(\Delta_2^2 = q^2 V_f^2 / 2\) \(\ldots\) \(4\)

with \(V_f\) represents the Fermi velocity.

The ionic polarizability is

\[
P_i(q, \omega) = \varepsilon_0 \frac{\omega_{LO}^2 - \omega_{TO}^2}{\omega_{TO}^2 - \omega^2}
\]

\(\ldots\) \(5\)

where \(\omega_{LO}\) and \(\omega_{TO}\) are the frequencies of LO and TO breathing vibrations. For the sake of simplicity, single optical phonon whose vibrational frequencies are independent of wave vector \((q)\) has been considered.

The model dielectric function for the polarized waves with the above description becomes

\[
\varepsilon(q, \omega) = \varepsilon_0 + \frac{D_1}{\Delta_1^2 - \omega^2} + \frac{D_2}{\Delta_2^2 - \omega^2}
\]

\(\ldots\) \(6\)

\[
\varepsilon(q, \omega) = \varepsilon_0 \left[ 1 + \frac{A_1}{\Delta_1^2 - \omega^2} + \frac{D_2}{\Delta_2^2 - \omega^2} \right]
\]

\(\ldots\) \(6\)

Here, \(A_1\) denotes a screened plasma frequency, \(\Delta_1 = \omega_{LO}^2 - \omega_{TO}^2\) and \(\Delta_2^2\) as \(\omega_{TO}^2\), respectively. The spectral intensity of the polarized wave is expressed as

\[
\eta(q, \omega) = -\frac{1}{\pi} \text{Imag} \frac{\varepsilon_0}{\varepsilon(q, \omega)}
\]

\(\ldots\) \(7\)

where, the dielectric constant is given by Eq.(6). Physically it corresponds to the excitation density of the polarized waves.

The main input parameter about the concerned material which determines the critical transition temperature, is the dynamic interaction potential \(V(q, \omega)\) or equivalently \(\varepsilon^{-1}(q, \omega)\) of the system. If to the first approximation, \(\varepsilon^{-1}(q, \omega)\) is identified with the inverse longitudinal dielectric function of the system, it can be associated with different longitudinal modes, corresponding to the exchange of phonons, plasmons, having poles at the respective modes. Since the interest is in separation of the individual contributions of \(\varepsilon^{-1}(q, \omega)\) from different longitudinal modes, the inversions of Eq. (6) is done in the form

\[
\varepsilon^{-1}(q, \omega) = \varepsilon_0 \left[ 1 + \sum_{i=1}^{2} \frac{f_i}{\omega_i^2 - \Omega_i^2} \right]
\]

\(\ldots\) \(8\)

where \(\Omega_i\) are the frequencies of two longitudinal modes and the resonant frequencies are given by

\[
\left( \Omega_i^2 - \Delta_i^2 \right) \left( \Omega_i^2 - \Delta_i^2 \right) + A_i \left( \Delta_i^2 - \Omega_i^2 \right) = 0
\]

\(\ldots\) \(9\)

\[-D_i \left( \Omega_i^2 - \Delta_i^2 \right) = 0\]

The effective interaction potential \(V(q, \omega)\) is the sum of electronic and ionic contributions, \(V(q, \omega) = V_e(q) \varepsilon^{-1}(q, \omega)\) from the individual longitudinal modes. The oscillator strength is defined as

\[
f_i = \frac{2}{\pi} \frac{\Omega_i^2 - \Delta_i^2}{\mu_i^2} \frac{\Omega_i^2 - \Delta_i^2}{\mu_i^2}
\]

\(\ldots\) \(10\)

It is suffice to see that following sum rules are valid,

\[
\sum_{i=1}^{2} \Omega_i^2(q) = D_1 + D_2 + \Delta_1^2 + \Delta_2^2
\]

\(\ldots\) \(11\)

\[
\sum_{i=1}^{2} f_i(0) = \frac{\Omega_i^2(0)}{\mu_i^2(0)} = 1
\]

Here, \(f_i(0)/\Omega_i^2(0)\) is the limiting value of \(f_i(0)/\Omega_i^2(0)\) in the long wavelength limit.

This states that

\[
\varepsilon^{-1}(q \rightarrow 0, 0) \rightarrow 0 \text{ when } \omega = 0
\]

Zero’s of the model dielectric function will yield two modes of the polarized waves and the frequencies of the coupled mode in the long wavelength limit are

\[
2\Omega_i^2 = \left[ \Omega_p^2 + \Delta_i^2 + \omega_{LO}^2 \right]^{1/2}
\]

\(\ldots\) \(12\)

Further simplification yields

\[
\Omega_i^2 \equiv \Omega_p^2 + \Delta_i^2
\]

\(\ldots\) \(13\)

shows the 2D acoustic plasmon characteristics. The lower mode is expressed as

\[
\Omega_1^2 \equiv \frac{\omega_{LO}^2 + \omega_{TO}^2}{2 + (\omega_{LO}^2 + \Omega_p^2)}
\]

\(\ldots\) \(14\)

which is basically coupled charge oscillation with optical phonon mode.
The effective longitudinal dielectric function in terms of 2D acoustic plasmon mode (\(\Omega_2\)) and coupled charge oscillation with phonon-mode (\(\Omega_4\)) is now written as

\[
\varepsilon_{\text{eff}}(q, \omega) = \left( \frac{\omega^2 - \Omega_2^2}{(\omega^2 - \Omega_4^2)} \right) \left( \frac{\omega^2 - \Omega_4^2}{\omega^2} \right) \varepsilon_e \tag{15}
\]

and the interaction potential takes the form

\[
V(q, \omega) = V_e(q) \varepsilon_{\text{eff}}^{-1}(q, \omega) = \frac{2\pi e^2}{q \varepsilon_0} \left[ 1 + \frac{\Omega_2^2 (\Omega_4^2 - \Delta_4^2)}{(\omega^2 - \Omega_2^2) (\Omega_4^2 - \Delta_4^2)} \right] \tag{16}
\]

Physically, the interaction potential \(V(q, \omega)\) gives the coupling strength for scattering a Fermion from the \(K\) to \(K'\) state and it works to break Cooper pairs in the system and to stabilize the superconducting state. From Eq. (16) \(V_{KK'}\) takes three values, \(V_c\) and \(V_{pl}\), depending upon the regions of electron energy as \(V_{KK'} = V_{ph}\) for \(\omega < \Omega_4\), \(V_c\) for \(\Omega - |\omega| < E_F\), and \(V_{pl}\) for \(E_F < |\omega| < \Omega_4\). \tag{17}

Here, \(E_F\) denotes the Fermi energy. The terms \(V_c\), \(V_{ph}\), and \(V_{pl}\) express the Coulomb, electron-coupled phonon-plasmon and electron-plasmon interactions, respectively.

In the strong-coupling theory, the superconducting transition temperature \(T_c\) requires the information of the screened Coulomb's repulsive parameter \((\mu^*)\) and the coupling strength \((\lambda)\) between neighbouring electrons through phonons. The averaged Coulomb repulsive parameter

\[
\mu = \frac{N(O)}{2K_F^2} \int_0^{K_F} \text{Real } V(q, \omega) q d q \tag{18}
\]

to get

\[
\mu = \frac{1}{a_B K_F} \left[ \frac{\ln(1 + a_B K_F^2)}{a_B K_F^2} \right] \tag{19}
\]

where \(a_B = (e / \omega_F^2 n/m^*)\) is the Bohr radius and \(N(O) = (m^*/2\pi \hbar^2)\) denotes the electronic density of states at the Fermi level. Finally, the screened Coulomb repulsive parameter \((\mu^*)\) represents the Coulomb electron-electron interaction as

\[
\mu^* = \frac{\mu}{1 + \mu \ln(E_F / \hbar \Omega_4)} \tag{20}
\]

The coupling parameter \((\lambda)\) is related to the Eliashberg function \(\alpha^2(\omega) F(\omega)\) through

\[
\lambda = \int \frac{\alpha^2(\omega) F(\omega) d\omega}{\omega} \tag{21}
\]

and the Eliashberg function is defined as

\[
\alpha^2(\omega) F(\omega) = \frac{N(O)}{2K_F^2} \int_{\omega}^{2K_F} \text{Imag } V(q, \omega) q d q \tag{22}
\]

to give \(\lambda\) as

\[
\lambda = \frac{2m^* e^2}{\hbar^2 K_F^2} = \frac{\Omega_4^2}{(\omega_F^2 - \omega_T^2)} \tag{23}
\]

Using the screened Coulomb parameter and the coupling strength, at the maximum value of coupled charge oscillations with longitudinal optical phonon frequency. \(T_c\) has been calculated for BaPbBiO superconductor using

\[
T_c = 0.7 \Omega_4 \exp \left[ \frac{1}{\lambda - \mu^*} \right] \tag{24}
\]

Results and Discussion

In order to compute the superconducting state parameters at maximum doping concentration, i.e., \(x=0.25\) in BaPb\(_{1-x}\)Bi\(_x\)O\(_3\) compound, the realistic physical parameters based on the experimental data have been used. The effective mass of the charge carrier (electron) is evaluated as

\[
\frac{m^*}{m_e} = \frac{N(E_F)}{N(E_F^*)} \tag{25}
\]

with \(N(E_F)\) as the band density of states calculated from the electronic specific heat coefficient \((\gamma)\) data\(^9\) as 1.5 mJ mol\(^{-1}\)K\(^{-2}\). The value of \(N(E_F^*^2) = 1.38 \times 10^{30}\) states/mJ/mol has been used as reported earlier by Itoh \textit{et al.}\(^b\) to obtain \(m^* = 1.5 m_e\). The background dielectric constant \(\varepsilon_\infty\) is taken as 4.0 (ref. 10). The Fermi velocity is deduced as 2.26x10\(^7\) cm s\(^{-1}\).

The Coulomb interaction among the adjacent ions in an ionic crystal is expressed in terms of the potential\(^20\).
\[ \Phi(r) = -(Ze)^2 \left[ \frac{1}{r} - \frac{a}{r^n} \right] \] \hspace{1cm} \ldots (26)

where \( a \) is the repulsion force parameter between the ion cores. The effective ion charge is denoted as \( Ze \) and is taken as \(-1.7e\). The elastic force constant \( k \) can be derived from the \( \Phi(r) \) at the equilibrium interionic distance \( r_0 \) as

\[ k = \left[ \frac{\partial^2 \Phi}{\partial r^2} \right]_{r_0} = (Ze)^2 \left[ \frac{n-1}{r_0^n} \right] \] \hspace{1cm} \ldots (27)

where \( n \) is the index number of the repulsive potential and \( r_0 \) is taken as 2.21 Å. The longitudinal and transverse optical breathing vibrations are expressed as

\[ \omega_{LO}^2 = \frac{1}{\mu(m)} [k + \beta^*] \] \hspace{1cm} \ldots (28)

and

\[ \omega_{TO}^2 = \frac{1}{\mu(m)} [k - \beta^*] \] \hspace{1cm} \ldots (29)

Here, the reduced mass \( (\mu) \) is represented as

\[ \mu(m) = \frac{M(\text{Pb}) M(\text{O})}{M(\text{Pb}) + M(\text{O})} \] \hspace{1cm} \ldots (30)

and is 14.84 amu. The force parameter \((\beta^*)\) is

\[ \beta^* = \frac{8\pi (Ze)^2}{3 \Omega} \] \hspace{1cm} \ldots (31)

with \( \Omega \) is the volume of unit cell and is taken to be 316.3 Å\(^3\) (ref. 7). The charge carrier density is \(3.2 \times 10^{21}\) cm\(^{-3}\) (ref. 21). The force parameters have been deduced as \( k = 6.169 \times 10^{14}\) g s\(^{-2}\) and \( \beta^* \) as \(1.763 \times 10^{14}\) g s\(^{-2}\) respectively.

Using these realistic physical parameters based on experimental observations, \( h \Omega \) and \( h \Omega_2 \) modes have accepted. The scattering of charge carriers at the Fermi surface is considered for all values of scattering angle. The wave vector \( q = (2K_F \sin \theta) \) can therefore take maximum values up to \( 2K_F \). It is evident from Eqs (13) and (14) that \( h \Omega(q) \) is a characteristic 2D acoustic plasmon mode and \( h \Omega_2 \) shows the coupled charge oscillations with optical phonon behaviour. The maximum 2D acoustic plasmon energy \( (\hbar \Omega_2) \) is obtained as 0.86 eV and coupled mode \( (\hbar \Omega) \) is deduced as 37.00 meV. The nature of interaction potential \( V_{KK-1} \) is shown in Fig. 1. It is inferred that for the range \( \omega < \Omega \) and \( E_\gamma < |q| < K \), the interaction potential shows the attractive characteristic while for \( \Omega < |q| < E_\gamma \), it is repulsive.

The values of \( E_\gamma \) and \( \mu \) have been obtained as 0.217 eV and 0.39 respectively. Estimated coupling strength in between the neighbouring electrons is 0.84 which favours the weak to moderate coupling theory. The screened Coulomb repulsive parameter is calculated as \( \mu^* = 0.22 \) for the maximum value of coupled frequency (37.00 meV) which shows the poor screening. With these parameters, \( T_c \) has been deduced as 15.50 K, which is higher by 16% than the reported \( T_c \) of 13 K. This allows one to propose that the charge oscillations with longitudinal optical phonons plays a key role and make a good explanation of the mechanism of superconductivity in Ba-Pb-BiO\(_3\) compounds. Besides, evaluating \( T_c \) at maximum doping concentration, attempt has also been made to obtain at different values of doping concentration. The obtained results are, \( x = 0.15 \).
Fig. 3—Variation of $T_c$ with $\lambda$ for a constant $\mu^*=0.22$ value

$T_c=10.35$ K (9 K), $x=0.20$, $T_c=12.76$ K (11 K) and $x=0.30$, $T_c=13.22$ K (11.5 K). The experimental data are given in brackets. These results on $T_c$ with $\lambda$ in BaPbBiO superconductors are although higher but within the range of experimental reported data. Furthermore, efforts have been made to obtain a relationship between $\lambda$, $\mu^*$ and $T_c$ in the proposed approach. In this context taking $\lambda=0.847$ as constant and $\lambda$ on varying $\mu^*$, it was observed that for this value of $\lambda$, $T_c$ decreases with the increased value of $\mu^*$ depicting that for the higher values of $T_c$, the screening parameter should possess low values (Fig. 2). Besides this, the dependence of $T_c$ on $\lambda$ for a fixed value of $\mu^*$ (0.22) has been worked out and is plotted in Fig. 3. It is observed that $T_c$ increases with the increasing value of coupling parameter ($\lambda$). The dependence of $\mu^*$ on $\lambda$ for a fixed value of $T_c=15.5$ K is shown in Fig. 4. It is noticed that $\mu^*$ monotonically increases for the high values of $\lambda$. From these observations, it may clearly be seen that $T_c$ depends on $\lambda$ as well as $\mu^*$. Thus it has been proposed that for high $T_c$ values, $\mu^*$, must be smaller and $\lambda$ values will be higher than 1.0. The low value of $T_c$ for $\lambda=0.84$, $\mu^*=0.22$ and $\Omega=37.00$ meV is in the weak to moderate coupling theory and the choice of parameters is reasonable for Ba-Pb-BiO superconductors.

Conclusions

In this paper, the cubic perovskite BaPb$_{1-x}$Bi$_x$O$_3$ ($T_c=13$ K, $x=0.25$) has been studied with emphasis on the coupled oscillations of electronic charge and breathing vibrations of oxygen. Doping of Ba$^+$ in place of Pb$^+$ introduces free electrons in the empty Pb (6s) band and a strong Coulomb interaction acts between electrons. These electrons couple with the breathing vibration of oxygen as well as charge oscillations in the system. The interaction generates oscillations of the electronic charge and the optical phonons. For simplicity, a single optical phonon mode has been considered whose vibrational frequencies are independent of wave number. The spectral intensity of the charge oscillations is extremely strong to the bare optical phonons. The superconducting transition temperature ($T_c$) has been investigated critically. The appropriateness of the present approach depends on the proper care of the charge oscillation and breathing vibrations. Due to its simplicity, the estimated value of $T_c$ is within the range of reported observations. Deduced values of $\lambda=0.84$ and $\mu^*=0.22$ for maximum $\hbar\Omega=37.00$ meV are quite reasonable and is a good set of physical parameters estimated from the experimental observations to yield high $T_c$ values as of 13 K despite of the low values of the charge carrier density as well as the density of the states at the Fermi level. The main conclusion is that the BaPb$_{1-x}$Bi$_x$O$_3$ is a weak to moderate coupled superconductor ($\lambda$ is nearly 1.0 or less) with strong interaction between electrons and high energy coupled charge oscillations and breathing modes of oxygen ($\hbar\Omega=37.00$ meV). The physical parameters other than $T_c$ in conventional superconductors are extremely varied, but those of highest $T_c$ are characterized by a large density of states at the Fermi level, which leads to a comparatively large value of $\lambda$, and thus to high value of $T_c$. Thus the nature of superconducting state as well as pairing mechanism in BaPb$_{0.75}$Bi$_{0.25}$O$_3$ is well explained by
the coupled charge oscillations with longitudinal optical phonons.

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SUPERCONDUCTIVITY IN BaPb$_{1-x}$Bi$_x$O$_3$ CUBIC OXIDE: A COUPLED CHARGE OSCILLATION WITH OPTICAL PHONON MODEL

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Abstract—The nature of pairing mechanism in cubic perovskite BaPbBiO$_3$ is theoretically investigated. A model potential is developed which includes the Coulomb e-e, electro-optical phonon e-ph) as well as electron-plasmon (e-pi) interactions to elucidate the superconducting state. The presence of these e-e, e-ph and e-pi interactions allows a coherent interpretation of their properties. The estimated value of the coupling parameter $\lambda^* = 0.73$ is consistent with an attractive electron-electron interaction. The screened Coulomb repulsive parameter $\mu^* = 0.31$ suggests poor screening of charge carriers with low concentration and hence reflects the small density of states $N(0)$. The superconducting transition temperature $T_c$ of the system is calculated from the McMillan formula and is consistent with earlier observations. The reduced energy gap of $\Delta/K_bT_c$ is found to be 3.53 which is close to the predicted value of BCS weak coupling theory ($\Delta/K_bT_c = 3.5$). The oxygen isotope shift of $T_c$ is then calculated and the characteristic exponent ($\alpha$) defined as $T_c \times M^{\alpha}$ ($M$ is the oxygen atomic mass) is evaluated as 0.227. These observations on BaPb$_{1-x}$Bi$_x$O$_3$ ($x = 0.25$) suggest that a weak to moderate coupling exists and the coupling of electrons with the coupled charge oscillation-optical phonon mode could be a reason for the superconductivity. © 1998 Elsevier Science Ltd. All rights reserved.

