LATTICE DYNAMICS OF $HGBA_2CUO_{4+\delta}$

V.N. POPOV and V.G. HADJIEV

Faculty of Physics, University of Sofia,

5 James Bourchier blvd., 1126 Sofia, BULGARIA

Abstract

The lattice dynamics of the recently synthesized high-T_c superconductor $HgBa_2CuO_{4+\delta}$ is studied in the framework of a shell model using transferrable parameters. The results of the calculations are compared with the available optical data and with the calculated and observed modes in the structurally similar compound $Tl_2Ba_2CuO_6$. It is concluded that the model yields reasonable description of the measured optical phonons and predicts the frequency and vibration patterns of the remaining modes..

The recently discovered superconductor $HgBa_2CuO_{4+\delta}$ [1] attracted much attention because of its unusually high transition temperature of 94K. This compound belongs to the tetragonal system with space group $P4/mmm$ (D^1_{4h}) [2]. It is structurally similar to $Tl_2Ba_2CuO_6$ in that both are built out of CuO_6 octahedra with Ba atoms embedded between the octahedra. These compounds differ, however, in the presence of separating Hg and TlO layers. Beside the possible involvement of phonons in the mechanism of superconductivity, it is impotant to reveal in what way the structural features of the two compounds reflect on their lattice vibrations. Raman observations on $HgBa_2CuO_{4+\delta}$ have already been announced [3,4]. However, since there still exist contradictions in the assignment of the Raman active modes and no infrared frequencies have been measured yet, it is of special interest to try to predict these modes on the basis of lattice dynamical calculations. Here such calculations were carried out within a shell model using parameters transferred from metal oxides and cuprates [5].

The results of the calculations along with the availing optical data for $HgBa_2CuO_{4+\delta}$ and $Tl_2Ba_2CuO_6$ are presented in Table 1. The Raman A_{1g} modes are clearly devided in two groups: low frequency barium and thallium modes and considerably higher oxygen O_2 and O_3 ones. While the apex oxygen A_{1g} mode in the thallium compound has a value that is typical for almost all layered copper oxides, the measured frequency of this mode in $HgBa_2CuO_{4+\delta}$ of 592 cm^{-1} is higher by about 100 cm^{-1}. The E_g modes are again low frequency barium and thallium ones and higher O_2 ones. The apex mode would hardly differ much from that in $YBa_2Cu_3O_7$ - 210 cm^{-1}, and the calculated here values are reasonable. The infrared active modes of A_{2u} symmetry in both compounds except for the additional O_3 mode in the thallium cuprate correspond to one another, the modes in the mercury cuprate being higher by about 30-50 cm^{-1}. The lowest two infrared E_u modes are metal ones, while the higher modes with this symmetry are of oxygen type. The O_2 mode in $HgBa_2CuO_{4+\delta}$ splits in $Tl_2Ba_2CuO_6$ into in-phase and out-of phase (O_2,O_3) modes. The rest two modes are Cu-O_1 bond-bending and bond-stretching ones and they can be compared directly with the corresponding modes in most of the cuprates.

Table 1. Experimentally observed and calculated frequencies (in cm^{-1}) of the Γ-point phonons of $HgBa_2CuO_{4+\delta}$ and $Tl_2Ba_2CuO_6$. The prime denotes a 'counter-phase' displacement.

	$HgBa_2CuO_{4-\delta}$			$Tl_2Ba_2CuO_6$		
mode	exp.		vibration	exp.	calc.	vibration
	[4]	calc.	pattern	[6]		pattern
A_{1g}	161	142	Ba	125	140	Ba
A_{1g}				165	150	Tl
A_{1g}	592	582	O_2	485	478	O_2
A_{1g}				603	585	O_3
E_g	75	73	Ba	—	47	Ba
E_g				—	104	Tl
E_g	168	225	O_2	—	235	O_2
E_g				—	340	O_3
A_{2u}	—/—	125/126	Cu,Ba,Hg'	—/—	83/102	Cu,Ba,Tl'
A_{2u}	—/—	231/253	Cu,Ba'	—/—	196/210	Cu,Ba'
A_{2u}	—/—	404/444	O_1 (O_2)	—/—	374/430	O_1 (O_2)
A_{2u}	—/—	578/588	O_2 (O_1')	—/—	481/500	O_2 (O_1')
A_{2u}				—/—	577/580	O_3
B_{2u}	—/—	236	O_1	—	265	O_1
E_u	—/—	47/47	Cu,Hg'	—/—	62/73	Cu,Tl'
E_u	—/—	92/103	Cu,Ba'	—/—	97/135	Cu,Ba'
E_u				—/—	135/210	O_2,O_3
E_u	—/—	222/282	O_2	—/—	336/350	O_2,O_3'
E_u	—/—	380/415	O_1 bend.	—/—	374/415	O_1 bend.
E_u	—/—	618/631	O_1 stretch.	—/—	636/643	O_1 stretch.

In conclusion, the lattice dynamics of $HgBa_2CuO_{4+\delta}$ and $Tl_2Ba_2CuO_6$ is studied within a shell model and it is shown that the results of the calculations are in reasonable agreement with the existing optical data.

Acknowledgments

This work was supported by Contracts F1/19 and F13/2002 from the Bulgarian Ministry of Education and Science and CIPA-CT93-0032 of the Commission of EC.

References

1. Putilin, S.N., Antipov, E.V., Chmaissem, O., and Marezio, M. (1993) Superconductivity at 94 K in $HgBa_2CuO_{4+\delta}$, *Nature* **362**, 226-228.

2. Wagner, J.L, Radaelli, P.G., Hinks, D.G., Jorgensen, J.D., Mitchell, J.F., Dabrowski, B., Knapp, G.S., and Beno, M.N. (1993) Structure and Superconductivity of $HgBa_2CuO_{4+\delta}$, *Physica* C **210**, 447-454.

3. Hur, N.H., Lee, H.-G., Park, J.-H., Shin, H.-S., and Yang, I.-S. (1993) Raman studies on single-phasic $HgBa_2CuO_{4+\delta}$ superconductors, *Physica* C **218**, 365-368.

4. Krantz, M.C., Thomsen, C., Mattausch, Hj., and Cardona, M. (1994) Raman-active phonons and mode softening in superconducting $HgBa_2CuO_{4+\delta}$, to appear in *Phys. Rev.* B **49**.

5. Popov, V.N. (1994) Lattice Dynamics of Layered Copper Oxides, submitted to *Phys. Rev.* B.

6. Burns, G., Crawford, M.K., Dacol, F.H., and Herron, N. (1990) Raman active phonons in Tl-based high-T_c superconductors, *Physica* C **170**, 80-86.