Elastic properties of La_2CuO_4 under pressure

2000 J. Phys.: Condens. Matter 12 1199

(http://iopscience.iop.org/0953-8984/12/7/305)

J. Phys.: Condens. Matter **12** (2000) 1199–1207. Printed in the UK PII: S0953-8984(00)04931-6

Elastic properties of La_2CuO_4 under pressure

A E Nikiforov, S Yu Shashkin and A Yu Zaharov†

Department of Physics, Urals State University, Lenin Avenue 51, Ekaterinburg 620083, Russia

E-mail: anton.zaharov@usu.ru

Received 2 June 1999, in final form 23 November 1999

Abstract. Within the framework of the pair potential approximation and the shell model including the Jahn–Teller contribution to the crystal energy we have studied the elastic properties of La_2CuO_4. The strong anisotropic correlation between the lattice deformations e_{xx} and e_{zz} and the internal displacements of the accompanying sublattices within the La_2O_2 layers are shown to be responsible for the giant anisotropy of the elastic moduli in the xz-plane. We have predicted the softening of several elastic moduli in the orthorhombic phase region near the pressure-induced structural phase transition. But we have not observed the softening of c_{11}, c_{12}, and c_{66} in the tetragonal phase region that was measured near the temperature-induced structural phase transition.

1. Introduction

The elastic properties of $La_{2-x}Me_xCuO_4$ (Me = Sr, Ba) as well as those of the parent material La_2CuO_4 have attracted considerable interest during the last few years. Nevertheless, until now there have been some contradictions in the available experimental and theoretical results. The experimental data obtained in [1, 2] for a single crystal of La_2CuO_4 showed only a very small anisotropy of the elastic properties in the xz-plane (see table 1). On the other hand, the elastic moduli measured in [3] for a single crystal of La_2CuO_4 as well as the results of theoretical calculations for La_2CuO_4 [4, 5] provided evidence of giant anisotropy in the xz-plane (see table 1). By referring to the 'giant anisotropy' of the elastic moduli of La_2CuO_4, we mean that the anisotropy of the elastic properties is much more pronounced than the anisotropy of the structural parameters. In fact, the structural anisotropy $(a - b)/(a + b)$ in the xz-plane is equal to 0.8% [6] (a, b are lattice constants) whereas the anisotropy of the elastic moduli $(c_{11} - c_{33})/(c_{11} + c_{33})$ is equal to 19.2% [3]. The origin of such a noticeable difference has not been understood, and the prime objective of this work is to determine the microscopical reasons for the giant anisotropy of the elastic moduli.

Another point regarding which there are some problems with interpretation of experimental data is the behaviour of the elastic moduli of both La_2CuO_4 and $La_{2-x}Me_xCuO_4$ near the tetragonal–orthorhombic structural phase transition (SPT). In particular, the temperature dependences of several elastic moduli measured experimentally (see below) show their softening, but up to now there has been no complete theoretical explanation for this effect. In view of this, it seems to be useful to study the pressure dependence of the elastic moduli near the tetragonal–orthorhombic SPT—the more so because there are no experimental data on this point.

† Author to whom any correspondence should be addressed.

0953-8984/00/071199+09$30.00

Table 1. Elastic moduli of La_2CuO_4 (GPa).

	c^r_{11}	c^r_{12}	c^r_{13}	c^r_{22}	c^r_{23}	c^r_{33}	c^r_{44}	c^r_{55}	c^r_{66}
This work	285	106	137	355	115	165	94	125	79
Experimental (at 44 K) [1]	169	71	100	200	73	167	71	104	66
Experimental (at 300 K) [2]	175	90	90	265	98	173	66	99	67
Experimental (at 77 K) [3]	230	102	98	276	92	156	75	102	64
Calculation [4]	369	140	65	380	129	199	128	131	131
Calculation [5]	340	120	57	392	123	210	125	117	72

