Phonon anharmonicity and structural instability of the $YBa_2Cu_3O_7$ crystal lattice under hydrostatic compression

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(Submitted 9 June 1995)
Zh. Éksp. Teor. Fiz. **109**, 1704–1723 (May 1996)

We model the potential function of the $YBa_2Cu_3O_7$ crystal lattice, describing the lattice's structural evolution and dynamical processes under conditions of hydrostatic compression, including macroscopic elastic properties, the pattern of variation of interatomic distances, and the baric dependences of vibrational frequencies. We predict a structural phase transition induced by hydrostatic pressure. The effect is found to be related to the lowering of the frequency of the dispersion branch that is flat along the $\Gamma(0,0,0)\rightarrow Z(0,0,0.5)$ direction in the Brillouin zone. The soft mode corresponds to a strain vibration along the x axis of a linear $-Cu1-O_{Cu1}-Cu1-$ chain. Softening of this vibration is caused by stresses generated in the chain under compression. We analyze the symmetry properties of the $YBa_2Cu_3O_7$ structure at $P>P_c$. *© 1996 American Institute of Physics.* [S1063-7761(96)01505-3]

1. INTRODUCTION

Most high-T_c superconductors known today belong to the class of perovskite-like compounds. The common property of such compounds is the tendency toward structural phase transitions.[1] These transitions usually are caused by an essentially anharmonic effect—condensation of the soft vibrational mode—which suggests that strong anharmonicity is a characteristic feature of the phonon subsystems of perovskite-like crystals.

This fact is a cornerstone of general discussions about the role of phonons in the mechanism of high-T_c superconductivity, since the anharmonicity of atomic vibrations is considered to be a factor responsible for strong electron–phonon coupling and, therefore, it affects the value of T_c (see, e.g., Refs. 2–5 and the review by Lemanov and Kholkin[6]). This explains the interest in vibrational-spectrum studies of high-T_c superconductors.

Among perovskite-like superconductors the most studied one is the $YBa_2Cu_3O_7$ compound. The literature to this compound is vast, and the phonon properties, especially their anharmonicity, occupy the central place in such discussions. Special attention is focused in this connection on vibrations of the linear component in this crystal, the $-Cu1-O_{Cu1}-Cu1-$ chain (see Fig. 1 below). The results of some researchers (see Refs. 3 and 7, and also Ref. 8 and the literature cited therein) suggest that the local potential in which transverse displacements of the atoms in this component take place contains a large anharmonic term destabilizing the linear chain. The growth of this potential (under an external agent acting on the crystal) stimulates the soft-mode behavior of vibrations generating such displacements.

Attempts to prove the existence of such properties by direct experiments have failed, however. In particular, studies of the temperature behavior of the individual low-frequency dispersion branches of the $YBa_2Cu_3O_7$ lattice by inelastic neutron scattering have revealed no traces of soft-mode behavior in the temperature range from 300 to 20 K (see Ref. 9). Here the frequency of the dispersion mode that is flat in the $(0,\xi,0)$ direction ($167\,cm^{-1}$ at $T=300$ K), which mode Pyka *et al.*[9] identified as the strain vibration of the chain, was found to grow only slightly.

Thus, the situation with this problem became fraught with controversy. However, in the current discussion attention has been focused on only one external thermodynamic factor, the temperature.

The present paper studies a model in which the anharmonicity of the phonon subsystem of the $YBa_2Cu_3O_7$ lattice is induced by hydrostatic compression. In relation to objects of this type the compression can be considered an alternative to lowering the temperature: pressure stimulates the transition of $YBa_2Cu_3O_7$ into the superconducting state (T_c is observed to increase linearly up to pressures $P\simeq 10$ GPa, with $dT_c/dP\simeq 1\,K\,GPa^{-1}$; see Ref. 10), and at the same time is a factor destabilizing perovskite-like structures. Usually for such structures the derivative dT_c/dP is positive[11,12] in the case of the most typical phase transitions caused by condensation of rotational vibrations of complex octahedral anions. Note that in classical perovskites with the formula ABX_3 these vibrations can be interpreted as combinations of zigzag strain in $(X-B-X)_\infty$ chains. This suggests that the instability of the chains under such strain is the underlying property of perovskite-like structures responsible for the type of phase transition mentioned earlier.[13]

The theoretical prerequisites of our study were the conclusions drawn in Ref. 13, according to which compression of crystals, in view of the laws of mechanics, must weaken the elastic restoring forces acting on the atoms in their transverse displacements in the linear structural components of the crystal lattice. This may lead to a loss of mechanical

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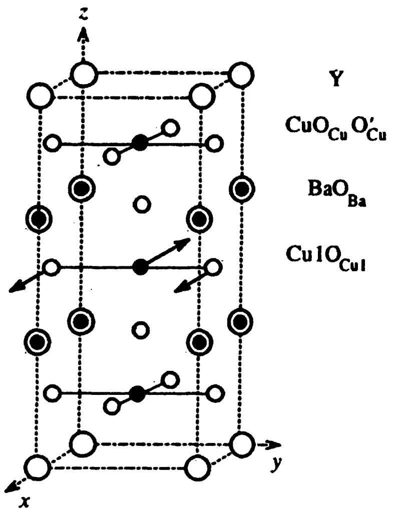

FIG. 1. The $YBa_2Cu_3O_7$ crystal structure and the schematic of strain vibrations of the $-Cu1-O_{Cu1}-Cu1-$ chain.

stability and to strain (zigzag fracture) in such components, i.e., to a structural phase transition.

A microscopic destabilizing factor in this effect is the stress in the interatomic bonds that emerges as a result of compression of the lattice. Note that the hypothesis of such a role of the static interatomic stress in perovskite lattices under normal pressure has been expressed earlier.[14] In Sec. 2 we use an approach based on the dynamical crystal theory to discuss the behavior of the vibration frequencies of an infinitely long linear chain of atoms in conditions of uniform compression and the case of a three-dimensional lattice. This approach forms the theoretical basis for studying the phonon subsystem of the $YBa_2Cu_3O_7$ crystal lattice. In this investigation we use the model of the valence-force potential function suggested earlier in Refs. 15 and 16 for describing the vibrational spectra and the elastic properties of this crystal at $P=0$.

For the present study the model was modified so as to allow for two competing anharmonic contributions to the potential function that determine the dynamic response of the system to a decrease in volume:

(1) the stabilizing contribution of the existing anharmonicity (using the terminology of Ref. 17) of the interatomic potentials caused by the increase in the force constants as the interatomic distances decrease;

(2) the destabilizing contribution determined by the stress in the interatomic bonds, i.e., static two-center repulsive forces that appear when the atoms in the compressed lattice move closer.

2. THE ANHARMONICITY OF VIBRATIONS OF A SYSTEM OF COUPLED POINTS UNDER HYDROSTATIC COMPRESSION

We start with the case of vibrations of an infinitely long linear single-spacies atomic chain consisting of ideal springs of length r characterized by a modulus of elasticity K when a longitudinal external force F acts on the chain. The compression (elongation) of the chain with respect to the free state can be described in terms of the absolute variation of the spring length, Δr, or in terms of macroscopic uniform strain

$$U\equiv\Delta r/r. \qquad (1)$$

To establish the properties of interest to us we restrict our discussion to the problem of short-wave (band-edge) vibrations, when the neighboring atoms in the chain are displaced in antiphase. The harmonic approximation presupposes that only the quadratic term is retained in the potential function $V(X)$ (i.e., in the expansion of the internal energy density V of the system in a Taylor series in the Cartesian displacements x of the atoms). Differentiating the quantity $V(r)$ twice with respect to X, we find the coefficient of the quadratic term, which is known as the atomic harmonic force constant, in the form

$$V_{\alpha\beta}=V''_{rr}\frac{\partial r}{\partial X_\alpha}\frac{\partial r}{\partial X_\beta}+V'_r\frac{\partial^2 r}{\partial X_\alpha\partial X_\beta}, \qquad (2)$$

where X_α are the Cartesian displacements of an atom along the α axis, and V'_r and V''_{rr} are the first and second derivatives of V with respect to r. Equation (2) is the general expression for the quantities $V_{\alpha\beta}$ in the case of an arbitrary potential of short-range forces.[18] The first term in (2) is known as the radial component of $V_{\alpha\beta}$ and the second as the tangential component.

