IOSR Journal of Engineering (IOSRJEN) **www.iosrjen.org**
ISSN (e): 2250-3021, ISSN (p): 2278-8719
Vol. 14, Issue 2, February 2024, ||Series -I|| PP 30-37

Phonon Frequency Spectrum of HTSC La_2BaCuO_5Through Lattice Dynamics and Normal Co-ordinate Analyses.

SONAMUTHU. K*, GEENA VIDYA . S
*(*J N R Mahavidayalaya, Port Blair, South Andaman, India.744104*
Sathyabamal Engineering College, Chennai-600066)
Received 28 February 2024; Accepted 12 Marc 2024

Abstract
In the present investigation the lattice dynamical calculations and normal coordinate analysis yield same phonon frequency a bridge between Solid State Physics and Spectroscopy to understand the mechanism of superconductivity. Raman and infrared studies of these HTSC have contributed significantly to their understanding. The assignment of the spectral features to specific lattice vibrations would be an important step in understanding their role in superconductivity. The lattice dynamics method is suited to determine the phonon frequencies in the proximity of the Brillouin zone centre only. But , the force constants obtained from that analysis do not provide a stable dynamics throughout the Brillouin zone. However, it is indispensable to have a precise knowledge of the zone
–boundary phonons to investigate the contribution of electron-phonon coupling to Tc which can be achieved by neutron scattering techniques. The most commonly employed model is the valence force field model for computing phonon frequencies based on stretching bond and bending bond coordinates. Such models have the advantage of being well adopted to describe a covalent bonding but ignored the long–range Coulomb forces and wave vector dependence of the phonon spectrum.
Key Words: Lattice dynamics ,Normal Coordinate Analysis , High Temperature Superconductors(HTSC),La_2BaCuO_5,Brillouinzone, Three Shell Model(TSM), Symmetry, Raman phonon frequencies, Infrared(IR),etc.,

I. INTRODUCTION

The introduction of superconductivity above 30 K in CuO-pervoskites by Bednorz Muller[1-3] initiated tremendous efforts in solid state physics and material sciences with the aim to isolate the phases which are responsible for the superconductivity.

One direction of experiments has the intention to find out what is the contribution of lattice vibrations to the superconductivity. Neutron scattering, as the method to determine the vibration spectrum throughout the whole Brillouin zone, could at the beginning of these activities only measure the phonon density of states, as shown by Ramirez et al. [4], Renker

et al.[5,6], Bruesch et al.[7],Burer et al.[8], and Belushkin et al.[9], because large single crystals were not available. Raman and infrared (IR)-spectroscopy, however, can yield at least some of the phonon frequencies, namely the long wavelength optical phonons at the center of the Brillouin zone, from polycrystalline materials. Even tiny single crystals embedded in polycrystalline samples can be investigated in Raman experiments with theuse of microscope.

The published results of experimental work on Raman and IR-Spectroscopy have detailed information about the lattice vibrations of the superconducting materials and their dependence on oxygen contents, element substitution and impurity phases, which appeared in various samples and partly yielded controversial results. In addition, the temperature variations of the optical phonon spectrum and the superconducting gap have been investigated[10]. .

The study of normal coordinate analysis and the free carriers is important for the understanding of the physical nature of high temperature superconductors. Raman and far- infrared studies of these superconductors have contributed significantly to the understanding of new class of superconductors. Cardona and coworkers [11-18] studied the infrared and Raman spectra of the super conducting cuparate perovskites $MBaCu_2O_2$ (M = Nd, Er, Dy, Tm and Eu) and reported the possible origins of phonon softening and the systematic variation of phonon

frequencies with the ionic radius. Where PED is the combination of the i-th symmetry coordinate to the potential energy of the vibration whose frequency is $\lambda_k = 4\pi^2 C^2\upsilon^2$ VkFij are potential constants, Lik are L matrix elements and .Recently, anomalous behavior of the phonon band vibrating in the c-axis direction has attracted much interest [40-43], and strong coupling theory of phonon and free carriers hasbeen reported [19-20].