2. The model

The equilibrium structural parameters for a crystal under hydrostatic pressure P can be found as a result of the minimization of the enthalpy $H = E + PV$ (V is the unit-cell volume). The crystal energy E is presented in the form of the sum of lattice and Jahn–Teller contributions:

$$E = E_{\rm lat} + E_{\rm JT}. \tag{1}$$

The ions Cu^{2+} have degenerate (quasi-degenerate) ground states; therefore it is necessary to take into account the interaction of these ions with low-symmetry local lattice distortions (the Jahn–Teller effect). The method of including the multi-body Jahn–Teller contribution to the energy and dynamical matrix of the crystal has been developed in our previous papers [7,8]. Note that the Jahn–Teller energy contribution plays a very important role in the crystal structure formation of K_2CuF_4 [9] which has the same layered perovskite structure as La_2CuO_4, discussed in this work. The Jahn–Teller energy contribution was also found to be important for the correct simulation of the structure and lattice dynamics of La_2CuO_4 [10] and this term determined the difference in physical properties between La_2CuO_4 and La_2NiO_4 [11]. We think that taking into account the multi-body Jahn–Teller contribution to the crystal energy of La_2CuO_4 is preferable from the physical point of view to describing the Jahn–Teller effect by including the anisotropic Cu^{2+}–O^{2-} pair potential (see, for example, [12]) or by considering the scaled Cu^{2+}–O^{2-} pair potential involving apical oxygen (see [5])†.

Within the framework of the pair potential approximation and the shell model, the lattice energy can be expressed as follows:

$$E_{\rm lat} = \frac{1}{2}\sum_{\substack{i,j\\ i\neq j}} V_{i,j} + \frac{1}{2}\sum_i k_i|\vec{s}|^2 \tag{2}$$

where the index i numbers all the ions in the unit cell, index j numbers all the crystal ions, k_i is the core–shell force constant, and $\vec{s}_i$ is the 'i'-ion shell displacement relative to its core. For the interionic pair potential $V_{i,j}$, we use the expression

$$V_{ij} = \frac{X_iX_j}{r} + \frac{Y_iX_j}{|\vec{r}_{ij}-\vec{s}_i|} + \frac{X_iY_j}{|\vec{r}_{ij}+\vec{s}_j|} + \frac{Y_iY_j}{(|\vec{r}_{ij}-\vec{s}_i+\vec{s}_j|)} + C_{ij}\exp(-D_{ij}|\vec{r}_{ij}-\vec{s}_i+\vec{s}_j|) - \lambda_{ij}/|\vec{r}_{ij}-\vec{s}_i+\vec{s}_j|^6 + f_{ij}(r) \tag{3}$$

with X_i, Y_i are the charges of an 'i'-ion core and shell respectively ($Z_i = X_i + Y_i$), and $r = |\vec{r}_{ij}|$ is the distance between the ion cores. The term

$$f_{ij}(r) = -A_{ij}\exp(-B_{ij}r)/r \tag{4}$$

† In [4] the calculations of the structural and elastic properties of La_2CuO_4 were performed without making any Jahn–Teller corrections.

describes the short-range electrostatic screening of the overlapping electron shells. The values of all of the constants (i.e. C_{ij}, D_{ij}, λ_{ij}, k_i, A_{ij}, and B_{ij}) needed to simulate La_2CuO_4 as well as the methods used to determine them are given in our previous paper [10], devoted to the calculation of the structural properties of La_2CuO_4 under pressure.

We approximate the multi-body Jahn–Teller contribution to the crystal energy as in [13] by the sum of expressions for the lower branches of CuO_6 cluster adiabatic potentials:

$$E_{\mathrm{JT}} = -\sum_k |V_e|(Q_\theta^2 + Q_\epsilon^2)^{1/2} \tag{5}$$

where the index k numbers all of the copper ions in the unit cell and the symmetrized coordinates Q_θ, Q_ϵ characterize the e_g distortion of the oxide octahedra around the copper ions (for more details, see [10]). Evaluation of the linear Jahn–Teller coupling constant V_e for the CuO_6 cluster with the distance R(Cu–O) $= 0.21$ nm (the average Cu–O distance in La_2CuO_4) with the aid of the method of [14] gives $V_e = -2.5$ nN.

As soon as the equilibrium crystal structure at constant pressure has been determined, the elastic properties of a crystal may be calculated using the second derivatives of the crystal energy E, equation (1), with respect to the lattice deformations and the corresponding sublattice internal displacements. This means that when a lattice deformation is applied, the value of the crystal energy E is found as a result of minimization of E with respect to all symmetry-permitted sublattice internal displacements.