When the configuration of the chain is time-independent, the forces acting on the atoms are zero (in view of symmetry), and the condition of equilibrium under macroscopic stresses with (1) taken into account is reduced to the equality

$$F=V'_r=K\Delta r=KUr, \qquad (3)$$

which means that the external force F is balanced by the internal stresses in the system.

Assuming that the Cartesian y axis is directed along the chain and using Eqs. (2) and (3), we find that

$$V_{xx}=2V'_r/r=2kU, \qquad (4a)$$

$$V_{yy}=2V''_{rr}\equiv 2K. \qquad (4b)$$

Thus, the frequency ν_y of the longitudinal oscillator of the chain is determined solely by the radial part of the $V_{\alpha\beta}$ matrix,

$$m\nu_y^2=V_{yy}=2K \qquad (5)$$

(m is the mass of the atom), and is independent of the state of the system, in full agreement with the properties of a harmonic oscillator.

The frequency ν_x of the transverse oscillator behaves differently. The oscillator's equation of motion has the form

$$m\nu_x^2=V_{xx}=2V'_r/r=2KU. \qquad (6)$$

It implies that ν_x is determined by the tangential part of $V_{\alpha\beta}$ and is a variable depending on the value of the uniform strain of the chain. Thus, the transverse oscillator of the chain is essentially anharmonic. When the chain is compressed $(U<0)$, ν_x is imaginary and the system loses stability with respect to transverse displacements of the atoms.

Let us now examine a three-dimensional periodic lattice consisting of N atoms coupled by ideal springs whose elastic properties are specified by a matrix K. In Born's theory[19] the space of true lattice strains has $3N+3$ dimensions, because it has $3N-3$ internal degrees of freedom and six external degrees of freedom. The latter correspond to macroscopic uniform strain. The difficulties of examining the dynamics of uniform strain in the basis space of absolute atomic displacements are well known (see, e.g., Ref. 19, Sec. 25). Bearing this in mind, we use the space of variations of the relative atomic positions,[20] which we call the **q**-space of natural coordinates.

Suppose that the lattice, which initially was free, has been deformed by an isotropic pressure P. In the natural coordinate space (which in our case is simply the set of variations of the interatomic spring lengths) the microscopic strain vector $\mathbf{q}_0$ corresponding to the new state is related to the macroscopic strain vector $\mathbf{U}$ and pressure P in the following way:[21,22]

$$\mathbf{q}_0 = L\mathbf{U} = L\kappa P, \tag{7}$$

where L is the uniform strain matrix, and κ is the crystal's linear compressibility tensor.

In a strained lattice the following forces (stresses) $\mathbf{F}$ appear in the lattice:

$$\mathbf{F} = K\mathbf{q}_0 = KL\mathbf{U} = KL\kappa P, \tag{8}$$

these balance the external pressures and are mutually balanced in the action on each atom.

The variation of the density V of the lattice's internal energy brought on by new strains q with respect to the equilibrium state contains (in the case of ideal springs) only two terms:

$$V(q) = Fq + \frac{1}{2}\, qKq. \tag{9}$$

To go from (9) to the standard notation for the potential function in the space of $3N$ absolute Cartesian displacements X_α of the atoms, we expand q in a power series in these displacements[23] (summation over repeated indices is assumed everywhere):

$$q = B_\alpha X_\alpha + \frac{1}{2} B_{\alpha\beta} X_\alpha X_\beta + \frac{1}{3!} B_{\alpha\beta\gamma} X_\alpha X_\beta X_\gamma + \cdots, \tag{10}$$

where all the coefficients are determined by the geometry of the structure.

Substituting (10) into (9) and collecting the terms with the same powers of X_α, we obtain the potential function in the form of an infinite series:

$$V(X) = \frac{1}{2} V_{\alpha\beta} X_\alpha X_\beta + \frac{1}{3!} V_{\alpha\beta\gamma} X_\alpha X_\beta X_\gamma + \cdots, \tag{11}$$

where the absence of a linear term corresponds to the equilibrium condition. We see that the potential function of a lattice constructed of ideal springs proves anharmonic, since it contains higher-order terms. If in (11) we keep only the first term, we have a quadratic potential energy, which by definition[17] describes lattice dynamics in the harmonic approximation.

In this approximation the oscillatory system of the crystal consists of a set of $3N-3$ independent oscillators. This means that their frequencies are independent of the internal strains of the lattice. However, below we show that this property is not valid for external uniform strain. Indeed, the coefficient $V_{\alpha\beta}$ in (11) obtained as a result of substituting (10) into (9) is defined as

$$V_{\alpha\beta} = B_\alpha K B_\beta + F B_{\alpha\beta}. \tag{12}$$

Similar to Eq. (2), the first and second terms on the right-hand side are, respectively, the radial and tangential components of the force constant.

Allowing for (8), we reduce (12) to

$$V_{\alpha\beta} = B_\alpha K B_\beta + KLUB_{\alpha\beta} = B_\alpha K B_\beta + KL\kappa P B_{\alpha\beta}, \tag{13}$$

which implies that the force matrix $V_{\alpha\beta}$ and, hence, the values of the vibration frequencies depend on the size of the uniform strain of the lattice, U, i.e., on the hydrostatic pressure P.

Note that in the dynamical theory of crystals such behavior of the vibration frequencies is defined as being a purely anharmonic property.[17] We can therefore say that our system possesses anharmonicity induced by uniform strain of the lattice under hydrostatic compression. The microscopic nature of this anharmonicity can be related to the interatomic static forces emerging as a response to changes in interatomic distances that such strain produces.

The bearer of this property is the tangential component of the force-constant matrix $V_{\alpha\beta}$. It determines the forces in the equations of the vibrational motion in directions perpendicular to the lines connecting the interacting atoms.[18] Note that the stresses in the interatomic bonds corresponding to lattice compression introduce (through this component) negative contributions to the characteristic numbers of the dynamical matrix. Thus, there is always a factor in the dynamics of the lattice that lowers the lattice's stability under compression. The factor is model-independent, i.e., is present in all physically consistent model descriptions of crystals as systems of elastically coupled atoms and hence is an inherent mechanical property of crystal lattices.

At the same time, as the interatomic distances decrease, the stiffness of the "interatomic springs" must increase in view of the substantial anharmonicity of the real interactions between atoms. In contrast to the forces generated in the springs, this effect increases (through the radial part of $V_{\alpha\beta}$) the characteristic numbers $\lambda \equiv \nu^2$ of the dynamical matrix and stabilizes the structure.