1. INTRODUCTION

The occurrence of superconductivity [1] in a perovskite oxide BaPb$_{1-x}$Bi$_x$O$_3$ with an anomalous high superconducting transition temperature $T_c \approx 13$ K provides an opportunity to understand the mechanism of pairing as well as the nature of superconducting states. The interest in this system has become increased due to the recent findings of superconductivity [2] in Ba$_{1-x}$K$_x$, Rb$_x$BiO$_3$ with a critical temperature up to 30 K. which is similar to those of the high temperature Lanthanum based copper oxides (La$_2$Sr$_n$CuO$_{4n}$). The cubic oxide based superconductors are highly anisotropic in their physical properties due to the two-dimensional (2D) character of the conducting copper oxide (CuO$_2$) planes. However, the non-transition metal compound BaPb$_{1-x}$Bi$_x$O$_3$ (BPBO) is isotropic as the oxygen octahedra form a three-dimensional (3D) network. The parent compound La$_2$CuO$_4$ is an antiferromagnetic insulator, instead BaBiO$_3$ is semiconducting with a low density of states at the Fermi level. The high values of $T_c$ despite essential differences in the copper and bismuth families have raised serious queries regarding the common pairing mechanism.

The parent compound BaBiO$_3$ is semiconducting, the breathing mode is completely softened and the static displacements of the oxygen atoms have been observed from crystallographic studies [3]. The chemical substitution of Pb in place of Bi introduces free charge carriers, and the BiO lattice is modified. The resistivity and Hall-coefficient measurements [4] revealed that the system BaPb$_{1-x}$Bi$_x$O$_3$ shows a metallic behaviour in the compositional range $0.0 \leq x \leq 0.35$. The superconductivity [1] is observed for $0.05 \leq x \leq 0.35$ with a maximum $T_c \sim 13$ K at $x = 0.25$, despite the fact that the charge carrier density [5] ($n = 10^{21}$ cm$^{-3}$) and the density of states at the Fermi level [6] (0.1 states/eV unit cell spin) are much smaller than in conventional superconductors with similar $T_c$'s. The metal to semiconductor transition in BPBO occurs at $x = 0.35$ and the material exhibits semiconducting characteristics in the range $0.35 \leq x \leq 0.5$. The doping concentration $x$ dependence of $T_c$ follows almost the same behaviour as the variation of charge carrier density ($n^{*}$) with $x$ [4].

Band structure calculations on BaPb$_{1-x}$Bi$_x$O$_3$ have been performed by Mattheiss and Hamann [7]. According to their studies this cubic alloy possesses a single broad conduction band that comes from the $\pi$-antibonding mixture of Pb—Bi($6s$) and O($2p$) states. They stress the presence of a complex of hybridized states near the Fermi energy, giving a low density of states. These electrons couple strongly to optical breathing vibration modes occurring between neighbouring oxygen and lead-bismuth atoms. The Raman study of lattice vibrations together with infrared spectroscopy results [8], confirm...
the presence of LO and TO breathing vibrations in Ba–Ph–BiO perovskites. They point out that the resonant Raman effect is caused by the charge transfer via the Forchlich type electron-phonon interaction. The electron-lattice interaction of Ba–Ph–BiO is studied microscopically by using the realistic electronic bands of BaBiO reproduced by the tight binding model [9]. The superconductivity was discussed in the framework of strong coupling theory of electron-lattice interactions caused by the longitudinal modes of oxygen stretching breathing vibration. These observations and the low density of states at the Fermi level, have led to the question of whether the strong interaction of electrons with oxygen breathing mode alone is the primary mechanism of pairing in these cubic oxides to account for the high $T_c$.

Reflectivity measurements have been carried out by Taiima et al. [10] over a wide energy range and also over the whole compositional range in BaPb$_{1-x}$Bi$_x$O$_3$ superconductors. The phonon structure is observed by far-infrared optical and Raman scattering measurements and plasma excitations are seen in the visible and near infrared region. They have focused their attention on the plasmon behaviour determined from the reflectivity spectra on single crystals as well as polycrystalline samples at the Bi concentration ($x \geq 0.27$), where the system shows semiconductor characteristics. It is suggested that electrons supplied by the Bi atoms are involved in this collective excitation (plasmons) although an energy gap is formed at the Fermi surface. The existence of plasmons is well confirmed by this group [11] from the electron-energy loss spectroscopy (EELS) at the bismuth dopant level ($x = 0.27$). This suggests the participation of a collective excitation besides optical phonons in the pairing mechanism in BaPb$_{1-x}$Bi$_x$O$_3$ superconductors. However, the presence of an oxygen isotope effect [12] (coefficient $\alpha = 0.22$) and the energy gap ratio ($\Delta = 2\Delta/K_BT_c \approx 3.5 \pm 0.5$), now clearly indicate that the usual electron-phonon interaction plays an important role. All these results are suggestive of the presence of ionic excitations as well as the electronic excitations. Furthermore, the substantial attractive interaction caused by charge oscillations with optical phonon modes in the metallic phase would bring high $T_c$ superconductivity in Ba–Ph–BiO systems. Batlogg et al. [12] have suggested that anomalous high $T_c$ in BiO superconductors is not due to conventional strong electron-phonon coupling but that the pairing is mediated by electronic excitations which involve the atomic displacements as a result of charge redistribution [13]. Also, the apparent absence of magnetic ordering in Ba–Ph–BiO and the significant presence of oxygen isotope effect with high $T_c$ favours the idea of a pairing mechanism via phonons and plasmons.

Looking to the earlier experimental observations and theoretical studies, a creative approach is required to associate the standard phonon model with an exotic model that can explain the observed $T_c$ and associated physical parameters. During the recent past the plasmon mechanism [14] has emerged as a central theme in the formation of additional pairing and could lead to high $T_c$ values in copper oxides. Recently, Varshney and Singh have made an attempt to study the joint phonon and plasmon mechanism in the lanthanum copper oxides based on a free electron layered electron gas model [15]. Deduced results from the above approach on superconducting state parameters of La-(Ba/Sr) CuO are consistent with the experimental observations. The purpose of the present communication is to study the role of charge oscillations as well as of the phonon breathing mode in the cubic perovskite Ba–Ph–BiO and to see what set of parameters can explain the experimental measurements in the normal metallic state. In the present studies, we have confined ourselves to the metallic state; the semiconducting state of this system will be studied separately. Such studies on Ba–BiO systems have wide potential as the $T_c$ is high and resembles that of CuO based superconductors. Earlier, Tachiki and Takahashi [16] explained the superconductivity in copper oxides, when the pairing interaction is mediated by the charge transfer oscillations associated with LO phonons and suggested a similar mechanism in Ba–Ph–BiO superconductors. In view of the earlier experimental and theoretical findings a model potential is developed including Coulombic, electron-plasmon interactions to look for the pairing mechanism as well as physical parameters in the superconducting state. The approach is used to work out (a) the coupling strength ($\lambda$), (b) the screened Coulomb repulsive parameter ($\mu^*$), (c) the 2D acoustic plasmon energy ($h\Omega_{pd}$) and (d) the coupled oscillations of electronic charge associated with longitudinal optical phonon energy ($h\Omega_{lo}$) in bismuth oxides. Finally, the transition temperature for maximum $T_c$ doping concentration ($x$) is evaluated.

The plan of this paper is as follows: In Section 2 we formulate the interaction potential by considering breathing modes of oxygen and charge oscillations developed by the electrons supplied from the Bi atoms in Ba–Ph–BiO. The polarizability is included through a model dielectric function which fulfils the $\varepsilon$-sum rule. The model parameters ($\lambda$ and $\mu^*$) are deduced and for a set of these parameters the superconducting transition temperature $T_c$ is then calculated. We also calculate the decrease of $T_c$ when $^{17}$O is completely replaced by $^{18}$O in the bismuth oxide. The energy gap parameter is also estimated. The details of numerical analysis and results obtained are discussed in Section 3. Finally, in Section 4, we present our conclusions.
2. ESSENTIAL FORMALISM

The parent BaPbO₃ compound is regarded as a semimetal. The empty Pb(6s) band slightly overlaps with the O(2p) band. Chemical substitution of Bi⁺⁺ in place of Pb⁺⁺ introduces one electron per Bi atom in the empty Pb(6s) band which are the active charge carriers (electrons) of effective mass m* and will participate in the pairing mechanism. Besides these active charge carriers the contraction and expansion of oxygen octahedra around the Bi or Pb atoms will give rise to breathing modes of phonons. The Bi atom has two stable ionic states in the form of Bi⁺⁺ and Bi⁺⁺, which allows the valence of Bi atoms to fluctuate even in the Pb⁺⁺ matrix. We first consider a two component plasma. In terms of its dielectric function ε(q,ω), the electron–electron matrix element between the states |k⟩ and |k'⟩ corresponding to the energies E(k) and E(k′) is

\[ V_{kl} = e^2 q q' e(q, ω_{kl}) \]  

with \( q = k - k' \) and \( ω_{kl} = |E(k) - E(k')|/ħ. \)

The dielectric function of the oxide is given by a sum of ionic and electronic polarizabilities. The model dielectric function is represented by

\[ ε(q, ω) = ε_e + Ω_{LO}^2 / (q^2 - ω^2) + ε_e [ω_{TO} - ω_{TO}] / (ω_{TO} - ω^2) \]  

Here, \( Ω_{LO}^2 = q^2 V_F^2 / 2 \) with \( V_F \) the Fermi velocity. The symbols \( ω_{LO} \) and \( ω_{TO} \) are the frequencies of LO and TO breathing vibrations. For the sake of simplicity, we have considered a single optical phonon whose vibrational frequencies are independent of wave vector \( q \). In the above equation the first term is the polarizability of ionic core-electrons. In the frequency region of interest, \( ε_{ion} \) is assumed to be a constant (= ϵ_0) and is independent of frequency. The electronic and ionic polarizabilities are represented by the second and third terms, respectively. When an ionic semimetal is doped with a small number of electrons or holes, the crystal becomes metallic and the current carriers also contribute to the dielectric constant. A realistic calculation of \( P(q,ω) \) requires a rigorous many body treatment for the behaviour of charge carriers [17].

The model dielectric function for the polarized waves with the above description becomes

\[ ε(q, ω) = ε_e \left[ 1 + \frac{D_1}{ω - ω'} - \frac{D_2}{ω - ω''} \right] \]  

Here, \( D_1 = \Omega_{LO}^2 / 2 \) denotes a screened plasma frequency and \( D_2 = ω_{TO}^2 / 2 \) with \( ω_{TO} \) respectively. The spectral intensity of the polarized wave is expressed as

\[ Ρ(q, ω) = \frac{1}{π} \text{Imag} \frac{ε_e}{ε(q, ω)} \]  

where the dielectric function is given by eqn (3). Physically it corresponds to the excitation density of polarized waves.

The main input parameter which determines the critical transition temperature, is the dynamic interaction potential \( V(q,ω) \) or equivalently \( ε(q,ω) \) of the system. If to the first approximation, \( ε(q,ω) \) is identified with the inverse longitudinal dielectric function of the system, it can be associated with different longitudinal modes, corresponding to the exchange of photons or plasmons, having poles at the respective modes. Since we are interested in separating the individual contributions of \( ε(q,ω) \) from different longitudinal modes, we do the inversion of eqn (3) in the form

\[ ε(q,ω) = ε_e \left[ 1 + \sum_{i=1}^{∞} \frac{f_i}{ω - ω_i} \right] \]  

where \( f_i \) are the frequencies of two longitudinal modes and the resonant frequencies are given by

\[ (Ω_i^2 - δ_i^2)(ω_i^2 - δ_i^2) - D_1 (δ_i^2 - δ_i^2) + D_2 (δ_i^2 - δ_i^2) = 0 \]  

Thus, the effective interaction potential \( V(q,ω) \) is the sum of electronic and ionic contributions, \( V(q,ω) = V_e(q,ω) + V_i(q,ω) \)

The following sum rules are valid:

\[ \sum_{i=1}^{∞} Ω_i^2 = D_1 + D_2 \]  

\[ \sum_{i=1}^{∞} f_i(q) = D_1 - D_2 \]  

\[ \sum_{i=1}^{∞} f_i(0) / Ω_i^2(0) = 1 \]

Here, \( f_i(0) / Ω_i^2(0) \) is the limiting value of \( f_i(q) / Ω_i^2(q) \) in the long wavelength limit.

This implies that

\[ ε(q,ω) \rightarrow ε_e + 1 / ω \]  

when \( ω \rightarrow 0 \) and \( ε_e \) \( \rightarrow \) \( 1 / 2 \).

Zeros of the model dielectric function will yield two modes of the polarized waves and the frequencies of the coupled mode in the long wavelength limit are: 

\[ Ω_±^2 = (Ω_{LO}^2 - δ_i^2) \]  

\[ ± \sqrt{(Ω_{LO}^2 - δ_i^2) - 4(ω_{TO}^2 - ω_{TO}^2) δ_i^2} \]

Further simplification yields

\[ Ω_±^2 \equiv Ω_{LO}^2 - δ_i^2 \]

where \( δ_i = \sqrt{δ_i^2} \).
showing the 2D acoustic plasmon characteristic. The lower mode is expressed as
\[ \Omega_{\pm}^2 = \frac{\omega_{\pm}^2 + \omega_{\mp}^2}{2} \] (14)
which is basically a coupled charge oscillation with optical phonon mode.

The effective longitudinal dielectric function in terms of the 2D acoustic plasmon mode \( \pm \) and coupled charge oscillation with phonon-mode \( \Omega_{\pm} \) is now written as
\[ \varepsilon_{\text{eff}}(q, \omega) = \frac{(\omega^2 - \Omega_{\pm}^2)(\omega^2 - \delta^2)}{(\omega^2 - \delta^2)(\omega^2 - \delta^2)} \] (15)
and the interaction potential takes the form
\[ V(q, \omega) = V_c(q) \frac{1}{\varepsilon_x} \left( \Omega_{\pm}^2 - \delta^2 \right) \]
\[ = \frac{4\pi e^2}{\varepsilon_x} \left[ \frac{1}{\varepsilon_x} \frac{\Omega_{\pm}^2 - \delta^2}{\Omega_{\pm}^2 - \delta^2} \frac{\delta^2}{\Omega_{\pm}^2 - \delta^2} - \frac{\delta^2}{\Omega_{\pm}^2 - \delta^2} \right] \] (16)

Physically, the interaction potential \( V(q, \omega) \) gives the coupling strength for scattering a Fermion from the \( k \) to \( k' \) state. Here, the first term in the right-hand side represents the direct Coulomb repulsion \( V_c(q) \) and second term is the interaction from exchange of electronic excitations \( \delta \) denoted as \( V_{\text{ex}} \). The third term \( V_{\text{ph}} \) is contributed from the exchange of ionic excitations \( \Omega_{\pm} \).

The Coulomb repulsive parameter is written as
\[ \mu^* = \frac{\mu}{1 + \mu \ln(eF/\Omega_{\pm})} \] (17)
where \( \mu = a^2 \ln[(1 + a^2)/a^2] \), \( a^2 = K_f^2/4K_F^2 \). \( K_f^2 = 4\pi e^2N(0) \) is the Thomas–Fermi wave vector and \( K_F^2 \) is the Fermi wave vector. The density of state at Fermi energy \( N(0) \) in three dimensions is
\[ N(0) = \frac{N(E_F)}{2\pi^2} \frac{m_e^*}{h^2} = \frac{N(E_F)}{2\pi^2} \frac{m_e^*}{h^2} \] (18)
with Fermi energy \( E_F = h^2(3\pi^2 n)^{1/3}/2m \).

The dimensionless coupling strength is
\[ \lambda = N(0)(\lambda^2)/M(\Omega_{\pm}^2) \] (19)
where \( \lambda > 1 \) is expressed as
\[ \langle \lambda^2 \rangle = \left[ \frac{\lambda^2}{2\pi^2} \frac{m_e^*}{h^2} \right] [V(k,k')V(k,k')]^2 \]
\[ \times \delta E_{k'} - \delta E_{k} \delta E_{k'} - \delta E_{k} ([V(2\pi)^2]) \int d^3k \]
\[ \times \left[ \int d^3k' \delta E_{k'} - \delta E_{k} \delta E_{k'} - \delta E_{k} ([N(0)])^2 \right] \]
\[ \times \int_0^{2K_F} q dq/2K_F \left[ V(q) \right]^2/[N(0)]^2 \]
\[ \times \int_0^{2K_F} q dq/2K_F \right] \times \int_0^{2K_F} q dq/2K_F \right] \times \int_0^{2K_F} q dq/2K_F \right] \times \int_0^{2K_F} q dq/2K_F \right] \times \int_0^{2K_F} q dq/2K_F \right] (20)
Here, \( V(q) \) is the screened Coulomb potential \( V(q) = V_0(q)/\epsilon(q) \) with \( V_0(q) \) is bare Coulomb potential. \( \epsilon(q) \) is the static dielectric function in the low \( q \) limit from eqn (2) and is \( \epsilon(q) = 4me^2K_F/\pi\hbar^2q^2 \). Thus, we have
\[ \frac{V(q)}{\epsilon(q)} = \frac{4\pi Ze^2/\Omega_{\pm}^2}{4me^2K_F/\pi\hbar^2q^2} = \frac{h^2 \pi^2 Z}{mK_F \varepsilon_x \Omega} \] (21)
where \( \Omega \) is the volume of the cell and \( Z \) denotes effective ionic charge.

Finally, we obtained
\[ \langle \lambda^2 \rangle = \frac{1}{\varepsilon_x^2 K_F \Omega_{\pm}^2} \left[ h^2 \pi^2 Z/\Omega_{\pm}^2 \right] \]
\[ = 2/h^2 \pi^2 Z/\Omega_{\pm}^2 \] (22)
Thus, the coupling strength is now written as
\[ \lambda = 2N(0)(\lambda^2)/M(\Omega_{\pm}^2) \] (23)
here. \( \Omega_{\pm}^2 \) is the normalized coupled charge oscillation-optical phonon frequency and \( M \) denotes the ionic mass.