3. Results and discussion

Before proceeding to the results obtained let us discuss the point of which coordinate systems are used. Presenting the elastic moduli, we use two different Cartesian systems of coordinates: 'orthorhombic' (see figure 1(a)) and 'tetragonal' (see figure 1(b)). The 'orthorhombic' coordinate system is preferable for determining the elastic moduli of La_2CuO_4 which is in the orthorhombic phase (space group D_{2h}^{18}). The 'tetragonal' coordinate system is useful for describing the tetragonal–orthorhombic SPT (see below). Throughout the text, for elastic moduli determined in the 'orthorhombic' coordinate system we use superscript r (for example, in c_{12}^{r}), and for elastic moduli determined in the 'tetragonal' coordinate system we use superscript t (for example, in c_{12}^{t}).

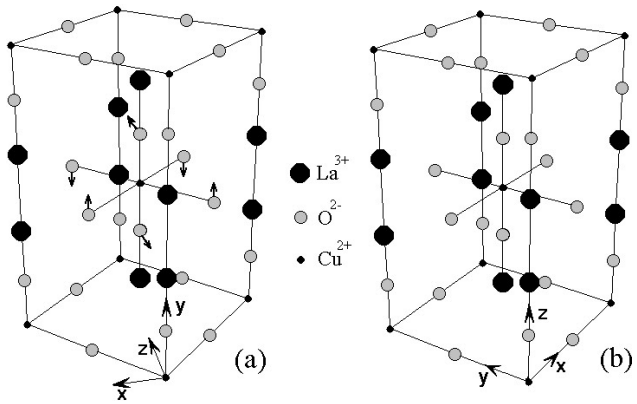

Figure 1. Cartesian coordinate systems used for determining the elastic moduli of La_2CuO_4.

3.1. Microscopical reasons for the giant anisotropy of the elastic moduli in the xz-plane

The calculated elastic moduli of La_2CuO_4 as well as the available experimental data and the results of the previous theoretical calculations are collected in table 1.

First of all, the noticeable differences between the experimentally measured elastic moduli presented in [1, 2] and in [3] are worth emphasizing. We are inclined to agree with Fil *et al* that such a discrepancy in the experimental results is explained by the fact that in [3] an especially untwinned single crystal of La_2CuO_4 was used for the measurements. On the other hand, in [1, 2] twinned crystals of La_2CuO_4 were evidently considered. So it becomes obvious that the calculation results should be compared with the experimental data given in [3], since within the framework of the theoretical models used in our work and in [4, 5] only untwinned crystals were considered. One can see from table 1 that our calculated elastic moduli are in good agreement with the experimental ones, although our calculations predict harder elastic properties of La_2CuO_4 than follow from the experiment. It should also be noted that our calculations describe the experimental results better than previously reported calculations [4,5]. But we would like to emphasize the fact that the results of our calculations as well as previously reported calculations [4,5] have reproduced correctly the main peculiarity of the elastic moduli of La_2CuO_4—their giant anisotropy in the xz-plane. Since in [4] the Jahn–Teller correction to the crystal energy was not taken into consideration while, on the other hand, in [5] and in the present study the Jahn–Teller correction was considered (although in a different way), we have grounds for saying that the Jahn–Teller effect does not play a crucial role in the explanation of the peculiarities of the elastic properties La_2CuO_4.

The most interesting result obtained by Fil *et al* is the giant anisotropy of the elastic moduli in the xz-plane. This anisotropy can be expressed quantitatively as $\sigma = (c^{\mathrm{r}}_{11} - c^{\mathrm{r}}_{33})/(c^{\mathrm{r}}_{11} + c^{\mathrm{r}}_{33})$. From [3], $\sigma = 19.2\%$, and our calculations give $\sigma = 26.5\%$. It is interesting to note again that the anisotropy of the elastic properties in the xz-plane is large enough, although the lattice distortions of La_2CuO_4 in the orthorhombic phase are rather small (see above).