2. Calculation of Lattice Dynamical by Using Three Shell Model (TSM) of HTSC La_2BaCuO_5.

The calculations of Lattice Dynamical vibration frequencies of La_2BaCuO_5 system is performed by Three-Body Force Shell Model (TSM). The Lattice Dynamical calculations based on modified TSM reproduce the observed frequencies of Raman and infrared active modes reasonable which are given in table 3 . The calculated frequencies are in good agreement with the available experimental values. The lowest calculated Raman active A1g mode frequency at 154 cm^{-1} is due to the vibration of La atoms and this agrees very well with the experimental frequency at 150 cm^{-1}. Similarly the calculated Raman frequency is A1g symmetry at 231 cm^{-1} and 554 cm^{1} are due to the vibration of Ba and O(3) atoms respectively and the observed frequencies at 231 and 554 cm^{-1} agrees very well with the calculated frequency. The highest calculated Raman frequency 554cm^{-1} in A1g symmetry isdue to the vibration of O(3) atoms which also agrees very well with the observed frequencyat 554 cm^{-1} The calculated Raman phonon frequencies at 173 and 418 cm^{-1} in B1g symmetry are due the vibration of La and Ba atoms respectively and the observed frequencies at 172 and 420 cm^{-1} agrees very well with the calculated phonon frequencies

The evaluated phonon frequency at 185 cm^{-1} in B2g symmetry is due to the vibration of La atom. The Cu and O(1) atoms vibrates at 180° out of phase to La atoms. Similarly the calculated Raman phonon frequencies at 332 cm^{-1} is due the vibration of O(2) atom which is out of phase to O(1) atom and its observed frequency at 330 cm^{-1}agrees vey well with the calculated phonon frequency. The Calculated Raman phonon frequency at 436 cm^{-1} is due to the vibration of O(1) atom and it performs bending bond vibration in the O(3) atom and Ba atom is out of phase to O(1) and O(3) atoms. The observed frequencies at 436 cm^{-1} agrees very well with the calculated phonon frequencies.

The calculated Raman phonon frequencies in Eg symmetry at 155 cm^{-1}, 287 cm^{-1}, 418 cm^{-1} and 572 cm^{-1} are due the vibration of La , Ba, Cu and O(1) atoms respectively and it agrees very well with the observed frequencies at 155, 287, 425 and 575 cm^{-1} respectively.

The calculated Infrared (IR) phonon frequencies in A2u symmetry at 160 cm^{-1}, 356 $cm^{-1}$and 420 cm^{-1} are due the vibration of O(1), O(2) and O(3) atoms respectively and it agrees very well with the observed frequencies at 155 cm^{-1} , 360 $cm^{-1}$and 419 cm^{-1} respectively .

The calculated infrared frequency in Eu symmetry at 155 cm^{-1} and 179 cm^{-1} are due to the vibration of Ba and O(1)atoms .The frequency at 238 cm^{-1} is due to the vibration of Ba atom. The frequencies at 428 cm^{-1} is due to the vibration of La atom. Similarly the frequency at 456 cm^{-1} is due to the vibration of O(1) and La atoms vibrates at 180° out of phase to O(1) and O(2) atoms. Its observed frequency at 460 cm^{-1} agrees very well with the calculated phonon frequency . The Calculated IR frequency 554 cm^{-1} is due to the vibration of O(1) atom whereas O(1) atom vibrates at 180°out of phase to Cu and O(2) atoms. The highest frequency in Eu symmetry is 608 cm^{-1} is due to the vibration of O(3) atom and its observed frequency at 608 cm^{-1}agrees vey well with the calculated frequency due to the stretched vibration of Cu(1)-O(1) atoms

