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Utilization of a Highly Correlated Cluster Model for
Interpretation of Electronic Spectroscopic Data for
The High-Temperature Superconductors

By

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UTILIZATION OF A HIGHLY-CORRELATED CuO_2 CLUSTER MODEL TO
INTERPRET ELECTRON SPECTROSCOPIC DATA FOR THE HIGH-
TEMPERATURE SUPERCONDUCTORS

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ABSTRACT

We have consistently interpreted electron spectroscopic data for the high temperature superconductors utilizing a highly-correlated CuO_2 cluster model, and an extended Hubbard Hamiltonian which includes the inter-site Cu-O U_{pd} and O-O U_{pp} parameters. The data indicate much larger U_p and U_{pp} values than found in other typical highly conductive metals. Previously unassigned features in the data are now assigned within the model.

INTRODUCTION

In this work we summarize results of an interpretation of electron spectroscopic data for the high temperature superconductors. The data interpreted include the valence band (VB), Cu 2p, and O 1s photoelectron data (UPS and XPS), the Cu $L_{2,3}VV$, Cu $L_{2,3}M_{2,3}V$, and O KVV Auger data, and the O K and Cu $L_{2,3}$ x-ray absorption and emission (XANES and XES) data. Published data for polycrystalline and single crystal samples of $\text{La}_{1-x}\text{Ba}_x\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ (herein referred to as the La and 123 HTSC's) are considered along with that for CuO and Cu_2O .

The basic electronic structure of the HTSC's can be described with the Anderson Hamiltonian utilized by Sawatzky and coworkers^{1,2}. It includes the transfer or hopping integral t , the Cu and O orbital energies ϵ_d and ϵ_p , the core polarization energy Q_d , and the intra-site Coulomb repulsion energies U_d and U_p (the latter sometimes are assumed to be zero). This model is most useful when the U 's are large relative to the band widths¹, i.e. when correlation effects dominate hybridization effects. A CuO_2 ^(2D-1D) cluster model, which is also reasonably valid when $U \gg t$, simplifies the model further¹. We utilize an extended Hubbard model by adding the inter-site repulsion energies U_{dp} and U_{pp} ³ (i.e. between neighboring Cu-O and O-O atoms). The addition of these interactions is important for understanding many of the features in the data.

RESULTS

Our results for the Hubbard parameters are summarized at the top of Table 1. Other estimates of these Hubbard U and c parameters have been reported previously for the HTSC's¹⁻⁴. These were obtained empirically from the Cu 2p XPS and the VB UPS data utilizing the Anderson model. Our optimal extended Hubbard

^aSupported in part by the Office of Naval Research.

TABLE 1 Summary of hole states revealed in the spectroscopic data, and estimated energies using the following optimal values for the Hubbard parameters in eV:

$\delta_1 = 2$	$c_d = 2$	$U_p = 12, 13$	$U_d = 9.5, 10.2$
$\delta_2 = 0.5, 0.8$	$c_p = 2, 3$	$U_{pp^*} = 4.5, 4$	$U_{dp} = 1$
$\Gamma = 2$	$U_{pp^*} = 0.$	$U_{cp^*} = 2$	$Q_d = 9$
$\alpha = 1, 0.5$	$\beta = 2$	$\Delta = 0, 1.$	$K = 4$