In order to clarify the point of what microscopical reasons are responsible for such a large anisotropy in the xz-plane, we have carried out a series of elastic modulus calculations without taking into account the internal displacements of some sublattices of La_2CuO_4. For La_2CuO_4 one can distinguish three sublattices as being of importance from the point of view of elastic modulus calculations: the sublattice of La^{3+} ions (La_{sub}), the sublattice of O^{2-} ions within La_2O_2 layers (O^{apex}_{sub}), and the sublattice of O^{2-} ions within CuO_2 layers (O^{basal}_{sub}). The internal displacements of the Cu^{2+} sublattice are not taken into account since they belong to odd irreducible representations of the space group D^{18}_{2h} while the deformation tensor components belong to even irreducible representations of the same group. Since in our work the main attention is focused on the elastic moduli c^{r}_{11} and c^{r}_{33}, it should be said that the internal displacements of all three sublattices mentioned above influence the values of c^{r}_{11}, and c^{r}_{33}, as among all of the symmetry-permitted ion displacements of these sublattices there are ones which belong to the A_g representation, to which the lattice deformations e_{xx} and e_{zz} also belong. The results obtained are collected in table 2. One can see that the neglect of any internal displacements leads to drastic changes in the elastic properties of La_2CuO_4, and the elastic modulus anisotropy σ is changed completely. On the basis of this result, we conclude that the microscopical reason for the large anisotropy of the elastic moduli lies in the internal displacements of the sublattices accompanying the crystal deformations. It can be seen from series 2, 3, and 4 that among the three sublattices of La_2CuO_4 the crucial role as regards the anisotropy is played by O^{apex}_{sub}. Furthermore, one can conclude from series 5, 6, and 7 that the main contribution to the elastic anisotropy is associated with the correlated internal displacements of O^{apex}_{sub} and La_{sub}. From table 2 it becomes obvious that the internal

Table 2. The elastic modulus anisotropy $\sigma = (c^r_{11} - c^r_{33})/(c^r_{11} + c^r_{33})$ and the elastic moduli c^r_{11} and c^r_{33} (GPa) for La_2CuO_4.

Series	1[a]	2[b]	3[c]	4[d]	5[e]	6[f]	7[g]	8[h]
σ	−9.3%	−3.9%	8.1%	−9.5%	19.7%	−3.0%	16.1%	26.5%
c^r_{11}	292	289	288	289	285	289	287	285
c^r_{33}	351	312	244	350	191	307	207	165

[a] Without taking into account any internal displacements.
[b] Taking into account only La_{sub} internal displacements.
[c] Taking into account only O^{apex}_{sub} internal displacements.
[d] Taking into account only O^{basal}_{sub} internal displacements.
[e] Taking into account La_{sub} and O^{apex}_{sub} internal displacements.
[f] Taking into account La_{sub} and O^{basal}_{sub} internal displacements.
[g] Taking into account O^{apex}_{sub} and O^{basal}_{sub} internal displacements.
[h] Taking into account internal displacements for all sublattices.

displacements of the sublattices have a much more profound influence on c^r_{33} than on c^r_{11}.

Thus, the large difference between c^r_{11} and c^r_{33} measured experimentally and calculated within the framework of the pair potential approximation and shell model is evidently a consequence of the strong anisotropic correlation between the lattice deformations e_{xx} and e_{zz} and the accompanying internal displacements of the sublattices within the La_2O_2 layers. On the other hand, CuO_2 layers do not significantly influence the elastic properties of La_2CuO_4 in the xz-plane.

3.2. The influence of pressure on elastic moduli

We have also carried out an investigation of the influence of hydrostatic pressure (up to 10 GPa) on the elastic moduli of La_2CuO_4. The hydrostatic pressure was experimentally observed to have a profound influence on the structural properties of La_2CuO_4, decreasing tilt angles of the CuO_6 octahedra and the difference between the lattice constants a and b [6]. The critical pressure P_{SPT} at which the SPT from the orthorhombic phase (space group D^{18}_{2h}) to the tetragonal phase (space group D^{17}_{4h}) must have taken place has not been achieved experimentally at low temperatures. According to our calculations [10], the value of the critical pressure P_{SPT} for La_2CuO_4 at $T = 0$ K is equal to 5 GPa.

