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Electronic and vibrational excitations in layered high T_c superconductors

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Abstract. In the series of the layered high T_c superconductors $(A)_{1,2}\ B_2Ca_{n-1}Cu_nO_{2n+3,4}$ (A = Tl or Bi; B = Ba or Sr), with n = number of consecutive Cu-O layers, the electron energy states of some of the Tl-based systems have been investigated. The electron and phonon dispersion curves have been obtained. The electronic states near the Fermi level are dominated by the hybridized Cu(d) and the O(p) orbitals. The dispersion curves are highly two-dimensional with very small dispersion along c-axis. The number of bands is enhanced with increase in the number of the consecutive Cu-O planes (n). The present results agree with those obtained earlier for other superconducting phases. The phonons are overall dominated by the vibrations of the light mass oxygen atom modes both lying in or outside the Cu-O planes. The low-frequency phonons involve the motions of the heavier Tl, Ba atoms etc.

Keywords. Electronic excitation; vibrational excitation.

1. Introduction

A tight-binding description of the electronic structure or a study of phonons in a Born lattice dynamical model of high T_c materials employed here is advantageous in the sense that it provides a convenient starting point for further theoretical studies in several directions such as various models of superconductivity, the calculation of physical properties and the effects of defects or impurities on them.

2. Electrons

For the electronic structure, we employ a set of (s, p) orbitals for O and Ca; (d, s) for Cu and (d, s, p) for Tl and Ba. The various intra- and interatomic matrix elements for Cu are taken over from Richert and Allen (1988) who obtained them by fitting the band structure of self-consistent calculations for La_2CuO_4. The value of s orbital energy E_s thus obtained for Cu is seen to be shifted from its atomic energy by $-5{\cdot}0$ eV. For various orbital energies, E_s, E_p and E_d for O, Ba and Ca, the atomic values have been used. For Tl, similar to Cu, we take the orbital energies equal to the atomic energies after shifting them by $-5{\cdot}0$ eV.

The computed electron dispersion curves in the different symmetry directions for $TlBa_2Ca_{n-1}Cu_nO_{2n+3}$ ($n = 1, 3$) are presented in figures 1–3. The zero of the energy has been fixed at the Fermi level E_F.

The important sub-bands are the hybridized Cu(d)-O(p) ones. Some of them have been numbered as (1) and (2) in figures which lie in the neighbourhood of E_F or cross it in the vicinity of the symmetric point $X(110)$ in Γ-X-D region. They are highly two-dimensional having very small dispersion along the c-axis. The multiplicity of these bands increases with the number of Cu-O layers (n). For each Cu layer, there

