Slab phonons in systems of the type A–Ba–Cu–O

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Slightly dispersive slab phonons, which are accompanied by an electric polarization along the conducting CuOII planes, were found to exist in $ABa_2Cu_3O_7$ systems.

The discovery of high-T_c superconductivity in La–(Ref. 1) Y–Ba–(Ref. 2) Cu–O systems has raised many questions regarding the role the CuO layer plays in the appearance of high critical temperature T_c. We will show that a layered (slab) system $ABa_2Cu_3O_7$ (A = Y, Ho, Eu, etc.[3]) has optical phonon modes which propagate along the layers whose transverse vibrations are symmetric with respect to the planes of the mirror symmetry of A and CuOI (Fig. 1). The characteristic features of such phonons—the accompanying electrical polarization **P** along the "metallic" CuOII planes and the slight dispersion which accounts for the large value of the phonon state density (Fig. 2)—suggest that there is a strong electron-phonon coupling in the layers, which may account for the high-T_c in such slab systems.

Let us consider the lattice vibrations which propagate along the slabs of the system, with the wave vector $\mathbf{q} = (q_x, q_y)$. We base our analysis on the analogy with the slab phonons in a superlattice consisting of two materials[4]: In our experiment we used CuOII–A and CuOII–(BaO–CuOI–BaO) with thicknesses $d_1 \approx a$ and $d_2 \approx 2a$ [$c = d_1 + d_2$, $a \approx b$ (Ref. 3) are the dimensions of the unit cell of the system]. We will

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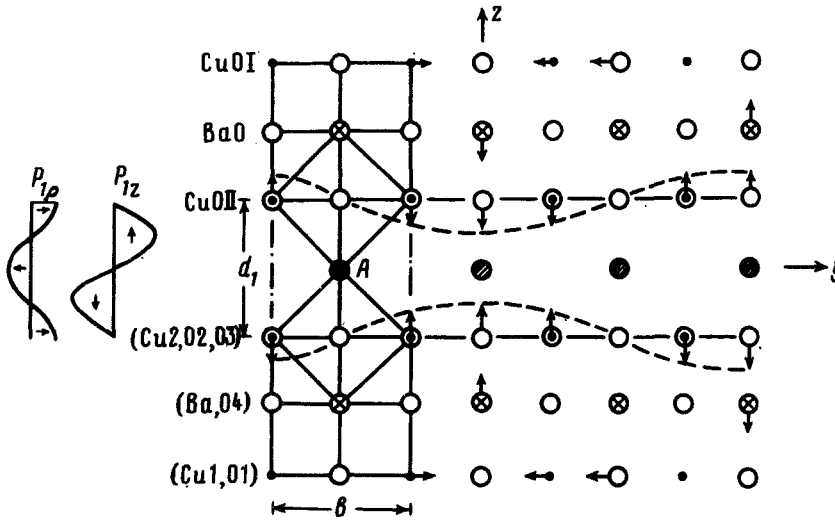

FIG. 1. Schmatic diagram of the $ABa_2Cu_3O_7$ structure and of its symmetric vibrations of the layers. ⓓ—A; ⊗—Ba; ●—Cu; ○—O.

consider the symmetric modes, in which the atomic vibrations in the CuOII and BaO layers are quasitransverse and out-of-phase relative to the average A and CuOI planes, where the atomic vibrations occur in the plane itself (Fig. 1). This choice was dictated by the fact that the vector **P** runs in the same direction in all the layers of CuOII. Working from the solution of the problem of polarization $\mathbf{P}(z,\rho,t)$ in a superlattice,[4] we find that at the frequency of the longitudinal (along the **z** axis) optical phonon the electric polarization vector of the first material [the dielectric constant is $\epsilon_1(\nu = \nu_{L1}) = 0$] has the constants

$$\begin{Bmatrix} P_{1\rho} \\ P_{1z} \end{Bmatrix} = B \begin{Bmatrix} iq\cos 2\pi z'/d_1 \\ 2\pi/d_1 \sin 2\pi z'/d_1 \end{Bmatrix} e^{i(\vec{q\rho} - 2\pi\nu t)}, \quad |z'| \leqslant d_1/2 ; \tag{1}$$

$$P_{2z} = 0, \quad P_{2\rho} = Biq\, e^{i(\vec{q\rho} - 2\pi\nu t)} \quad |z'| < d_2/2. \tag{2}$$