The calculated pressure dependences of the elastic moduli of La_2CuO_4 (determined in the 'orthorhombic' coordinate system) are shown in figure 2. According to the simulation results, most of the elastic moduli—c^r_{11}, c^r_{12}, c^r_{13}, c^r_{22}, c^r_{55}, and c^r_{66}—harden upon the pressure increase. But several moduli—c^r_{33}, c^r_{23} (when $P > 3.2$ GPa), and c^r_{44} (when $P > 3.8$ GPa)—soften upon pressure increase. In our opinion, the softening of these moduli can be explained by the correlation between the lattice deformations and those internal displacements of the La^{3+} sublattice and O^{apex} sublattice which soften near the SPT. The crucial importance of the internal sublattice displacements for the softening of the elastic moduli should be emphasized again, since our calculations performed without taking into account the internal sublattice displacements predict only a very small softening of c^r_{33} and no sign of softening for c^r_{23} and c^r_{44}.

The SPT observed in La_2CuO_4 is generally understood as being a result of freezing of the zone-edge phonon mode corresponding to the almost rigid tilting of the CuO_6 octahedra. The Landau theory of phase transitions is usually used to explain this transition, with the tilt angles of the octahedra as the order parameters. In order to study the behaviour of the elastic moduli near the SPT, the Landau free energy must be generalized to include the elastic energy for a

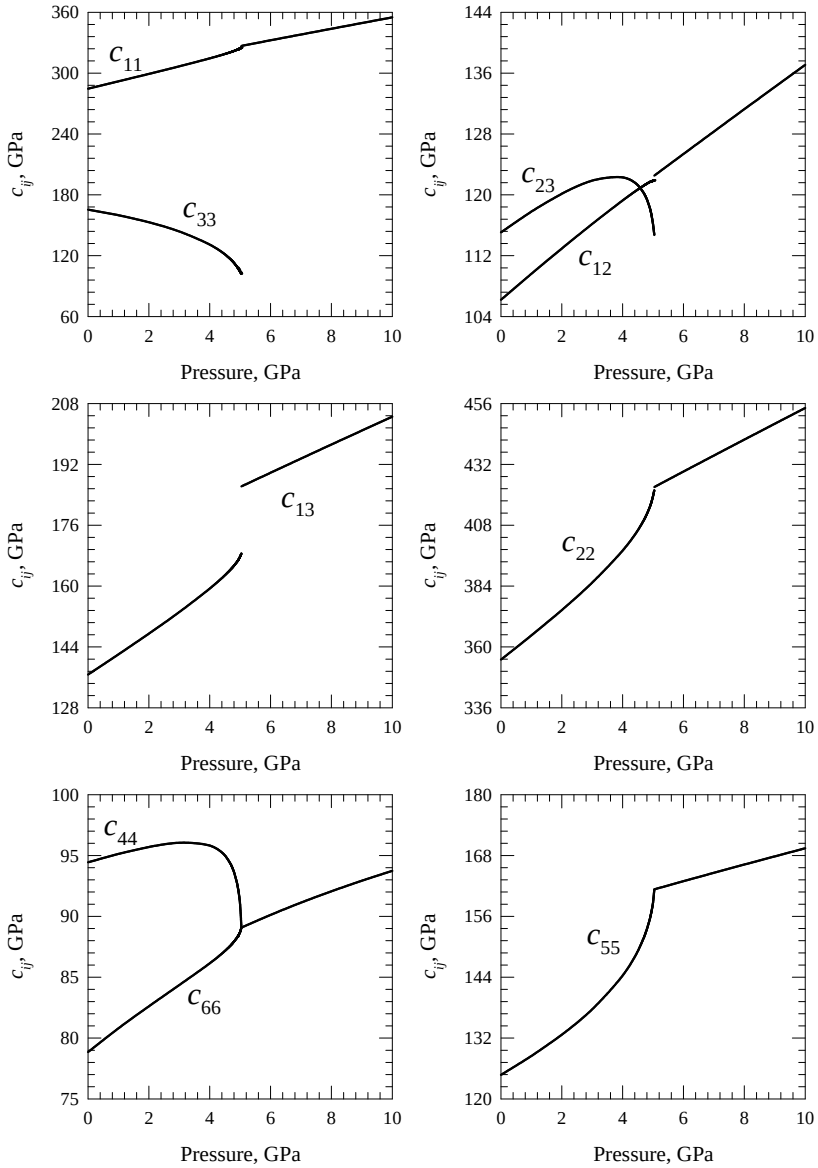

Figure 2. The pressure dependences of the elastic moduli of La_2CuO_4 calculated in the 'orthorhombic' coordinate system (see the text).

