Comment on “Strain and High Temperature Superconductivity: Unexpected Results from Direct Electronic Structure Measurements in Thin Films”

Mrkonjić, Ivana; Barišić, Slaven

Comment on "Strain and High Temperature Superconductivity: Unexpected Results from Direct Electronic Structure Measurements in Thin Films"

The angle-resolved photoemission spectroscopy (ARPES) measurement on the lanthanum system $La_{2-\delta}Sr_{\delta}CuO_4$ (LSCO) [1,2] reveal two important and qualitatively new results: the evolution of the Fermi surface (FS) from holelike to electronlike, accompanied by the transfer of the spectral weight from the lower to the conducting band upon doping. More specifically, recent ARPES measurements on thin films of LSCO under strain [1] show the same topology of the FS as the crystal samples [2], shifted to the smaller values of doping. Quite surprisingly, the change of the topology under strain is accompanied by the drastic change of the bandwidth, deduced from the experimental data. More specifically, at $\delta = 0.15$ doping, the bandwidth of the system under strain is almost doubled, compared to the one of the relaxed sample, although the Cu-O (apex) distance varies by 2.9%.

We argue here that this increase is the artifact of the inappropriate choice of the fitting regime. The analysis [1], as well as the band fits, is based on

$$\varepsilon(\mathbf{k}) = -2\tilde{t}[\cos(k_x a) + \cos(k_y a)] + 4\tilde{t}'\cos(k_x a)\cos(k_y a), \quad (1)$$

called the tight-binding (TB) fit. The origin of the drastic change in the bandwidth is the consequence of the change of the ratio $\tilde{t}'/\tilde{t}$, which is taken 6 times larger in the unstrained crystal. From the physical point of view, Eq. (1) can be related to the nonmagnetic limit of either the single-band (one site) extended Hubbard model or the charge-transfer (CT) three-band extended Emery model, sufficiently close to the Brinkmann-Rice (BR) transition point [Eq. (27) of [3] taken at $t < \Delta_{pf}$]. In both cases, the effective overlaps $\tilde{t}$ and $\tilde{t}'$, denoting Cu-Cu hopping, should renormalize in the same way with doping. The strain (small or large) is not expected to considerably change their ratio, except in the neighborhood of the BR point at small doping. These arguments imply that the fits based upon Eq. (1), with drastic variation of $\tilde{t}'/\tilde{t}$, are physically meaningless and can therefore be regarded only as an eye guideline.

The alternative explanation of the observed change of the topology of the FS can be obtained from the asymptotic limit of the extended Emery model which was already successfully used to predict the evolution of the band structure upon doping in LSCO crystals [3]. In this regime, the dispersionless Cu level comes in anticrossing with one O band [Anderson lattice case, Eq. (20) of [3]] or two O bands [full Emery case, Eq. (14) of [3]]. The precursor to the anticrossing (relevant for small doping) is a modified Eq. (1) with $\tilde{t}$ and $\tilde{t}'$ themselves $\mathbf{k}$ dependent [Eq. (21) of [3]]. The corresponding band fits are shown in Fig. 1. Values of the parameters are $t' = -0.45$, $t = 0.47$, and $\Delta_{pf} = 1.93$ eV for the unstrained crystal and

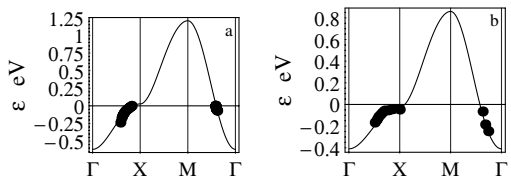

FIG. 1. Band fits of the data presented in [1]: (a) strained film; (b) crystal.

$t' = -0.48$, $t = 0.51$, and $\Delta_{pf} = 2.04$ eV for the strained film. They imply the increment of approximately 8% with respect to the unstrained values. At the same time, the effective bandwidth is only 8% larger. It should be finally stressed that these are only preliminary numbers, since more precise analysis would require simultaneous adjustment of the FS and the band dispersion. Unfortunately, there exists an obvious inconsistency in Fig. 2(c) of [1] related to strained film [4]. Therefore, the implication [1] that the Luttinger sum rule (LSR) is preserved in strained film should be reexamined [5]. If the LSR is obeyed, it speaks in favor of the $U = \infty$ limit [6]. This would rule out, in particular, the single-band Hubbard model, where the electron doping is strictly forbidden when $U = \infty$, which cannot be reconciled with the phase diagram of the single-layered cuprates exhibiting the approximate symmetry with respect to $\delta = 0$.

Finally, the importance of the choice of the appropriate fitting regime is more than just academic. The respective weights of the Cu and O components in the electronic states close to the Fermi level and the corresponding coherence factors are important for the understanding of both magnetic and superconducting properties of the high-T_c cuprates.

We gratefully acknowledge the authors of [1], D. Pavuna in particular, for many useful discussions, as well as for providing the experimental data.

Ivana Mrkonjić* and Slaven Barišić
Department of Physics, University of Zagreb, Bijenička 32, POB 331, 10002 Zagreb, Croatia

Received 30 July 2003; published 26 March 2004
DOI: 10.1103/PhysRevLett.92.129701
PACS numbers: 74.78.Bz, 68.60.Bs, 74.72.–h, 79.60.–i

*Electronic address: ivanam@phy.hr

[1] M. Abrecht, D. Ariosa, D. Cloetta, G. Margaritondo, and D. Pavuna, Phys. Rev. Lett. 91, 057002 (2003).
[2] A. Ino, C. Kim, M. Nakamura, T. Yoshida, T. Mizokawa, Z.-X. Shen, A. Fujimori, T. Kakeshita, H. Eisaki, and S. Uchida, Phys. Rev. B **65**, 94504 (2002),
[3] I. Mrkonjić and S. Barišić, Eur. Phys. J. B **34**, 69 (2003).
[4] D. Pavuna (private communication).
[5] I. Božović, G. Logvenov, I Belca, B. Narimbetov, and I Sveklo, Phys. Rev. Lett. **89**, 107001 (2002) reports the additional incorporation of oxygen.
[6] I. Mrkonjić and S. Barišić, Eur. Phys. J. B **34**, 441 (2003).