State ^b	Energy expression	Calc. E. eV ^{c,d}	Exp. E. eV ^c	Remark
<u>G.S. and IPES, v</u>				
†a) d	$c_d - \delta_1 \mp \Gamma$	0 \mp 2	-	heavily mixed
†b) p	$c_p + \delta_1 \mp \Gamma$	4 \mp 2	-	mixed
<u>UPS and XES, v²</u>				
1)° pp [*]	$c_p + \Delta - \delta_2 + \alpha$	2.5	2.5	heavily mixed
2)° dp	$c_p + U_{dp} + \delta_2 + \alpha$	4.5	4.2	mixed
3) pp [*] _a	$c_p + \Delta + U_{pp^*} - \Gamma + \alpha$	5.5	5.	
4) pp [*] _b	$c_p + \Delta + U_{pp^*} + \Gamma + \alpha$	9.5	9.5	mystery peak
5) d ²	$c_d + U_d + \alpha$	12.5	12.5	Cu sat.
6) p ²	$c_p + \Delta + U_p + \alpha$	15	16	
<u>Cu 2p XPS, cv</u>				
d → cp	$c_c + \Delta + \alpha$	$c_c + 1$	E_{1p}	main
cd	$c_c + Q_d + \alpha$	$c_c + 10$	$E_{1p} + 9.2$	sat.
<u>Cu 2p XPS for NaCuO₂, pp[*] → cv²</u>				
pp [*] -cpp [*]	$c_c + \delta_2 + \beta$	$c_c + 2.5$	$c_c + 2.2$	main
cpp [*] _a	$c_c + U_{pp^*} - \Gamma + \delta_2 + \beta$	$c_c + 4.5$	$c_c + 5$?
cpp [*] _b	$c_c + U_{pp^*} + \Gamma + \delta_2 + \beta$	$c_c + 8.5$	$c_c + 9$?
cdp	$c_c - \Delta + Q_d + U_{dp} + \delta_2 + \beta$	$c_c + 11.5$	$c_c + 11$	sat.
cp ²	$c_c + U_p + \delta_2 + \beta$	$c_c + 15.5$	$c_c + 14$	sat.?
<u>O 1s XPS, cv</u>				
d → cd	$c_c + \alpha$	$c_c + 1$	E_{1s}	main
cp [*]	$c_c + \Delta + \alpha$	$c_c + 1$	E_{1s}	main
cp [*]	$c_c + \Delta + U_{cp^*} + \alpha$	$c_c + 3$	$E_{1s} + 2$?	tail
cp	$c_c + \Delta + Q_p + \alpha$?	?	not obs
pp [*] -cdp [*]	$c_c - \Delta + U_{dp} + \delta_2 + \beta$	$c_c + 3.5$	$E_{1s} + 2$?	tail
<u>Cu L_{2,3}VV ABS, v²</u>				
dpp [*]	$2c_p + 2U_{dp} + \alpha$	7	7	2 cent.
dpp [*]	$2c_p + U_{pp^*} + 2U_{dp} + \alpha$	11.5	-	no mix
d ² p	$c_d + c_p + U_d + 2U_{dp} - \delta_2 + \alpha$	16	15.5	main
dp ²	$2c_p + U_p + 2U_{dp} + \delta_2 + \alpha$	19.5	18-25	sat.

TABLE 1 (cont.)

State ^b	Energy expression	Calc. E. eV ^{c,d}	Exp. E. eV ^c	Remark
<u>Cu L_{2,3}V AES, cv²</u>				
cdp	$c_c + c_p + Q_d + U_d + \sqrt{K} + \alpha$	$c_c + 9$	$E_{2p} + 10$	main, ¹ L
		$c_c + 17$	$E_{2p} + 18$	main, ² L
cp ³	$c_c + c_p + \Delta + U_p + \alpha$	$c_c + 15$	-	not
cd ²	$c_c - c_d + U_d + 2Q_d + \alpha$	$c_c + 30.5$	-	obs.
<u>Cu L_{2,3} EELS, c</u>				
d → c	$c_c - c_d + \delta_1$	$E_{2p} - 1$	$E_{2p} - 1.4$	edge
cpCB	$c_c + \Delta - CB + \alpha$	$E_{2p} - CB$	$E_{2p} + 1.2$	upper
pp ⁴ → cp	$c_c - c_p + \delta_2 + \beta$	$E_{2p} - 0.5$	E_{2p}	middle
<u>O K EELS, c</u>				
d → c	$c_c - c_d + \delta_1$	$E_{1s} - 1$	E_{1s}	edge
cdCB	$c_c - CB + \alpha$	$E_{1s} - CB$	$E_{1s} + 1.7$	upper
pp ⁴ → cd	$c_c - \Delta - c_p + \delta_2 + \beta$	$E_{1s} - 0.5$	-	not obs

^aParameters for 123 indicated first, those for CuO second.

^bThe dominant character in the hybridized states is given.

^cThe Calc. E and Exp. E columns indicate the results for 123, except for the "Cu 2p XPS, pp⁴ → cv²" section, which is for NaCuO₂.

^dThe calculated E is defined relative to the ground v¹ (d) state energy = $c_d - \alpha$, or to the v² (pp⁴) ground state energy = $2c_p - \delta_2 - \delta$. The v¹(d) energy defines the Fermi level relative to the vacuum level at zero.