Generally, the λ contain contributions from both parts of $V_{\alpha\beta}$, and lattice compression generates two effects: the stabilizing and the destabilizing. Usually the first is greater than the second and the vibration frequencies increase under compression of the lattice. But if the lattice structure is such that for some vibrations the tangential component is predominant, these frequencies may manifest their "anomalous" soft-mode nature under compression of the lattice. Primarily this is related to a purely geometric factor, in view of which the radial and tangential parts of the dynamical matrix separate. This situation realizes itself most vividly, as noted earlier, in the case of a linear chain.

TABLE I. Force constants, structural parameters, and baric dependences of bond lengths, dl/dP, for the $YBa_2Cu_3O_7$ crystal lattice under hydrostatic compression.

			$P=0$ GPa		$P=15$ GPa		$P=30$ GPa	
		dl/dP	Length or angle	Constants	Length	Constants	Length	Constants
S_1	$Cu1-O_{Ba}$	47	1.837	1.80; 0	1.766	2.49; −0.0630	1.696	3.39; −0.126
S_2	$Cu-O_{Cu}$	60	1.931	1.35; 0	1.841	1.79; −0.0705	1.751	2.70; −0.141
S_3	$Cu1-O_{Cu1}$	44	1.943	1.30; 0	1.877	1.60; −0.0495	1.811	1.99; −0.099
S_4	$Cu-O'_{Cu}$	51	1.961	1.25; 0	1.885	1.57; −0.0525	1.808	2.03; −0.105
S_5	$Cu-O_{Ba}$	96	2.315	0.70; 0	2.171	0.85; −0.0435	2.027	1.12; −0.087
S_6	$Y-O'_{Cu}$	39	2.384	0.55; 0	2.326	0.79; −0.0375	2.267	1.03; −0.075
S_7	$Y-O_{Cu}$	37	2.400	0.55; 0	2.345	0.74; −0.0360	2.289	0.95; −0.072
S_8	$Ba-O_{Ba}$	70	2.743	0.27; 0	2.638	0.36; −0.0120	2.533	0.46; −0.024
S_9	$Ba-O_{Cu1}$	80	2.880	0.23; 0	2.760	0.27; −0.0090	2.640	0.34; −0.018
S_{10}	$Ba-O'_{Cu}$	140	2.960	0.20; 0	2.750	0.28; −0.0150	2.540	0.46; −0.030
S_{11}	$Ba-O_{Cu}$	127	2.996	0.20; 0	2.806	0.25; −0.0120	2.615	0.37; −0.024
S_{12}	$O_{Cu}-O_{Cu}$	5	2.817	0.20; 0	2.810	0.20; −0.0005	2.802	0.21; −0.001
S_{13}	$O'_{Cu}-O'_{Cu}$	−13	2.854	0.20; 0	2.874	0.19; +0.0030	2.893	0.18; +0.006
S_{14}	$Cu-Y$	84	3.207	0.10; 0	3.081	0.15; −0.0030	2.955	0.19; −0.006
S_{15}	$Cu1-Ba$	91	3.474	0.20; 0	3.337	0.25; −0.0075	3.201	0.28; −0.015
S_{16}	$Ba-Ba$	97	3.853	0.10; 0	3.707	0.15; −0.0030	3.561	0.19; −0.006
S_{17}	$Cu1-Cu1$	97	3.853	0.10; 0	3.707	0.15; −0.0030	3.561	0.19; −0.006
B_1	$O_{Cu}-Cu-O'_{Cu}$		88.9	0.45		0.56		0.66
B_2	$O_{Ba}-Cu1-O_{Cu1}$		90.0	0.45		0.56		0.66
B_3	$O_{Ba}-Cu-O'_{Cu}$		97.7	0.15		0.19		0.22
B_4	$O_{Ba}-Cu-O_{Cu}$		98.4	0.15		0.19		0.22
H_1	S_1-S_1			−0.20		−0.24		−0.28
H_2	S_6, S_7-S_6, S_7			0.13		0.18		0.22

[a] *Note*: The force constants are given in the following units: S_i, mdyn/Å^{-1}, B_i, mdyn/Å, and H_i, mdyn/Å^{-1}. The distances are given in angstroms, the angles in degrees, and the quantity dl/dP in units of Å $(10^4$ GPa$)^{-1}$.

It is the presence in the $YBa_2Cu_3O_7$ lattice of such a structural component as the $-Cu1-O_{Cu1}-Cu1-$ chain (Fig. 1) that provided us with arguments in favor of the hypothesis concerning the existence in the lattice's spectrum of soft modes induced by hydrostatic compression and, as a corollary, the tendency of the lattice toward becoming destabilized under pressure. In view of the complexity of the structure of the given compound, verifying the hypothesis required doing quantitative model calculations that allow for both of the above-mentioned factors (the stabilizing and the destabilizing).

3. BUILDING THE DYNAMICAL MATRIX OF THE $YBa_2Cu_3O_7$ CRYSTAL LATTICE UNDER CONDITIONS OF HYDROSTATIC COMPRESSION

The calculations done in this paper are based on Born's theory,[19] whose central concept is that of the dynamical matrix $D_{\alpha\beta}$ of a crystal lattice. The approach to building such a matrix is described in detail in the literature (see, e.g., Ref. 24).

In our calculations we used the CRYME package.[25] With it the (generally) complex-valued matrix $D_{\alpha\beta}$ is built for each wave vector separately and satisfies the corresponding properties of translational and point symmetries. The eigenfrequencies and vibration modes (polarization vectors) were found by diagonalizing the matrix, while the elastic constants of the lattice were determined by the long-wave method.[19] In the potential function of the crystal we allowed only for short-range forces, considered in the basis space of two- and three-center (angular) internal coordinates q (see Refs. 24 and 26), which automatically ensures that all the conditions of invariance following from the physical meaning of this quantity are met.[20] New conditions are added when pressure P is applied to the lattice—those of equilibrium in relation to the internal and external degrees of freedom of the crystal. This means that the resultant of the forces acting on the atoms is zero and that the external pressure is balanced by the totality of all inner stresses in the lattice.

The crystal lattice of $YBa_2Cu_3O_7$ ($D_{2h}^1=Pmmm$ and $z=1$) is depicted in Fig. 1. The notation system for the atoms used below corresponds to that adopted in the reviews by Evarestov *et al.*[27] and Kitaev *et al.*[28] and in Refs. 15 and 16 and allows for the layered structure of this compound: an oxygen atom belonging to a definite metal–oxygen layer contains a label of the corresponding metal. In calculations we used the structural data of Molchanov *et al.*[29]

The model of the force field suggested earlier in Refs. 15, 16, 30, and 31 for describing the dynamical properties of the $RBa_2Cu_3O_{7-\delta}$ compounds at $P=0$ incorporates three types of constants: S, B, and H (Table I). The constants S describe diagonal two-center interactions at distances no greater than 3.9 Å. The constants B determine diagonal three-center interactions, i.e., the elasticities of the angles (the model allows for elasticity of the O–Cu–O angles). Finally, the constants H describe the dynamical interactions of two bonds with a common atom (two types of interaction were considered: through the Cu1 atom, $O_{Ba}-Cu1/Cu1-O_{Ba}$, and through the Y atom, $O_{Cu}-Y/Y-O_{Cu}$).

In the present study the set of constants used in Refs. 15 and 16 was augmented by two other constants, S_{16} and S_{17}

TABLE II. Experimental and calculated values of the elastic constants C_{ik} (GPa) in $YBa_2Cu_3O_7$ compounds.

