ELSEVIER

Physica C 249 (1995) 117–122

PHYSICA C

Gap anisotropy and van Hove singularities in high-T_c superconductors

J. Bouvier *, J. Bok

Laboratoire de Physique du Solide UPR 5 CNRS, ESPCI, 10, rue Vauquelin, 75231 Paris cedex 05, France

Received 19 April 1995

Abstract

We compute the superconducting gap Δ_k using a simple band structure of the CuO_2 planes in the high-T_c materials. We suppose that for maximum T_c, the van Hove singularities lie close to the Fermi level as is confirmed by many photoemission experiments. We use a electron–phonon interaction with weak screening; we find a strong gap anisotropy. For Bi 2212, Δ is maximum along the 001 and 010 directions with values of the order of 22 meV and minimum along 011 with a value of 6 meV. These values are in agreement with experiments.

1. Introduction

Many recent experiments of angle-resolved photoemission spectroscopy (ARPES) have confirmed the existence of saddle points (vHS) at the Fermi level in five different copper oxide compounds by three different groups, in Stanford [1], in Argonne [2] and in Wisconsin [3]. These observations have been made in the following compounds: $Bi_2Sr_2CuO_6$ (Bi 2201), $Bi_2Sr_2CaCu_2O_8$ (Bi 2212), $YBa_2Cu_3O_7$ (Y123), $YBa_2Cu_4O_8$ (Y124) and $Nd_{2-x}Ce_xCuO_{4+\delta}$ (NCCO). These experiments establish a general feature: in very high-T_c superconductors cuprates ($T_c \sim$ 90 K) van Hove singularities are present near the Fermi level. This is probably not purely accidental and we think that any theoretical model must take into account these experimental facts. The origin of a high T_c in the cuprates is still controversial and the role of these singularities in the mechanism of high-T_c superconductivity is not yet established, but we want to stress that the model of 2D itinerant electrons in the presence of vH singularities in the band structure has already explained a certain number of experimental facts, i.e. high T_c's, anomalous isotope effect [4], marginal Fermi-liquid effects [5] and the very small values of the coherence length [6]. It has also been shown that the singularity is in the middle of a wide band and that in these circumstances, the Coulomb repulsion μ is renormalized and μ is replaced by a smaller number; the effective electron–phonon coupling is $\lambda_{eff} = \lambda - \mu^*$ and remains positive [7]. More recently, we have interpreted, using this same model, the results of NMR experiments of ^7Li in YBCO 123, where the Knight shift ΔK obeys a logarithmic law versus the inverse of the temperature, $\Delta K \approx \ln 1/T$ [8,9].

The purpose of this paper is to show by a detailed calculation that the 2D band structure of the cuprates, with a vHS at the Fermi level can explain the

* Corresponding author.

0921-4534/95/$09.50 © 1995 Elsevier Science B.V. All rights reserved
SSDI 0921-4534(95)00294-4

observed gap anisotropy, in the case of a weak screening of the electron–phonon interaction. Such a prediction has been made by Abrikosov [10] on the basis of an extended saddle-point singularity in the electron energy spectrum, lying close to the Fermi level, but he did not give any quantitative calculation of the gap. We show that, without adjustable parameter, we find the measured values of the gap in various crystallographic directions of the cuprate compounds.

2. Electron band structure and electron–phonon interaction

The simplest band structure we can take for a square lattice of dimension a is

$$\varepsilon_k = -2t(\cos k_x a + \cos k_y a), \tag{1}$$

where t is a transfer integral between nearest neighbours, k_x and k_y the components of the wave vector along the 1, 0 and 0, 1 axis. This gives a square Fermi surface, and the vHS corresponds, in this approximation, to half filling (Fig. 1). Also this leads to the logarithmic density of state near a saddle point [4]:

$$n(\varepsilon) = \frac{N}{\pi^2 D} \ln \frac{D}{|\varepsilon|}, \tag{2}$$

where D is the width of the vHS, in the case of the CuO_2 planes of the cuprates $N = 8$ per Cu atom, and with formula (1) $D = 16t$.