^eThe dominant character switches as described in the text, and thus the sign in front of δ_2 is the opposite for CuO.

parameters in Table 1 were obtained by considering this same data plus XANES, Auger and XES data. Although we are in general agreement with the reported magnitudes for most of the parameters, our U_d value is larger by about 2-3 eV so that it is consistent with the AES data. In Table 1, we indicate the location of two valence holes by d (Cu 3d) or p (O 2p). In the case of two holes on the oxygens, we distinguish two holes on the same O (p²), on ortho neighboring O atoms (pp⁴), or on para O atoms (pp⁴) of the cluster. Furthermore, neighboring pp⁴ holes can dimerize⁵, so we distinguish between two holes in bonded (pp⁴) and antibonded (pp⁴) O pairs.

The magnitudes of the U parameters are critical to the mechanism for the superconductivity. As a consequence, much effort has also gone into theoretically calculating these parameters, but wide disagreement still exists over the magnitudes. Theoretical values for U_d in the range 6.5-10 eV, U_p (actually $U_p - U_{pp}^4$) in the range 7-14 eV, and U_{pp}^4 in the range 0.6-1.6 eV have been reported⁶, with the smaller results favored based on the quality of the calculations. No results for U_{pp}^4 have been reported. Our empirical

notation pp^* . We use $2c_p - d_s - s$ as the energy of the pp^* ground state relative to the vacuum level, where $s = 2$ eV is the energy shift between the principal pp^* UPS final state at 2.5 eV and the lowest ground pp^* states around 0.5 eV from the Fermi level.

The correlation between the calculated energies and experimental features, utilizing the indicated optimal Hubbard parameters is very good. Details of this work are published elsewhere³. Figs. 1 and 2 show examples of the UPS and Cu AES data for 123 and CuO, which reveal some of the features itemized in Table 1; the remaining data are published elsewhere.

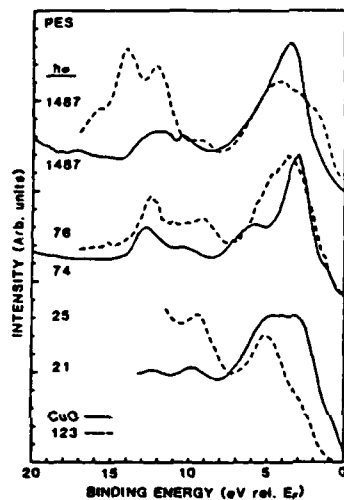


Figure 1. Comparison of UPS spectra for CuO and 123 taken with the indicated photon energies in eV. Data for CuO from refs. 10 ($h\nu = 1487$), 11 ($h\nu = 74$) and 12 ($h\nu = 21$). Data for 123 from ref. 13 ($h\nu = 25$ and 74) and 14 ($h\nu = 1487$).

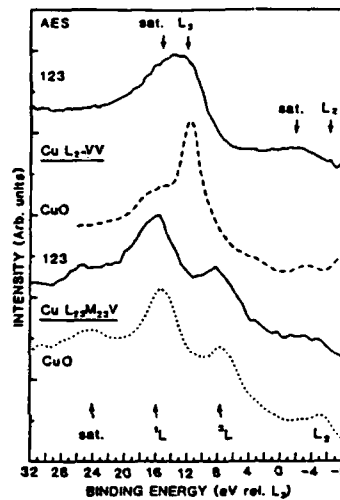


Figure 2. Comparison of Auger data for the materials indicated. $L_{23}VV$ data for CuO and 123 from ref. 15. $L_{23}M_{23}V$ data for CuO from ref. 16 and for 123 from Ref. 9. The $L_{23}VV$ data is on a 2-hole binding energy scale = $E_{L_2} - E_{k_1}$, and the $L_{23}M_{23}V$ on a 1-hole scale = $E_{L_2} - E_k - E_{M_2}$, where $E_{L_2} = 933.4$ and $E_{M_2} = 77.3$ eV^{11,12}.