In the case of small wave numbers, $qa \ll 1$, a vibration of this sort has the nature of a transverse optical mode: $|P_{1z}/P_{1\rho}| \gg 1$, but it oscillates at a frequency ν_{L1}. This frequency may be determined by the vibration frequencies along the z axis of the O2 and O3 oxygen atoms, ν_O, or along z of the Cu2 copper atoms, ν_{Cu}, in the CuOII layer. Here the polarization $P_{1\rho}$ is at a maximum and is proportional to the diplacement of the atom, u_z^α [$\alpha = 0$, Cu; $B \sim u_z$ (Ref. 4)]:

$$P_{1\rho}^{\alpha}(z' = \pm d_1/2, \quad \rho \in \text{CuOII}) = e^{\alpha} qiu_z^{\alpha}. \tag{3}$$

This result follows from the symmetry of the structure $ABa_2Cu_3O_7$: The CuOII plane

in the neighborhood of the A and BaO layers [the local symmetry is a 4 mm (Ref. 5)] lacks a mirror symmetry. A local longitudinal polarization may therefore appear in the case of a transverse deformation of the layer—an effect similar to the piezoelectric effect. The constant e in (3) can be compared with the components of the piezoelectric tensor of the local 4mm structure: $e'_{15} = e'_{24} \sim e$. The value of e can be estimated from $e_{15} = 18 \times 10^{-12}$ C/H for a crystal of such symmetry Ba_2SiTiO_3 (Ref. 6), which is comparable with the same constant of a strong piezoelectric CdS. A more accurate determination of this constant requires a calculation of the transverse effective charge.[7]

An important point in the case of electron-phonon coupling in the layers is that polarization (3) is isotropic in the CuOII plane. A polarization similar to (3) also occurs in the case of the displacement u_z of the Ba and O4 atoms in the BaO layer of the second material at the frequencies $\nu_{L2} = \nu_{\mathrm{Ba,O4}}$ and also at the frequencies ν_F of vibration of the group of oxygen atoms, e.g., the O1–O4–O1–O4 "frames" (Ref. 8) when $\epsilon_2(\nu = \nu_{L2}) = 0$.

Let us now consider the structural features of the spectrum $\nu(\mathbf{q})$ of the slab phonons. On the basis of the strength constants[8,9] which indicate that the atomic bond in the CuO and BaO layers is stronger than that between them, we will single out from the complete system of equations for the vibration amplitudes of all the atoms in the unit cell a block of equations for the displacement along the z atoms: Cu2–U and O2(O3)–$\nu_{x,y}$, with allowance for the coupling with the A atom, and through it, $v'_{x,y}$; the neighboring Ba–V, with allowance for the coupling with other Ba–V' through the CuOI layer. Here the amplitudes of the symmetric vibrations of the atoms in the lower and upper (primed) halves of the cell (Fig. 1) are related by the relation

$$U' = -U, \quad V' = -V, \quad v'_{x,y} = -v_{x,y}. \tag{4}$$

These equations can be isolated because (a) the displacement U^A_ρ is small because of the large mass, M_A, compared with the masses of the neighboring (in terms of the binding) O2 and O3 atoms, and because $U^A = 0$ when the slab modes undergo a transition ($\mathbf{q} \to 0$) to the A_g modes at frequencies ν_α (Ref. 8) and (b) the modes at $\nu_{\mathrm{Ba,Cu,O}} \approx 130$, 200, and 330 cm^{-1} are far from the modes at $\nu_{\mathrm{O4,F}} \cong 450$ and 600 cm^{-1} (Refs. 8 and 9). A slight difference in the critical temperatures, $T_c = 88 \pm 6$ K, accompanied by a variation of the A atom in the system, $M_A = 89$–170 a.u.,[3] also suggests that the slab modes of the vibration of Ba, Cu, and O atoms play the key role.

Solutions of a truncated dynamic matrix of equations for the amplitudes U, v_x, and v_y are shown in Fig. 2a for the [100] and [110] directions. We see that the branches $\nu_\alpha(\mathbf{q})$ have a small dispersion, suggesting that their spectral state density is large and that the vibration amplitude of the αth mode peaks in the α layer. A small dispersion of such a phonon can be explained in terms of its belonging to the highest branch of the mode, which is associated with the vibration of the layers of atoms of the same type: This is illustrated by the $\nu(q_z)$ curve in Fig. 2b, which corresponds to the second "convoluted" phonon mode in the triatomic linear-chain model (cf. Ref. 4). The dispersion of a slab phonon is seen in the 90° (ZX or ZY) Raman-scattering geometry of the type that is observed in the slab modes in the superlattice.[4]