C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	
230	-	150	50	-	85	100	100	-	Experiment[36]
207	-	63	31, 36	-	85	-	-	-	Experiment[37]
-	-	160	25	-	85	66	-	-	Experiment[38]
231	268	186	49	37	95	132	71	95	Experiment[39]
181	235	167	50	47	59	50	94	82	Calculation[16]
206	261	167	50	47	59	50	94	82	Calculation*

**Note*: Results of the present work.

(see Table I), corresponding to the weak Ba–Ba and Cu1–Cu1 interactions between the closest translationally equivalent atoms in the xy plane. Allowing for these interactions made it possible to improve (in comparison to the results of Ref. 16) the similarity between the calculated results and experimental data on elastic constants (see Table II below).

In modeling the response of this force field to the hydrostatic compression of the crystal we allowed for two factors related to the decrease in the interatomic distances in the lattice:

(1) an increase in the values of the force constants S, B, and H caused by the substantial anharmonicity of the interatomic potentials;

(2) the generation of stresses, i.e., interatomic forces F balancing the outer pressure and ensuring that the atoms in the deformed lattice are in equilibrium.

For this we used the calculated values of the absolute variations in interatomic distances found for each new value of P (Table I). This made it possible to allow for the first factor by introducing anharmonic corrections for the values of the force constants S with the use of the S vs r dependence, which was found from the sets of respective constants obtained earlier in calculations of the dynamical properties of the $YBa_2Cu_3O_7$, $YBa_2Cu_3O_6$, $GdBa_2Cu_3O_7$, and $GdBa_2Cu_3O_6$ compounds at $P=0$ (see Refs. 15, 16, 30, and 31). In favor of this was the fact that these compounds contain a set of chemically single-type bonds of varying length. For instance, the $RBa_2Cu_3O_7$ compound contains five symmetry-nonequivalent Cu–O bonds, four Ba–O bonds, and two Y–O bonds, all corresponding to different distances r (Table I). Using the sets of constants for the four compounds, we found $S_{\mathrm{Cu-O}}$, $S_{\mathrm{Ba-O}}$, and $S_{\mathrm{Y-O}}$ as functions of r. Furthermore, as Fig. 2 shows, all three functions form a common "universal" empirical S vs r curve. On its basis we estimated the other two-center force constants for which there was no way of obtaining the S vs r dependence at $P=0$. Figure 2 gives an example of the baric dependence of $S(\mathrm{Cu-Y})$ built in this way (in the linear approximation).

Since the literature contains no data on the behavior of B and H under strains of the corresponding structural components, we calculate their variations caused by lattice compression as linear functions of pressure according to the best fit of the calculated baric dependences of the frequencies of vibrations of the A_g symmetry and the experimental data.

The second factor mentioned above (the destabilizing one) determines the variation of the tangential part of the force-constant matrix $V_{\alpha\beta}$ for $P>0$. To allow for it, we substituted the values of the uniform strains U and their shapes L, determined for a given value of P from the geometry of the problem and the force matrix according to the scheme developed in Ref. 21, into the second term on the right-hand side of Eq. (2).

Thus, the dynamical properties of the crystal lattice were found from the dynamical matrix $V_{\alpha\beta}(P)$, which at $P=0$ was determined only by the first term $V_{\alpha\beta}(0)=B_\alpha K(0)B_\beta$ in Eqs. (12) and (13) and for a fixed hydrostatic pressure $P \neq 0$ assumed the form

$$V_{\alpha\beta}(P)=B_\alpha K(P)B_\beta+K(0)L\kappa PB_{\alpha\beta}, \qquad (14)$$

where $K(0)$ corresponds to the initial (at $P=0$) set of the force parameters S, B, and H, and $K(P)$ to the set of these quantities determined in the above way for a compressed lattice.

By way of an example, Table I lists the force constants of the $YBa_2Cu_3O_7$ lattice at $P=0$, 15, and 30 GPa found in this manner. Here for each two-center interaction at $P \neq 0$ we list two parameters: one determining the elasticity of a spring for a given value of P, i.e., the value of S with allowance for the anharmonic correction, and the other the magnitude of the force F on a given spring.

Note that the variation of both terms in (14) corresponds to allowing in the potential function for two anharmonic factors of an entirely different nature. As noted in the Introduction, the first is determined by the "substantial" anharmonicity of the interatomic potentials, and for a two-center

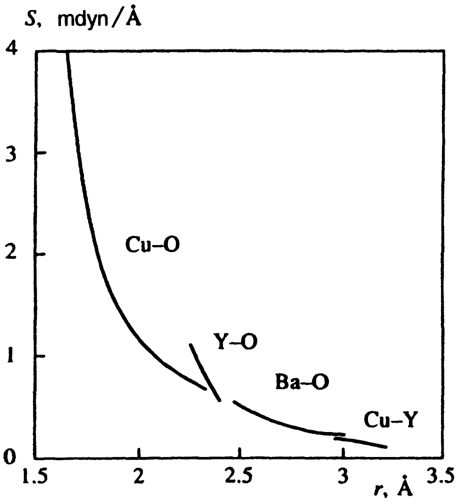

FIG. 2. The force constants $S(\mathrm{Cu-O})$, $S(\mathrm{Y-O})$, $S(\mathrm{Ba-O})$, and $S(\mathrm{Cu-Y})$, as functions of the interatomic distance r.

interaction was numerically estimated from the diagram in Fig. 2. The second describes the anharmonicity that is in no way related to the nature of the interatomic forces and is present even in the simplest dynamical model consisting of hard spheres and ideal springs. To clarify its meaning we note that from the viewpoint of physics the anharmonicity of atomic movements in a crystal means the existence of a nonlinear relationship between the absolute displacement of an atom and the restoring force that is generated in the process. Earlier it was shown[32] that due to the curvature of the space of the internal coordinates q the variation of the coefficients in the linear terms in the expansion (9), i.e., the generation of forces F, leads to nonlinear effects in the expansion (11), i.e., to a change in the quantities $V_{\alpha\beta}$, $V_{\alpha\beta\gamma}$, etc., which constitutes an inherently anharmonic effect. In Ref. 33 it was noted that these effects should be related to the cubic terms of the X^2U type in the expansion of the energy V in the $3N+N$-dimensional total space of true (by the terminology of Ref. 9 strains of the crystal, the space consisting of $3N-3$ internal strains X (the vibrational coordinates) and six external macroscopic strains U.

Thus, both anharmonic factors were numerically allowed for in our predictive calculations without introducing explicitly any anharmonic terms in the expansion (11), in contrast to the common way of introducing higher-order terms into the potential for reproducing the experimental results (e.g., the phase transition of β-quartz into an incommensurate structure[34] or destabilization of the La_2CuO_4 lattice[35]).

4. RESULTS OF CALCULATIONS

4.1. Dynamical properties of the $Yba_2Cu_3O_7$ lattice at $P=0$

Since modeling the behavior of the $YBa_2Cu_3O_7$ structure under external mechanical stresses was of a predictive nature, it was done together with calculations of a broad spectrum of dynamical characteristics of the structure. These characteristics included, in particular, nine independent elastic constants C_{ik} and 39 fundamental vibrations of the $YBa_2Cu_3O_7$ lattice, which are distributed over the irreducible representations at the center of the Brillouin zone as follows (see, e.g., the review articles by Evarestov *et al.*[27] and Kitaev *et al.*[28]):

$$\Gamma(D_{2h}^1)=5A_g+5B_{2g}+5B_{3g}+8B_{1u}+8B_{2u}+8B_{3u}. \tag{15}$$

Note that vibrations that are even with respect to the inversion center are active only in Raman scattering (RS) spectra, while odd optical vibrations are active only in IR spectra.