tetragonal phase and the proper coupling of the strain and order parameter [15]. Summarizing the results given in [15] and taking into account the difference between the coordinate systems used in [15] and in our work, it should be said that the behaviour of the elastic moduli near the SPT must be as follows: c^{r}_{44}, c^{r}_{55}, and c^{r}_{66} are unaffected by the transition, while c^{r}_{11}, c^{r}_{12}, c^{r}_{13}, c^{r}_{22}, c^{r}_{23}, c^{r}_{33} must show a steplike jump. The results of our calculations given in figure 2 and in table 3 are seen to follow the prediction of the Landau theory. But it should be noticed that near the SPT (in the orthorhombic phase) the errors in the structural parameter calculations become large, leading to the large errors in the calculated elastic moduli.

Table 3. Differences between the elastic moduli of La_2CuO_4 in the tetragonal phase ($P > P_{SPT}$) and in the orthorhombic phase ($P < P_{SPT}$) near the structural phase transition ($\Delta c_{ij} = c_{ij}(P > P_{SPT}) - c_{ij}(P < P_{SPT})$) (GPa).

Δc^r_{11}	Δc^r_{12}	Δc^r_{13}	Δc^r_{22}	Δc^r_{23}	Δc^r_{33}	Δc^r_{44}	Δc^r_{55}	Δc^r_{66}
2	1	18	1	8	225	0	0	0

As mentioned in the introduction, some peculiarities of the temperature dependence of elastic moduli near the SPT are measured experimentally. A striking anomalous decrease of Young's modulus near the SPT was observed for $La_{2-x}Sr_xCuO_4$ [16, 17]. An analogous decrease was measured for c^t_{66} for $La_{1.86}Sr_{0.14}CuO_4$ [18]. A careful study of the elastic moduli [2] (except c^t_{13}) for La_2CuO_4 and $La_{2-x}Sr_xCuO_4$ showed that c^t_{11}, c^t_{12}, and c^t_{66} decreased as $1/(T - T_{SPT})$ for $T > T_{SPT}$, c^t_{33} showed a steplike drop, and c^t_{44} was unaffected by the transition (T_{SPT} is the temperature at which the temperature-induced SPT takes place).

A few theoretical models have been suggested to explain the elastic softening near the SPT. Migliori *et al* [18] attempted to explain the c^t_{66}-softening by order parameter fluctuations, but the source of the large temperature range (about 100 K) for the c^t_{66}-softening was not understood. Sarrao *et al* [2] pointed to the dopant-induced symmetry breaking as a possible cause for the elastic softening, but within this model it was not possible to explain the observed softening in stoichiometric La_2CuO_4. In order to suggest a model suitable for both stoichiometric and non-stoichiometric La_2CuO_4, Sarrao *et al* [2] speculated that the in-plane distortion of the CuO_6 octahedra which is usually neglected might be significant enough to explain the elastic properties. Kwon *et al* [19] accounted for the elastic softening of c^t_{66} by electronic redistribution between the strain-split itinerant p bands and also between the strain-shifted energy pockets, but they did not try to explain the elastic softening of c^t_{11} and c^t_{12}.

The behaviour of the elastic moduli of La_2CuO_4 under pressure near the SPT has not been measured yet, although it would be very useful to know whether the peculiarities of the elastic modulus behaviour near the SPT mentioned above can be observed for a SPT induced by the pressure or not. The calculated pressure dependences of the elastic moduli of La_2CuO_4 (determined in the 'tetragonal' coordinate system) are shown in figure 3. The results obtained are in good agreement with predictions of the Landau theory [15]. Only one modulus—c^t_{44}—is unaffected by the phase transition, and other moduli must show discontinuities at the point of the phase transition. According to the results obtained, we do not observe the softening of c^t_{11}, c^t_{12}, and c^t_{66} measured experimentally near the SPT induced by the temperature—although we do predict the large steplike drop of these moduli (see figure 3) near the SPT induced by the pressure. We are inclined to explain the disagreement between the experimental data mentioned above and our predictions by the underlying difference between the mechanism of the SPTs in La_2CuO_4 induced by temperature and induced by pressure. We do not believe that the problem is that we have neglected the order parameter fluctuations near the phase transition. Anyway, we think that the in-plane distortion of CuO_6 octahedra, fully taken into consideration in our calculations, cannot account for the elastic modulus softening as had been suggested by Sarrao *et al* [2].

