Phys. Status Solidi B **253**, No. 3, 486–493 (2016) / **DOI** 10.1002/pssb.201552465

physica status solidi b
www.pss-b.com
basic solid state physics

Effect of external pressure on the normal and superconducting properties of high-T_c cuprates

K. A. Sidorov[1,2], V. A. Gavrichkov[1,2], S. V. Nikolaev[*,1,2], Z. V. Pchelkina[3], and S. G. Ovchinnikov[1,2]

[1] L.V. Kirensky Institute of Physics, SB RAS, 660036 Krasnoyarsk, Russia
[2] Siberian Federal University, 660041 Krasnoyarsk, Russia
[3] Institute of Metal Physics, UB RAS, 620219 Ekaterinburg, Russia

Received 19 July 2015, revised 16 September 2015, accepted 9 October 2015
Published online 6 November 2015

Keywords cuprates, electronic structure, Fermi surface, Lifshitz transitions, strongly correlated electrons, superconducting properties

[*] Corresponding author: e-mail svinikolaev@sfu-kras.ru, Phone: +7-391-2062117, Fax: +7-391-2912967

The pressure effects on the normal state electronic structure, the superexchange interaction, and the critical temperature of d-type superconductivity mediated by magnetic pairing have been studied within the multielectron hybrid scheme LDA+GTB that takes into account electron correlations in CuO_2 planes. We have found the changes of the multiband p–d model parameters at 3% compression of different symmetry: (i) hydrostatic, (ii) along the c-axis, and (iii) in a–b plane. We have studied the changes of the Fermi surface under external pressure for different hole doping concentration x. In general, this effect is too small except two critical concentrations $x_{c1} \approx 0.15$ and $x_{c2} = 0.24$ where the Lifshitz transitions occur with the change of the Fermi surface topology. In the vicinity of the critical concentration, we have found the giant change of the Fermi surface area up to 100% related to the pressure-induced Lifshitz transition. The effects of pressure on the antiferromagnetic coupling J and the mean-field value of T_c are obtained in a good agreement to experimental data.

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1 Introduction In spite of a remarkable progress in physics of high-T_c superconducting cuprates, our understanding of the unusual normal state in a wide doping and temperature range as well as the origin of superconducting pairing is far from being complete. In this situation, experimental study under external pressure P is exceptionally valuable as an *in situ* way to probe the electronic structure and the temperature T_c response [1]. The maximal value of T_c for cuprates has been achieved in the optimally doped three-layer compound $HgBa_2Ca_2Cu_3O_{8+y}$ (Hg-1223) with $T_c \approx 134$ K at ambient pressure [2], reaching a value near 160 K at hydrostatic pressure 30 GPa [3]. A combination of the hydrostatic and uniaxial pressures results in a separation of different structural effects on the electronic structure parameters and the hydrostatic dT_c/dP and uniaxial pressure derivatives dT_c/dP_i ($i = a, b, c$) [4–6].

Empirically, several correlations of T_c and structural parameter changes under pressure have been revealed [1, 7, 8]. Two key structural quantities have been suggested: the CuO_4 placket area (or the bond length l between copper and in-plane oxygen), and the Cu-apical oxygen distance h_o. The role of the apical oxygen on the electronic properties has been addressed in several theoretical works [9–13] as the effect of interlayer coupling in the phonon-mediated BCS-like theory [14].

Recently, the time-frequency-resolved spectroscopy [15] has revealed a dominant role of the nonretarding electronic mechanism of pairing. The antiferromagnetic nearest neighbor exchange interaction J is one of the candidates for the electronic pairing. The experimental studies [1, 16, 17] have found $dJ/dP > 0$ under hydrostatic pressure. However, we did not find any publications concerning the uniaxial pressure effect on J. The normal state electronic properties as the electronic band structure and the Fermi surface under external pressure are less studied. It is clear that a consistent theoretical description and new predictions of the pressure effects on the properties of both normal and superconducting phases may results in a more profound understanding of the unsolved problems of the high-T_c cuprates.

In this paper, we have realized this program within the hybrid multielectron approach LDA+GTB [18, 19], where LDA is the conventional local density approximation to the

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