In discussing our results of calculating center-zone vibration frequencies at $P=0$ for $YBa_2Cu_3O_7$ (Refs. 15 and 16), $YBa_2Cu_3O_6$ (Ref. 30), $GdBa_2Cu_3O_7$ (Ref. 16), and $GdBa_2Cu_3O_6$ (Ref. 31) we have already noted their good agreement with a large set of experimental data known from RS and IR-reflection spectra. Adding the constants $S_{16}(\mathrm{Ba-Ba})$ and $S_{17}(\mathrm{Cu1-Cu1})$ to the model of Ref. 16 has no effect on the properties of center-zone vibrations but considerably improves the description of elastic properties (Table II).

The main idea of our study of the possibility of destabilizing the $YBa_2Cu_3O_7$ lattice by hydrostatic compression presupposes the existence in the lattice's spectrum of a phonon that either totally or to a considerable extent corresponds to the strain vibration of an isolated $-\mathrm{Cu1}-\mathrm{O_{Cu1}}-\mathrm{Cu1}-$ chain. Symmetry considerations imply that when the chain is directed along the y axis, the two components of such a vibration polarized along the z and x axes must belong to the representations B_{1u} and B_{3u}, respectively.

An analysis of the shapes of the calculated vibrations (the eigenvectors of the dynamical matrix) given in Table VI of Ref. 15 suggests that the B_{3u}-mode with the frequency $126\ \mathrm{cm}^{-1}$ has the most easily discernible features of a strain vibration of the chain (see Eq. (16) below). To a lesser extent this is true of the vibration with the frequency $336\ \mathrm{cm}^{-1}$ of the B_{1u} symmetry. Thus the question of the low-frequency region in the IR spectrum with the polarization $\mathbf{E}\|\mathbf{x}$ where vibrations of the B_{3u} symmetry are active is of primary importance.

Note that in studying the IR spectra of the superconductor $YBa_2Cu_3O_7$ there is the problem of separating the vibrations from the background of strong plasma reflection (primarily in the $\mathbf{E}\perp\mathbf{z}$ polarization). It is for this reason that the corresponding data are absent even from the most thorough review of the IR spectroscopy of superconductors.[40] As the carrier concentration decreases (as the oxygen content in the $\mathrm{O_{Cu1}}$ position decreases), phonon screening also decreases, in view of which fairly reliable spectra of IR reflection for $YBa_2Cu_3O_6$ in the $\mathbf{E}\perp\mathbf{z}$ polarization were obtained.[40] However, the $YBa_2Cu_3O_6$ structure does not contain $\mathrm{Cu1}-\mathrm{O_{Cu}}-\mathrm{Cu1}$ chains. We known of only one work (Ref. 41) devoted to the study of B_{2u}- and B_{3u}-vibrations in single crystals of $YBa_2Cu_3O_{6+\delta}$ with considerable oxygen content δ. Three new lines (as compared to the spectra of $YBa_2Cu_3O_6$) were discovered in the IR spectra of such crystals with an oxygen content $0.2<\delta<0.4$, which is in full agreement with the result of symmetry analysis. The line $147\ \mathrm{cm}^{-1}$ for the $\mathbf{E}\perp\mathbf{z}$ polarization was related to the strain B_{3u}-vibration of the chain along the x axis discussed here.

The results of studies of the dispersion of phonon branches in $YBa_2Cu_3O_{7-\delta}$ crystals by the method of inelastic neutron scattering can be found in Refs. 9, 36, 42, and 43 and are compared with the data of optical experiments and the results of dynamical calculations in the review of Litvinchuk *et al.*[40] Unfortunately, not all 39 dispersion branches have been detected in the neutron spectra, but in the spectral range of interest to us a number of vibrations were observed; namely, the vibrations that at point Γ have the frequencies 120, 140, 153, and $167\ \mathrm{cm}^{-1}$. Allowing for the results of Ref. 41, we select two of these vibrations, 140 and $153\ \mathrm{cm}^{-1}$, which can be related to the strain vibration of chains along the x axis in $YBa_2Cu_3O_7$ crystals.

4.2. Comparison of experimental data and results of calculations for $P>0$

Let us now discuss the agreement between the experimental data and the calculated elastic characteristics of the crystal and the estimate of strain for different structural components of the $YBa_2Cu_3O_7$ lattice under hydrostatic compression, since these quantities form the basis for a model description of the anharmonic contributions to the potential function. Moreover, such an analysis is a cornerstone in modeling the potential function of crystal lattices since there exists the possibility of solving the problem of reproducing an eigenvalue (in the given case the bulk modulus) and eigenvector (the microstrain patterns of the structural components of the lattice) of the dynamical matrix of the crystal.[21] This is in sharp contrast to the situation in vibrational spectroscopy, where studying such a problem is fraught with difficulties, since measuring the eigenvectors of phonons in multicomponent objects usually constitutes a complicated experimental problem. In our studies the good agreement of the calculated polarization vectors at $P=0$ and those determined from experiments (say, in studying Raman scattering in samples with isotopic substitution) was noted in Refs. 16 and 31 and in the review article by Kitaev *et al.*[28]

The experimental picture of micro- and macro-strains in the $YBa_2Cu_3O_7$ lattice under pressure has been fully determined in structural studies.[34] The results obtained in the 0–0.6GPa range suggest that the nature of the internal relaxation of the lattice has prominent special features: the variation of interatomic distances along the z axis within the elementary cell is of an undulating nature. In particular, the relative variations of the lengths of the O_{Cu}–O_{Cu} and O'_{Cu}–O'_{Cu} bonds in the $YBa_2Cu_3O_{6.93}$ lattice for $P>0$ prove to be considerably smaller than the similar variation of the parameter c of the cell, i.e., the quantity $(\partial c/\partial P)/c$. In $YBa_2Cu_3O_{6.60}$ this effect manifests itself even stronger: the lengths are practically independent of pressure in the studied pressure range. This picture of internal relaxation resembles the undulating structural transformation of the lattices $RBa_2Cu_3O_{7-\delta}$ observed under variations of their chemical composition.[16,27]

In our calculations the bulk modulus $B=120$ GPa for all practical purposes coincides with the experimental value of 123 GPa (Ref. 44), and the above-mentioned undulating behavior of the lattice clearly manifests itself for $P>0$: the pressure derivative of the interatomic distance in O'_{Cu}–O'_{Cu} even proves to be a small negative quantity, which explains the anomalous behavior of the corresponding force constant S_{13} when the lattice is compressed (see Table I).

Since an important component in our calculation scheme is the fact of allowing for substantial anharmonicity in the potential function, we paid special attention to reproducing the experimentally established baric dependences of the frequencies of a number of vibrations at the center of the Brillouin zone. Unfortunately, the relevant experimental information is restricted to the most intense vibrations of the totally symmetric representation in RS spectra. For instance, in the case of $YBa_2Cu_3O_{6.9}$ single crystals under pressure, the behavior of the frequencies of two A_g-vibrations (435 and 498 cm^{-1} at $P=0$) have been studied[45] (Fig. 3), while for ceramic samples of the $YBa_2Cu_3O_7$ composition the baric dependences of the frequencies of four A_g-vibrations (145, 338, 440, and 540 cm^{-1} at $P=0$) have been obtained for pressures up to 16 GPa.[45] These frequencies increase with pressure, and the higher the vibration frequency the greater the value of the parameter $d\nu/dP$ (Fig. 3). We also note that Syassen *et al.*[46] observed a line that splits away from the band at 338 cm^{-1} as the pressure grows and exhibits a weak negative baric dependence.