The experimentally revealed softening of $(c^t_{11} - c^t_{12})/2$ starting from about 50 K in $La_{1.86}Sr_{0.14}CuO_4$ [20] is also worth mentioning. Analogous behaviour of $(c^t_{11} - c^t_{12})/2$ is predicted by our calculations under pressure (see figure 3). Such behaviour of these elastic moduli can be interpreted as a consequence of the structural instability of the orthorhombic phase La_2CuO_4 and the possibility of the transition to the low-temperature tetragonal phase (space group D^{16}_{4h}) observed experimentally in $La_{2-x}Ba_xCuO_4$ [21] and predicted from the total-energy calculations [22].

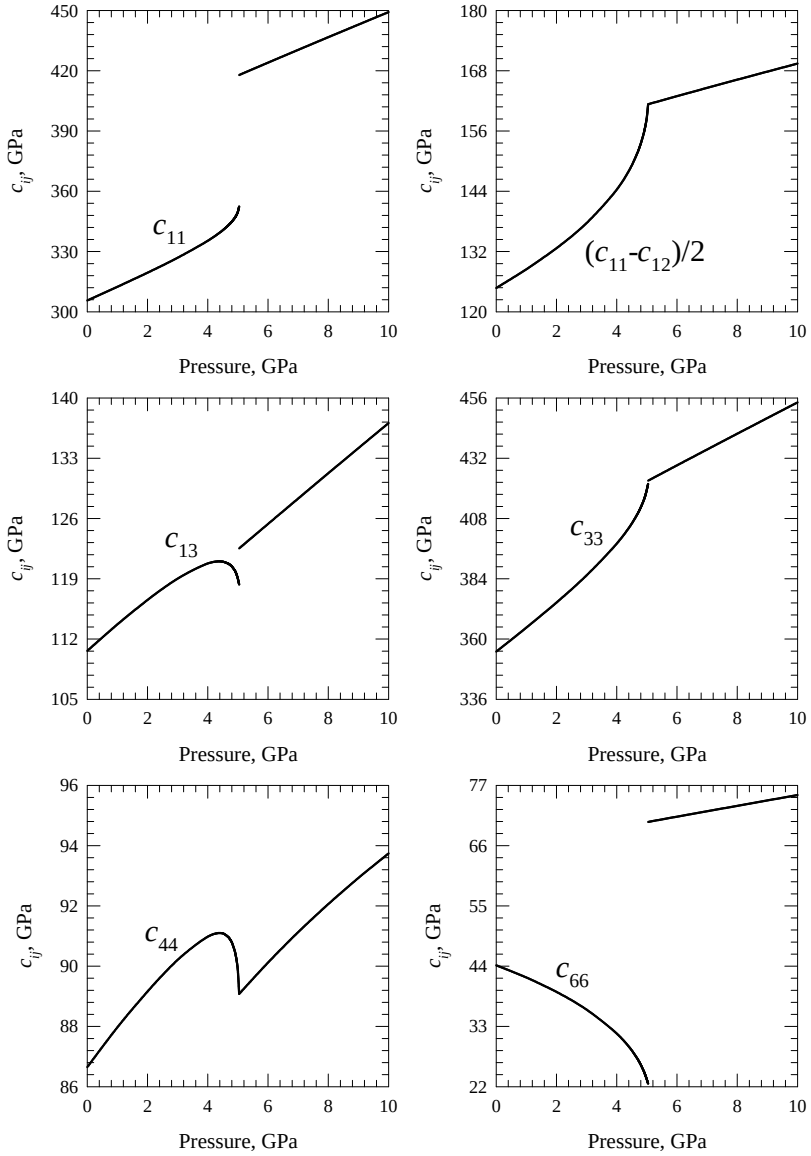

Figure 3. The pressure dependences of the elastic moduli of La_2CuO_4 calculated in the 'tetragonal' coordinate system (see the text).