3. Normal Co-ordinate Analysis of The Zero Wave-Vector Vibration of La_2BaCuO_5

The study of lattice vibrations and the free carriers is important for the understanding of the physical nature of high temperature superconductors. Raman and far-infrared studies of these superconductors have contributed significantly to the understanding of new class of superconductors. Cardona and coworkers [21] studied the infrared and Raman spectra of the super conducting cuparate perovskites $MBaCu_2O_2$ (M = Nd, Er, Dy, Tm and Eu) and reported the possible origins of phonon softening and the systematic variation of phonon frequencies with the ionic radius. Here an attempt has been made to perform the normal coordinate analysis for the phonon frequencies and the form of the zero wave vector vibrations for the La_2BaCuO_5 Superconductors.

The high Tc superconductor **La_2BaCuO_5** System crystallizes in the body-centered tetragonal (bct) system, which belongs to the space group P_4/mmm (D^1_{4h}) The body-centered tetragonal (bct) unit cell of **La_2BaCuO_5** and the numbering of the atoms are shown in Fig. 1. The 09 atoms of the unit cell yield a total of 27 optical vibrational modes. All the above calculations are made at q=0. Once of A_{2u} and E_u modes corresponds to acoustic vibrations with frequency ω = 0. These normal modes are distributed as follows.

$A_{1g}+B_{1g}+B_{2g}+E_g+A_{2u}+E_u$ □ from the motion of 2 La atoms

E_g+E_u □ from the motion of Ba atom

$A_{2u}+E_u$ □ from the motion Cu (1) atoms

$A_{1g}+B_{1g}+B_{2g}+E_g+A_{2u}+2E_u$ □ from the motion O (1) atoms alone c-axis

$A_{1g}+B_{2g}+E_g+A_{2u}+2E_u$ □ from the motion O (2) atoms alone b-axis

$A_{2u}+2E_u$ □ from the motion O (3) atoms alone a-axis

Subtracting the translation modes $A_{2u} + E_u$ the q = 0 optical modes involved in an irreducible representation are as follows.

$$\Gamma_{opt} = 3A_{1g}+2B_{1g}+3B_{2g}+4E_g+3A_{2u}+8E_u$$

The species belonging to A_{1g} , B_{1g} , B_{2g} and E_g Raman active modes whereas A_{2u} and E_u are infrared active modes. The A_{2u} and A_{1g} modes involve displacement along crystallographic c-axis, the B_{2u} and E_g modes along the b-axis and E_u modes along the a-axis.

The normal coordinate calculation was performed using the programs GMAT and FPERT given by Fuhrer et al [22]. The general agreement between the evaluated and observed normal frequencies of **La_2BaCuO_5** is good. The calculated force constants using the above programs are given in Table 3. It is interesting to note that the evaluated frequencies given in Table 3, agree favorably with the experiment values.

To check whether the chosen set of vibrational frequencies makes the maximum contribution to the potential energy associated with the normal coordinate frequencies of the super conducting material, the potential energy distributions was calculated using the equation.

$$PED = (F_{ij} L^2_{ik})/ \lambda_k$$

Where PED is the combination of the i-th symmetry coordinate to the potential energy of the vibration whose frequency is $V_kF_{ij}$are potential constants, L_{ik} are L matrix elements and $\lambda_k = 4\pi^2 C^2 \upsilon^2_k$.

4. Calculation by using Normal coordinate analysis of HTSC La_2BaCuO_5 :

The G-matrix elements have been calculated from the equilibrium geometry. The initial force constants were taken from the related molecules. The final sets of potential constants provide the stability of the crystal in relation to all vibrational modes. The vibrational frequencies and potential energy distribution values are presented in this work. The potential energy distribution indicates the contribution of an individual force constant to the vibrational energy of normal modes. It clearly indicates that there is mixing of the internal displacement coordinates..