Using the screened Coulomb parameter and the coupling strength, for the renormalized value of coupled charge oscillations with optical phonon frequency, we have calculated \( T_c \) for BaPbBiO using \[ T_c = 0.7\Omega_{\pm} \exp \left[ \frac{1}{\lambda - \mu^*} \right] \] (24)
The isotope effect exponent is
\[ \alpha = \frac{\ln(T_c)}{\ln M} = \frac{1}{\ln(\lambda - \mu^*)} \] (25)
The energy gap parameter \( \beta \) is expressed as
\[ \beta = \frac{2\lambda}{K_F \Omega_{\pm}} = 3.52[1 + 5.3(T_c/\Omega_{\pm})^2]/\ln(\Omega_{\pm}/T_c) \] (26)
Using the developed expressions, the superconducting transition temperature \( T_c \) and \( \alpha \) in BaPbBiO (\( x = 0.25 \)) are computed in the next section.

3. RESULTS AND DISCUSSION

In order to compute the superconducting state parameters at maximum doping concentration, i.e. \( x = 0.25 \) in BaPbBiO, we have used realistic physical parameters based on the experimental data as follows. The effective mass of the charge carrier (electron) is evaluated as
\[ m^* / m_e = N(E_F)/N(E_F^2) \] (27)
with \( N(E_F) \) is the band density of \( s^* \) states calculated from the electronic specific heat coefficient \( (\gamma) \) data as \( 1.5 \, \text{mJ} \cdot \text{mol}^{-1} \cdot \text{K}^{-2} \) [19]. We use the value of \( N(E_F^2) = 1.38 \times 10^{19} \, \text{states} \cdot \text{m}^{-1} \cdot \text{mol}^{-1} \), as reported earlier by Itoh et al. [6] to obtain \( m^* = 1.5 m_e \). The background dielectric constant \( \varepsilon_x \) is taken as 40 [10]. The Fermi velocity is deduced as \( 3.496 \times 10^7 \, \text{cm} \cdot \text{s}^{-1} \). The Coulomb interaction...
among the adjacent ions in an ionic crystal is expressed in terms of the potential \[ \Phi(r) = -(Ze)^2 \left( \frac{1}{r} - \frac{1}{r_0} \right) \] (28)

where \( a \) is the repulsion force parameter between the ion cores. The effective ion charge is denoted as \( Ze \) and is taken as \(-1.7e\). The elastic force constant \( k^* \) can be derived from the \( \Phi(r) \) at the equilibrium interionic distance \( r_0 \) as

\[ k^* = \left[ \frac{d^2\Phi}{dr^2} \right]_{r_0} = (Ze)^2 \left( \frac{1}{r_0^3} - \frac{1}{r^3} \right) \] (29)

where \( n \) is the index number of the repulsive potential and \( r_0 \) is taken as 2.21 Å. The force parameter \( \beta^* \) is

\[ \beta^* = \frac{8\pi(Ze)^2}{3} \frac{\Omega}{n} \] (30)

with \( \Omega \) is the volume of unit cell and is taken to be 316.3 Å\(^3\). The longitudinal and transverse optical breathing vibrations are expressed as

\[ \omega_{LO} = \frac{1}{\mu(m^*)} (k^* - \beta^*) \] (31)

and

\[ \omega_{TO} = \frac{1}{\mu(m^*)} (k^* - \beta^*) \] (32)

Here, the reduced mass \( (\mu) \) is represented as

\[ \mu(m) = \frac{M(Pb)M(O)}{M(Pb) + M(O)} \] (33)

and is 14.84 amu. The charge carrier density is \( 2.2 \times 10^{21} \) cm\(^{-2}\) [21]. We deduce first the force parameters \( k^* = 30.844 \times 10^4 \) g cm\(^{-2}\) and \( \beta^* = 1.763 \times 10^4 \) g cm\(^{-2}\) from eqns (29) and (30). Here, we have used \( n = n \) for BaPbBiO\(_3\) superconductors. For most ionic crystals, the index number of repulsive potential has been reported to be \( n = 0 \sim 5 \) [22]. Furthermore, \( \omega_{LO} \) and \( \omega_{TO} \) are then estimated from eqns (31) and (32) using the above description.

Using these realistic physical parameters based on experimental observations, we have computed the \( \hbar\Omega_L \) and \( \hbar\Omega_T \) modes. The scattering of charge carriers at the Fermi surface is considered for all values of scattering angle \( \theta \). The wave vector \( q \) is given as \( 2K \cos \theta \), which is consistent with the earlier data [8]. The calculated Coulomb repulsive parameter is deduced as \( \alpha^* = 0.31 \) for the renormalized value of coupled frequency (73.47 meV) which shows poor screening. With these parameters, we deduce \( T_c \sim 9.7 \) K, which is consistent with the reported \( T_c \sim 13 \) K [1]. This allows one to propose that the scattering of charged oscillations with longitudinal optical phonons plays a key role and provides a good explanation of the mechanism of superconductivity in BaPbBiO\(_3\) compounds.

The proposed model calculation also predicts the existence of an oxygen isotope effect [10]. An oxygen isotope effect has been observed [12] as \( \alpha = 0.22 \) in a BPBO system although with a smaller value than in the BCS limit. Since the mass of oxygen directly influence-

### Table 1: Calculated physical parameters of BaPb\(_{1-x}\)Bi\(_x\)O\(_3\)

<table>
<thead>
<tr>
<th>Sample no.</th>
<th>Quantity</th>
<th>Unit</th>
<th>Formula</th>
<th>BaPb(_{1-x})Bi(_x)O(_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>( m^*m )</td>
<td></td>
<td>( \mu )</td>
<td>( 28 \times 10^{-4} )</td>
</tr>
<tr>
<td>2.</td>
<td>( \omega^* )</td>
<td>( \mu )</td>
<td>( 28 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>3.</td>
<td>( \alpha )</td>
<td>( 10^9 )</td>
<td>( 29 )</td>
<td></td>
</tr>
<tr>
<td>4.</td>
<td>( \beta )</td>
<td>( 10^9 )</td>
<td>( 30 )</td>
<td></td>
</tr>
<tr>
<td>5.</td>
<td>( \Theta_{LO} )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>6.</td>
<td>( \Theta_{TO} )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>7.</td>
<td>( \Theta_{LO} )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>8.</td>
<td>( \Theta_{TO} )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>9.</td>
<td>( \Theta )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>10.</td>
<td>( \Theta )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>11.</td>
<td>( \epsilon )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>12.</td>
<td>( \epsilon )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
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</tr>
<tr>
<td>13.</td>
<td>( \epsilon )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
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</tr>
<tr>
<td>14.</td>
<td>( \epsilon )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>15.</td>
<td>( \epsilon )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>16.</td>
<td>( \alpha )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>17.</td>
<td>( \alpha )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>18.</td>
<td>( \beta )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
<tr>
<td>19.</td>
<td>( \beta )</td>
<td>( \mu )</td>
<td>( 29 \times 10^{-4} )</td>
<td></td>
</tr>
</tbody>
</table>
the optical phonon frequencies and hence the \( T_c \), one may expect a reasonable oxygen isotope effect. Equation (25) estimates \( \alpha \) as 0.227, which is consistent with the experimental value. Although the pure BCS value of \( \alpha \) is 0.5, the theoretically calculated values suggest the crucial role of oxygen breathing vibrations and their coupling to the electronic states at the Fermi level. The smaller value of \( \alpha \) might be due to the choice of superconducting state parameters of the system in the proposed approach. Besides transition temperature and oxygen isotope effect, the energy gap parameter \( (\beta) \) has also been estimated. The BCS gap ratio \( 2\Delta/K_bT_c \) is evaluated at 3.53, which is in agreement with the reported value of 3.5 \pm 0.5 for bismuth compounds [12]. Recently, Navarro [23] has presented the results of thermodynamical analysis on BaPb\(_{0.99}\)Bi\(_{0.01}\)O\(_3\), and found that the value of energy gap ratio \( (\beta = 2\Delta/K_bT_c) \) is 3.57, close to the BCS result.

4. CONCLUSIONS

In this communication, we have discussed our efforts to study the cubic perovskite BaPb\(_{1-x}\)Bi\(_x\)O\(_3\) \((T_c = 13\, K, x = 0.25)\) by emphasizing the coupled oscillations of electronic charge and breathing vibrations of oxygen. Doping of Ba\(^{2+}\) in place of Pb\(^{2+}\) introduces free electrons in the empty Pb\(_{6s}\) band and a strong Coulomb interaction acts between electrons. These electrons will couple with the breathing vibration of oxygen as well as other charge oscillations in the system. The interaction will generate oscillations of the electronic charge and the optical phonons. For simplicity, we have considered a single optical phonon mode whose vibrational frequencies are independent of wave number. The spectral density of the charge oscillations is extremely strongly coupled to the bare optical phonons. We have investigated critically, the superconducting state parameters, i.e. (a) transition temperature \( (T_c) \), (b) oxygen isotope effect \( (\alpha) \), and (c) energy gap parameter \( (\beta) \). The appropriateness of the present approach depends on the proper care of the charge oscillation and breathing vibrations. Despite its simplicity, the estimated value of \( T_c \) is within the range of reported observations. Deduced values of \( \lambda = (0.73) \) and \( \mu^* = (0.31) \) for maximum \( K \Omega_2 = 73.47 \, \text{meV} \) are quite reasonable and provide a good set of physical parameters estimated from the experimental observations, which yield high \( T_c \) value of 10 K despite of the low values of the charge carrier density as well as the density of the states at the Fermi level. The main conclusion is that the BaPb\(_{1-x}\)Bi\(_x\)O\(_3\) is a weak coupling superconductor \( (\lambda \) is nearly 1.0 or less) with weak to moderate interaction between electrons and high energy coupled charge oscillations and breathing modes of oxygen \( (\Omega_2 = 73.47 \, \text{meV}) \). The physical parameters other than \( T_c \) in conventional superconductors are extremely varied, but those of highest \( T_c \) are mostly characterized by a large density of states at the Fermi level, which leads to a comparatively large value of \( \lambda \) and thus to high \( T_c \).

The optical phonon frequencies are predicted by the proposed approach to be a key feature, as confirmed by the presence of a large oxygen isotope effect. The value of \( \alpha \) as well as \( \beta \) fall into the weak to moderate coupling theory for admissible values of \( \Omega_2 \). These are consistent with a pure electron–phonon mechanism, which involves the vibrations of oxygen atoms. In conclusion, the nature of the superconducting state as well as the pairing mechanism in BaPb\(_{0.99}\)Bi\(_{0.01}\)O\(_3\) is well explained by the coupling of charge oscillations with longitudinal optical phonons. The energy gap ratio, oxygen isotope effect and the superconducting transition temperature in this system can be analyzed in terms of a weak to moderately coupled superconductors. As regard of Ba–K–BiO superconductors, it is believed that they are strongly coupling systems. The present approach is extended to Ba–K–BiO\(_2\) superconductors with high \( T_c \) value and this work will be reported in future.

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Current excited plasma instabilities in anisotropic cuprate superconductors

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Based on free electron layered electron gas (FELEG) model of quasi two dimensional planes (CuO₂) in anisotropic copper oxide superconductors, we examine the phenomenon of current excited plasma instabilities. A dielectric response function is developed with electron-ion plasmon and electron-electron plasmon interactions by properly incorporating the structure factor for layered systems in two temperature domains i.e., at low temperature \( T \ll 0 \) K and near the vicinity of \( T_c \). A cold beam type current excited instability is generated at low temperature as scattering effects are absent. Furthermore, near the vicinity of \( T_c \) an instability can be generated for sufficiently large drifts in these high \( T_c \) cuprate superconductors. This instability might occur due to Cooper pair breaking effects. For these anisotropic cuprate superconductors the \( T_c < \Delta \) as well as \( T_c < \phi \), the drift velocity does not exceed the phase velocity. Hence the damping will be associated with the single particle absorption in original plasma waves. The implications of the above analysis are discussed in view of recently discovered high \( T_c \) copper oxide superconductors.

1. Introduction

Much research activity is currently being focussed on the properties of high - \( T_c \) superconductors based on the oxygen deficient perovskites. The interest extends far beyond the solid state community as these materials hold great promise for a variety of futuristic technological importance. The early thrust has centered on the methods of preparation, study of structural features as well as the electromagnetic response of these materials. In spite of gigantic efforts made jointly by scientists all over the world, there is still no consensus on theoretical understanding among them. As major inroads are being made in these areas, the interest broadens to a wider spectrum of anomalous physical and chemical properties in the hope of providing a cohesive picture of superconducting state responsible for electron pairing at temperatures of the order of 100 K. One research area that is beginning to yield useful information is the plasma instabilities which are although well known in gaseous state but current excited plasma instabilities in high \( T_c \) superconductors are yet to explore.

The high \( T_c \) superconductors as Nd-Ce-CuO (Ref.2) \( [ \delta = 0.15, T_c \approx 17 \text{K (1.46 meV)} ] \) La-Sr-CuO (Ref.3) \( [ \delta = 0.15, T_c \approx 38 \text{K (3.27 meV)} ] \), YBaCuO(Ref.4) \( [ \delta = 0.0, T_c \approx 90 \text{K (7.75 meV)} ] \) and HgBaCuO(Ref.5) \( [ \delta = 0.08, T_c = 94 \text{K (8.10 meV)} ] \) are highly anisotropic in their physical properties due to two dimensional (2D) character of the conducting copper oxide (CuO₂) planes. These cuprates can be viewed as layered structure with a periodic stack of 2D electron gas layers with conducting as well as insulating planes. In the elemental unit cell of copper oxides, the active conducting CuO₂ planes are well separated by insulating building blocks. Indeed the main attention is focussed on the conducting (CuO₂)n planes which contain the free charge carriers as well as ions and are thought to be responsible for high \( T_c \) phenomenon. In the recent past, the semiconductor technology has led to the systems which are layered...
as well as two dimensional in character. Several attempts, so far unsuccessfully have been made to observe current driven plasma instabilities both in bulk and layered semiconductors. The problem is to reach the instability threshold i.e., the carrier velocity at which the transfer of energy from the current into plasma oscillations will begin. As the threshold velocity in semiconductor is high, one needs a mobile plasma for achieving amplification. Although this effect is possible as the current-plasma wave energy transfer to be limited due to an intrinsic absorption associated with the carrier phonon or carrier impurity scatterings. Naturally, to achieve a particular drift velocity, we have to constrain ourselves to the systems with low dimensionality as well as reduced carrier scattering. However, it has been shown in layered semiconductors the 2D plasma of very high mobility can be formed.

Collective oscillations in superconductors were studied since late fifties. It was shown by Bogolyubov and Anderson that the free oscillations of the phase of the superconducting order parameter would have an acoustic spectrum provided that the electron gas is ignored. However, the perturbation of the electron density creates Coulomb forces and therefore, transforms such oscillations into a plasma mode whose energy is much larger than the superconducting energy gap ($\Delta$). Thus the resulting oscillations are nearly identical to usual plasma oscillations in a normal metal. The plasma oscillations may also appear in highly anisotropic layered superconductors like high $T_c$ superconductors. The high $T_c$ cuprates can be considered as a stack of quasi 2D superconducting layers with Josephson interlayer coupling which was confirmed by experimental reports of the Josephson effect. Therefore, plasma oscillations analogous to these in Josephson tunnel junction arrays are present in layered cuprate superconductors. Plasma oscillations through Josephson junctions were studied in a pioneering paper by Dinter for clean superconductors ($\omega << 2\Delta$) in the vicinity below $T_c$.

In the present paper, the possibility of current excited plasma instabilities in a superconducting plasma has been studied. As this instability has earlier been studied in semiconductors, we planned to study the copper oxide superconductors by considering two temperature regimes. For low temperatures i.e., $T \approx 0$ K, where the carrier scattering effects are negligible near the vicinity of critical temperatures, where the plasma oscillations of superconducting electrons exist in the superconducting state. These plasma oscillations are damped due to the absorption of energy associated with the Cooper pair breaking effects. In the vicinity below $T_c$, we make use of the dielectric function formalism developed by Dinter and properly introduced the structure factor for layered systems to obtain the drift velocity. Such an approach allows one to take strictly into account the influence of normal as well as superconducting electrons. In addition, this approach permits us to elucidate the dispersion of plasma waves in terms of drift velocity for both temperature domains.

2 Essential Formalism

The layered cuprates such as La$_{2-x}$Sr$_x$CuO$_4$, Nd$_{2-x}$Ce$_x$CuO$_4$, and HgBa$_2$CuO$_4$ contain conducting isolated planes of CuO$_2$ which have a significant number of free charge carriers. These charge carriers are developed by way of chemical substitution (x) or oxygen content (6) in the parent compound. The developed free charge carriers interact by way of Coulomb law with charges on nearby CuO$_2$ planes and the resulting potential has a strong effect particularly in the long wavelength limit ($q \rightarrow 0$). We treat the elemental unit cell of cuprates consisting of two dimensional (2D) layers in the x-y plane with relatively weak coupling between the planes in the perpendicular z direction (c axis). The periodic array of La$_{2-x}$Sr$_x$CuO$_4$, Nd$_{2-x}$Ce$_x$CuO$_4$, and HgBa$_2$CuO$_4$ with single CuO$_2$ plane in a unit cell can be described by the layers (Fig. 1) with a varying degree of interlayer coupling. To a first approximation these layers are well separated and treated as non-interacting. We consider the screened Coulomb potential for a series of identical CuO$_2$ planes separated by a distance $d (=c/2)$. Furthermore, both electronic as well as ionic excitations in the conducting CuO$_2$ planes will contribute to the superconducting mechanism. The effective interaction between charge carriers is expressed as:

$$V(q,\omega,T) = Vc(q) / \varepsilon(q,\omega,T)$$ ... (1)
Here $V_C(q)$ is the bare Coulomb potential between the charge carriers, $\varepsilon(q, \omega, T)$ is the dielectric function for a single band of charge carriers and $q$ is the in-plane wave vector.