4. Conclusions

In summary, we have presented a determination of the complete set of elastic moduli of La_2CuO_4 within the framework of the pair potential approximation and the shell model including the Jahn–Teller contribution to the crystal energy. We have shown that the internal displacements of the sublattices within the La_2O_2 layers accompanying the lattice deformations have a profound influence on the elastic properties of La_2CuO_4, leading to the giant anisotropy of the elastic moduli in the orthorhombic phase region and the softening of some elastic moduli near the tetragonal–orthorhombic structural phase transition.

Acknowledgment

This work was supported by the Russian Foundation for Basic Research (Grant No 96-03-32130a).

References

[1] Migliori A, Visscher W V, Brown S E, Fisk Z, Cheong S W, Alten B, Ahrens E T, Kubat-Martin K A, Maynard J D, Huang Y, Kirk D R, Gillis K A, Kim H K and Chan M H W 1990 *Phys. Rev.* B **41** 2098
[2] Sarrao J L, Mandrus D, Migliori A, Fisk Z, Tanaka I, Kojima H, Canfield P C and Kodali P D 1994 *Phys. Rev.* B **50** 13 125
[3] Fil V D, Bezugly E V, Burma N G, Kolobov I G, Vitebsky I M, Knigavko A N, Lavrinenko N M, Barilo S N, Zhigunov D I and Soshnikov L E 1994 *Physica* C **235–240** 1215
[4] Allan N L and Mackrodt W C 1988 *Phil. Mag.* A **58** 555
[5] Allan N L and Mackrodt W C 1990 *J. Chem. Soc. Faraday Trans.* **86** 1227
[6] Takahashi H, Shaked H, Hunter B A, Radaelli P G, Hitterman R L, Hinks D G and Jorgensen J D 1994 *Phys. Rev.* B **50** 3221
[7] Nikiforov A E, Shashkin S Yu, Levitan M L and Agamaluan T H 1983 *Phys. Status Solidi* b **118** 419
[8] Shashkin S Yu and Nikiforov A E 1987 *Fiz. Tverd. Tela* **29** 3133
[9] Mitrofanov V Ya, Nikiforov A E and Shashkin S Yu 1997 *Solid State Commun.* **104** 499
[10] Nikiforov A E, Shashkin S Yu and Zaharov A Yu 1999 *Phys. Solid State* **41** 1096
[11] Nikiforov A E, Shashkin S Yu and Zaharov A Yu 1997 *Z. Phys. Chem.* **201** 597
[12] Piveteau B and Noguera C 1991 *Phys. Rev.* B **43** 493
[13] Nikiforov A E and Shashkin S Yu 1995 *Phys. Solid State* **37** 719
[14] Nikiforov A E, Shashkin S Yu and Krotkii A I 1980 *Phys. Status Solidi* b **97** 475
[15] Ting W, Fossheim K and Lagreid T 1990 *Solid State Commun.* **75** 727
[16] Lee W K, Lew M and Nowick A S 1990 *Phys. Rev.* B **41** 149
[17] Slaski M, Steinsvoll O, Samuelsen E J, Nes O M, Ting W, Lagreid T, Fossheim K and Hidaka Y 1991 *Solid State Commun.* **77** 945
[18] Migliori A, Visscher W V, Wong S, Brown S E, Tanaka I, Kojima H and Allen P B 1990 *Phys. Rev. Lett.* **64** 2458
[19] Kwon T S, Park J C, Nahm K, Noh H S and Kim C K 1994 *Phys. Rev.* B **49** 4388
[20] Nohara M, Suzuki Y and Fujita T 1993 *Phys. Rev. Lett.* **70** 3447
[21] Axe J D, Moudden A H, Hohlwein D, Cox D E, Mohanty K M, Moodenbaugh A R and Xu Y 1989 *Phys. Rev. Lett.* **62** 2751
[22] Pickett W E, Cohen R E and Krakauer H 1991 *Phys. Rev. Lett.* **67** 228