The calculated Raman phonon frequency at 152 cm^{-1} in A1g symmetry agrees very well with the observed frequency at 150 cm^{-1}. This is the lowest phonon frequency due to the vibration of La atom and is due to the bending vibration of O(2)-Cu-O(3),which is confirmed by the potential energy distribution calculation. The calculated Raman phonon frequencies at 232 cm^{-1} and 530 cm^{-1} are due to the vibration of Ba and O(2) atoms, both the oscillation are due to the bending vibrations. Both the frequencies agrees very well with the observed frequencies at 231cm^{-1} and 554 cm^{-1}. Respectively.

The calculated Raman phonon frequencies in B1g symmetry at 174 cm^{-1} and 418 cm^{-1} are due the vibration of La atom and Ba atoms respectively. Both the frequencies agrees very well with the observed frequencies at 172cm^{-1} and 420 cm^{-1}respectevly.

The calculated Raman phonon frequencies in B2g symmetry at 184 cm^{-1} , 330 cm^{-1} and 430 cm^{-1} are due the vibration of Ba, Cu and O(1) atoms respectively. The observed frequencies at 190 cm^{-1}, 330 cm^{-1} and 436 cm^{-1} agrees very well with the calculated frequencies respectively.

The calculated Raman phonon frequencies in Eg symmetry are at 155 cm^{-1} , 285 cm^{-1}, 418 cm^{-1} and 572 cm^{-1} are due the vibration of La , Ba , Cu and O(1) atoms respectively. The observed frequencies at 155 cm^{-1}, 287 cm^{-1}, 425 cm^{-1} and 575 cm^{-1} agrees very well with the calculated frequencies respectively. All these vibrations are bending vibration which is confirmed by the potential energy distribution calculation. .

The calculated infrared phonon frequencies in A2u symmetry at 160 cm^{-1} and 357cm^{-1} are due to the vibration of Cu(1) and O(1) atoms and due to the stretched vibration.. The infrared phonon frequencies at 156cm^{-1}, 357cm^{-1} and 421cm^{-1} are due to the vibration of Cu(1),O(1) and O(3) atoms respectively. The frequency at 421cm^{-1} in this symmetry is due to the bending vibration of O(2)-Cu-O(1). The calculated phonon frequencies at 156 cm^{-1}, 357 cm^{-1}, and 421 cm^{-1} agrees very well with observed frequencies at 155 cm^{-1}, 360 cm^{-1}, and419 cm^{-1} respectively.
The calculated infrared phonon frequencies in Eu mode are at 156 cm^{-1} ,179 cm^{-1}, 239 cm^{-1}, 428 cm^{-1}, 460 cm^{-1},555 cm^{-1}, 580 cm^{-1} and 605 cm^{-1} are due to the vibrations of La, Ba, Cu, O(1),O(2), O(3),O(4), O(5) respectively, which agrees very well with the observed phonon frequencies at 156 cm^{-1} ,180 cm^{-1}, 240 cm^{-1}, 430 cm^{-1}, 460 cm^{-1}, 555 cm^{-1}, 580 $cm^{-1}$and 608cm^{-1} respectively which are confirmed by the Potential Energy Distribution calculation.

5. RESULT AND DISCUSSION:

5.1 The comparative studies between Lattice dynamics and normal coordinate analysis of high temperature superconductors La_2BaCuO_5.

The lattice dynamics of high temperature of high temperature superconductor have been performed by using rigid ion model. The modified three body shell model adopted in the lattice dynamical study gives favourable phonon frequencies. The lattice dynamical calculation based on modified TSM reproduce the observed frequencies of Raman and infrared active modes reasonably which are given in table 3. along with calculated normalcoordinate analysis frequencies and the observed frequencies.