The Fourier transformed interaction potential is:

$$V(q, q_2, \omega, T) = \frac{2\pi e^{-2}}{q\varepsilon_0} \varepsilon(q, q_2, \omega, T)$$

with $S(q, q_2)$ is the structure factor for layered cuprates with single conducting CuO$_2$ plane sandwiched between insulating planes of the elemental unit cell and is given as:

$$S(q, q_2) = \frac{\sinh(qd)}{\cosh(qd) - \cos(q_2d)}$$

In terms of polarizability, $\varepsilon$ is defined as:

$$\varepsilon(q, q_2, \omega, T) = 1 + P(q, \omega, T)S(q, q_2)$$

with

$$P(q, \omega, T) = -\frac{2\pi e^{-2}}{q\varepsilon_0} \Pi(q, \omega, T)$$

and $\varepsilon_0$ is the background dielectric constant of the surrounding material.

The cuprates have anisotropic physical properties and it is convenient to confine the effective potential between the charge carriers along the $a$-plane. Averaging $V(q, q_2, \omega)$ over $q_2$, the effective potential along the conducting plane is:

$$V(q, \omega, T) = \frac{d}{2\pi} \int_{-\pi d}^{\pi d} V(q, q_2, \omega, T) dq_2$$

and to get

$$V'(q, \omega, T) = \ldots$$
\[ -2\pi e^2 \frac{D(q,\omega,T)\sinh(qd)}{D(q,\omega,T) - 1} \left\{ \sqrt[4]{\frac{D(q,\omega,T)}{2}} \right\} \] \hspace{1cm} (7)

with

\[ D(q,\omega,T) = \sinh(qd) P(q,\omega,T) + \cosh(qd) \] \hspace{1cm} (8)

For small \(qd\) values, we do write:

\[ D(q,\omega,T) \approx 1 + (qd)P(q,\omega,T) \] \hspace{1cm} (9)

The dynamic polarizability of a layered electron gas in the cuprates is due to the active charge carriers of effective mass \(m^*\) along the a-b plane as the chemical substitution as well as the addition of oxygen content in the parent compound introduces free charge carriers in the conducting plane which are the active participants. Besides these charge carriers ions will also contribute. The model dielectric function at low temperatures for the polarized waves in the long wavelength limit is expressed as:

\[ D(q,\omega) = 1 - \left[ \frac{\omega P_e^2}{\omega^2 + \omega P_i^2} \right] q d \] \hspace{1cm} (10)

where \(\omega_p\) (\(\omega_i\)) denotes the 2D electron (ion) plasmon frequency. Eq.(10) signifies the dielectric function at \(T \approx 0\) K and is used to study the electromagnetic response of a superconductor. As there are no carrier-carrier and carrier-ion scattering effects present at low temperatures, a cold beam type instability will generate in the system when there is a relative drift between two components of a uniform plasma. To do so, we assume two superconducting plasmas, one filling a half space \(z > 0\) and drifting with velocity \(V_{dr}\) parallel to \(z = 0\) interface and a second stationary which occupies the half space \(z < 0\). For the sake of simplicity, we only consider the relative drift of charge carriers (electrons / holes) and assuming the massive ions as stationary in the Jellium model. Also, neglecting 1 in comparison to \(\omega P_e^2/\omega^2\) write the dielectric response function of a non-drifting plasma as:

\[ \varepsilon_1(q,\omega) = -\frac{\omega P_e^2 q d}{\omega^2} \] \hspace{1cm} (11)

and for drifting plasma:

\[ \varepsilon_2(q,\omega) = -\frac{\omega P_e^2 q d}{(\omega - q V_{dr})^2} \] \hspace{1cm} (12)

As there are no scattering effects at low temperature, the entire electron distribution function acquires a uniform drift and the denominator of Eq.(12) represents the shifted frequency due to relative drift. The solution of Eq.(12) in the two domains are plane waves given as:

\[ E_1(z) = E_1^\pm \exp \left( i k_1 z \right) + E_1^\pm \exp \left( -i k_1 z \right) \] \hspace{1cm} \( z < 0 \)

\[ E_2(z) = E_2^\pm \exp \left( i k_1 z \right) \] \hspace{1cm} \( z > 0 \)

where, \(k_1(= 1,2)\) is the wavevector along z direction as:

\[ k_j = \left[ (\omega^2 F_1/c^2) - q^2 \right]^{1/2} \] \hspace{1cm} (13)

with \(c\) as the velocity of light. The reflection amplitude is \(r = E_1^+/E_1^-\) which is given by:

\[ (\varepsilon_1 K_2 - \varepsilon_2 K_1)/(\varepsilon_1 K_2 + \varepsilon_2 K_1) \] which has a pole i.e. \((\varepsilon_1 K_2 + \varepsilon_2 K_1) = 0\) or

\[ \varepsilon_1 \left[ (\omega^2 \varepsilon_2 c^2) - q^2 \right]^{1/2} + \varepsilon_2 \left[ (\omega^2 \varepsilon_1 c^2) - q^2 \right]^{1/2} = 0 \] \hspace{1cm} (15)

The analytical solution of Eq.(15) is:

\[ \omega \approx q V_{dr} \frac{1 + \sqrt{(ha + \beta)}}{1 + \alpha + \beta} \] \hspace{1cm} (16)

where \(\alpha = \omega P_{e_2}^2/\omega P_{e_1}^2\) and \(\beta = \omega P_{e_2}^2/dq c^2\).

This shows the dispersion of an acoustic mode and possess two waves, one amplified (plus sign) supports an instability while the other is damped (minus sign). In the long wavelength, the amplified mode is acoustic with resonant frequency:

\[ \omega_r = Re(\omega) = \frac{q^3 c^2 V_{dr}}{q^2 c^2 + \omega P_{e_1}^2} \] \hspace{1cm} (17)

and the growth rate:

\[ \gamma = Im(\omega) = \frac{q^3 c^2 + \omega P_{e_1}^2 V_{dr}}{q^2 c^2 + \omega P_{e_1}^2} \] \hspace{1cm} (18)

\[ \frac{q^3 c V_{dr}}{\omega P_{e_1}} \] \hspace{1cm} (19)

The practical upper limit on \(V_{dr}\) is obtained by the Cooper pair breaking energy \(\Delta\) as \(V_{dr} = \Delta/K_F = V_F(\Delta/2e_F)\). Thus the maximum achievable growth rate is:

\[ \gamma_{max} \equiv V_F q^2 c \Delta / (2 e_F \omega P_{e_1}) \] \hspace{1cm} (20)

with \(K_F\) and \(e_F\) are Fermi wave vectors and Fermi energy, respectively.

The free electron layered electron gas model is used to look for the plasmons below \(T_c\) in the frequency range \(h \omega \leq 2 \Delta \leq q V_F < K_F T < K_B T_c\), where \(\Delta\) is the binding energy of the Cooper pair. Strictly, the plasmons can exist only in superconductor with an energy gap much larger than the product of temperature and the pair breaking parameter. In the vicinity below \(T_c\) the longitudinal plasma oscil-
lations can propagate and get damped by the single particle absorption associated with the normal electrons. To generate an instability a relative drift is introduced in between the normal and superconducting electrons of the plasma. As far as the 2D polarizability of layered electron gas is concerned, it is a difficult task to calculate $P(q, \omega, T)$ from first principles, as it needs summation over several diagrams which contribute to the effective potential. To have a simple description for the paired and unpaired (normal) electrons, we obtain a phenomenological expression for $P(q, \omega, T)$ from the polarization function of a three dimensional (3D) electron gas as derived by Dinter. The 3D polarization function is modified in such a manner that in the limiting case it yields a correct value of 2D polarization for a normal electron. Thus, the polarization of charge carriers $P_r$ in the frequency range $h \omega \leq 2 \Delta \leq q V_F < K_B T < K_B T_c$ is:

$$
P_r(q, \omega, T) \equiv \frac{2}{q a^*} \left[ \left( \frac{1}{q V_F} - \left( \frac{1}{q V_F} - \frac{1}{\Delta} \right) \right) \frac{1/3 \rho_s}{(\alpha \Delta - T) - (\omega/q V_F)^2} \right]$$

where $a^*$ is the effective Bohr radius, $\alpha = 0.21$, $\rho_s = n_s$, $n$ is the fraction of superfluid $n = n_s + n_0$, where $n_s$ is the number of superconducting electrons which vary with $T$ and $n_0$ represents the number of normal electrons per unit area. The fraction of superfluid near $T_c$ is expressed as $\rho_s = \eta (\Delta T)^2$. For high $T_c$ superconductors, it is convenient to use the empirical relation based on the two-fluid model as:

$$
\rho_s = \frac{n_s}{n} = \left[ 1 - \frac{T}{T_c} \right]^{1/3} \left[ 1 - \frac{T}{T_c} \right]^{2/3}
$$

The ionic contribution to the polarizability is:

$$
P_i(q, \omega, T) = -\alpha^2 \nu_s^2 / \omega^2
$$

with $\nu_s$ as the velocity of sound. In cuprates the electron plasmon energy is higher by at least two order of magnitude than ion-plasmon energy, so we consider the contribution of electrons as dominating. In Eq.(21), the second term represents the contribution due to superconducting electrons and have a crucial role in the vicinity of $T_c$. With these the dielectric function in the frequency range $h \omega \leq 2 \Delta \leq q V_F < K_B T < K_B T_c$ for anisotropic copper oxide superconductors becomes:

$$
\epsilon(q, \omega, T) \equiv \frac{2}{q a^*} D \left( q, \omega, T \right) + \frac{1/3 \rho_s}{(\alpha \Delta - T) - (\omega/q V_F)^2}
$$

With the use of Eq.(9) $D(q, \omega, T)$ is defined as:

$$
D(q, \omega, T) \equiv 1 - \frac{\Delta}{2T} + \frac{\omega}{q V_F} \left( 1 - \frac{\Delta}{2T} \right)
$$

Zero's of Eq.(24) will yield the frequency of plasmon mode as $\omega = \nu_s V_F$ which is acoustic in nature with $\eta$ as number. We now introduce the drift term by inducing dc current. The superconducting electrons will drift much faster than normal electron in the frequency region of interest and hence, we do write:

$$
\epsilon(q, \omega, T) \equiv \frac{2}{q a^*} D \left( q, \omega, T \right) + \frac{1/3 \rho_s}{(\alpha \Delta - T) - (\omega/q V_F)^2}
$$

The minimum drift velocity needed for the plasma mode is evaluated from the zero's of $\epsilon(q, \omega, T)$ (Eq.26) and is:

$$
\nu_d = V_F \left[ \frac{\alpha \Delta}{T} + \frac{1/3 \rho_s}{(1 - \Delta/2T)} \right]
$$

The minimum drift velocity needed for the plasma mode is:

$$
\nu_d = \nu_s \left[ 1 - (1/2) \left( \frac{T}{T_c} \right)^{1/3} \right]
$$

is approximately the phase velocity of the driftless mode. Furthermore, the amplification is possible in the domain $T \approx T_c$ when the drift velocity exceeds the phase velocity of the original plasma wave. On the contrary at $T \approx T_c$ a minimum drift velocity is needed for the current driven plasma instability. No doubt in the former case the dependence is on the Cooper pair breaking energy. The estimation of the following for the anisotropic cuprates are presented.

3. Results and Discussion

One can evaluate the maximum achievable growth rate for electrons at $T_c \approx T_c$ using Eq.20. Let us consider the case of NdCeCuO$_4$ superconductor. The realistic physical parameters are used as effective mass and the charge carrier density for the condition of optimized pairing. The parameters are as follows: $n = 2.74 \times 10^{23}$ cm$^{-3}$, $\nu_s = 4.9 \times 10^6$ cm sec$^{-1}$ to get $\epsilon_s = 333$ meV, $\omega \nu_s = 2.83$ eV and $\Delta = 4.02$ meV. The $T_c$ of NdCeCuO$_4$ is 1.46 meV. In fact, the scattering of charge carriers at the Fermi surface is considered for all possible values of scattering angle.
The wavevector along the plane \( q = 2K_F \sin \theta \) can therefore take the maximum value up to \( 2K_F \). We obtained \( \gamma = 9.3 \text{ eV} \). It is inferred from the Eq. (20) when \( q = 0 \), \( \gamma \) is zero and it increases with the increased value of \( q \). In other words the maximum instability grows at \( q = 2K_F \). We find that in low temperature domain, no carrier – carrier and carrier - carrier- phonon scattering effects are there. Thus a simple cold beam instability will grow when there is a relative drift between two components of a uniform plasma. Similar are the cases for La\(_{2-x}\)Sr\(_x\)CuO\(_4\) (\( T_c = 3.27 \text{ meV} \)) and HgBa\(_2\)CuO\(_{4+\delta}\) (\( T_c = 8.1 \text{ meV} \)). The parameters used are as follows \( n_c = 2.28 (0.47) \times 10^{14} \text{cm}^{-2} \). \( V_F = 2.2 (0.33) \times 10^7 \text{cm sec}^{-1} \) to get \( \varepsilon_F = 136 (19) \text{ meV} \), \( \omega_D = 1.73 (0.63) \text{ eV} \) and \( \Delta = 8.18 (6.7) \text{ meV} \) for LSCO (HBCO) superconductor respectively\(^{13,14}\). The maximum achievable growth rates are 28.47 eV (LSCO) and 14.16 eV (HBCO).

Now, we consider the another temperature domain i.e., when \( T \) is in the vicinity below \( T_c \). In the superconducting state, the superconducting electrons are dominant and the energy gap (\( \Delta \)) is larger than transition temperature (\( T_c \)). From Eq. (27) it is clear that the second term is negative as \( \Delta > T_c \) for NCCO, LSCO and HBCO superconductors, so the drift velocity is approximately the phase velocity of the driftless mode. This is a condition for inverse Landau damping. The amplification is possible when \( V_{dr} > \varepsilon_F \) exceeds the phase velocity. However, the growth is accompanied by single particle excitations of the normal electrons and hence a negative energy wave is developed. Furthermore, it is required to check whether the current driven instabilities can be practically possible in high temperature copper oxide superconductors. The Cooper pair breaking threshold is \( V_{dr} = V_F \Delta / 2\varepsilon_F \) and we need \( \alpha(\Delta/T) V_F < |\varepsilon/\Delta| / 2\varepsilon_F \) which is not fulfilled because \( T_c \varepsilon_F << 1 \).

On the contrary in the earlier case when \( T = OK \), a minimum drift velocity is required to achieve the current excited plasma instability. It is thus argued that at temperature \( T = T_c \), the current driven plasma instability can only be possible when \( \varepsilon_F \) is considerably reduced or in other words reduced charge carrier density and increased effective mass besides higher value of \( T_c \).

The current excited plasma instability in high temperature cuprate superconductors in two temperature domains is studied. A cold beam type of instability is generated in a system of two superconductors by introducing a relative drift at low temperature (\( T \approx OK \)). In the vicinity near \( T_c \) the superconducting electrons have significant contribution. The deduced drift velocity is higher than phase velocity as \( T_c < \varepsilon_F \) and \( T_c < \Delta \) so an increase in \( V_{dr} \) leads to the growth of the plasma wave associated with the single particle excitations in a single superconductor. Thus inverse Landau damping related instability arises in the vicinity of near critical temperature for sufficiently large drift.

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References

Superconductivity and normal state resistivity of Ba$_{0.6}$K$_{0.4}$BiO$_3$: an optical phonon approach

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We discuss the nature of the pairing mechanism and the physical properties associated with the normal as well as the superconducting state of cubic perovskites Ba$_{0.6}$K$_{0.4}$BiO$_3$ using the strong coupling theory. An interaction potential which includes the Coulomb, electron–optical phonon and electron–plasmon interactions is developed to elucidate the superconducting state. A model dielectric function is constructed with these interactions fulfilling the $\varepsilon$-sum rule. The screening parameter ($\mu^* = 0.26$) infers the poor screening of charge carriers. The electron–optical phonon strength ($\lambda$) estimated as 0.98 is consistent with an attractive electron–electron interaction and supports the moderate to strong coupling theory. The superconducting transition temperature of Ba$_{0.6}$K$_{0.4}$BiO$_3$ is then estimated as 32 K. Ziman’s formula of resistivity is employed to analyse and compare this with the temperature-dependent resistivity of a single crystal. The estimated contribution from the electron–optical phonon together with the residual resistivity clearly infers a difference when a comparison is made with experimental data. The unsubtracted data infer a quadratic temperature dependence in the temperature domain ($30 \leq T \leq 200$ K). The quadratic temperature dependence of $\rho = \rho_{\text{res}} - (\rho_0 + \rho_{\text{el-ph}})$ is understood in terms of 3D electron–electron inelastic scattering. The presence of these el–el and el–ph interactions allows a coherent interpretation of the physical properties. Analysis reveals that a moderate to strong coupling exists in the Ba$_{0.6}$K$_{0.4}$BiO$_3$ system and the coupling of electrons with the high-energy optical phonons of the oxygen breathing mode will be a reason for superconductivity. The implications of the above analysis are discussed.

Key words: optical phonon, normal-state resistivity, bismuth oxides.

1. Introduction

The discovery of superconductivity in the multiphased Ba–K–BiO by Mattheiss et al. [1] at 22 K and later the identification of the superconducting component as Ba$_{0.6}$K$_{0.4}$BiO$_3$ ($T_c = 30$ K) by Cava et al. [2] provides an opportunity to understand the nature of the pairing mechanism as well as that of normal-state electronic properties. The mechanism of electron pairing in a copper-free phase remains elusive as the aikali metal.

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K. chemically substituted on the Ba sites does not participate in the conduction band while Ba(Pb, Bi)O₃ is made superconducting by the substitution of Pb on electronically active Ba sites. Unlike the current high 𝑇𝑐 compounds which structurally contain two-dimensional (2D) layered CuO planes. (Ba, K)BiO₃ [BKBO] has a cubic structure in its superconducting phase. The Bi-oxides are three-dimensional (3D) in contrast to the layered structure of all the CuO₂ superconductors; the parent cuprate materials are also antiferromagnetic insulators. BaBiO₃ is a diamagnetic charge-ordered insulator, the Bi ions have zero magnetic moment. This would imply that neither the dimensionality nor the antiferromagnetism can be the origin of the pairing mechanism.