SUMMARY AND CONCLUSIONS

This work has allowed us to assign some previously unassigned features in the data, and greatly increased our understanding of the

dynamical electronic processes which produce these features. We itemize our conclusions as follows:

1) A switch in the character of state 1 (see Table 1) from more dp^2 to pp^2 and vice versa for state 2 between CuO and 123 arises because Δ decreases from 1 eV to 0 eV. The smaller Δ in 123, due to a smaller ϵ_c , polarization energy, is consistent with the Cu 2p XPS and XES data (the latter showing this effect dramatically)^{17,18}. Since state 1 is more of pp^2 character in the SC's, the "charge carrier holes" (present in the La after Sr doping and in the 123 when $7-x$ is greater than 6.5) spend more time on the oxygens in 123 than in CuO.

2) The pp^2 state is believed to be responsible for the "mystery" peak found at 9.5 eV in the UPS. Figure 1 indicates that such a feature also appears for CuO^{11,12}. This feature does not appear for Cu₂O, as expected since UPS reflects the one-hole DOS in Cu₂O. Thus this feature is not unique to the SC's; it naturally appears for those systems with two-hole photoemission final states.

3) Although Cu₂O, CuO, and NaCuO₂ have a formal Cu valence of +1, +2, and +3, in the current picture they reflect the cv^2 DOS, with $n=0, 1, \text{ and } 2$. Furthermore, we consistently predict the "chemical shifts" in the primary Cu 2p XPS peaks. Whereas, Cu₂O exhibits just a primary core hole c state at energy ϵ_c , CuO has its primary cd feature energy shifted by $\Delta+\alpha$ relative to ϵ_c , and the primary cpp^2 feature for NaCuO₂ by $\delta_1+\delta$ (Table 1), which is consistent with the experimental data¹⁷. The width of the primary feature is seen to correlate with the intensity of the satellite, and is not due to the O p band width as suggested by others¹⁸.

4) The increased "satellite" feature at 19 eV in the Cu L₂₃VV Auger line shape for the HTSC's compared with CuO^{15,16} (see Fig. 2) arises because of increased final-state configuration mixing between the d^2p and dp^2 states. Its intensity is increased in 123 relative to CuO because the energy separation (before hybridization) between d^2p and dp^2 has decreased from 3.8 eV in CuO to 2.5 eV in 123. We have indicated this mixing in Table 1 by adding the hybridization shifts δ_2 to the energy expressions for these two states.

5) We find that the initial-core shakeup (ICSU) process, which is known to be responsible for the satellite features in the Cu 2p XPS data¹, does not produce satellites in the AES or XES data, because the ICSU states generally "relax" to the primary states of the same symmetry before the core level decay. Such a relaxation is expected when the ICSU excitation energy is larger than the core level width¹⁹. Previously, vanderLaan et al.¹, for the Cu halides, suggested that the intensity of these ICSU states in the XPS should be quantitatively reflected in the intensity of the Auger satellites found in the L₂₃VV lineshapes. The data do not indicate this however. We previously¹⁵ indicated that a fraction of these ICSU states probably resulted in Auger satellites for the HTSC's, and that this fraction becomes larger as the covalency of the HTSC material increases. This work indicates rather that the ICSU states relax before the core level decay to states of the same symmetry, provided they have a ICSU excitation energy that is much greater

than the core level width. We believe this to be a general result, at least in the Cu²⁺ materials.

6) The EELS and XANES data^{20,21} reflect the contributions from three possible transitions; the dominant d → c contribution nearest the Fermi level, the pp² → cv (v = d or p) contribution resulting from the carrier hole states, as well as the cvCB contribution well above the Fermi level²². Here CB represents an electron present in the higher Cu 4sp or O 3p "conduction band". The latter two contributions are not always resolved, and sometimes have been confused in the literature²⁰⁻²².

7) All of the temperature effects seen in the spectroscopic data²³⁻²⁶ can be attributed to a single phenomenon, namely a decrease in ϵ_p due to increased metallic screening, or long range polarization. This is consistent with the decrease in the primary cp peak energy in the Cu 2p XPS, while the cd satellite remains unshifted. The larger energy separation between the cd and cp states decreases the mixing which causes the satellite to decrease in intensity and the main peak to get narrower. Although the primary cd peak does not shift in the O 1s XPS, a slight shift to lower energy is seen in the cp² and cp² contributions at lower temperature, as expected with a decrease in ϵ_p . The UPS spectra show a skewing toward the Fermi level at lower temperature, as expected with a decrease in ϵ_p . Finally the growth of the satellite intensity in the Cu L_{2,3}VV Auger lineshape is consistent with a decrease in ϵ_p . The increased metallic like screening or polarization which appears to occur at lower temperature, reducing ϵ_p , probably involves the grain boundaries, since the more recent data for the single crystal samples do not change with temperature²⁷.