The calculated Raman phonon frequency of Lattice dynamics at 154 cm^{-1} in A1g symmetry is due to the vibration of La atom which agrees very well with the normal coordinate analysis's frequency at 152 $cm^{-1}$and it is due to the bending vibration of O(2)- La -O(3) which is confirmed by the potential energy distribution calculation. The highest phonon frequency in this symmetry of lattice dynamical is 554 $cm^{-1}$and is equal to 550 cm^{-1} in normal coordinate analysis is due to the vibration of O(2) atom and it also shows stretched vibration of O(2) atom.

The phonon frequency in B1g symmetry at 173 cm^{-1}in lattice dynamics is more or less equal to the phonon frequency at 174 cm^{-1}obtained by the normal coordinate analysis. This phonon frequency is due to the bending vibration. Similarly, The phonon frequency 418 cm^{-1} in lattice dynamical calculation agrees very well with the frequencies obtained by the normal coordinate analysis at 418 cm^{-1}.

The evaluated phonon frequency at 185 cm^{-1} in B2g symmetry is due to the vibration of La atom. The Cu and O(1) atoms vibrates at 180° out of phase to La atoms that agrees very well with the frequencies obtained by the normal coordinate analysis frequency at 184 cm^{-1} . The calculated phonon frequencies of Lattice dynamics at 332 $cm^{-1}$and 436 cm^{-1} in B2g symmetry are due to the vibration of Cu and O(1) atoms that agrees very well with the frequencies obtained by the normal coordinate analysis frequency at 330 $cm^{-1}$and 430 cm^{-1} respectively.

The calculated Raman phonon frequencies in lattice dynamical calculation at 155 cm^{-1}, 287 cm^{-1}, 418 $cm^{-1}$and 572 cm^{-1}in Eg symmetry are due to La, Ba, Cu and O(1) atoms agrees very well with the calculated phonon frequencies obtained by the normal coordinate analysis at 155 cm^{-1}, 285 cm^{-1}, 418 cm^{-1}, 575 cm^{-1}respectively which is confirmed by the PED calculation.

The minimum infrared phonon frequency in A2u symmetry at 160 cm^{-1}in lattice dynamical calculation is due to the vibration of Cu atom which agrees very well with the frequency obtained by the normal coordinate analysis at 160 cm^{-1}which is performed by stretching vibration and it is confirmed by the potential energy distribution calculation. The maximum frequency of Lattice dynamic calculation in this symmetry is 420 cm^{-1} that agrees very well with the frequency obtained by the normal coordinate analysis at 421 $cm^{-1}$is due to the stretched vibration of O(2) atom and is confirmed by PED calculation.

The calculated phonon frequency of lattice dynamics at 155 cm^{-1},179 cm^{-1}, 238 cm^{-1}, 428 cm^{-1}, 456 cm^{-1}, 554 cm^{-1}, 580 cm^{-1} and 608 cm^{-1}in Eu symmetry are due to the vibration of La, Ba, Cu, O(1),O(2), O(3),O(4), O(5) atoms respectively which agrees very well with the frequency obtained by the normal coordinate analysis at 156 cm^{-1},179 cm^{-1}, 239 cm^{-1}, 428cm^{-1}, 460 cm^{-1} , 555 cm^{-1}, 580 cm^{-1} and 605 cm^{-1}which is confirmed by the PED calculation.

6. Conclusion

In this work, two different methods viz, lattice dynamical study and normal coordinate analysis yielded the same phonon frequency for high temperature superconductor La_2BaCuO_5. the agreements between the calculated and observed frequencies wherever available are very good for the systems under consideration. Therefore, it is concluded that metal - oxide (Cu-O) plays an important role for the occurrence of superconductivity. The Raman scattering has provided direct evidence for strong electron−phonon interaction in the high Tc superconducting oxides. The vibrational frequencies calculated by the methods of Lattice Dynamics and Normal Coordinate Analysis are compared and they appear to be in good agreement, which is confirmed by the Potential Energy Distribution calculation.