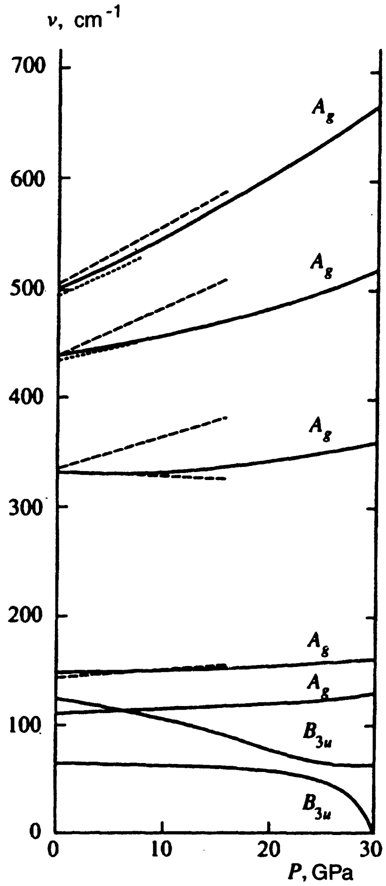

FIG. 3. Baric dependences for the vibrational frequencies of $YBa_2Cu_3O_7$ crystals in the center of the Brillouin zone. The solid curves represent the results of calculations (for vibrations of the A_g symmetry and for two low-frequency B_{3u} modes), the dashed curves to the experimental data of Syassen *et al.*,[46] and the dotted curves correspond to the experimental data of Kulakovskiĭ *et al.*.[45]

The results of our calculations (Fig. 3) reproduce fairly well the behavior of the experimental ν vs. P curves, including the increase in their slope $d\nu/dP$ as we move from one vibration to another with a higher frequency.

To obtain a full picture of the variation of the vibrational spectrum of $YBa_2Cu_3O_7$ under pressure we calculated the dispersion branches along all the high-symmetry directions in the Brillouin zone, namely,

$$\Gamma(0,0,0)\to(\xi,0,0)\to X(0.5,0,0),$$

$$\Gamma\to(0,\xi,0)\to Y(0,0.5,0),$$

$$\Gamma\to(0,0,\xi)\to Z(0,0,0.5),$$

$$\Gamma\to(\xi,\xi,0)\to S(0.5,0.5,0),$$

$$\Gamma\to(\xi,0,\xi)\to U(0.5,0,0.5),$$

$$\Gamma\to(0,\xi,\xi)\to T(0,0.5,0.5),$$

$$\Gamma\to(\xi,\xi,\xi)\to R(0.5,0.5,0.5).$$

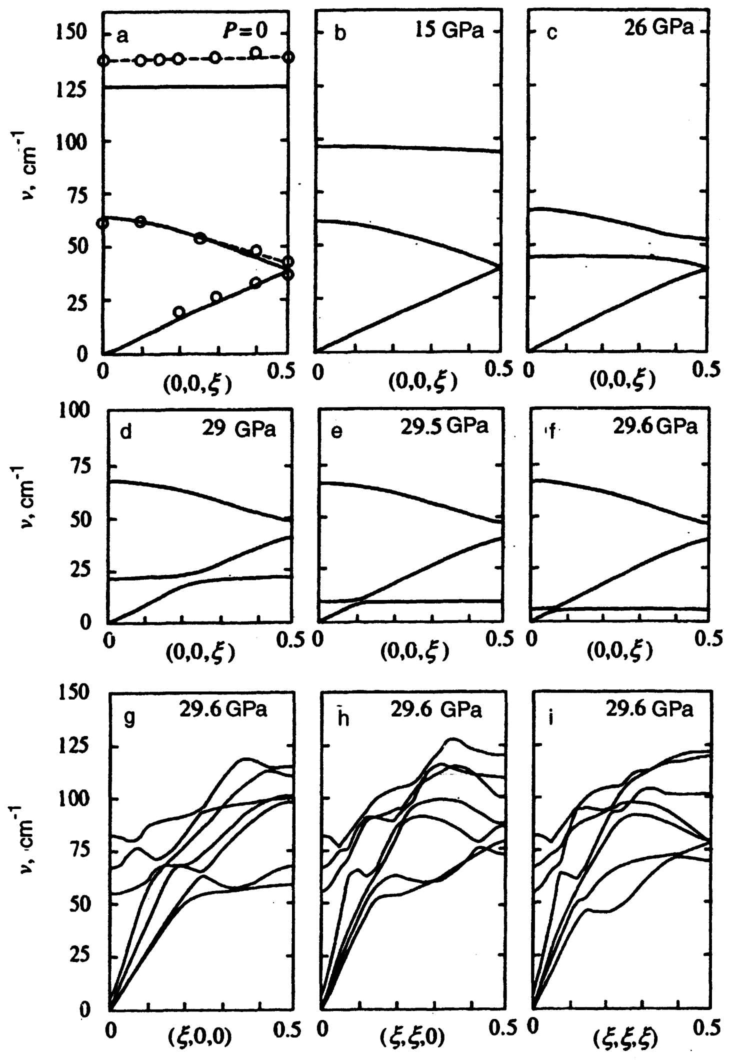

FIG. 4. Dispersion of the vibrational branches in the $YBa_2Cu_3O_7$ crystal: (*a*)–(*f*) baric dependences of the dispersion branches in the $\Gamma(0,0,0)\rightarrow Z(0,0,0.5)$ direction for the vibrations of the B_{3u} symmetry at point Γ (solid curves represent the results of calculations, and the circles linked by dashes correspond to the experimental data of Reichardt *et al.*[36]); (*g*)–(*i*) the dispersion of branches without separating the vibrations by their symmetry (the results of calculations).

(The notation for the singular points corresponds to that adopted in Ref. 47.)

Note that all the calculated vibrations in the medium- and high-frequency ranges of the spectrum become considerably stiffer under hydrostatic compression of the lattice, demonstrating in this way the ordinary baric dependence caused by the essential anharmonicity of interatomic interactions. Within the present model the effect has a simple explanation: this spectral range contains what is known as valency vibrations, for which the tangential contributions to the force constants are either zero or so small that they play no noticeable role.

4.3. Prediction of the appearance of a soft mode at $P>0$

The behavior of low-frequency vibrations for $P>0$ constitutes the most interesting aspect in our study. According to calculations, the situation in this range differs dramatically from the one discussed in Sec. 4.2: the frequency of a number of vibrational branches decreases (softening of vibration modes) as the pressure increases. For instance, the vibration frequencies at the edge of the Brillouin zone at point $S(0.5,0.5,0)$, which at normal pressure are 85, 93, and 97 cm^{-1}, at $P=30$ GPa lower to 68, 77, and 87 cm^{-1}, respectively.

The most dramatic changes, however, occur in the dispersion branch along the $(0,0,\xi)$ direction, whose center-zone point corresponds to an IR-active vibration of the B_{3u} symmetry with a calculated frequency of 126 cm^{-1} at $P=0$. Exhibiting practically no dispersion along $(0,0,\xi)$, this branch "descends," as the pressure grows, with a rate $\Delta\nu/\Delta P$ that is greater than that of the above-noted vibrations by a factor of ten, and at $P_c\simeq30$ GPa it actually touches the horizontal axis over the entire $\Gamma\rightarrow Z$ interval (Fig. 4), demonstrating in this way the reduction in the stability of the lattice for the set of points $(0,0,\xi)$ of the Brillouin zone, with $0\leqslant\xi\leqslant0.5$.