We have taken a classical electron–electron interaction potential $V_{kk'}$ between two electron states of wave vector $\boldsymbol{k}$ and $\boldsymbol{k}'$, respectively, via electron–phonon coupling. From BCS theory [11] this matrix element may be written

$$V_{kk'} = \frac{|g_q|^2}{q^2 + q_0^2} \frac{(\hbar\omega_q)^2}{\varepsilon_{kk'}^2 - (\hbar\omega_q)^2}, \tag{3}$$

where $\boldsymbol{k}' - \boldsymbol{k} = \boldsymbol{q}$ is the phonon wave vector, $|g_q|^2$ is the square of an electron–phonon interaction matrix element, $\varepsilon_{k'k} = \varepsilon_{k'} - \varepsilon_k$ is the electron energy difference and ω_q is the phonon frequency; q_0 is a screening vector, q_0^{-1} is the screening length. In the cuprates, the important phonons are the optical ones, so we take the usual approximation, $\omega_q = \omega_0 =$ constant.

The interaction between electrons is attractive $V_{kk'} < 0$, as long as the energy variation $|\varepsilon_{kk'}|$ is less than $\hbar\omega_0$. In most models the last term of Eq. (3) is taken as -1. In our case, this is even more justified since the important contributions to Δ will come from states of vector $\boldsymbol{k}$ near the saddle points taken on the Fermi surface, that is for energy differences close to zero. Abrikosov [10] has done the same approximation.

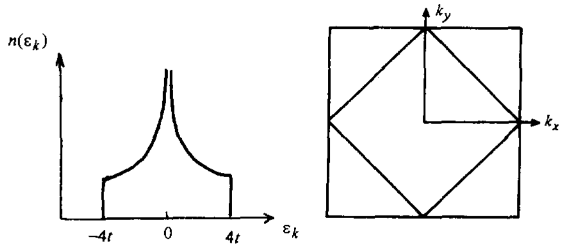

Fig. 1. Density of states $n(\varepsilon)$ and Fermi surface for a band given by Eq. (1).

3. Anisotropic BCS gap equation

We first solve the problem at zero temperature, $T = 0$ K, in which case the BCS equation giving the gap Δ_k reads

$$\Delta_k = -\frac{1}{2} \sum_{k'} \frac{V_{kk'} \Delta_{k'}}{\sqrt{\varepsilon_{k'}^2 + \Delta_{k'}^2}}, \tag{4}$$

with

$$V_{kk'} = \frac{-|g_q|^2}{q^2 + q_0^2} < 0$$

and

$$-\hbar\omega_0 < \varepsilon_{kk'} < +\hbar\omega_0.$$

Eq. (4) may be rewritten, replacing the sum by an integral:

$$\Delta_k = -\frac{1}{2} \int\int \frac{V_{kk'} \Delta_{k'}}{\sqrt{\varepsilon_{k'}^2 + \Delta_{k'}^2}} \, \mathrm{d}k'_x \, \mathrm{d}k'_y. \tag{5}$$

It is useful to introduce tangential and normal coordinates $\mathrm{d}k_t$ and $\mathrm{d}k_\perp$. $\mathrm{d}k_t$ is tangential to the constant energy curve Γ and $\mathrm{d}k_\perp$ is normal to this curve. We obtain

$$\mathrm{d}k_t\,\mathrm{d}k_\perp = \frac{\mathrm{d}k_\perp}{\mathrm{d}\varepsilon}\,\mathrm{d}\varepsilon\,\mathrm{d}k_t \tag{6a}$$

but

$$\hbar\,|v_k| = \frac{\mathrm{d}\varepsilon}{\mathrm{d}k_\perp}$$

so that

$$\hbar\frac{\mathrm{d}k_\perp}{\mathrm{d}\varepsilon} = \frac{1}{|v_k|} = \frac{\hbar}{2ta\sqrt{\sin^2 k_x a + \sin^2 k_y a}}; \tag{6b}$$

for $\varepsilon = cte$ and Eq. (1) we find

$$\mathrm{d}k_t = \frac{\sqrt{2}}{2}\frac{\mathrm{d}k_x}{\sin k_y a}\sqrt{\sin^2 k_x a + \sin^2 k_y a} \tag{6c}$$

and finally

$$\sin k_y a = \left[1 - \left(\frac{\varepsilon}{2t} - \cos k_x a\right)^2\right]^{1/2} \tag{6d}$$

by combining Eqs. (4), (5) and (6) we obtain for the gap

$$\Delta_k = \lambda_{\mathrm{eff}}\int_0^{\hbar\omega_D}\mathrm{d}\varepsilon\int_\Gamma \frac{\mathrm{d}k'_x a}{\left[1 - ((\varepsilon/2t) - \cos k'_x a)^2\right]^{1/2}} \times \frac{(q_0 a)^2}{(qa)^2 + (q_0 a)^2}\frac{\Delta_{k'}}{\sqrt{\varepsilon_{k'}^2 + \Delta_{k'}^2}}. \tag{7}$$

λ_{eff} is a numerical parameter with no dimension; it includes an effective interaction V and an average density of states $N/\pi^2 t$.