REFRENCES

[1]. J.G.Bednorz and K.A.Muller. Z.Phys.B 64(1986)189
[2]. M.K.Wu,J.R.Ashbirn,C.J. Torng, P.H Hor,R.LMeng,L.Gao, Z.J.Huang, Y.Q Wangand C.W. Chu,. Phys. Rev. Lett. 58(1987)908.
[3]. Z.Z.Sheng, A.MHermann,A.Elali,C.Almasan,J.Estrada,T.Datta and R.J.Matson, Phys. Rev Lett.60(1988)937.
[4]. A.P.Ramirez, B.Batlogg, G.Aeppli R,J.Cava, E.Rietman, A.Goldman and G.Shirane, Phys.Rev B35(1987)8833.
[5]. B.Renker,F.Gompf,E.Gering,N.Nucker,D.Ewert,W.Reichardt and H. Rietchel, Z. Phys. B 67(1987)15.
[6]. B.Renker, F.Gompf, E.Gering, G.Roth, D.Ewert, and W.Reichardt, Z.Phys.B 71(1988)437.
[7]. P.Bruesh and W.Buhrer, Z.Phys.B 70(1988) 70.
[8]. P.Bruesh and W.Buhrer,P.Unternaehre and A.Taylor,Physica C 153-155(1988) 300.
[9]. A.V.Belushkin, E.A.Goremychkin, Inatkaniec, I.L.Sashin, W.Zajac, A.R.Kadyrbaev and B.P.Michailov, Physica C 156(1988) 259.
[10]. S.Sugai, M.Sato. S.Hosoya, S.Uchida, H.Takagi, K.Kitazawa and S.Tanaka, Jpn. J.Appl. Phys. Part 2, Suppl.26-3(1987)1003.
[11]. K.Ohbayashi,N.Ogita,M.Udagawa,Y.Aoki,Y.Maeno and P.Fujita,Jpn. J.Appl.Phys.Part 2,25(1987) L423.
[12]. Torben Burn,M.Grimsditch, K.E.Gray,R.Bhadra,V.Maroni and C.K.Loong, Phys.Rev B35(1987)8837.
[13]. S.Sugai, M. Sato, S.Hosoya, Jpn.J.Appl.Phys.Part 2,.26 (1987)L495.
[14]. S.Blumenroder, E.Zirngiebl, J.D. Thompson, P.Killough, JL Smith and Z.Fisk Phys.Rev B35(1987)8840.
[15]. M.Copic, D.Mihailovic, M. Zgonit, M. Prester, K. Biljakovic, B. Oreal and N.Brnicevic, Solid State Commun. 64 (1987)297.
[16]. B.Batlogg, G.Kourouklis, W.Weber,R.J.Cava, A.Jayaraman, A.E. White, K.T.Short, L.W.Rupp and E.A.Rietmann. Phys. Rev. Lett.59(1987)912.
[17]. G.A.Kourouklis, A.Jayaraman, W.Weber, J.P Remeika, G.P.Espinosa, A.S.Cooper and R.G.Maines Sr., Phys.Rev B36(1987)7218.
[18]. K.B.Lyons, P.A.Fleury, J.P Remeika, A.S.Cooper and T.J.Negeren, Phys.Rev b 37 (1988)2353.
[19]. S.Zhang, He-Tian Zhou,Chongde Wei and Qin Lin, Solid State Commun. 66 (1988) 1085.
[20]. A.I Maksimov, O.V.Misochko, I.T.Tartakovosky, V.V.Timofeev, J.P.Remeika, A.S.Cooper and Z.Fisk Solid State Commun. 66 (1988) 1077.
[21]. Friedl B, Thomsen C, Cardona M, Phys. Rev. Lett., 65:915, (1990)
[22]. H.Fuhrer, V.V.Kartha, K.G.Kidd, P.J.Krueger, and H.H.Mantasch, Computer Programmes for infrared Spectrometry, Vol.V, Normal Cordinate Analysis National Research Council of Canada, Ottawa1976.