In summary, an interpretation of the data utilizing a highly correlated Cu₂O cluster model shows that a single set of Hubbard parameters predicts all of the state energies. Changes in the data between CuO and the HTSC's arises primarily from a reduction in ϵ_p ; this reduction continues with decreasing temperature in the HTSC's due to increased metallic screening. Compared with CuO, the HTSC's show an increased covalent interaction between the Cu-O bonds. The large size of U_{pp}²⁸, and the temperature dependence, reveal that metallic screening is incomplete, and hence that the DOS at the Fermi level in the HTSC's is relatively small.

REFERENCES

1. G. vanderLaan et al., Phys. Rev. 24, 4369 (1981); G.A. Sawatzky et al., Phys. Rev. Lett. 53, 2339 (1985); J. Zaanen et al., Phys. Rev. B33, 8060 (1986).
2. Z. Shen et al., Phys. Rev. B36, 8414 (1987).
3. A. Fujimori et al., Phys. Rev. B35, 8814 (1987).
4. J.C. Fuggle et al., Phys. Rev. B37, 1123 (1988).
5. R.A. de Groot, H. Gutfreund, and M. Weger, Sol. State Commun. 63, 451 (1987); W. Folkerts et al., J. Phys. C: Solid State Phys. 20, 4135 (1987); A. Manthiram, X.X. Tang, and J.B. Goodenough, Phys. Rev. B37, 3734 (1988).

6. C.F. Chen et al., unpublished; A.K. McMahan, R.M. Martin, and S. Satpathy, unpublished; M. Schluter, M.S. Hybertsen, and N. E. Christensen, Proc. Intn. Conf. High Tc. Superconductors and Materials and Mechanisms of Superconductivity, J. Muller and J.L. Olsen, Eds., (Interlaken, Switzerland, 1988).
7. G. Klopman, *J. Am. Chem. Soc.* **86**, 4550 (1964).
8. J. Redinger et al., *Phys. Lett.* **124**, 463 and 469 (1987).
9. D.E. Ramaker, N.H. Turner, and F.L. Hutson, submitted.
10. A. Rosencwaig and G.K. Wertheim, *J. Elect. Spectrosc. Related Phenom.* **1**, 493 (1972/73).
11. M.R. Thuler, R.L. Benbow, and Z. Hurych, *Phys. Rev.* **B26**, 669 (1982).
12. C. Benndorf et al., *J. Electron. Spectrosc. Related Phenom.* **19**, 77 (1980).
13. N.G. Stoffel et al., *Phys. Rev.* **B37**, 7952 (1988); **B38**, July (1988).
14. D.C. Miller et al., in Thin Film Processing and Characterization of High Temperature Superconductors, J.M. Harper, J.H. Coiton, and L.C. Feldman, Eds., AVS Series No. 3 (AIP: New York, 1988) p 336.
15. D.E. Ramaker et al., *Phys. Rev.* **36**, 5672 (1987).
16. P.E. Larson, *J. Electron Spectrosc. Related Phenom.* **4**, 213 (1974).
17. P. Steiner et al., *Z. Phys. B- Condensed Matter* **67**, 497 (1987).
18. D.D. Sarma, *Phys. Rev.* **B37**, 7948 (1988).
19. J.W. Gadzuk and M. Sunjic, *Phys. Rev.* **B12**, 524 (1975).
20. D.D. Sarma et al., *Phys. Rev.* **B37**, 9784 (1988).
21. N. Nucker et al., *Z. Phys. B: Cond. Matter* **67**, 9 (1987); *Phys. Rev.* **37**, 5158 (1988).
22. A. Bianconi et al., *Solid State Commun.* **63**, 1009 (1987); *Intn. J. Modern Phys.* **131**, 853 (1987).
23. N.S. Kohiki and T. Hamada, *Phys. Rev.* **B36**, 2290 (1987).
24. B. Dauth et al., *Z. Phys. B- Condensed Matter* **68**, 407 (1987).
25. D.H. Kim et al., *Phys. Rev.* **B37**, 9745 (1988).
26. A. Balzarotti et al., *Phys. Rev.* **B36**, 8285 (1987).
27. J. Weaver and P. Steiner, private communication.

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