Eq. (7) is an integral equation which is not easy to solve. But we know from symmetry considerations, that Δ_k will have a four-fold symmetry; we can expand it in a Fourier series of the form

$$\Delta_k = \Delta_0 + \Delta_1 \cos 4\Phi + \dots, \tag{8}$$

where Φ is the angle between $\boldsymbol{k}_x$ and $\boldsymbol{k}$.

We solve Eq. (7) by iteration, we first replace in the integral Δ_k by its average value Δ_0, then compute Δ_1, introduce Δ_1 in the integral, etc.

We shall present here only the first two steps: calculation of Δ_0 and Δ_1; a detailed calculation will be given in a following paper. To compute Δ_0 and Δ_1, we use the following procedure. Let us first take $\boldsymbol{ka}$ at point A $(0, \pi)$ (see Fig. 2). We have

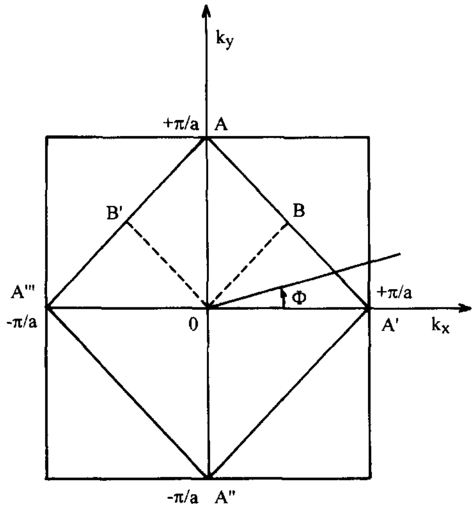

Fig. 2. Square Fermi surface and the interesting points (A, A', B, B').

$$\Delta_A = \Delta_{\mathrm{maximum}} = \Delta_0 + \Delta_1;$$

then at point B $(\pi/2, \pi/2)$

$$\Delta_B = \Delta_{\mathrm{minimum}} = \Delta_0 - \Delta_1.$$

For Δ_A, the vector $\boldsymbol{k}'$ must circumscribe the whole contour AA'A''A''' but we see that this is twice the contour AA'A''. For large values of q the integral is very small, so in a first approximation, we neglect large q values and integrate only from A to B and multiply by two. We thus obtain

$$\Delta_{\max} = \lambda_{\mathrm{eff}}\int_0^{u_{\max}}\frac{\Delta_0}{\sqrt{u^2 + u_0^2}} I_A(u)\,\mathrm{d}u \tag{9a}$$

with

$$I_A(u) = \int_0^{x'_0}\frac{\mathrm{d}x'}{\left[1 - (u - \cos x')^2\right]^{1/2}} \times \frac{2(q_0 a)^2}{2x'^2 + (q_0 a)^2}, \tag{9b}$$

$$\Delta_{\min} = \lambda_{\mathrm{eff}}\int_0^{u_{\max}}\frac{\Delta_0}{\sqrt{u^2 + u_0^2}} I_B(u)\,\mathrm{d}u, \tag{10a}$$

with

$$I_{\mathrm{B}}(u)=\int_0^{x'_0}\frac{\mathrm{d}x'}{\left[1-(u-\cos x')^2\right]^{1/2}}\times\frac{2(q_0a)^2}{2\left(x'-\frac{\pi}{2}\right)^2+(q_0a)^2}\tag{10b}$$

where $x'=k'_xa$, $x'_0=\arccos(u/2)$, $u=\varepsilon/2t$, $u_0=\Delta_0/2t$, and $u_{\max}=\hbar\omega_0/2t$.

λ_{eff} in these integrals is the isotropic part of the electron–phonon interaction; it is of the order of 0.5. These results allow one to make a first qualitative comparison between $\Delta_{\max}$ and $\Delta_{\min}$. In the integrals $I_{\mathrm{A}}(u)$ and $I_{\mathrm{B}}(u)$, the dominant contribution is that for which the velocity v_k goes to zero, i.e. the limit $x'\to 0$. We see that the multiplicative factor is 1 ($q=0$) in the case of I_{A} and of the order of $\frac{1}{6}$ to $\frac{1}{7}$, in the other case, $q=\pi/2a$. We see that the physical origin of the gap anisotropy comes from the fact that in certain directions there are saddle points where $|v_k|\to 0$ and Δ_k is large and other directions for which $|v_k|$ is always finite and Δ_k is smaller. At finite temperature T, Eqs. (9) and (10) are replaced by Eq. (11):

$$\Delta_{(\max,\min)}=\lambda_{\mathrm{eff}}\int_0^{u_{\max}}\frac{\Delta_0(T)}{\sqrt{u^2+u_0^2(T)}}I_{(\mathrm{A,B})}(u)\times\tanh\left(\frac{\sqrt{u^2+u_0^2(T)}}{k_{\mathrm{B}}T/t}\right)\mathrm{d}u.\tag{11}$$