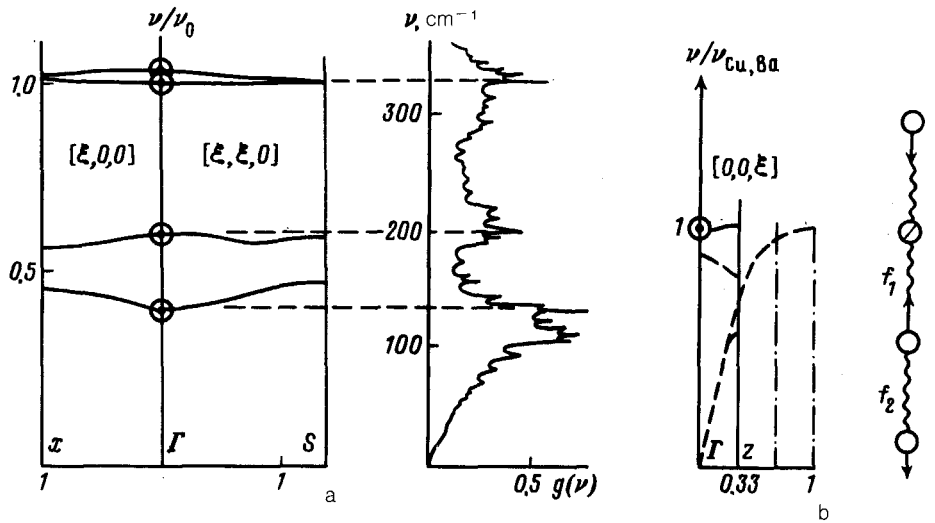

FIG. 2. (a) Dispersion curves for slab phonons, $\nu_\alpha(\mathbf{q})$, directed along $[\xi,0,0]$ and $[\xi,\xi,0]$ ($\nu_{Cu}/\nu_0 = 0.6$, $\nu_{Ba}/\nu_0 = 0.4$); at the right—calculated phonon state density of $YBa_2Cu_3O_7$ (Ref. 10). (b) Dispersion curves for phonons "convoluted" along the $[0,0,\xi]$ direction in a linear Cu2–Cu2–Cu1 chain, $f_2 > f_1$, $\nu_{Cu} = \sqrt{3f_2/M_{Cu}}$ (or Ba–Ba–A, $f_{1,2} = f$, $\nu_{Ba} = \sqrt{3f/M_{Ba}}$, f is the strength constant); at the right—its vibration at a frequency ν_α. $\xi = qa/\pi$; ⊙—origin of the slab mode, $\nu_\alpha(\mathbf{q}=0) \equiv \nu_\alpha$.

The phonon dispersion curves for the principal directions $[\xi,0,0]$, $[0,\xi,0]$, and $[0,0,\xi]$, which have been recently obtained by numerical calculations,[10] support our qualitative model: Slightly dispersed modes have been observed at the frequencies mentioned above, as have peaks in the phonon state density (Fig. 2a). The phonon spectrum, however, has not been explained in detail, nor has it been determined whether phonons can contribute to the electron-phonon coupling.

In multilayer structures in which the "metallic" layers [CuO_2 in $ABa_2Cu_3O_7$ or BiO_2 in $K_{0.4}Ba_{0.6}BiO_3$ (Ref. 11); see also the recently discovered Bi and Tl systems[12]] are situated in the layer facings with different atoms, a strong electron-phonon coupling can thus occur through the electric field which accompanies the slab phonons and which has an appreciable component along these layers.

The following experimental results, which can be explained in terms of the model under consideration, have recently been published: (1) A strong anisotropy of thermal vibrations, corresonding to the slab-phonon scheme, has been detected (Fig. 1): The Cu2, O2(O3), and (O4 atoms vibrate preferentially in the z direction and the CuI and O1 atoms vibrate preferentially in the x,y plane.[13,14] (2) The phonon state density, determined from the inelastic neutron scattering,[15] has strong peaks at the frequencies close to $\nu_{Ba,Cu2,O2(O3),F}$ (Fig. 2), confirming the conclusion that there is a strong phonon concentration in the layers. (3) In the study of polarization Raman scattering in crystals,[16] the IR reflection, and the dynamic conductivity[17] vibrations were detected at $\nu_{Ba,Cu2,O2(3)}$, to which the frequencies of the slab modes $\nu_\alpha(\mathbf{q}\to 0)$ undergo a transition. (4) There is no high-T_c superconductivity in metallic structures which

contain the same atoms as those found in the superconducting structures without a layered order[18] and hence without slab phonons.

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