The parent compound BaBiO₃ is diamagnetic and the chemical substitution of the monovalent alkali metal. K. at the Ba sites makes the system metallic. The formal charge valence of Bi ions of BaBiO₃ is +4 and since neutral Bi atoms have five valence electrons, one valence electron exists at each Bi site. Neutron powder diffraction studies [3] suggested that potassium might enter the compound only in an oxygen-deficient environment. At lower compositions, i.e. 𝑥 < 0.3, the system displays semiconductor properties. Superconductivity occurs only in the cubic phase (𝑥 ⩾ 0.37) and has an undistorted cubic perovskite structure. For 𝑥 = 0.35, a transition from the cubic to orthorhombic phase occurs between 200 and 100 K. Within this cubic phase 𝑇𝑐 is highest for the composition 𝑥 ≈ 0.4 at 30 K. Band structure calculations on the cubic phase of Ba–K–BiO have been performed by Mattheiss and Hamann [4]. According to their studies the antibonding Bi(6s)–O(2p) conduction of BKBO (𝑥 = 0.3) is nearly the same as in BaBO₃. It is pointed out that the doping at the Ba sites extends the metallic range of BaBiO₃ closer to half filling than the doping at Bi sites does and hence maximizes the electron–phonon interaction. They stress that K doping at Ba sites increases not only the coupling of conduction electrons to the bond stretching oxygen phonons but also 𝑇𝑐 in the framework of a conventional phonon mechanism. The augmented plane wave method within the tight binding model is used to determine the McMillan–Hopfield parameter, 𝜂, and it is found that the values are sufficiently large to indicate the coupling of electrons with soft phonon modes resulting in a 𝑇𝑐 in the observed range [5]. Shirai et al. [6] have studied the electron–lattice interaction of both BPBO and BKBO using realistic electronic bands of BaBiO₃ reproduced by the tight binding model and superconductivity was successfully discussed in the framework of the strong coupling theory of electron–phonon interactions caused by the longitudinal modes of oxygen stretching/breathing vibrations.

Raman spectroscopic studies [7] of superconducting BaKBO₃ reveal a Raman peak at 348 cm⁻¹ (43 meV) that exhibits the distinctive Fano line shape which results from significant coupling between the optical phonons and electronic states in superconducting Ba₀.₅K₀.₄BiO₃ but not in Ba₀.₆K₀.₂BiO₃. The Raman peak at 348 cm⁻¹ excludes the possibility of scattering from acoustic phonons since acoustic phonons occur below ~140 cm⁻¹. Although the studies could not detect the expected longitudinal optical branch of breathing-type vibrations of O octahedra, a scattering intensity was, however, found at 340 cm⁻¹ in a longitudinal geometry for phonon wavevectors away from the Γ point. Photoemission and inverse photoemission studies have been performed by Wagener et al. [8] for the occupied and unoccupied electronic states of Ba₁₋ₓKₓBiO₃₋ᵥ. The results indicate a metallic characteristic with a low density of states on either side of the Fermi energy. Low-energy plasmon features appear in the core level spectrum [8] which are similar to those observed in high 𝑇𝑐 cuprates. High-resolution tunnelling spectroscopy on BaKBO₃ (𝑥 = 0.375. 𝑇𝑐 = 29 K) has been reported by Zasadzinski et al. [9]. Tunnelling phonon structures between 40 and 65 meV are the most strongly coupled and these correspond to the optical modes of oxygen atoms. The tunnelling data exhibit strong features which correspond to the peaks in the phonon density of states of BKBO obtained from Raman spectroscopy [7]. The tunnelling results strongly suggest that the electron–optical phonon is the mechanism for superconductivity in BKBO systems with the electron–optical phonon strength as 1.0. At this stage it is clear from band structure studies [4–6] and spectroscopic data [7–9] that high-energy optical phonons play a significant role in the pairing mechanism for superconducting states in the Ba₀.₆K₀.₄BiO₃ system.

Affronte et al. [10] have reported resistivity data for a single crystal of Ba₁₋ₓKₓBiO₃ (0.35 < 𝑥 < 0.4) and found that the resistivity (ρ) shows a metallic temperature dependence. The ρ versus 𝑇 behaviour of a single
crystal, prepared by the electrochemical process, shows the lowest residual resistivity \( \rho_0 = 0.57 \text{ m}^2\text{cm} \). The behaviour is not simply linear as is observed in most superconducting oxides and it looks similar to that of more conventional metals. They have fitted the resistivity data between 35 K and room temperature with an explicit form of the Bloch–Grunensein expression using \( T_E = 233 \text{ K} \). Subsequently, Hellman and Hartford Jr [11] have measured the normal-state resistivity of epitaxial films of Ba–K–BiO; the temperature dependence of films as grown by the molecular beam epitaxy (MBE) technique shows nearly linear temperature dependence. The lowest resistivity films are quite metallic, with resistivity ratios \( \rho(300)/\rho(30) \) as high as 1.9, but the temperature dependence of the resistivity becomes more semiconductor-like as the resistivity increases. The high resistivity and its semiconductor-like temperature dependence is interpreted using the concept of parallel conductivity channels: a metallic channel responsible for the conductivity at low temperature and a semiconducting channel that freezes out at low temperatures. They have fitted the resistivity data using \( \rho_0 = 0.224 \text{ m}^2\text{cm} \) and a scaling factor as fitting parameters. The fit is reasonably good and the estimation of the coupling strength \( \lambda \) from the temperature dependence would be revised down to about 1.0.

Recently, the resistivity of single crystals of cubic \( \text{Ba}_{0.8}\text{K}_{0.2}\text{BiO}_3 \) with \( T_c = 30 \text{ K} \) has been reported in the temperature range 4.2–300 K [12]. The temperature dependence of the resistivity of a single crystal displays a metal-like behaviour. The experimental data are well approximated in the framework of the electron–phonon model of resistivity by a Gruneisen-type dependence using the phonon spectrum in the form of an acoustic branch and a widely separated narrow optical peak. Analysis reveals that \( \rho \) as a function of temperature is quadratic at low temperature \( (T < 180 \text{ K}) \) and rises linearly with temperature when \( T > 200 \text{ K} \). The quadratic temperature dependence of \( \rho \) is interpreted in terms of the dominant electron–electron interaction at low temperatures. Characteristic Debye and Einstein temperatures are, respectively, estimated to be 320 K and 680 K from the generalized phonon density of states as obtained from neutron experiments. Furthermore, the optical phonons of the oxygen breathing mode yield a relatively larger contribution to the resistivity as well as to the electron–phonon interaction, \( \lambda \).

Looking at the earlier experimental and theoretical information on the superconducting-state parameters and normal-state resistivity, a creative approach is required to explain both the pairing mechanism and the physical properties associated with the normal and superconducting state in cubic, magnetic free ion, high \( T_c \) Ba–K–BiO superconductors. Keeping in mind the dominant role of the high-frequency oxygen breathing vibrations and the presence of low-energy plasmons, we develop a coupled model which could explain the electron pairing and the observed properties. The plan of the present investigations is as follows. In Section 2, we formulate a 3D interaction potential for the cubic, magnetic free ion Ba–K–BiO by considering the breathing modes of oxygen in BiO octahedra and charge oscillations developed by the charge transfer from unstable Bi atoms. The polarizability of the charge carriers is included through a model longitudinal dielectric function which fulfils the \( f \)-sum rule. The coupling parameters such as the interaction strength, \( \lambda \), and the Coulomb repulsive parameter, \( \mu^\ast \), are then deduced for a renormalized optical phonon frequency to predict the transition temperature. Ziman’s formula is used to analyse the temperature-dependent part of the electron–optical phonon resistivity. The zero-temperature-limited resistivity is deduced from the scattering rate using an experimental value of the critical magnetic field and the theoretically developed coupling parameters. Section 3 is devoted to results and discussions. The main findings of the present analysis include: (a) the significant participation of optical phonons in the pairing as well for predicting the physical properties and (b) the contribution of 3D inelastic electron–electron scattering from low to moderate temperatures. Finally we conclude in Section 4.

## 2. The model

### 2.1. Interaction potential

The parent \( \text{BaBiO}_3 \) system is regarded as an insulator and the valence configuration is \( \text{Ba}^{2+} \) and three \( \text{O}^{2-} \). The charge of the Bi ions of \( \text{BaBiO}_3 \) is \( -4 \) and since the neutral Bi atoms have five valence electrons, two
6s and three 6p), an average of one valence electron is left at each Bi atom, making BaBiO₃ a system with a half-filled band. Chemical substitution of the monovalent alkali metal K (six 3p and one 4s) at the donor site Ba (six 5p and two 6s) introduces free electrons in the conduction band and the doped system Ba₁₋ₓKₓBiO₃ becomes metallic. The free electrons of effective mass, m*, actively participate in the pairing mechanism. In addition, the contraction and expansion of oxygen octahedra around the Bi atoms leads to breathing modes.

As a first step, we write the electron–electron matrix element between the states |K⟩ and |K'⟩ in terms of the dielectric function as

$$V_{KK'} = \frac{4\pi e^2}{q^2 \varepsilon(q, \omega_{KK'})}$$

where $$q = K - K'$$, $$\omega_{KK'} = \frac{[E(K) - E(K')]h}{\hbar}$$ and E(K), E(K') denote the corresponding energies of the states.

The dielectric function of a metal oxide, considered as two-component plasma, will be the sum of the contributions of the electronic and ionic polarizabilities. The model dielectric function is

$$\varepsilon(q, \omega) = \varepsilon_{\infty} + \frac{\omega_p^2}{(A_1^2 - \omega^2)} + \frac{\varepsilon_{\infty}(\omega_{LO}^2 - \omega_{TO}^2)}{(\omega_{LO}^2 - \omega^2)}.$$  

Here, $$A_1^2 = q^2 V_F^2/2$$ with V_F the Fermi velocity and $$\omega_{LO}$$ and $$\omega_{TO}$$ are the usual frequencies of the longitudinal and transverse optical phonons. In a true sense, the Bi atom has two stable ionic states in the form of Bi³⁺ and Bi⁵⁺ and the bond stretching oxygen displacements lead to a charge density wave distortion in which the oxygen octahedra surrounding adjacent Bi sites alternatively expand or contract. It is useful to consider a single optical phonon whose vibrational frequencies are independent of the wavevector (q). The first term in the previous equation is the polarizability of core electrons and in the frequency region of interest it is independent of frequency and is constant, denoted as $$\varepsilon_{\infty}$$. The second and third terms are the electronic and ionic polarizabilities, respectively. The model dielectric function for the polarized waves becomes

$$\frac{\varepsilon(q, \omega)}{\varepsilon_{\infty}} = \left[1 + \frac{D_1}{A_1^2 - \omega^2} + \frac{D_2}{A_2^2 - \omega^2}\right]$$

where $$D_1 = \omega_p^2$$ is the screened plasma frequency. $$D_2 = \omega_{LO}^2 - \omega_{TO}^2$$ and $$A_2^2$$ is $$\omega_{TO}^2$$, respectively. The main input parameter, which determines the superconducting and normal-state transport parameters, is inhibited in the dynamic interaction potential $$V(q, \omega)$$ or, equivalently, $$\varepsilon^{-1}(q, \omega)$$ of the system under consideration. The inverse dielectric function is associated with different longitudinal modes, corresponding to the exchange of ionic as well as electronic excitations. The separation of individual contributions from different longitudinal modes can be made possible by inverting eqn (3) into the following form:

$$\varepsilon_{\infty}\varepsilon^{-1}(q, \omega) = \left[1 + \sum_{i=1}^{2} \frac{f_i}{\omega^2 - \Omega_i^2}\right]$$

with $$\Omega_i$$ are the frequencies of the two longitudinal modes and the resonant frequencies are expressed as

$$(\Omega_1^2 - A_1^2)(\Omega_2^2 - A_2^2) + D_1(A_2^2 - \Omega_2^2) + D_2(A_1^2 - \Omega_1^2) = 0.$$  

The effective interaction potential $$V(q, \omega)$$ is the sum of the electronic and ionic contributions, i.e. $$V(q, \omega) = V_e(q)\varepsilon^{-1}(q, \omega)$$ from the individual longitudinal modes. The oscillator strength is defined as

$$f_i = \prod_{i=1}^{2} \frac{[\Omega_i^2 - A_i^2]}{\prod_{i=j}^{2} (\Omega_i^2 - \Omega_j^2)}.$$
The following \( f \)-sum rules are valid:

\[
\sum_{i=1}^{n} \Omega_i^2(q) = D_1 - D_2 - A_1^2 + A_2^2.
\]

(7)

\[
\sum_{i=1}^{n} f_i(q) = D_1 - D_2.
\]

(8)

\[
\sum_{i=1}^{n} f_i(0)/\Omega_i^2(0) = 1.
\]

(9)

where \( f_i(0)/\Omega_i^2(0) \) is the limiting value of \( f_i(q)/\Omega_i^2(q) \) in the long wavelength limit. This implies that \( e^{-1}(q \rightarrow 0, 0) \rightarrow 0 \), when \( q \rightarrow 0 \).

Zeros in the model dielectric function will lead to two modes of the polarized waves and the frequencies of the coupled mode in the long wavelength limit can be expressed as

\[
2\Omega_{\pm}^2 = \left[ \omega_0^2 - A_1^2 + \omega_{\pm}^2 \right] \pm \sqrt{\left[ \omega_0^2 - A_1^2 + \omega_{\pm}^2 \right]^2 - 4A_1^2\omega_{\pm}^2}\left[ \omega_0^2 - A_1^2 \right]^{1/2}
\]

(10)

Simple algebra yields

\[
\Omega_{\pm}^2 \approx \omega_0^2 - A_1^2
\]

(11)

which infers the acoustic plasma characteristics. The lower mode can be expressed as

\[
\Omega_{\pm}^2 \approx \frac{(\omega_{\perp}^2 + \omega_{\parallel}^2)\omega_0^2}{\left(2\omega_0^2 - \omega_{\perp}^2\right)}
\]

\[
\approx 0.78\omega_{\perp}^2
\]

(12)

which is a longitudinal optical phonon mode in the adiabatic approximation, i.e. \( \omega_\parallel > \omega_{\perp} \) and \( \omega_{\perp} \) a.

The modelled longitudinal dielectric function in terms of the lower \( n\Omega_{\pm}^2 \) and upper \( n\Omega_{\pm}^2 \) modes is

\[
\varepsilon(q, \omega) \approx \frac{(\omega_{\perp}^2 - \Omega_{\pm}^2)(\omega_{\parallel}^2 - \Omega_{\pm}^2)}{\omega_{\parallel}^2(\omega_{\parallel}^2 - A_1^2)}
\]

(13)

and the interaction potential takes the following form

\[
\mathcal{V}(q) = \mathcal{V}_2(q)e^{-(1)}(q, \omega)
\]

\[
\approx \frac{4\pi e^2}{\varepsilon_0} \left[ \frac{\Omega_{\perp}^2}{\omega_{\perp}^2 - \Omega_{\perp}^2(\Omega_{\perp}^2 - A_1^2)} - \frac{\Omega_{\parallel}^2}{\omega_{\parallel}^2 - \Omega_{\perp}^2(\Omega_{\perp}^2 - A_1^2)} \right]
\]

(14)

which essentially describes the coupling strength for scattering a fermion from the \( K \) to \( K' \) state in the long wavelength limit. To justify the above approach for BaKBiO\(_4\) superconductors, the parameters describing the superconducting states are investigated in the next subsection.

2.2. Superconducting states parameters

In the strong coupling theory, the superconducting transition temperature \( T_c \) requires information about the coupling constants such as the electron-phonon coupling strength and the Coulomb repulsive parameters. In the traditional approach to the theory of superconductivity, the phonon-mediated interaction strength is usually treated first and the direct Coulomb interaction is subsequently introduced in terms of the Morel-Anderson pseudopotential, \( \mu^* \). In a true sense, from the viewpoint of considering the energy scales, it might appear more reasonable to take into account first the large electron-electron interaction and to incorporate
the electron–phonon interaction strength later. The effect of screening of electrons is determined by the renormalized Coulomb repulsive parameter:

$$\mu^* = \frac{\mu}{1 + \mu \ln(\epsilon_F / h\Omega)}$$

with $h\Omega$ as the longitudinal optical phonon energy and $\mu$ the repulsive parameter obtained from the Thomas–Fermi wavevector ($K_s$) as

$$\mu = \alpha^2 \ln \left( \frac{(1 + \alpha^2)}{a^2} \right).$$

Here, $\alpha^2 = K_s^2 / 4k_F^2$ with the screening length $K_s^2 = 4\pi^2e^2N(\epsilon_F)$. The density of states at Fermi energy $N(\epsilon_F)$ in three dimensions is

$$N(\epsilon_F) = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \epsilon_F^{1/2}.$$  \hfill (16)

Inelastic neutron scattering measurements and the superconducting tunnelling spectroscopy yields the electron–phonon spectral weight $\alpha^2 F(\omega)$ from a strong-coupling inversion procedure, and hence, the electron–phonon coupling strength with great accuracy. Alternately, the coupling strength can also be evaluated from the McMillan expression which is related to the mean square electron–ion matrix element, $(I^2)$, the density of states at the Fermi level, $N(\epsilon_F)$, the ionic mass, $M$, and the renormalized phonon frequency, $(\omega^2)^{1/2}$. The use of the McMillan expression in the present system Ba–K–BiO seems to be appropriate because of the large density of states as well as the greater mass difference between Bi and O. The dimensionless electron–phonon coupling strength is $[13]$

$$\lambda = \frac{N(\epsilon_F)(I^2)}{M(\omega^2)},$$  \hfill (17)

The mean square electron–ion matrix element is

$$\langle I^2 \rangle = \frac{\Omega_{cell}^2}{(2\pi)} \int d^3k \int d^3k' (k - k')^2 |V(k - k')|^2 \delta(E_k - \epsilon_F) \delta(E_{k'} - \epsilon_F)$$

$$\langle I^2 \rangle = \frac{[N(\epsilon_F)]^2}{[N(\epsilon_F)]^2} \int_{k_F}^{k_F} \frac{q dq / 2k_F}{q^2} V(q)^2,$$

$$\langle I^2 \rangle = \frac{\Omega_{cell}^2}{(2\pi)} \int_{k_F}^{k_F} \frac{q dq |V(q)|^2}{q^2}$$

where $V(q)$ is the screened Coulomb potential and the static dielectric function. $\epsilon(q)$ is obtained from eqn (2) as

$$\epsilon(q) \approx \frac{4m^*e^2k_F}{(\pi\hbar^2q^2)}.$$  \hfill (19)

Thus, the screened Coulomb potential is

$$V(q) = \frac{4\pi Ze^2 / (q^2\Omega_{cell}\epsilon_{\infty})}{4m^*e^2k_F / (\pi\hbar^2q^2)}$$

$$V(q) = \frac{\hbar^2\pi^2Z}{m^*k_F\Omega_{cell}\epsilon_{\infty}}$$

where $\Omega_{cell}$ is the volume of the cell and $Ze$ denotes the effective ionic charge and is $-2e$.  \hfill (20)
The mean square electron–ion matrix element using eqns (19) and (20) becomes

\[ (I^2) = \frac{1}{2k_F^2} \left[ \frac{\hbar^2 \pi^2 Z}{\varepsilon_{\infty} m^* k_F \Omega_{\text{cell}}} \right]^2 \int_0^{2k_F} q^2 dq \]  

(21)

and the electron–phonon coupling strength is

\[ \lambda = \frac{2N(\varepsilon_F)}{M} \left[ \frac{\hbar^2 \pi^2 Z}{m^* \Omega_{\text{cell}} \varepsilon_{\infty}} \right]^2 \frac{1}{\langle \Omega_{\text{eff}}^2 \rangle} \]  

(22)

Using the screened Coulomb repulsive parameter, \( \mu^* \), and the electron–phonon coupling strength, \( \lambda \), for the renormalized phonon frequency, we have estimated \( T_c \) for BKBO in the strong coupling theory as [14]

\[ T_c = 0.25 \langle \Omega_{\text{eff}} \rangle^{1/2} \left[ \exp(2/\lambda_{\text{eff}}) - 1 \right]^{-1/2} \]  

(23)

with the effective coupling strength expressed as

\[ \lambda_{\text{eff}} = (\lambda - \mu^*)[1 + 2\mu^* + \lambda \mu^* \tau(\lambda)]^{-1} \]  

(24)

and the numerical function, \( \tau(\lambda) \), having the form

\[ \tau(\lambda) = 1.5 \exp(-0.38\lambda) \]  

(25)

The approach is further applied to investigate the normal-state transport properties and, in particular, the electrical resistivity in the following subsection.