4. Results and discussion

We evaluate numerically Δ_{A} and Δ_{B} using the two integral equations (9) and (10). To do that we have to choose two parameters, the phonon frequency ω_0 and the transfer integral t. We could consider them as adjustable parameters to find the values of $\Delta_{\max}=20\pm 3$ meV, $\Delta_{\min}=5\pm 5$ meV and $T_{\mathrm{c}}=86\pm 2$ K observed experimentally [2,12] for Bi 2212. For $YBa_2Cu_3O_{7-x}$ or $Y_bBa_2Cu_3O_{7-x}$ single crystals, tunneling effects show a two-gap structure [13]; with values for the maximum gap

Table 1
Several sets of parameters for the calculated gap, for $\hbar\omega_0=60$ meV and with two choices for the integral transfer.
(a) $t=0.20$ eV

	$\hbar\omega_0=60$ meV	$t=0.20$ eV				
q_0a	λ_{eff}	Δ_{A} (meV)	Δ_{B} (meV)	Δ_0 (meV)	T_{c} (K)	$2\Delta_0/k_{\mathrm{B}}T_{\mathrm{c}}$
0.18	0.57	22	6	14	88.5	3.7
0.12	0.785	22	5	13.5	84.4	3.7
0.13	0.37	20	7	13.5	84.5	3.7
0.08	1.10	22	4	13	81.5	3.7
0.23	0.45	20	6	13	82	3.7
0.05	1.67	22	3	12.5	78.5	3.7
0.15	0.62	20	5	12.5	78.5	3.7

(b) $t=0.25$ eV

	$\hbar\omega_0=60$ meV	$t=0.25$ eV				
q_0a	λ_{eff}	Δ_{A} (meV)	Δ_{B} (meV)	Δ_0 (meV)	T_{c} (K)	$2\Delta_0/k_{\mathrm{B}}T_{\mathrm{c}}$
0.19	0.50	22	6	14	87.5	3.7
0.13	0.67	22	5	13.5	84.5	3.7
0.35	0.31	20	7	13.5	85	3.7
0.085	0.94	22	4	13	81.5	3.7
0.25	0.39	20	6	13	82	3.7
0.045	1.60	22	3	12.5	77.5	3.7
0.165	0.53	20	5	12.5	78.5	3.7

between 26 and 30 meV and for the minimum gap between 0.5 and 11 meV.

But on the contrary we have taken ω_0 and t from experimental measurements and we show that we obtain correct values for Δ and T_c. So our model contains no adjustable parameter, but leads to a low value of $q_0 a$; we discuss this point in the last part of this work.

(1) Choice of t. t has been estimated theoretically by band-structure calculations [14]. We prefer experimental determinations. From ARPES measurements t is estimated to be between 0.20 and 0.25 eV [15,16].

(2) Choice of $\hbar\omega_0$. Many authors have determined several mode frequencies of phonons which should play a major role in the superconductivity mechanism. The modes involved are mainly the breathing modes of the $Cu-O_6$ complex, with an important implication for the apical oxygen. Here we cite these modes for the most known HTSC's. For example in La_2CuO_4 the oxygen breathing modes frequencies are in the range 400–640 cm^{-1} [17]; and for $YBa_2Cu_3O_7$ in the range 340–610 cm^{-1} [18]. In this compound the 340 cm^{-1} mode frequency seems to play a particular role [19]. Then in $Bi_2Sr_2CaCu_2O_8$ the mode frequencies assigned to the axial phonon ($\parallel c$) and involved in an electron–phonon interaction are 445 cm^{-1} and 594 cm^{-1} [20]; other phonons seem to play an important role, like the 587.2 cm^{-1} mode frequency due to the phonons in the Bi–O plane and the 645.2 cm^{-1} associated with those in the Cu–O plane [21].