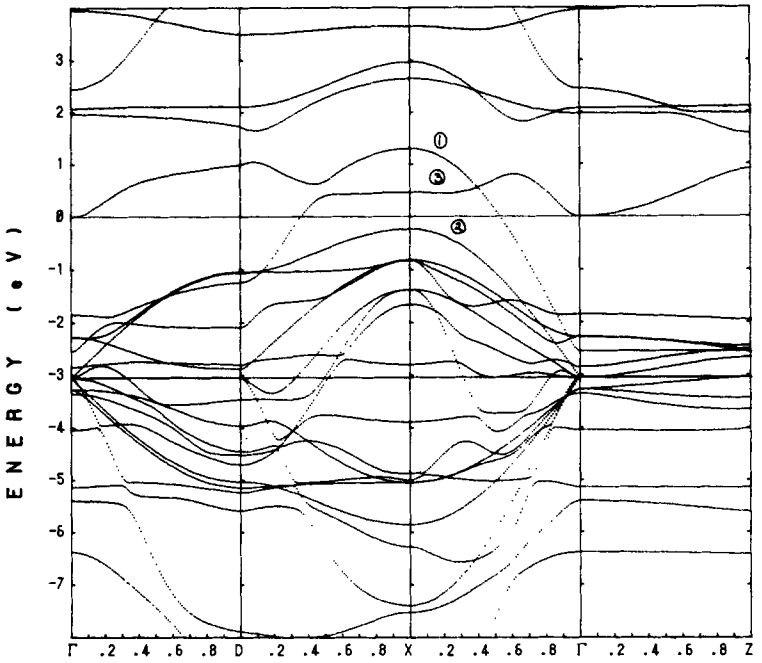

Figure 1. Electronic energy bands for $TlBa_2CuO_5$

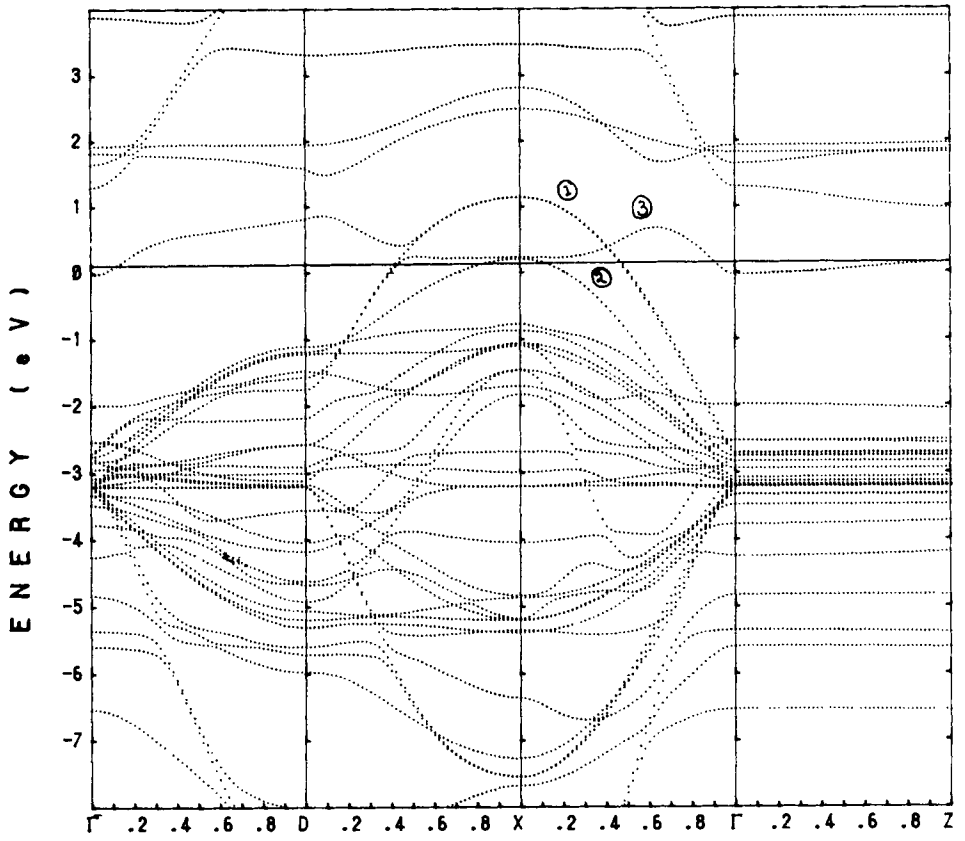

Figure 2. Electronic energy bands for $TlBa_2CaCu_2O_7$

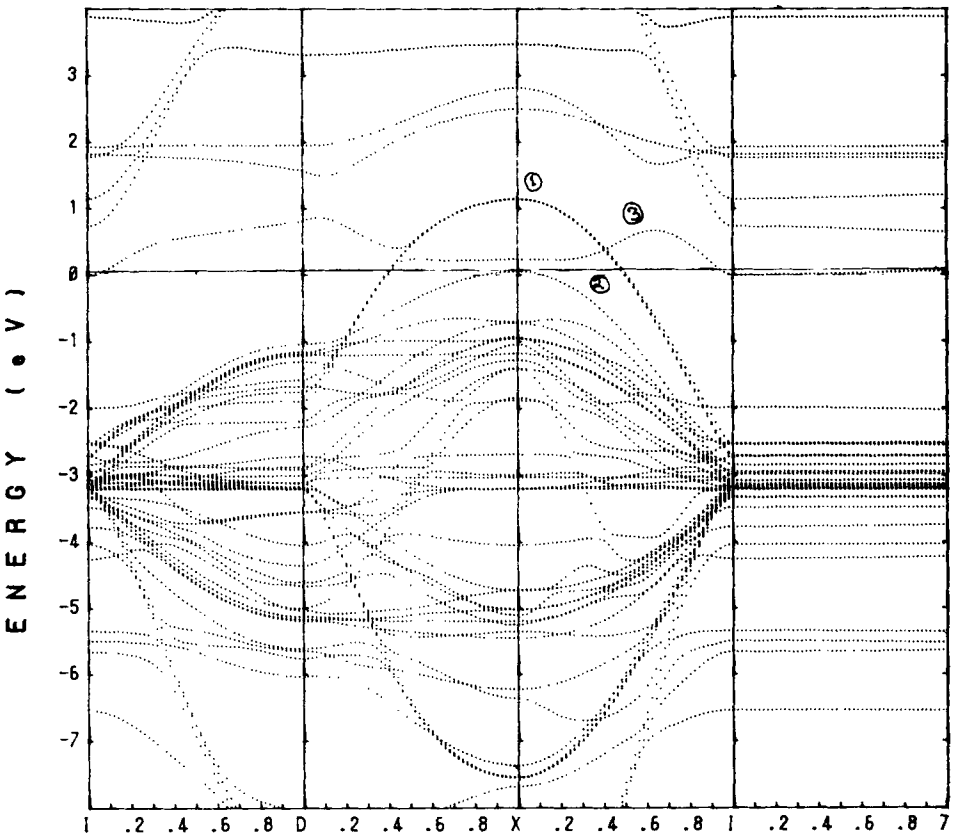

Figure 3. Electronic energy bands for $TlBa_2Ca_2Cu_3O_9$.

appears one conduction band (1) which crosses E_F, whereas others either touch E_F or lie below it. The active bands (1) which possess the mixed Cu($dx_2 - y_2$)-O($p_{x,y}$)σ-antibonding character have maximum at X.

There are a number of Cu(d)-O(p) bands which lie above or just below the Fermi level and are degenerate at more symmetric k-points like Γ(000) or D(100). However, their degeneracies are lifted as one moves away from these symmetry points or directions.

A number of Cu(d)-O(p) bands are quite narrow. Some of them are very close to E_F and sometimes slightly overlap E_F (numbered (2)). In case, some portion of these bands lies above E_F, hole pockets are introduced. On account of the flatness of these bands and their multiplicity, the induced hole concentration may be quite large even for a very small overlap.

Another feature common to all members of the family is the occurrence of one Tl-O band numbered as (3) arising from one Tl-O layer and the associated pyramidal apex O atoms. This band has a dispersion of about 1 eV and lies on average about 1 eV above E_F. However, this band goes down near the Γ point. For $n = 1$, it just touches E_F, but for $n = 2$, it crosses the Fermi level along the Γ-Z direction. The portion of the band below E_F will create electron pockets and will make Tl-O layer metallic, otherwise it is insulating.

Table 1. Comparison of the calculated and measured optical modes for $TlBa_2CuO_5$ in cm^{-1}.