Here for the other directions of the Brillouin zone at $P\simeq30$ GPa not a single vibration has a frequency close to zero. This fact is illustrated in Figs. 4(g)–(i), where by way of an example we depict the dispersion of the branches along the $(\xi,0,0)$, $(\xi,\xi,0)$, and (ξ,ξ,ξ) directions.

Note that the results of experimental investigations of the dispersion of the vibrations along the $\Gamma\rightarrow Z$ direction in the relevant spectral range are known only for the mode with a frequency of approximately 140 cm^{-1} at $P=0$. According to Ref. 36, this vibration has no dispersion along the $(0,0,\xi)$ direction [Fig. 4(a)].

As the frequency drops, the "soft" branch crosses two branches with the same symmetry: the optical branch emerging at the center-zone vibration 64 cm^{-1}, and the acoustic. Hence, for a clearer understanding of the mechanism of lattice strain for $P>P_c$ related to the shape of the soft-mode vibration we will examine the results more carefully.

5. ANALYSIS OF THE STRUCTURAL INSTABILITY OF THE $YBa_2Cu_3O_7$ LATTICE UNDER CONDITIONS OF HYDROSTATIC COMPRESSION

The practically flat shape, obtained as a result of calculations, of the soft mode along the $\Gamma \rightarrow Z$ direction makes it impossible to provide a unique value for the wave vector $\mathbf{K}$ at which phonon condensation, which determines the phase transition and the property of the low-symmetry structure, occurs. From symmetry considerations it follows that three variants are possible: (1) $\mathbf{K}=0$, (2) $\mathbf{K}=(0,0,0.5)$, and (3) $\mathbf{K}=(0,0,\xi)$ with $0<\xi<0.5$. We examine these cases separately.

5.1. Phase transition is induced at the center of the Brillouin zone by condensation of a polar vibration of the B_{3u} symmetry

This effect leads to a phase transition in which the symmetry changes from D_{2h}^1 to C_{2v}^1 but the size of the elementary cell is retained. The soft mode becomes a vibration of a totally symmetric polar representation A_1 of a low-symmetry structure. From symmetry considerations it follows that in the new phase the lattice can have a dipole moment, i.e., exhibits ferroelectric properties.

Let us examine the evolution of the properties of low-frequency vibrations of the B_{3u} type as the pressure grows from zero to P_c.

We note that optical vibrations in layered perovskite-like multicomponent compounds separate into interlayer modes that exhibit considerable dispersion in all directions of the Brillouin zone, and intralayer modes, which are characterized by the absence of any dispersion in the $\Gamma \rightarrow Z$ direction perpendicular to the layer xy plane (Ref. 15; see also the review by Kitaev *et al.*[28]). The vibration with a frequency of 126 cm^{-1} must also be classified as belonging to such intralayer modes; to a great extent it is determined by the displacements of atoms in a single layer (in the present case the layer is the one formed by chains). This vibration, like all other vibrations of the B_{3u} symmetry, is caused by the displacement of atoms along the x axis and has the following shape:[15]

$$(11\text{Cu1}-4\text{O}_{\text{Cu1}})-(2\text{Ba}+3\text{O}_{\text{Ba}})+(1\text{Cu}+1\text{O}_{\text{Cu}}). \quad (16)$$

It can be classified as an essentially strain vibration of $-\text{Cu1}-\text{O}_{\text{Cu1}}-\text{Cu1}-$ chains (see Fig. 1).

At $P=0$ in the spectrum of $YBa_2Cu_3O_7$ the calculated optical mode of the B_{3u} symmetry with the lowest frequency, 64 cm^{-1}, is clearly an interlayer vibration, since its shape is

$$(4\text{Cu1}+3\text{O}_{\text{Cu1}})+(3\text{Ba}+3\text{O}_{\text{Ba}})-5Y-(5\text{Cu}+5\text{O}_{\text{Cu}}+5\text{O}'_{\text{Cu}}), \quad (17)$$

which corresponds to antiphase displacements along the x axis of the Cu1O_{Cu1} and BaO_{Ba} layers with respect to the layers of Y atoms and $\text{CuO}_{\text{Cu}}\text{O}'_{\text{Cu}}$.

TABLE III. Calculated values of the frequencies ν and the relative displacements along the x axis of Cu1 and O_{Cu1} atoms corresponding to two low-frequency vibrations of the B_{3u} symmetry at the center of the Brillouin zone for different pressures P.

		Amplitudes			Amplitudes	
P,GPa	ν,cm^{-1}	Cu1	O_{Cu1}	ν,cm^{-1}	Cu1	O_{Cu1}
0	64	+4	+3	126	+11	−4
5	62	+5	+3	117	+11	−5
10	61	+5	+3	106	+11	−7
15	61	+5	+2	96	+10	−8
20	59	+7	+1	79	+9	−9
22	57	+9	−2	72	+7	−9
24	54	+11	−4	69	+5	−8
26	43	+11	−6	65	+1	−7
28	33	+11	−7	65	0	−6
29	21	+11	−8	66	−1	−5
29.5	10	+11	−8	66	−1	−5

Thus, in contrast to the strain mode at 126 cm^{-1}, the 64 cm^{-1} mode contains translational movements of chains along the x axis. According to our calculations, as the pressure grows, the frequency of the strain mode decreases, while the frequency of translational mode increases very slightly. As a result of these two vibrations of the same symmetry moving closer to each other and interacting, mixing or even inversion occurs (see Fig. 3). The data listed in Table III shows how the characteristic vectors of these vibrations are transformed in the interaction process. Table III gives only the contributions of the Cu1 and O_{Cu1} atoms to these vibrations, since the displacements of other atoms play no significant role and depend on pressure only slightly over the entire pressure range from zero to 30 GPa. Clearly, at $P \simeq 21$ GPa the shape of the vibrations of a chain in the low-frequency mode changes from translational to strain, and in the 21–28 GPa range the spectrum contains two vibrations of the B_{3u} symmetry with antiphase displacement of the Cu1 and O_{Cu1} atoms in the chains. At $P \simeq 28$ GPA the vibration with the higher frequency acquires the shape of a translational vibration: the displacements of Cu1 and O_{Cu1} atoms are now in phase. Hence inversion ("exchange") of vibration shapes occurs, and the low-frequency mode, which becomes softer under a further increase in pressure, is a strain vibration of a chain.

In addition, as the pressure is increased from zero to 30 GPa, the soft optical branch moves closer to the acoustic branch of the same symmetry. Their interaction results in an observable effect similar to the one described above for the case of two optical B_{3u}-vibrations. The overall behavior of the dispersion branches is depicted in Fig. 4.

At $P_c \simeq 30$ GPa the frequency of the soft mode vanishes, and its shape is determined by the following components of the displacements of atoms along the x axis:

$$(11\mathrm{Cu1}-8\mathrm{O}_{\mathrm{Cu1}})-(1\mathrm{Ba}+3\mathrm{O}_{\mathrm{Ba}})-1Y-(1\mathrm{Cu}+1\mathrm{O}_{\mathrm{Cu}}+1\mathrm{O}'_{\mathrm{Cu}}), \qquad (18)$$

i.e., practically coincides with the vibration 126 cm^{-1} at $P=0$.

Note that the calculated value of P_c is determined by a number of parameters with no experimental verification, so that the obtained value of 30 GPa can only be thought of as being a rough estimate.

5.2. Condensation of a vibration at point Z (0,0,0.5) at the edge of the Brillouin zone

We immediately note that for all points of the dispersion branch with a wave vector $\mathbf{K}=(0,0,\xi)$ directed at right angles to the plane in which the Cu1 and $\mathrm{O}_{\mathrm{Cu1}}$ atoms are displaced, the shape of the strain vibration along the x axis is retained.