Moreover, we know that the mode frequencies are screened by the carriers and renormalized in the interaction. Therefore, we have chosen an arbitrary average phonon of 480 cm^{-1} or 60 meV, which is in the range 335–640 cm^{-1}, for $\hbar\omega_0$ in our calculations.

We have tried other values for $\hbar\omega_0$ of the same order of magnitude, and we have observed no significant change in the results. This observation confirms the anomalous isotope effect already observed and explained in these materials [4].

The numerical results are presented in Table 1. We see that there is a good agreement between our computation and the experimental values. The set of parameters ($t = 0.20$ eV, $\hbar\omega_0 = 60$ meV) has been chosen in Fig. 3, where we plot the gap $\Delta(\Phi)$ as a function of the angular coordinate Φ, using the first two terms in the Fourier expansion

$$\Delta(\Phi) = \Delta_0 + \Delta_1 \cos 4\Phi,$$

with $\Delta_0 = 14$ meV and $\Delta_1 = 8$ meV, for $T_c = 88.5$ K (solid line); and with $\Delta_0 = 12.5$ meV and $\Delta_1 = 7.5$ meV, for $T_c = 78.5$ K (dashed line).

The black dots represent the experimental values for several samples as published by Shen et al. [12], and Ding et al. [2]. The agreement seems very good

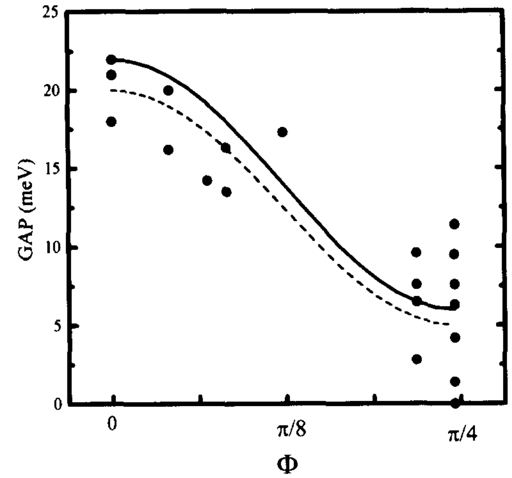

Fig. 3. Angle-dependent calculated gap $\Delta(\Phi)$ for two sets of parameters: $\Delta_0 = 14$ meV, $\Delta_1 = 8$ meV, for $T_c = 88.5$ K (solid line), and $\Delta_0 = 12.5$ meV, $\Delta_1 = 7.5$ meV, for $T_c = 78.5$ K (dashed line); experimental values from Refs. [2] and [12] (black dots).

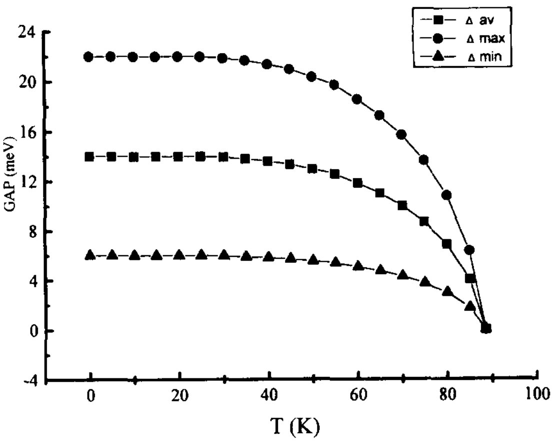

Fig. 4. Temperature-dependent maximum (full circle), average (full square) and minimum (full triangle) gaps at $T = 0$ K, for $\Delta_{av} = \Delta_0 = 14$ meV, $\Delta_1 = 8$ meV, and for a T_c of 88.5 K.

considering the experimental precision of ARPES measurements and the approximations made in our theory. Fig. 4 gives the variation of the average gap Δ_0, the maximum gap Δ_{max} (22 meV at $T = 0$ K), the minimum gap Δ_{min} (6 meV at $T = 0$ K), with the temperature T. Here we obtain a T_c value of 88.5 K, close to the experimental one. We find that $2\Delta_0/k_B T_c = 3.7$ (very close to the BCS value), $2\Delta_{max}/k_B T_c = 5.8$ and $2\Delta_{min}/k_B T_c = 1.6$. This perhaps explains the different values observed in various experiments.

5. Conclusion

We have calculated the gap anisotropy in the high-T_c cuprates using an itinerant electron model in a two-dimensional periodic potential leading to van Hove singularities. We assume that the vHS lies close to the Fermi level and we use a weakly screened electron–phonon interaction potential.

