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INFLUENCE OF CuO_2 LATTICE STRAIN ON THE ELECTRONIC STRUCTURE OF HIGH-T_C CUPRATE FAMILY

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There is material dependence of superconducting transition temperature of the HTSC cuprates [1]. One of the most likely structural control parameter causing this material dependence is lattice parameter of CuO_2 layer. In this work we theoretically investigate effect of CuO_2 lattice parameter variation on the electronic structure of HTSC cuprate $La_{2-x}Sr_xCuO_4$ in the tetragonal phase at different concentration of doped holes.

HTSC cuprate $La_{2-x}Sr_xCuO_4$ is modelled by the plane of CuO_6 octahedra. Electronic system is described in the frameworks of five-band p-d model involving copper $d_{x^2-y^2}$-, $d_{3z^2-r^2}$-, planar oxygen p_x-, p_y- and apical oxygen p_z-orbitals. LDA+GTB method is used to get realistic parameters of Hamiltonian and to correctly take into account strong electronic correlations [2]. On-site energies and hopping integrals are calculated using the procedure of LDA eigenfunctions projection onto Wannier functions basis of the chosen model for the undoped La_2CuO_4 for the set of lattice deformations $\delta a/a_0$: -1, -0.5, 0, 0.5, 1, 1.5, 2.5, 3.5, 4.15 %. Generalized tight-binding (GTB) method [3] is cluster form of perturbation theory in the terms of Hubbard operators, it provides representation of electron as set of quasiparticle excitations between multiparticle eigenstates of finite cluster. Electronic structure of quasiparticle excitations in the effective two-band Hubbard model is obtained with equation of motion method for the matrix Green function. System of equations of motion is decoupled within generalized Hartri-Fock approximation by applying the Mori-type projection technique with taking into account spin-spin and kinematic correlation functions.

Valence (VB) and conductivity (CB) bands of quasiparticle excitations can be presented as result of hybridization of high-intensity single band of free electrons in the antiferromagnetic lattice and shadow low-intensity band [4]. Spectral weight is inhomogeneously distributed over dispersion surface throughout the whole Brillouin zone. Fermi contour (FC) of underdoped compound is four small hole pockets with inhomogeneous spectral weight. Hole doping changes dispersion, spectral weight distribution and shifts chemical potential deeper to VB. Reconstruction of bands includes growth of energy at point $\mathbf{k} = (\pi, \pi)$ in the VB caused by damping of spin correlations and decrease of energy at point $(0, 0)$ in the CB. Inhomogeneity of spectral weight on the opposite sides of the hole pocket relative to the boundary of the antiferromagnetic Brillouin zone increases with hole doping. Low spectral weight on the one side potentially can be reason of its absence in the ARPES. Hole pockets are transformed to large hole and electron contours with doping and then only large hole contour around $\mathbf{k} = (\pi, \pi)$ with almost homogeneous spectral weight distribution remains. Change of FC topology appears at critical concentrations x_{c1} and x_{c2} corresponding to quantum phase transitions (QPT) of Lifshits type.

Main effects of CuO_2 lattice strain on band structure are k-dependent energy shift of the VB and CB and shrink of their bandwidths. Concentrations of the first and second QPT are shifted with strain increasing (Table 1). Strain dependence of the characteristics determining superconducting temperature T_c within the mean-field theory with exchange mechanism of pairing, DOS and antiferromagnetic exchange constant J, was obtained (Table 1). The singularity of the DOS at the level of chemical potential

at concentration of first QPT $N_{\max}(\mu_{c1})$ demonstrates monotonic growth with lattice parameter $a\,(b)$ increasing. Exchange constant J monotonically decreases with strain increasing as well as resulting effective exchange constant $JN_{\max}(\mu_{c1})$ in the T_c equation.

Table 1. Concentrations of the first and second quantum phase transitions (x_{c1} and x_{c2}), superexchange parameter (J), DOS maximum at chemical potential for concentration x_{c1} ($N_{\max}(\mu_{c1})$) and their product ($JN_{\max}(\mu_{c1})$) at different values of the strain $\delta a/a_0$. First row shows HTSC compound with lattice parameter $a\,(b)$ corresponding to a given strain, experimental $T_{c\max}$ of the related compound is in second row

Compound	$T_{c\max}$, K	$\delta a/a_0, \%$	x_{c1}	x_{c2}	J (eV)	$N_{\max}$	$JN_{\max}$
–	–	-1	0.1604	0.285	0.168	3.3295	0.5594
$La_{2+x}Sr_xCuO_4$	40	0	0.1601	0.2828	0.156	3.499	0.5458
–	–	0.5	0.16	0.2815	0.15	3.5862	0.5379
$Bi_2Sr_2CaCu_2O_{8+x}$	82	1.5	0.1599	0.28	0.14	3.7355	0.5230
$HgBa_2Ca_2Cu_3O_{8+\delta}$	135	2.5	0.1594	0.277	0.127	3.9886	0.5066
$HgBa_2CaCu_2O_{6+\delta}$	127	2.7	–	–	–	–	–
$HgBa_2CuO_{4+\delta}$	97	3.1	–	–	–	–	–
–	–	4.15	0.1589	0.2735	0.112	4.3413	0.4862

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