2.3. Normal-state resistivity

The Bloch–Boltzmann theory based on the Migdal approximation, which is valid if the electron–phonon scattering process dominates, i.e. on the existence of the small parameter \( [N(\varepsilon_F)\hbar \Omega_{\text{ph}}] \), is understood to describe better the normal-state transport properties. The contribution to the normal-state resistivity \( \rho_n(T) \) due to electron–phonon scattering is calculated using Ziman’s resistivity formula [15]:

\[ \rho_{\text{e–ph}}(T) = \varepsilon_{\text{ph}} \left[ \frac{(4\pi)^{3/2} \hbar \omega_p}{\omega_p^2} \right] \int_0^{\omega_{\text{max}}} \frac{(\hbar\omega/k_BT)\alpha_F^2 F(\omega) d\omega}{[\exp(\hbar\omega/k_BT) - 1][1 - \exp(-\hbar\omega/k_BT)]} \]  

(26)

where \( \omega_{\text{max}} \) is the cut-off frequency of the phonon spectrum and \( \omega_p \) is the bare plasma frequency. At temperatures, \( k_BT > \hbar \omega_{\text{ph}} \), the resistivity expression can be reduced to

\[ \rho_{\text{e–ph}}(T) = \frac{8\pi^2 k_B \lambda_{\text{eff}} T}{\hbar \omega_p^2}. \]  

(27)

The bare plasma frequency is related to the density of states at the Fermi level through

\[ \omega_p^2 = \frac{4\pi^2 e^2}{3} 2N(\varepsilon_F)V_F^2. \]  

(28)

The transport electron–phonon coupling constant which is related to the resistivity requires the spectral weight \( \alpha_F^2 F(\omega) \) while the superconducting transition temperature depends on \( \alpha_F^2 F(\omega) \). The expressions for \( \alpha_F^2 F(\omega) \) and \( \alpha_F^2 F(\omega) \) seem to be quite similar except for the fact that the transport expression weighs the differences in the Fermi velocities between different points on the Fermi surface. Use of \( \alpha_F^2 F(\omega) \) is generally believed to result in no significant qualitative error [16]. However, there exists a noteworthy difference between \( \lambda \) and \( \lambda_{\text{eff}} \) for the case (a) of a strongly nested Fermi surface in which \( \lambda_{\text{eff}} \) is smaller than \( \lambda \) due to backscattering of electrons between the opposite sides of the Fermi surface; and (b) when the electron–phonon matrix has a
strong dependence on the wavevector \((q)\). The situation in BKBO is clear as the Fermi surface is not complex due to its isotropic nature. The high-energy optical phonons should exhibit very little dispersion which would suggest that electron–phonon coupling for these modes is isotropic in \(k\)-space. Thus, it is speculated that there is no substantial difference between \(\lambda\) and \(\lambda'\).

The temperature-dependent part of the normal-state resistivity can now be expressed using eqns (22) and (27) as

\[
\rho_{\text{e-ph}}(T) = \frac{8\pi^2 k_B}{h} \frac{2N(e_F)}{M} \left[ \frac{\hbar^2 \pi^2 Z}{m^* \Omega_{\text{cell}} e_F} \right]^2 \frac{1}{(\Omega^2 + \omega_n^2)} \frac{T}{\Omega^2}.
\]  

(29)

Besides electron–phonon scattering, other scattering mechanisms, such as electrons scattering off impurities, defects and disordered regions giving rise to a temperature independent contribution, are also possible. Knowledge of the zero-temperature scattering rate and bare plasma frequency will allow us to have an independent estimation of the zero-temperature-limited resistivity. The zero-temperature scattering rate is related through the upper critical magnetic field \(H_{c2}(0)\). Using the method described by Carbotte \[17\], we write

\[
\frac{1 + \lambda}{\lambda - \mu^*} = 2\pi \frac{T}{T_c} \sum_{i=0}^{N_c} x_i^{-1} \frac{1}{(2\tau^*)^{-1}}.
\]  

(30)

where

\[
N_c = \frac{1}{2} \left( \frac{\omega}{\pi T} + 1 \right)
\]  

(31)

and

\[
x_i = \frac{2}{\sqrt{\alpha^*}} \int_0^\infty \exp(-q^2) \tan^{-1}(\beta) dq
\]  

(32)

with

\[
\beta = \frac{q \sqrt{\alpha^*}}{[(2i + 1)\pi T/T_c] + [\tau^*/2]].
\]  

(33)

The symbols \(\lambda\) and \(\mu^*\) are the electron–phonon coupling strength and renormalized Coulomb repulsive parameter as expressed by eqns (22) and (15) respectively.

The upper critical magnetic field \(H_{c2}\) is related to \(\alpha^*\) through

\[
\alpha^* = \frac{eH_{c2} V_F^2}{2}.
\]  

(34)

The renormalized quantities are related to the coupling strength as \(H_{c2}^* = H_{c2}[(1 + \lambda)T_c]^{-1}\), \(V_F^* = V_F[(1 + \lambda)^{1/2} T_c]^{-1}\) and \(\tau^* = [1 + \lambda]T_c\). The zero-temperature-limited resistivity can now be expressed as

\[
\rho(0) = \frac{4\pi \tau^*-1}{\omega_n^2}.
\]  

(35)

The determination of the scattering rate essentially needs the Coulomb repulsive parameter, the electron–phonon coupling strength, the Fermi velocity, the plasma frequency and the upper critical magnetic field. We use the magnetization measurement data to estimate \(H_{c2}\) and the remaining parameters have been discussed earlier. This allows one to estimate the zero-temperature-limited resistivity and hence the two-component resistivity is modelled as \(\rho(T) = \rho(0) + \rho_{\text{e-ph}}(T)\).

Using the expression developed for the superconducting and normal-state parameters in high \(T_c\) Ba–K–BiO superconductors we have computed the model parameters and the results along with a discussion are presented in the following section.
3. Results and Discussion

In order to compute the physical parameters describing the superconducting and normal-state of high $T_c$ cubic $\text{Ba}_6\text{K}_4\text{Bi}_3\text{O}_{12}$ superconductors, we have used the following experimental data. Keeping in mind that the experimentally reported physical parameters provide constraints on any proposed approach, the effective mass of the charge carriers (electrons) is evaluated from the electronic specific heat coefficient ($\gamma$) by the expression

$$m^* = \frac{3h^2\gamma d}{\pi k_B^2}$$  \hspace{1cm} (36)

with $\gamma$ is used as $1.5 \text{ mJ mol}^{-1} \text{ K}^{-2}$ from the specific heat measurements [18] and the lattice parameter $d = 4.2932 \text{ Å}$ to obtain $m^* = m_e$. The background dielectric constant $\varepsilon_\infty$ is taken as $4.0$ [19]. The charge carrier density and the Fermi velocity are deduced as $3.1592 \times 10^{12} \text{ cm}^{-2}$ and $5.23 \times 10^4 \text{ cm s}^{-1}$, respectively. As a first step towards estimating the superconducting and normal-state electronic properties, we wish to estimate the breathing phonon frequency of $\text{Ba–K–BiO}$ superconductors, considering the system as an ionic solid. The Coulomb interaction among the adjacent ions in an ionic crystal is expressed in terms of the deformation potential as

$$\phi(r) = -(Ze)^2 \left[ \frac{1}{r} - \frac{1}{r^2} \right]$$  \hspace{1cm} (37)

where $a$ is the repulsion force parameter between the ion cores. The effective ion charge is $Ze$ and is $-Ze$. The elastic force constant ($K^*$) can be derived from the ionic potential, $\phi(r)$, at the equilibrium interionic distance ($r_0$) as

$$K^* = \left[ \frac{\partial^2 \phi}{\partial r^2} \right]_{r_0} = (Ze)^2 \left[ \frac{n - 1}{r_0^3} \right]$$  \hspace{1cm} (38)

where $n$ is the index number of the repulsive potential. We have used $n = 0$ for the BKBO system under consideration as in most ionic solids, the index number has been reported to be $6 \sim 8$ [20]. The equilibrium interionic distance $r_0$ is taken as $2.14 \text{ Å}$.

The force parameter ($\beta^*$) is

$$\beta^* = \frac{8\pi (Ze)^2}{3 \Omega_{\text{cell}}}$$  \hspace{1cm} (39)

where $\Omega_{\text{cell}}$ is the volume of the cell and is $316.52 \text{ Å}^3$. With this description the longitudinal and transverse optical phonon frequencies in terms of the elastic force constant and the force parameter can be expressed as

$$\omega_{\text{LO}}^2 = \frac{1}{\mu(M)} [K^* - \beta^*]$$  \hspace{1cm} (40)

and

$$\omega_{\text{TO}}^2 = \frac{1}{\mu(M)} [K^* - \beta^*].$$  \hspace{1cm} (41)

Here, the reduced mass, $\mu(M)$ is determined to be

$$\mu(M) = \frac{M(\text{Bi})M(\text{O})}{M(\text{Bi}) + M(\text{O})}$$  \hspace{1cm} (42)

and is $14.84 \text{ a.m.u}$. The basic premise of the interaction is inhibited in the BiO network where the charge carriers as developed with the chemical doping are dynamic and will lead to an attractive interaction. When the interaction is mediated by phonons, then the breathing phonon modes related to the contraction and expansion of oxygen octahedra around bismuth atoms will contribute the most and, in particular, the longitudinal modes will contribute effectively to the deformation potential. The force parameters are deduced...
Fig. 1. Variations in normal-state resistivity (ρ) with temperature in Ba$_{0.6}$K$_{0.4}$BiO$_3$ superconductors. The experimental data (closed circles) are taken from Affronte et al. [10]. The estimated values are represented by the straight line.

as $K^* = 23.293 \times 10^4$ gm s$^{-2}$ and $\beta^* = 2.439 \times 10^4$ gm s$^{-2}$. The estimated $\omega_{LO}$ is 67.21 meV which is consistent with the high-resolution tunnelling spectroscopy data [9].

With these realistic parameters based on experimental information we have computed the upper and lower modes, i.e. $\hbar \Omega_+$ and $\hbar \Omega_-$ respectively. The scattering of charge carriers at the Fermi surface is considered for all values of the scattering angle $\theta$. The wavevector $q = 2k_F \sin \theta$ can, therefore, take maximum values up to $2k_F$. The bare plasma frequency from eqn (28) is estimated as 1.47 eV. The acoustic plasmon energy using eqn (11) is deduced as 2.65 eV. The lower mode is 52.42 meV which is smaller than the bare longitudinal phonon frequency. The coupling strength between the electrons from the lower mode using density of states at the Fermi level and the McMillan-Hopfield parameter is obtained as 0.98. We estimated the density of states at the Fermi level from eqn (16) as 1.927 states/eV spin atom. The screened Coulomb repulsive parameter, $\mu^*$, is deduced as 0.26 for the renormalized optical phonon frequency (52.42 meV) which clearly infers poor screening. The numerical function, $t(\lambda)$, and effective coupling strength, $\lambda_{\text{eff}}$, are then obtained as 1.14 and 0.48 respectively, and, hence, the $T_c$ value is 32 K from Kresin’s expression of strong coupling theory [14]. The calculated value of $T_c$ is in reasonably good agreement with the reported experimental data of 30 K. This set of coupling parameters ($\lambda = 0.98$ and $\mu^* = 0.26$) for the renormalized optical phonon frequency (52.42 meV) will provide a good choice for estimating the superconducting transition temperature in cubic high $T_c$ BaKBiO$_3$ superconductors.

Switching to the normal-state resistivity, we first deduce the zero-temperature-limited resistivity, $\rho_0$. This naturally demands the estimation of the elastic scattering rate which essentially depends on the coupling parameters ($\lambda, \mu^*$), the Fermi velocity and the upper critical magnetic field $H_{c2}(0)$. The coupling parameters ($\lambda = 0.98, \mu^* = 0.26$) as well as the Fermi velocity ($V_F = 5.231 \times 10^7$ cm s$^{-1}$) were estimated earlier. We use the experimental value of $H_{c2}(0) = 22.7$ T [21] from the linear extrapolation of the upper critical field phase diagram. With the previously deduced model parameters, the zero-temperature elastic scattering rate is thus obtained as $2.285 \times 10^{14}$ s$^{-1}$. It is believed that the smaller the electron mass is, the larger the plasma frequency is and hence the zero-temperature elastic scattering rate is enhanced. We further estimate the zero-temperature mean free path, $L = \frac{V_F \tau}{2} = 23.189$ Å which is one-half of the zero-temperature coherence
Fig. 2. Variation in $\rho_{e-e}(10^{-4}\, \Omega\, \text{cm})$ with $T^2(10^4\, \text{K}^2)$ in the temperature range ($30 \leq T \leq 280\, \text{K}$).

length of $53 \pm 1\, \text{Å}$ [22]. The Mott–Ioff–Regel criterion for metallic conductivity is valid as the mean free path is several times larger than the Bi–O bond length ($\sim 2\, \text{Å}$). A significantly enhanced mean free path is indicative of metallic conduction as the product $k_FL(\sim 10.52)$ seems to be much larger than unity. The zero-temperature-limited resistivity ($\rho_0 = 0.5\, \text{mΩ\, cm}$) as deduced from the elastic scattering rate and plasma frequency is consistent with the single crystal result of $0.575\, \text{mΩ\, cm}$ [10].

Our numerical results for the temperature dependence of the resistivity of $\text{Ba}_0.6\text{K}_{0.4}\text{BiO}_3$ with the electron–optical phonon contribution together with the residual resistivity are plotted in Fig. 1 along with the single crystal data [10]. It is inferred from the plot that the estimated $\rho$ is lower than the reported data from $T_c$ to near room temperature. The deduced values of the temperature-dependent $\rho$ from Ziman’s formula [15] appear to be low as the values of $\rho_0$ and $\omega_p$ are constraints for the present analysis. Thus, the estimated model parameters [$\lambda, \mu^*, V_F, \omega_p, \tau(0)$ and $\rho(0)$] represent a good set of parameters for the estimation of the normal-state resistivity in high $T_c$ BKBO superconductors. Nevertheless, the role of high-frequency optical phonons is further explored and found to be significant not only for interpreting the superconducting state parameters but also the normal-state transport parameters. The difference between the measured and calculated $\rho(\omega_p - \rho_{e-ph})$ in the temperature range $30–280\, \text{K}$ is plotted in Fig. 2. A quadratic temperature dependence of $\rho$ is depicted at low as well as moderate temperature. It can be seen from the plot that the $T^2$ characteristic of $\rho$ occurs until $200\, \text{K}$ and it then deviates in the high-temperature limit. The quadratic temperature contribution is indeed from conventional three-dimensional electron–electron scattering, and hence, its magnitude essentially depends on the charge carrier density ($n$) as $n^{-5/3}$ and plasma frequency ($\omega_p$) as $\omega_p^{-10/3}$. It should be noted that in conventional metals, the electron–electron contribution to the resistivity can at best be seen only at very low temperatures due to its small magnitude when compared with the phonon contribution.

The temperature dependence of the resistivity ($\rho$) has been analysed by Golovashkin et al. [12] and they found that $\rho(T)$ is quadratic with respect to temperature ($T < 180\, \text{K}$) and rises linearly with temperature.
when \( T > 200 \text{ K} \). The existence of \( \rho(T) \propto T^2 \) over a wide temperature range \( 30 \leq T \leq 200 \text{ K} \) was previously interpreted in terms of electron–electron scattering for \( \text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4 \), superconductors [23]. In interpreting the resistivity data, Golovashkin et al. [12] used the values for the Debye and Einstein temperatures determined from the phonon density of states using neutron scattering data. On the other hand, in the present calculations, we have used the coupling strength for optical phonons as deduced from the density of states at the Fermi level and the McMillan–Hopfield parameter. The electron–ion matrix element in the McMillan–Hopfield parameter is derived from the Coulomb potential with the static dielectric function in the long wavelength limit. While determining the longitudinal optical phonon frequency, we have made an approximation that the vibrational frequencies are independent of wavevector \( (q) \), and used the nearest-neighbour ionic potential. Furthermore, Golovashkin et al. [12] have predicted a crossover from \( T^2 \) to \( T \) characteristic for the normal-state resistivity. It is argued that the dependence change from \( \rho(T) \propto T^2 \) at low temperature to \( \rho(T) \propto T \) at high temperatures as observed in electron doped cuprates [23] which is related to a 3D to 2D crossover is not true for BKBO systems which with its cubic structure and electron system is unlikely to change dimensionality. From the present analysis of normal-state resistivity in BKBO systems we support the argument made by Golovashkin et al. [12]. The 3D to 2D crossover concept, although applicable to anisotropic cuprates because of their low dimensionality, does not hold for 3D isotropic cubic BKBO superconductors. Furthermore, an analysis of normal-state resistivity reveals the significant participation of optical phonons from the oxygen breathing mode in the electronic transport mechanism which is consistent with the earlier explanation [12].