With that model, we predict for Bi 2212 for example, a minimum gap of 6 ± 2 meV and a maximum gap of 20 ± 3 meV. We use only experimentally determined parameters in our calculation, except a rather low isotropic value of $q_0 a$ that is essential to obtain a large anisotropy. The values obtained theoretically agree very well with the values determined by various experiments, ARPES and tunnel effect. We thus obtain an "extended s wave" gap and not a d wave pair function. The order parameter is never negative in our model. Abrikosov [22] has shown, however, that if a short-range repulsive interaction (which can represent either some part of the Hubbard repulsion at the copper sites or the interaction mediated by spin fluctuations) is added, then the order parameter can vary in sign and become negative at points of the Fermi surface distant from the singularity.

Such an approach may reconcile all the observations leading sometimes to s wave and other times to d wave symmetry of the order parameter.

References

[1] Z.X. Shen, W.E. Spicer, D.M. King, D.S. Dessau and B.O. Wells, Science 267 (1995) 343.

[2] H. Ding, J.C. Campuzano, K. Gofron, C. Gu, R. Liu, B.W. Veal and G. Jennings, Phys. Rev. B 50 (1994) 1333.

[3] J. Ma, C. Quitmann, R.J. Kelley, P. Alméras, H. Berger, G. Margaritondoni and M. Onellion, Phys. Rev. B 51 (1995) 3832.

[4] J. Labbé and J. Bok, Europhys. Lett. 3 (1987) 1225.

[5] D.M. Newns, C.C. Tsuei, P.C. Pattnaik and C.L. Kane, Comm. Cond. Matt. Phys. 15 (1992) 273.

[6] J. Bok and L. Force, Physica C 185–189 (1991) 1449.

[7] L. Force and J. Bok, Solid Stat. Commun. 85 (1993) 975.

[8] J. Bok and J. Bouvier, Physica C 244 (1995) 357.

[9] K. Sauv, M. Nicolas and J. Conard, Physica C 223 (1994) 145.

[10] A.A. Abrikosov, Physica C 222 (1994) 191.

[11] J. Bardeen, L.N. Cooper and J.R. Schrieffer, Phys. Rev. 108 (1957) 1175.

[12] Z.X. Shen, D.S. Dessau, B.O. Wells, D.M. King, W.E. Spicer, A.J. Arko, D. Marshall, L.W. Lombardo, A. Kapitulnik, P. Dickinson, S. Doniach, J. DiCarlo, A.G. Loeser and C.H. Park, Phys. Rev. Lett. 70 (1993) 1553.

[13] B.A. Aminov, M.A. Hein, G. Muller, H. Piel and D. Wehler, J. Supercond. 7 (1994) 361.

[14] H. Krakauer, W.E. Pickett and R.E. Cohen, Phys. Rev. B 47 (1993) 1002.

[15] D.S. Dessau, Z.X. Shen, D.M. King, D.S. Marshall, L.W. Lombardo, P.H. Dickinson, J. DiCarlo, C.H. Park, A.G. Loeser, A. Kapitulnik and W.E. Spicer, Phys. Rev. Lett. 71 (1993) 2781.

[16] A. Bansil, M. Linches, K. Gofron and J.C. Campuzano, J. Phys. Chem. Solids 54 (1993) 1185.

[17] C. Thomsen and M. Cardona, in: Physical Properties of High-Temperature Superconductors, ed. D.M. Ginsberg (World Scientific, Singapore, 1989) p. 409.

[18] I.I. Mazin et al., in: Lattice Effects in High-T_c Superconductors, eds. Y. Bar Yam, T. Egami, J. Mustre-de-Leon and A.R. Bishop (World Scientific, Singapore, 1992);
C. Thomsen, M. Cardona, B. Friedl, C.O. Rodringuez, I.I. Mazin and O.K. Andersen, Solid State Commun. 75 (1990) 219.

[19] K.F. McCarty, J.Z. Liu, R.N. Shelton and R.N. Radousky, Phys. Rev. B 41 (1990) 8792;
L.V. Gaparov, V.D. Kulubovskii, O.V. Misochka and V.B. Timofeev, Physica C 157 (1989) 341;
R.M. Macfarlane, H. Rosen and H. Seki, Solid State Commun. 63 (1987) 831.

[20] G. Ruani, C. Taliani, R. Zambeni, V.M. Burlakov and V.N. Denisov, Solid State Commun. 78 (1991) 979.

[21] H.C. Gupta, Physica C 157 (1989) 257.

[22] A.A. Abrikosov, Physica C 244 (1995) 243.