Calculated frequencies for $TlBa_2Cu_5$	Measured Raman and infrared frequencies for $Tl_2Ba_2CaCu_2O_8$
83	75
104	
110	108
133	130,142
158	158
	222
280	278
356	
407	407
458	460
495	494
520	525
547	565
558	
599	599

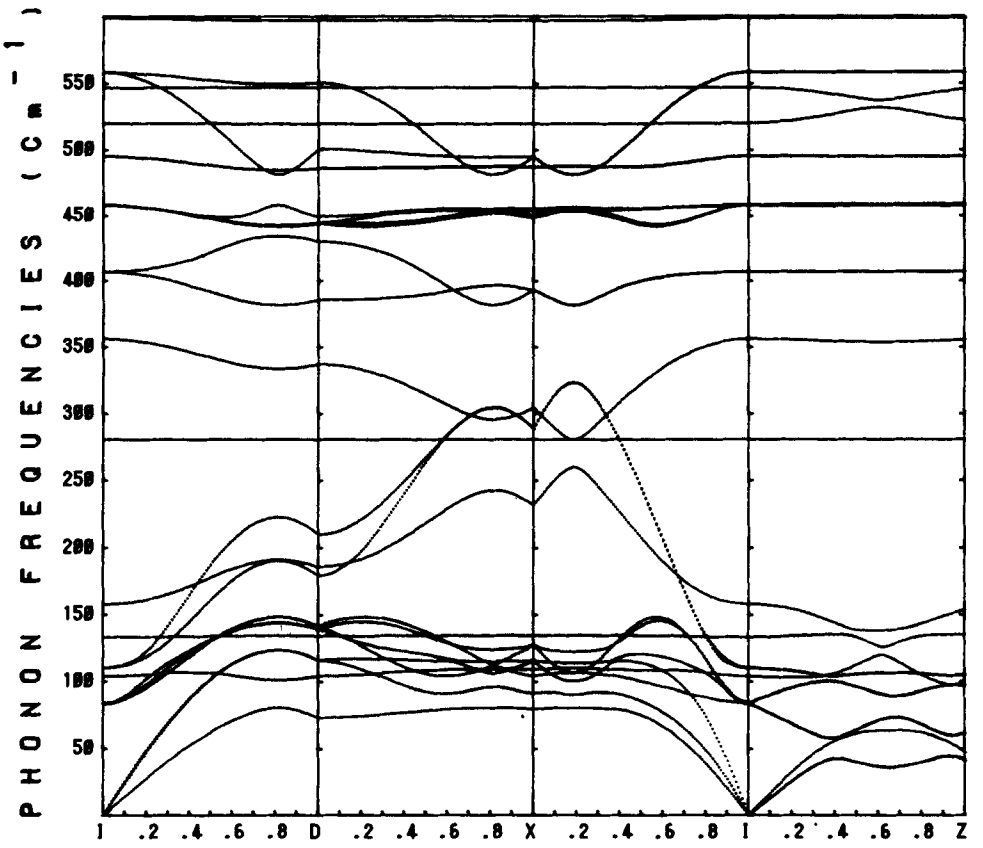

Figure 4. Phonon dispersion curves for $TlBa_2CuO_5$.

3. Phonons

An attempt has been made to reproduce the observed Raman and infrared peaks measured by McCarty *et al* (1988, 1989) and Renk *et al* respectively, using the Born model. We present the calculated frequencies for $TlBa_2CuO_5$ for $\mathbf{K} = \theta$ and compare them with the experimental results obtained for $Tl_2Ba_2CaCu_2O_8$ in table 1. A reasonably good agreement is seen. The phonon dispersion curves are shown in figure 4.

4. Conclusions

The electron states at E_F are dominated by the mixed Cu(d)-O(p) orbitals which have $2d$-character and their number increase with the number of layers. Both electron as well as hole pockets may be created. The high frequency phonons involve the motion of O-atoms whereas the low-frequency ones involve the other atomic vibrations.

Acknowledgements

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References

Harrison W A 1980 *Electronic structure and the properties of solids* (San Francisco: Freeman)
McCarty K F *et al* 1988 *Solid State Commun.* **68** 77
McCarty K F (private communication)
McCarty K F *et al* 1989 *Physica* **C157** 135
Renk K F *et al* (private communication)
Richert B A and Allen R E 1988 *Phys. Rev.* **B37** 7869