### 4. Conclusion

In this paper, we have reported our studies of the nature of the pairing mechanism, superconducting transition temperature and normal-state resistivity of alkali metal doped cubic 3D \( \text{Ba}_{1-x}\text{K}_x\text{BiO}_3 \) \((x = 0.4, T_c \approx 30 \text{ K})\) superconductors within the framework of the strong coupling theory. Treating the system as a two-component plasma, we have properly incorporated the electronic excitations (plasmons) as developed from the chemical substitution of monovalent alkali metal K at the donor site divalent Ba and the ionic excitations due to the oxygen breathing in the Bi–O bond. For the sake of simplicity, we have considered a single optical phonon whose vibrational frequencies are independent of the wavevector \( (q) \). This working assumption is appropriate because of the 3D network and five atoms per unit cell. Looking at various experimental spectroscopic results and electronic energy band structure studies, we speculate that the high-energy oxygen breathing mode is a key source of superconductivity in magnetic free ion \( \text{Ba–K–BiO} \) superconductors. We have critically examined the transition temperature and the nearly linear behaviour of the temperature-dependent normal-state resistivity. The appropriateness of the present analysis is based on the recognition of optical phonons from the oxygen breathing mode at the first step. The basic premise of the approach is that the model dielectric function and the developed model dielectric function fulfils the \( f \)-sum rule of polarizabilities in the long wavelength limit \( (q \to 0) \) and properly explores various interactions in the interaction potential. Simplification of the model dielectric function leads to two coupled modes, i.e. the acoustic plasmon mode and an optical phonon dressed with electronic excitations (plasmons). The acoustic plasmon energy is, in principle, higher by three orders of magnitude than that of the optical phonons and, hence, the lower mode is approximated as longitudinal optical phonons of the oxygen breathing mode within the adiabatic approximation. The static dielectric function describes the electron–optical phonon coupling strength with the use of electron–ion matrix element and density of states at the Fermi level. The effects of screening of electrons is determined by the renormalized Coulomb repulsive parameter. Due to the simplicity of the approach as well as proper utilization of the structural information and specific heat data, the estimated \( T_c \) with the electron–optical phonon interaction in the strong coupling theory seems to be reasonably good with the published data. Deduced data on the coupling strength \( (\lambda = 0.98) \) and repulsive parameter \( (\mu^* = 0.26) \) for the optical plasmon frequency \( (\hbar \Omega_\perp = 52.42 \text{ meV}) \) seems to be appropriate and gives us a meaningful set of physical parameters for high \( T_c \) BKBO systems with an enhanced density of states at the Fermi level. We identify the BKBO superconductor as a moderate...
to strongly coupled system. It is worth mentioning that the physical parameters other than $T_c$ in conventional superconductors are extremely varied, but those at higher $T_c$ are mostly characterized by a large density of states at the Fermi level, which leads to an enhanced value of $\lambda$, a reduced value of $\mu^*$ and thus to high $T_c$.

A central prediction of the proposed approach is the interpretation of the normal-state resistivity. We have first estimated the zero-temperature elastic scattering rate with the use of parameters ($\lambda$, $\mu^*$, $V_F$, $\tau$ and $\omega_{np}$) from the developed approach and the upper critical magnetic field from a magnetization measurement. The estimated zero-temperature-limited resistivity is consistent with the single crystal data. Furthermore, the zero-temperature mean free path is found to be one-half of the zero-temperature coherence length. The mean free path is several times larger than the Bi–O bond length and the product $k_F L > 1$ favours metallic conduction. Hence, the use of Ziman’s formula in estimating the electron–phonon contributions is found to be appropriate.

It is noted that the contribution from the electron–optical phonon together with the zero-temperature-limited resistivity is smaller than the published data on the single crystal. When the subtracted data are plotted as a function of $T^2$, a clear straight line is depicted until 200 K and then the resistivity varies linearly with temperature up to room temperature. The observation of the $T^2$ dependence is understood in terms of 3D electron–electron scattering. We have thus demonstrated that apart from electron–phonon (breathing modes of oxygen), electron–electron scattering is important in the temperature range $30 < T < 200$ K. The change in the power temperature law to a linear temperature law is not clearly understood as it does not indicate any crossover of the dimensionality in 3D BKBO superconductors. We speculate that the linear temperature dependence of $\rho$ in the temperature range $200 < T < 280$ K is due to high-energy oxygen breathing modes. The scattering lifetime at low temperatures is of the order of $10^{-14}$ s in high $T_c$ cuprates. For the high $T_c$ BKBO with higher resistivity we obtained a reduced lifetime ($10^{-15}$ s) which is a natural outcome of the present analysis. The mass difference between Bi and O is large so using the coupling strength from an electron–ion matrix element using the McMillan formula is appropriate and yields reasonably good results.

In conclusion, the nature of the pairing mechanism, superconducting transition temperature and normal-state resistivity of 3D cubic Ba–K–BiO superconductors is well understood by electron pairing mediated with high-energy optical phonons of the oxygen breathing mode. The same set of parameters used to interpret the published data on $T_c$ and $\rho$ suggest that Ba$_{0.6}$K$_{0.4}$BiO$_3$ is a strong coupling superconductor and both electron–electron and electron–phonon scatterings are significant.

References

Two-component model for optical conductivity in Y–Ba–CuO superconductors

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Abstract. The optical conductivity of optimized doped YBa$_2$Cu$_3$O$_{7-}\delta$ (\(\delta = 0.0, \ T = 92 \text{ K}\)) superconductors, which are frequency dependent, has been theoretically investigated based on two-component (Drude and mid infrared terms) approach within the Fermi liquid description. Our approach incorporates the Drude contribution as well as hopping of charge carriers in the model dielectric function along with the structure factor. It explains the anomalies observed in the optical measurements for the normal state as the frequency dependence of optical conductivity using the Drude term which gives a sharp peak at zero frequency, and a long tail at higher frequencies, i.e. in the infrared region. The extra term (hopping carriers) gives a peak value in the optical conductivity centred in the mid infrared region. The two species of charge carriers contribution to the conduction in the CuO chain layer as well as CuO$_2$ layer will account for the optical conductivity in the mid infrared as well as infrared frequency regions. The analysis reveals an interesting relation $\sigma_{\text{CuO layer}} = \sigma_{\text{chain layer}}$ and the nature for optical conduction with energy is similar qualitatively, the only difference is quantitatively. It is shown that the analysis is consistent with the published data on optical conductivity in optimized-doped YBa$_2$Cu$_3$O$_{7-}\delta$ superconductors.

Keywords. Optical conductivity; Drude term; hopping; YBCO superconductors.

1. Introduction

Since the discovery of high temperature superconductivity in cuprates, attempts have been made to identify the superconducting energy gap and other features responsible for the pairing mechanism, using infrared spectroscopy. Infrared spectroscopy provides valuable information on optical conduction of the charge carriers in the normal as well as superconducting states, which are not clearly understood and controversies remain to be unresolved (Tanner and Timusk 1992). Among various cuprates, 90 K Y–Ba–CuO system has been widely analysed experimentally, since good crystals with a very sharp superconducting transition at $T_c$ can be prepared from it. However, 90 K Y–Ba–CuO system has complex crystal structure as there exists single one-dimensional (1-D) CuO chain layer, two-dimensional (2-D) CuO$_2$ layer, and metal oxide layers. It is generally believed that superconductivity occurs primarily in the 2-D CuO$_2$ layer, and that the 1-D CuO chains are not so crucial. Recent experiments have indicated that the chain layer is metallic and contributes significantly to the transport of charge carriers (Bernhard and Tallon 1996). Exact mechanism of the binding of holes into Cooper pairs remains elusive and this concept has to be taken into account in attempting a theoretical discussion of this system.

Optical conductivity measurements in the mid- and near-infrared regimes can give valuable information regarding the properties of low-lying charge excitations in the metallic system. For optimized-doped 90 K YBCO, the optical conductivity, $\sigma(\omega)$, spectra shows a sharp peak at $\omega = 0$, and a long tail extending to higher frequencies in the infrared region where $\sigma(\omega)$ falls as $\omega^{-\beta}$ slower than $\omega^{-1}$ decay in the Drude spectrum. The origin of the mid-infrared (MIR) band is still unclear. When a Drude model is used, an extremely short mean free path should be used to fit the optical data, and the temperature dependence is much weaker than expected due to dc conductivity. It has been argued that the anomaly in MIR band may be caused by the coupling between the mid-infrared carriers and phonons. Furthermore, the optical spectra is mainly due to the 2-D CuO$_2$ layers (Tanner and Timusk 1992). While some authors attribute MIR band in part to trapped holes near dopant atoms, others claim that it is from the Cu–O chains of YBCO that most of the weight originates. It is therefore important to establish the role of CuO chain layer as well as CuO$_2$ layers in the optical conduction mechanism.
Extending the scenario, the idea of phonon-mediated force alone to meet high transition temperature in cuprates seems to be difficult, and the observed high $T_c$ may be associated with charge fluctuations other than the phonon, proposed earlier (Kresin et al 1993). Examples to support this include low-energy plasmons, or excitons which may play an important role in realizing high $T_c$ superconductivity. Optical conductivity measurements (Uchida et al 1991) and Raman scattering experiments (Sugai et al 1990) have suggested the strong density fluctuations in the mid-infrared region of optical spectra.

Optical conductivity can be obtained after a Kramers-Kroning analysis of the reflectance spectra, and many experimental studies of YBCO superconductors have been carried out in the recent past (Thomas et al 1988; Kamaras et al 1990; Orenstein et al 1990). While the far-infrared region depends strongly on temperature, especially below $T_c$, the mid-infrared region is temperature independent. There is a clear minimum at $\sim 2000 \text{ cm}^{-1}$ that can be easily seen at $T = 100 \text{ K}$ (Orenstein et al 1990). It is remarkable in this connection that the real part of the conductivity, which describes the absorption, provides a measure of the size of the superconducting gap. There has been an ongoing debate as to whether or not a superconducting gap is observable in the in-plane reflectivity spectrum. Conventional superconductors display an $s$-wave gap and are in dirty limit, while the high $T_c$ cuprates are different. Using the two-component model in which a spectrum is decomposed into a $T$-dependent Drude part and a $T$-independent mid-infrared absorption part, Kamaras et al (1990) claimed that a gap cannot be observed in the in-plane spectrum because of clean limit on superconductivity. Experimental results for optical conductivity (Terasaki et al 1990; Uchida et al 1991) in the superconducting copper oxides suggest that there exists at least two species of carriers, contributing to the conduction in CuO$_2$ layers over the infrared and the lower frequency regimes in the light of conductivity sum rules.

On the theoretical side, it may be noted that the normal state $\sigma(\omega)$ does not follow an ordinary Drude law in the infrared region. Schlesinger et al (1990) have analysed the $\sigma(\omega)$ data using one component model which considers the frequency dependent parameters $\omega(\omega)$ and $1/\omega(\omega)$, and obtained a gap of $500 \text{ cm}^{-1}$. The two-component analysis in which the $\sigma(\omega)$ spectrum is decomposed into an ordinary term (where all parameters are independent of frequency) at $\omega = 0$ plus an extra Drude contribution modelled by one or more lorentz oscillators centred at $\omega$ in the MIR region. Recently, Stevens et al (1997) have investigated the electronic excitations contribution to the superconducting gap function in YBCO systems using the Femto second time resolved spectroscopy. The optical response favours the two-component mode of high $T_c$ superconductivity in the YBCO systems. As mentioned earlier, the mid-infrared in the optical spectra is mainly due to the CuO$_2$ layers (Tanner and Timusk 1992). Guided by these experimental and analytical work, the role of 1-D CuO chain layer and 2-D CuO$_2$ layer contribution to optical conductivity as well as the underlying physics of observed MIR anomaly was investigated.

In § 2, we have discussed a model which we have developed using two species of charge carriers. The first channel to the conductivity is the coherent Drude component with temperature dependent damping. Secondly the hopping of charge carriers from one site to another site of the CuO$_2$ layer will contribute to the conductivity. Moreover, we assumed that in the metallic normal phase, $\sigma(\omega)$ consists of a Drude term centred at zero frequency whose shape depends on temperature, and the hopping term will contribute a peak value in the mid-infrared region, Role of chains and layers are well approximated, forming a layer stacking sequence structure of YBCO. § 3 deals with the estimation of parameter, along with results and discussion.

2. The model

The peculiarity of the high $T_c$ superconducting cuprates are in their structural complexity as well as topology of Fermi surface associated with the electronic band energy. For the calculation of the transport property, knowledge is required of both hole and phonon bands, construction of the Fermi surface, in addition to the operating superconducting mechanism. The high $T_c$ cuprates are layered, low-dimensional structures with anisotropic Fermi surface. The single crystal of Y-based cuprate superconductors can be modelled as an infinite array of two-dimensional (2-D) conducting CuO$_2$ planes and 1-D CuO chains, which have a significant number of charge carriers (holes) and are well separated by metal oxide reservoirs with interlayer distance $d > d_0, d_0$. In a unit cell, the layer stacking sequence is $Y, CuO_2, BaO, CuO_2, CuO_2, Y, \ldots$. The layers in the $a-b$ plane possess a relatively weak coupling between the planes in the perpendicular $c$ direction. To a first approximation, these layers are well separated and treated as non-interacting. We may regard such a system as a 2-D hole liquid which may be characterized as a collection of strongly correlated, but with the itinerant Fermi particles confined along $ab$ axis. Furthermore, these two species of carriers contribute to the conduction along the $ab$ axis, which is consistent with the earlier observations.

The free charge carriers, as developed from the chemical doping in the parent compound, are constrained to move within this 2D CuO$_2$ layer and hence the electron gas lies in this plane. We assume that for a non-interacting
system, copper and oxygen electrons are within the Fermi surface. The Fermi surface is anisotropic and is considered as open in the $k_z$ direction perpendicular to the layer plane, i.e. in the $z$-axis. Regarding the construction of the Fermi surface, we assume that the 2-D electron system contains a subgroup with a high density of states near the Fermi level. In this case, the Fermi curve has sections which are almost linear, and has a number of nesting states. As a result of the nesting of the Fermi surface, the scattering processes involve $2k_F$ scattering across the Fermi surface which dissipates momentum effectively. The energy of an electron with open Fermi surface has the following form.

\[
\epsilon(k) = \left(\frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^* d^*} \right) \left| 1 - \cos(k d) \right| \mu,
\]

where $k$ and $k_z$ are the 2-D momentum wave vector along and perpendicular to the CuO$_2$ plane. It appears that one can estimate the effective mass of the electron for their motion in respective directions using the band structure parameters based on local density approximation. The Fermi liquid picture provides the information along the plane only, as it utilizes the experimental data on electronic specific heat coefficient for the estimation of effective mass. We restrict ourselves to the case \( |k_{max}| = \pi/c \). The interplanar separation, $d$, is half of the lattice parameter $'c'$, and $\mu$ represents the chemical potential. Within this Fermi liquid picture (Varshney and Singh 1995; Varshney et al 1996), one can estimate the normal and superconducting state parameters using experimental information in a self consistent way.

As was said above, the electrons below the Fermi surface do interact with nearby charges and the resulting potential have a particularly strong influence in the long wavelength limit. We consider the screened Coulomb potential for a series of identical CuO$_2$ planes. Furthermore, we speculate that two species of carriers contribute to the electrical conduction along the $ab$ axis, which is consistent with the earlier observations (Timusk and Tanner 1989). The distance between two consecutive layers is $d = 2d_i + d_j$, between a CuO chain and a CuO$_2$ layer is $d_i$, and $d_j$ denotes the separation of two consecutive chains. The charged quasi particles are being scattered by the phonons as well as the electronic excitations (plasmons) and the impurities possess a finite damping rate $\Sigma$. The effective interaction potential between the electrons can be conveniently described by the perturbation approach. Performing the Fourier transformation and keeping in mind the periodicity of the layers, the $q_z$ integration ranges from $-\pi/d_z$ to $+\pi/d_z$, one does write the effective interaction potential as (Varshney and Singh 1995):

\[
V(q, q_z, \omega) = \frac{2\pi e^2}{q \epsilon(q, q_z, \omega)} S(q, q_z),
\]

where, $S(q, q_z)$ is the model dielectric function for a single band of charge carriers. $S(q, q_z)$ represents the static structure factor. The contribution from core electrons is $\epsilon_{\infty}$ and in the frequency region of interest it is independent of frequency.