The point symmetry of the wave vector $\mathbf{K}=(0,0,0.5)$ is described by the D_{2h} group, whose vibrational representations have the following form (see Table 8 in Ref. 22):

$$Z=7Z_1^+ +7Z_3^+ +7Z_4^+ +6Z_2^- +6Z_3^- +6Z_4^-$$

$$=7A_g+7B_{3g}+7B_{2g}+6B_{1u}+6B_{3u}+6B_{2u}, \qquad (19)$$

with the vibration of the soft-mode branch at point Z belonging to the representation $Z_4^+ \equiv B_{2g}$. When this vibration becomes condensed, there is induced a $D_{2h}^1 \rightarrow D_{2h}^5$ phase transition with doubling of the elementary cell along the z axis, and the symmetry of the soft-mode vibration changes from B_{2g} to A_g.

5.3. Condensation of vibrations with the wave vector $\mathbf{K}=(0,0,\xi)$, $0<\xi<0.5$

The point symmetry of the wave vector $\mathbf{K}=(0,0,\xi)$ is described by the C_{2v} group. For $P<P_c$ the vibrations with such a wave vector are distributed over the irreducible representations of this group as follows:

$$13A_1+13B_1+13B_2. \qquad (20)$$

The soft mode belongs to the B_2 representation.

This case corresponds to multiplication of the cell along the z axis. The modulation period of the structure is determined by the wavelength of the soft-mode vibration and generally is not an integral multiple of the lattice constant C of the D_{2h}^1 phase. The transition is into an incommensurate phase, whose symmetry, in accordance with the classification of Wolff *et al.*[48] is described by the four-dimensional space group $P_{1\,1\bar{1}}^{mmm}$.

6. DISCUSSION AND CONCLUSIONS

Let us estimate the objectivity of the obtained results on the basis of the relationship between the number of the adjustable parameters in the model and the volume of the experimental data described.

Note that in modeling the radial part of the potential function the principle by which the arbitrariness in the choice of the numerical values of the force constants should be reduced to a minimum was inherent in the very method of calculating these constants from a single "universal" empirical S vs. r dependence for two-center interactions (Fig. 2). The tangential part of the potential function, responsible for the destabilizing effect, is actually determined by the laws of mechanics and in this sense is model-independent.

Using the potential function constructed along these lines, we were able to describe in a fairly consistent manner practically all of the experimental data referring to the structural and dynamical properties of crystals of the $\mathrm{RBa_2Cu_3O_{7-\delta}}$ family. Briefly the data are as follows:

(a) the values of the elastic constants C_{ik} (Table II) and the value of the bulk modulus of the $\mathrm{YBa_2Cu_3O_7}$ lattice (see Ref. 44);

(b) the nontrivial undulating transformation of the structure of $\mathrm{YBa_2Cu_3O_7}$ under hydrostatic compression (Table I and the results of Ref. 44);

(c) the set of the experimentally established optical frequencies at the center of the Brillouin zone for the $\mathrm{YBa_2Cu_3O_7}$ compound (Refs. 15 and 16), the $\mathrm{YBa_2Cu_3O_6}$ compound (Ref. 30), the $\mathrm{GdBa_2Cu_3O_7}$ compound (Ref. 16), and the $\mathrm{GdBa_2Cu_3O_6}$ compound (Ref. 31);

(d) the baric dependences of the frequencies of vibration of the A_g symmetry in $\mathrm{YBa_2Cu_3O_7}$ crystals (Fig. 3);

(e) the values of LO–TO splitting in IR-active vibrations in $\mathrm{YBa_2Cu_3O_6}$ crystals (Ref. 30);

(f) the dispersion of the vibrational branches of the $\mathrm{YBa_2Cu_3O_7}$ lattice (Fig. 4*a*).[14]

We pay special attention to the discrepancy between our calculation results and the experimental data of Pyka *et al.*,[9] who in establishing the anharmonicity in the chain's vibrations focused exclusively on the 167 cm^{-1} vibration and the corresponding dispersion branch along the $\Gamma \rightarrow Y$ direction. Allowing for the results of studies[41] of the IR spectra of $\mathrm{YBa_2Cu_3O_{7-\delta}}$ and of calculations of the dynamical properties of the $\mathrm{YBa_2Cu_3O_7}$ lattice conducted by other researchers (see, e.g., Refs. 49 and 50), we conclude that classifying these vibrations as strain displacements of the chain along the x axis is not obvious, and it cannot be ruled out that the results of Ref. 9 are outside the scope of the present study.

As for other experiment, we note that the above-noted possibility of a phase transition of the $\mathrm{YBa_2Cu_3O_7}$ lattice to the ferroelectric phase is in qualitative agreement with the anomalies of the insulator properties of this lattice discovered by Testardi *et al.*[51] This case is especially interesting also because all known superconductors have centrally symmetric crystal lattices.

Here is another argument in favor of our conclusions. We note the agreement of our result with the structural features of the object being discussed. The crystal lattice of $\mathrm{YBa_2Cu_3O_7}$ (Fig. 1) consists of $\mathrm{BaO_{Ba}}$ and $\mathrm{CuO_{Cu}O'_{Cu}}$ layers, a layer of Y atoms, and $-\mathrm{Cu1}-\mathrm{O}_{\mathrm{Cu1}}-\mathrm{Cu1}-$ chains. The first three types of layers consist of atoms forming a quasisquare lattice ($a \simeq b$), which proves to be a considerably more stable structural element in conditions of hydrostatic compression than the $-\mathrm{Cu1}-\mathrm{O}_{\mathrm{Cu1}}-\mathrm{Cu1}-$ chain. The anisotropy of the vibrational properties of the chain is of clear origin: the Cu1 and $\mathrm{O}_{\mathrm{Cu1}}$ atoms in the chain are positioned at a small distance (on the y axis) from each other (1.94 Å), and the length of the bond along the z axis between the Cu1 and O_{Ba} atoms is even smaller (1.84 Å). The distance between the O_{Cu1} and Ba atoms in the adjacent layers along the z axis is characterized by an average value of 2.88 Å , while the distance between the chain atoms along the x axis is equal to the value of cell parameter of 3.82 Å . Because of this the potential relief for atomic displacements along the x axis has a mild slope, which makes the zigzag vibration of the chain in this direction the most "vulnerable" structural strain of the $YBa_2Cu_3O_7$ lattice under compression.

All of this suggests that the proposed potential function provides a fairly accurate description of the dynamical properties of the $YBa_2Cu_3O_7$ crystal lattice, a description that can be used to model the behavior of the vibrational subsystem of the lattice under varying external conditions.

The main results of the present work are the prediction of structural instability in the $YBa_2Cu_3O_7$ crystal lattice in conditions of high hydrostatic pressure and the description of the micromechanism of this phenomenon. According to our calculations, the optical vibrations belonging to the flat dispersion branch along the $\Gamma \rightarrow Z$ direction and the corresponding strain displacements along the x axis of the atoms in the $-Cu1-O_{Cu1}-Cu1-$ chain demonstrate soft-mode behavior as the pressure increases.

The authors are grateful to H. Lichtenstern and M. B. Smirnov for the help in calculations and V. P. Smirnov for determining the symmetry of the $YBa_2Cu_3O_7$ lattice for the case of an incommensurate phase transition with $P > P_c$. The study was supported financially by the Russian Fund for Fundamental Research (project 1V 95-02-061132a).

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Translated by Eugene Yankovsky