TABLE 1

Parameters of the model: a, b are Born-Mayer constants: Z,Y,K, ionic charge, shellcharge and on-site core-shell force constant of the ion, Va is the volume of the unitcell.

Interaction	a (eV)	b ($Å^{-1}$)
La-O(1) (Same plane)	3864	3.40
La-O(2) (adj plane)	3400	3.40
Ba-O(1)	3225	2.90
Cu-O(1)	3000	3.34
O(1)-O(2)	2764	6.71

ion	Z(|e|)	(|e|)	$k_x(e^2/Va)$	$k_y(e^2/Va)$	$k_z(e^2/Va)$
La	3.00	3.554	434	--	
Ba	2.00	2.32	2282	--	
Cu	2.60	3.22	1000	1000	1000
O ((1)	-1.85	-2.11	1000	1000	1000
O (2)	-1.85	-2.11	225	210	400
O (3)	-1.93	-2.70	441($K_{\parallel}$) 2264 ($K_{\perp}$)	--	--

Table. 2

Force Constants La_2BaCuO_5 (in units of 10^2 Nm^{-1})

(Stretching) and 10^{-18}Nm rad^{-2} (bending).

Force Constants	Bond Type	Distance (A^o)	Initial Value Constants
f_a	La-O(1)	1.625	--
f_b	La-O(2)	1.732	--
f_c	La-O(3)	1.852	--
f_d	Cu-O(1)	1.945	--
f_e	Cu-O(2)	1.827	--
f_g	Cu-O(3)	1.835	--
f_h	La-La	1.852	0.80
f_i	La-Ba	1.920	1.61
f_k	Ba-O(1)	2.030	1.85
f_l	Ba-O(2)	2.050	1.90
f_m	Ba-Cu	4.300	0.40
f_n	O(1)-O(1)	1.990	0.08
f_o	O(2)-O(2)	1.980	0.57
f_β	O(1)-O(2)	3.410	0.50
f_r	O(1)- Cu- O(2)	--	1.32
f_s	O(2)- Cu- O(3)	--	1.13

Table. 3

Calculated Phonon Frequencies of La_2BaCuO_5

(Values in the parentheses are experiment frequencies)

Symmetry species	Frequency(cm^{-1}) Using Lattice Dynamics	Frequency(cm^{-1}) Using Normal Coordinate analysis	Potential Energy Distribution(%)
A1g (Raman)	154(150)	152	fb (48) fk(21)
	231(231)	232	fi (67)fg(20)
	554(554)	530	fβ (47)fα(19)
B1g	173(172)	174	fe (56)fl(34)fk(21)
	418(420)	418	fd (38)fβ(21)fh(11)
B2g	185(190)	184	fβ (39)fm(22)fα(16)
	332(330)	330	fc (39)fα(29)fϒ (15)
	436(436)	430	fg (64)f∂(14)
Eg	155(155)	155	fm (59)fβ(16)fe(11)
	287(287)	285	fβ (42)fh(14)
	418(425)	418	fg(45) fa(31) fa (12)
	572(575)	575	fβ (42)fa (45)fe(16)
A2u (IR)	160(155)	156	fa(40)fc (21)f∂(23)
	356(360)	357	fβ(54)fϒ(32)fb(12)
	420(419)	421	fb (37)fc(26)
Eu	155(156)	156	fl (44)fh(26)fϒ(15)
	179(180)	179	fc (46)fb(21)fa(14)
	238(240)	239	fβ (51)fk(18)
	428(430)	428	fϒ (41)f∂(29)
	456(460)	460	fa (46)fβ(28)
	554(555)	555	fϒ (50) fc (19)
	580(580)	580	fβ (41)fα(21)fm(11)
	608(608)	605	fα (66) fn (21) fm(11)