The dielectric function, $\epsilon(q, q_z, \omega)$ in terms of polarizability is expressed as

\[
\epsilon(q, q_z, \omega) = 1 + P(q, \omega) S(q, q_z),
\]

with

\[
P(q, \omega) = \frac{-2\pi e^2}{q \epsilon_{\infty}} \Pi(q, \omega),
\]

and

\[
S(q, q_z) = \frac{\sinh(qd_z)}{\cosh(qd_z) - \cosh(qd) - \cos(qd)}. \tag{4}
\]

where, $q$ is the in-plane 2-D wave vector and $q_z$ is in the $z$ direction. The elastic properties along and perpendicular to the conducting planes are considerably different. To have the conduction along the $a-b$ plane, it is suffice to average (1) to get

\[
V(q, \omega) = \frac{d}{2\pi} \int_{-\infty}^{\infty} V(q, q_z, \omega) dq_z. \tag{5}
\]

The integral can thus be evaluated by using (1) and (5) to obtain

\[
V(q, \omega) = \frac{2\pi e^2}{q \epsilon_{\infty}} D(q, \omega) \sinh(qd_z) \sinh(qd) \tag{6}
\]

with

\[
D(q, \omega) = \cosh(qd) + P(q, \omega) \sinh(qd_z) \sinh(qd). \tag{7}
\]

The two-dimensional electronic polarizability in long wavelength limit ($q \rightarrow 0$) is

\[
P(q, \omega) = -\frac{2\pi e^2 \Sigma(\omega)}{\epsilon_{\infty} m^* \omega |\omega + i\Sigma(\omega)|} \tag{8}
\]

with $\Sigma(\omega)$ being the frequency dependent relaxation rate. We thus write the model dielectric function for two species of charge carriers as:

\[
D(q, \omega) = 1 - \sum \frac{Z_i n_i}{\epsilon_{\infty}} \frac{\Sigma(\omega)}{m^* \omega |\omega + i\Sigma(\omega)|}, \tag{9}
\]

where $n_i$ is the 2-D charge carrier contribution and $m^*$ the effective mass of the carriers. The sum of electronic and ionic bound charge is denoted as $Ze$. We represent

\[
e = a^* d_z.
\]
The frequency dependent relaxation rates are expressed in terms of memory functions as:

$$\Sigma_{\nu}(\omega) = \Sigma_{\nu}(0) + \left[\Sigma_{\nu}(\infty) - \Sigma_{\nu}(0)\right][1 - i\omega\Gamma_{\nu}(\omega)],$$

(10)
in terms of memory functions $\Gamma_{\nu}(\omega)$ (Yoshida and Takeno 1989). Here, we denote $\Sigma_{\nu}(0) = \gamma_{1\nu}$ and $\Sigma_{\nu}(\infty) = \gamma_{2\nu}$ as the low and high frequency limits of the relaxation rates, respectively. In order to satisfy the requirements of causality, the memory functions are:

$$\Gamma_{\nu}(\omega) = \int_{0}^{\infty} \Gamma_{\nu}(t)e^{-i\omega t} dt,$$

(11)
where $\Gamma_{\nu}(t = 0) = 1$ and $\Gamma_{\nu}(t = \infty) = 0$. Using the Gaussian forms of $\Gamma$ (Yoshida and Takeno 1989) for the memory function

$$\Gamma_{\nu}(t) = \exp(-t^2\gamma_{\nu}^2),$$

(12)
with $\gamma_{\nu}^2$ being the characteristic relaxation rates.

Using (9) and (10), the imaginary part of the dielectric function is

$$\text{Im}D(q, \omega) = 1 - \frac{2\pi\epsilon^2 q\epsilon}{\epsilon_{\infty}} \times \sum_{\nu} \frac{Z_{\nu}^2 n_{\nu}^2}{m_{\nu}^*\omega^2 - (\gamma_{1\nu}^2 + \gamma_{2\nu}^2)}.$$

(13)
The optical conductivity is expressed as:

$$\sigma(\omega) = \lim_{\Delta \rightarrow 0} \left[\frac{\omega\Delta}{2\pi q} \text{Im}\{D(q, \omega)\}\right] = \epsilon \sum_{\nu = 1}^{2} \frac{\omega\gamma_{\nu}^2}{2\pi} \frac{Z_{\nu}^2 n_{\nu}^2}{\omega^2 - (\gamma_{1\nu}^2 + \gamma_{2\nu}^2)}.$$

(14)
where $1$ is the number density of CuO$_2$ layers along c axis.

Using the developed expression for optical conductivity assuming two channels of optical within CuO chain layer as well as CuO$_2$ layer, we have computed optical conductivity for YBCO superconductors at $T = 100$ K. Deduced results along with discussions are presented in the following section.

3. Results and discussion

We have estimated the optical conductivity of YBa$_2$Cu$_3$O$_{6.5}$ superconductors at $T = 100$ K based on the experimental observations within the Fermi liquid description in the reciprocal space. Such a technique is of vital importance as the structural information of the system, i.e., lattice parameters as well as the specific heat measurements can be performed well on high quality single crystals, and the data yielded for any theoretical description are more reliable. For the YBCO superconductors, a stack of 2-D layers and 1-D chains which are well separated by average distances, the condition for optimized pairing suggests that 2-D charge carrier density in the layers will follow $n_{\parallel} = 1$, and for 1-D chains $n_{\perp} = 1$. Thus the volume concentration of the charge carriers will be $n = n_{\parallel}n_{\perp}/3$. The Fermi wave vector for the 2-D plane is $k_{\text{F2D}} = (2\pi n_{\parallel})^{1/2}$, and for 1-D chain it is $k_{\text{F1D}} = (2\pi n_{\perp})^{1/2}$.

Furthermore, the effective mass of the charge carriers can be well estimated from the electronic specific heat coefficient ($\gamma$) value for 2-D layers as $m^* = 3\hbar^2\pi^2K_{\text{F2D}}^{-2}$, and $m^*_c = 12\hbar^2\pi^2d^2nK_{\text{F1D}}^{-2}$ are used for the 1-D chains, respectively (Varshney et al 1996). It has been pointed out that incorporation of the realistic physical parameters, based on experimental observations in the Fermi liquid description, will lead to a clearer picture of the properties in the YBCO systems. The lattice parameter and separation distance of the YBCO unit cell are $a = 3.81\,\text{Å}$, $b = 3.88\,\text{Å}$, $c = 11.88\,\text{Å}$, $d = 6\,\text{Å}$, $d_{\perp} = 4.129\,\text{Å}$ and $d_{\parallel} = 3.422\,\text{Å}$ to deduce $n = 2.82 \times 10^{21}\,\text{cm}^{-3}$. Taking $\gamma = 12.6\,\text{mJ} \cdot \text{mol}^{-1} \cdot \text{K}^{-2}$ (Inderhees et al 1987), the effective mass $m^*_c = 6m_0$, and $m^*_c = 2m_0$ are deduced. With these realistic parameters based on experimental information, we attempted to estimate the plasma frequency in chain layer, using $\omega_p^c = 4\pi\epsilon^2\tilde{n}_c\hbar\epsilon_{\text{F}} = 4\pi\epsilon^2\tilde{n}_c\hbar\epsilon_{\text{F}}A_c$. Here, $n_c = N/2$, and area of unit cell $A_c$ is $'ca'$ to obtain $\omega_p$ as $1.146\,\text{eV}$. Similarly for 2-D CuO$_2$ layer, $\omega_p^c = 4\pi\epsilon^2\tilde{n}_c\hbar\epsilon_{\text{F}}/m_c$, with $\tilde{n}_c = 2n_c/c$ and $n_c = N/d$.$d$. Asssumed that one hole $N = 1$ enters into the number of holes in chain layer of length $d_{\perp}$, as well as area $A_c$ of 2-D CuO$_2$ layer.

From the above, it can be inferred that frequency of plasmons, as developed in 2-D CuO$_2$ layer, is enhanced by a factor of $1.7$ than that in 1-D CuO chain layer. The low value of plasma frequency in CuO chain layer is attributed to the reduced effective mass of holes as well as the hole carrier concentration in the one-dimensional conduction process. For the two-component model of optical conductivity, the effective mass ($m_e$) follows the relation $m_e = 8m$, for two species of charge carriers. The effective mass of charge carrier participating in hopping process is much larger due to weak Josephson coupling, and is difficult to determine because of short mean free path. The background dielectric constant, $\epsilon_c$, is taken as $4.5$. The sum of ionic and bound electronic charge is $Ze$. The optical conductivity essentially depends on the value of relaxation rates representing the life time of free charge carriers, and are roughly estimated as $\gamma_1 = \gamma_2 = 2-5 K_{\text{F}}T$ (Timusk and Tanner 1989).
4. Conclusion

In this communication we have devoted our efforts to understand: (i) role of chain layer and CuO,
layer in the optical conduction process, and (ii) the observed anomalous behaviour in the mid-infrared region of YBCO superconductors. To elucidate the contribution of chain layer and CuO,
layer, proper structure factor for layer stacking sequence of YBCO has been constructed which
utilizes the information of structural data within the Fermi liquid description. We speculate that phonons as well as low energy plasmons perhaps contribute to the superconducting pairing. Physically, the Drude carriers couple only weakly with phonons or low energy plasmons, giving rise to a sharp value at zero frequency. Using the memory function approach for frequency-dependent relaxation rates, we have systematically obtained the characteristic relaxation rates. In a true sense, the scattering rates are very large, and of the order of \( T \), in high \( T \) cuprates. Specific heat data is used to estimate the effective mass of the charge carriers (holes) participating in the \( a-b \) plane conduction process. The effective mass of the charge carrier in CuO chain layer is nearly 3-times smaller than that of CuO,
layer because of its one-dimensional characteristic.

Assuming two-channel of optical conduction, i.e. (i) Drude component with temperature-dependent relaxation rates which essentially describes the peak value centred at \( w = 0 \) as well as the long tail in the infrared region, and (ii) the hopping of the charge carrier from one site to another within the CuO,
layer—the interlayer effects, we interpret the anomalies observed in the optical measurements. Within this framework, we are able to understand the observed anomaly in the mid-infrared region. In principle, CuO chain layer as well as CuO,
layer actively participate in the optical conduction process and they differ in only the magnitude. The analysis reveals that \( \sigma_{\text{opt}} = 3\sigma_{\text{chain layer}} \). In conclusion, the two species of charge carriers, which were earlier observed experimentally, can describe the anomalies observed in the \( \sigma(\omega) \) spectrum as a sharp one at \( \omega = 0 \), a long tail in the infrared region and a peak value centred at mid infrared region (\( \omega = 1000 \text{ cm}^{-1} \)).

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Abstracts

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SUPERCONDUCTIVITY IN Ba-Pb\textsubscript{1-x}Bi\textsubscript{x}O\textsubscript{3} : A COUPLED 2D ACOUSTIC PLASMON-PHONON APPROACH

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We have explored our efforts to study the cubic pervoskites Ba-Pb-BiO ($T_c = 13K \pm 0.25$) by emphasizing the breathing vibrations of oxygen and charge oscillations in the system due to the chemical substitutions of Pb (6s) in place of Bi. The free electrons will coupled to the charge oscillations and the influence is strong enough. The interaction will generate two modes. One of them is 2D acoustic plasmon mode and the other is coupled plasmon - optical phonon mode. The spectral intensity of the charge oscillations is extremely strong to the bare phonons. Earlier, we have developed a Free electron layered electron gas model (FELEG) [1] which successfully describe the pairing mechanism and the superconducting state parameters of High $T_c$ Lanthanum cuprates. The approach facilitates the various interactions, the dielectric function and plasmon, phonon modes. The present approach [2] is able to explain the nature of pairing mechanism in Ba-Pb-BiO superconductors successfully. We work out the Frohlich coupling strength and the screened Coulomb parameter for maximum phonon frequency. Looking to the previous work on Lanthanum cuprates and present studies on Barium bismuthates, we propose that the superconductivity in High $T_c$ systems will be explained by the coupled charge transfer oscillations and the oxygen breathing vibrations.

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- TEN YEARS AFTER ITS DISCOVERY
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ABSTRACTS

Co-Organizers:
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TEMPERATURE DEPENDENCE OF ELECTRODYNAMIC PROPERTIES OF Y-Ba-CuO (248 & 123) SUPERCONDUCTORS

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The temperature dependence of electrodynamic properties of YBCO (123 & 248) superconductors have been estimated. The analysis is based on Electronic energy band structure studies (EEBS) [1] as well as Layered electron gas (LEG) approach [2]. Anisotropy of the Layered structure of YBCO is well reflected in the shape of Open Fermi surface. We have properly considered the two CuO planes and one 1D CuO chain in a unit cell of Y123 system and an extra 1D CuO chain in Y124 system. The transport parameters (m, n) estimated from EEBS yields smaller values of penetration depth (λ) as compared to the radio frequency surface impedance measurements on Y123 system [3], while higher values are obtained for Y124 system. On the other hand the transport parameters as deduced from the LEG approach which properly considers the layered structure for chains and layers yields a consistent data for Y123 and Y124 cuprates [4]. We argue that EEBS overestimates the transport parameters. Fig. 1 shows the temperature dependence of λ and predicts the similar nature as revealed from the experiments. Furthermore, the results on coherence length and critical magnetic fields are also presented and are consistent with the earlier reports.

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The Superconducting state parameters of electron doped Nd-Ce-CuO and hole doped La-Sr-CuO systems have been estimated. The analysis is based on Electron Energy band structure studies /1/. Anisotropy of the Layered structure is well reflected in the shape of open Fermi surface. The effective mass of the charge carriers is then worked out from the Fermi velocity. The model calculations yield smaller values of magnetic penetration depth than those revealed from the μSR measurements /2/. The coherence length (ξ^⊥ and ξ^∥) is evaluated and appears to be higher /3/. Temperature dependence of Ginzburg Landau parameter (κ) and magnetic penetration depth shows the same nature as those revealed from experiments (see Fig. 1). Furthermore, results on lower and upper critical magnetic field are also presented. It is concluded that results on magnetic properties of electron & hole doped superconductors are although consistent when band structure parameters are used and are in better agreement when the Fermi liquid approach /4/ is used.

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ABSTRACT

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CURRENT DRIVEN PLASMA INSTABILITIES IN CUPRATE SUPERCONDUCTORS

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Based on free electron layered electron gas (FELEG) model of quasi two dimensional layers of CuO\textsubscript{2} in Y-Ba-CuO (T\textsubscript{c}=90K) Superconductors a model dielectric function is developed with electron-ion plasmon and electron-electron plasmon interactions at low temperature (T=0K) and at temperature where T is closed to T\textsubscript{c}. At low temperature (T=0K) an instability (current driven) is generated in this layered structure as the charge carriers (holes) do not scattered. This plasma instability is of cold beam type. At the temperature when T=T\textsubscript{c} the electrons form a superconducting state where the carrier scattering effects are dominating. It is noticed that an inverse Landau damping related instability will generate in cuprate superconductors for sufficiently large drift. Indeed this current driven instability is due to the pair breaking effect near T\textsubscript{c} and it will grow only when Cooper pair energy (\epsilon) is greater than T\textsubscript{c} which todate is not practically achievable. We conclude from our analysis that the drift velocity does not exceed the phase velocity so a negative energy wave is observed.
THE 80K Superconductor Y-Ba-CuO (124) with double two dimensional (2D) CuO planes as well as one dimensional (1D) CuO chains is found as a distinctly ordered phase \cite{1}. We have devoted our efforts to develop a free electron layered electron gas model to elucidate the nature of interaction when electron-electron, electron-phonon and electron-plasmon interactions are present. Proper care of structure factor for both 2D planes and 1D chains have been incorporated in the effective interaction \(V_{\text{eff}}\) via polarisation function. Poles of \(V_{\text{eff}}\) will lead to three modes as \(\Omega_{+L} (\Omega_{+C})\) denotes 2D acoustic plasmon plane (chain) and \(\Omega_{-}\) as 2D acoustic phonon mode. We find that the polarisation term in \(V_{\text{eff}}\) for double planes and chains in unit cell will yield two plasmon modes which are acoustic in nature and deduced values are \(\Omega_{+L}=2.5\) eV and \(\Omega_{+C}=65\) meV, respectively. The chain plasmon is of low energy and will stabilise the charge carriers in the planes. The interaction potential \(V_{k,k'}\) will take three values as \(V_{k,k'}=-V_{\text{ph}}\) for \(\omega < \Omega_{-}\) = \(V_{c}\) for \(\Omega_{-} < \omega < \varepsilon_{F}\) and = \(-V_{\text{pl}}\) for \(\varepsilon_{F} < \omega < \Omega_{+L}\). The nature of \(V_{\text{eff}}\) with energy is shown in Fig.1. It is inferred that for the range \(\omega < \Omega_{-}\) and \(\varepsilon_{F} < \omega < \Omega_{+L}\) the interaction potential shows the attractive nature, while for \(\Omega_{-} < \omega < \varepsilon_{F}\) \(V_{\text{eff}}\) is repulsive. The attractive energy \(V_{\text{ph}}(V_{\text{pl}})\) have an upper cut off \(\Omega_{-}(\Omega_{+L})\). The results deduced on \(T_{c}\) as 33K with this effective potential \cite{2} which is consistent with the reported data of 80K/1/.


SUPERCONDUCTIVITY IN Ba-K-BiO : A COUPLED PHONON PLASMON APPROACH

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Since the discovery of Ba-K-BiO by Mattheiss et al. /1/ with a $T_c$ of 28K tremendous quantity of work has been carried out. The BaKBiO possesses a cubic three dimensional lattice and does not contain copper or any other magnetic atoms which is why particularities of BaKBiO could not be explained by the layered structure or magnetic properties of the system. We have devoted our efforts to understand the nature of pairing mechanism by developing a model for Ba-Pb-BiO /2/ which includes the Coulomb, electron-optical phonon and electron-plasmon interactions to elucidate the superconducting state. The presence of these electron-electron, electron-phonon and electron-plasmon interactions allows a coherent understanding of the pairing mechanism in these 3D systems. The longitudinal dielectric function follows the $f$-sum rule and the interaction will generate oscillations of the electronic charge coupled with optical phonon. On applying the above approach for Ba-Pb-BiO ($\Delta = 0.4$) superconductors, we have estimated the coupling parameter $\lambda$ as 1.30 which favours the strong coupling and screened Coulomb repulsive parameter ($\mu^* = 0.26$) for the characteristic frequency value $\Omega_- = 514.85$ cm$^{-1}$ and suggests the poor screening of charge carriers with low concentration. The $T_c$ is then estimated as 31.16K within the strong coupling theory and is consistent with a $T_c$ of 30K at $\Delta = 0.4$ /3/. Deduced values of $\lambda$ (1.30) and $\mu^*$ (0.31) for maximum $\Omega_- (=514.85$ cm$^{-1}$) are quite reasonable and provide a good set of physical parameter estimated from the experimental observations, which yield high $T_c$ value $\sim 31.16K$ despite of low values of charge carrier density and the density of states at Fermi level. The oxygen isotope effect and energy gap parameters are also evaluated and consistent with the reported data. In conclusion, the coupling of electrons with the coupled charge oscillations-optical phonon mode could be a reason for superconductivity in Ba-KBiO superconductors. The Ba-KBiO is a strong coupling superconductor ($\lambda > 1.0$) with weak to moderate interaction between electrons and high energy coupled charge oscillations and breathing modes of oxygen ($\Omega_- = 514.85$ cm$^{-1}$).