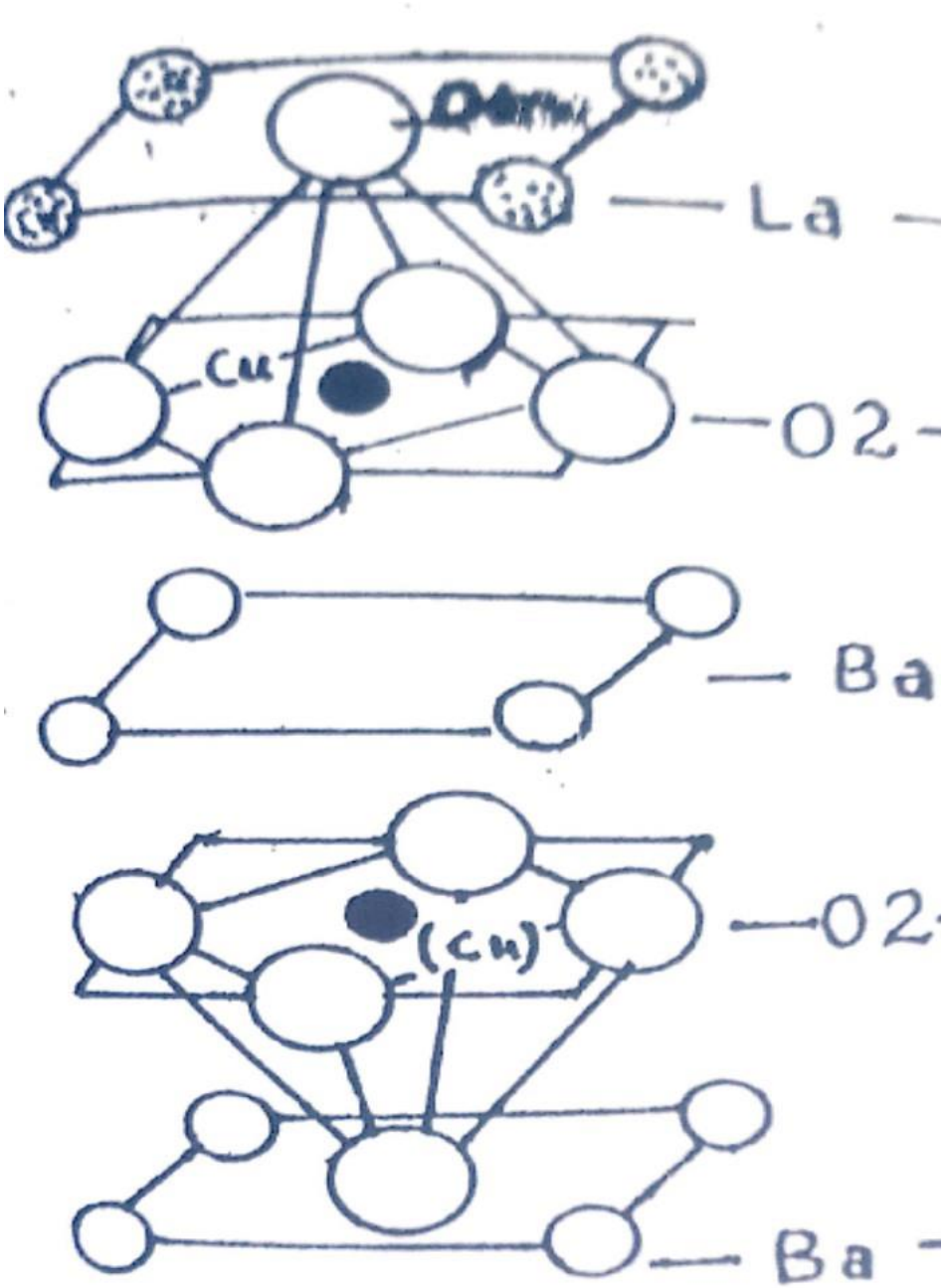

Fig. 1 Crystal Structure of La_2BaCuO_5