

Band Structure and Electron-Phonon Interaction of LaAgO₃

N. C. Bacalis² and D. A. Papaconstantopoulos¹

Received 1 January 1988

A comparison is made between the band structure of LaAgO₃ and LaCuO₃, which is the cubic counterpart of the high- T_c superconducting oxides. The electron-phonon parameter η is also calculated and is found to be larger for Ag and O in LaAgO₃ than for Cu and O in LaCuO₃.

KEY WORDS: band structure; electron-phonon interaction; superconductivity.

1. INTRODUCTION

A common feature of the new high- T_c superconductors is that they derive from the same basic structure, namely, the cubic perovskite LaCuO₃. In addition, recent band structure studies [1] suggest that the local environment of the copper and oxygen atoms is probably responsible for the high-temperature superconductivity. In an effort to explore these ideas further, we are performing a systematic study of the band structure of the cubic perovskites together with an evaluation of the electron-phonon parameter η . In previous work [2], we have studied the effects of substituting for La. In this article, we report on the effects of substituting Cu by Ag, which is in the same column of the periodic table just below Cu.

2. METHOD OF CALCULATION AND APPROXIMATION

The band structure calculation was performed using the self-consistent scalar-relativistic APW method in the muffin-tin approximation with the local density approximation for exchange and correlation described by

¹Naval Research Laboratory, Washington, DC 20375-5000.

²National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, 48 Vas. Constantinou Ave., Athens 116 35, Greece.

Hedin and Lundqvist [3]. The self-consistent potential was calculated using 10 k -points in the 1/48th of the 1st Brillouin zone (BZ) and the final band structure was found in 165 k -points by a symmetrized Fourier series interpolation [4] based on the APW eigenvalues at 35 k -points in the 1/48th BZ. The densities of states (DOS) were calculated with the tetrahedron method [5]. The muffin-tin sphere radii were taken for La (3.576 au) and for Ag and O (1.956 au). LaAgO₃ is an unknown material, very difficult to form in this structure [6]. We examined two lattice constants: $a_1 = 7.8234$ au, which is the same used [1] in LaCuO₃, and $a_2 = 7.88$ au. The core levels were treated in the "soft core" approximation, as explained elsewhere [7]. We also used our band structure results to calculate the strength of the electron-phonon interaction determining the McMillan-Hopfield parameter η , using the rigid muffin-tin approximation [8] of Gaspari and Gyorffy.

3. RESULTS AND DISCUSSION

The energy bands and total DOS are shown in Figs. 1 and 2, for LaAgO₃ with lattice constant a_1 and for LaCuO₃ with the same lattice spacing. We see that the band structure of LaAgO₃ is very similar to that of LaCuO₃. The main difference is that LaAgO₃ has a wider complex of Cu d - and O p -bands than LaCuO₃. The width of the occupied bands is ~ 0.52 Ry and ~ 0.42 Ry for LaAgO₃ and LaCuO₃, respectively. Above the Fermi level, E_F , we find, for both compounds, the very narrow La f -bands and a complex of La d -bands. The effect of the lattice constant change from a_1 to a_2 on the band width of LaAgO₃ is very small. We note that, as in LaCuO₃ near E_F , LaAgO₃ shows one band, consisting of mainly O (2p) and Ag (4d) orbitals. This band has a parabolic free electron-like shape similar to that found in the high-temperature superconductors La₂CuO₄ and Y₁Ba₂Cu₃O₇. As seen from Fig. 3, where the partial DOS are shown, the d -bands at E_F are of only e_g symmetry consisting of the Ag: d -orbitals ($x^2 - y^2$) and ($3z^2 - r^2$). These couple at E_F with O p -orbitals. Thus we see that the Fermi surface properties, including superconductivity, would involve bonding characteristics of Ag and O atoms. The La atom essentially does not contribute at the Fermi level.

These observations regarding the band structure of LaAgO₃ are the same as those noted in the study [2] of LaCuO₃ and consistent with the analysis [1] of the electronic structure of La₂CuO₄. The electron-phonon coupling parameter λ , which controls the value of T_c in the conventional theory of superconductivity, is given by $\lambda = \eta/F$ where F is a force constant giving the average stiffness of the crystal against phonon modes, and $\eta = \langle I^2 \rangle N(E_F)$ with $\langle I^2 \rangle$ being the average electron-ion scattering matrix

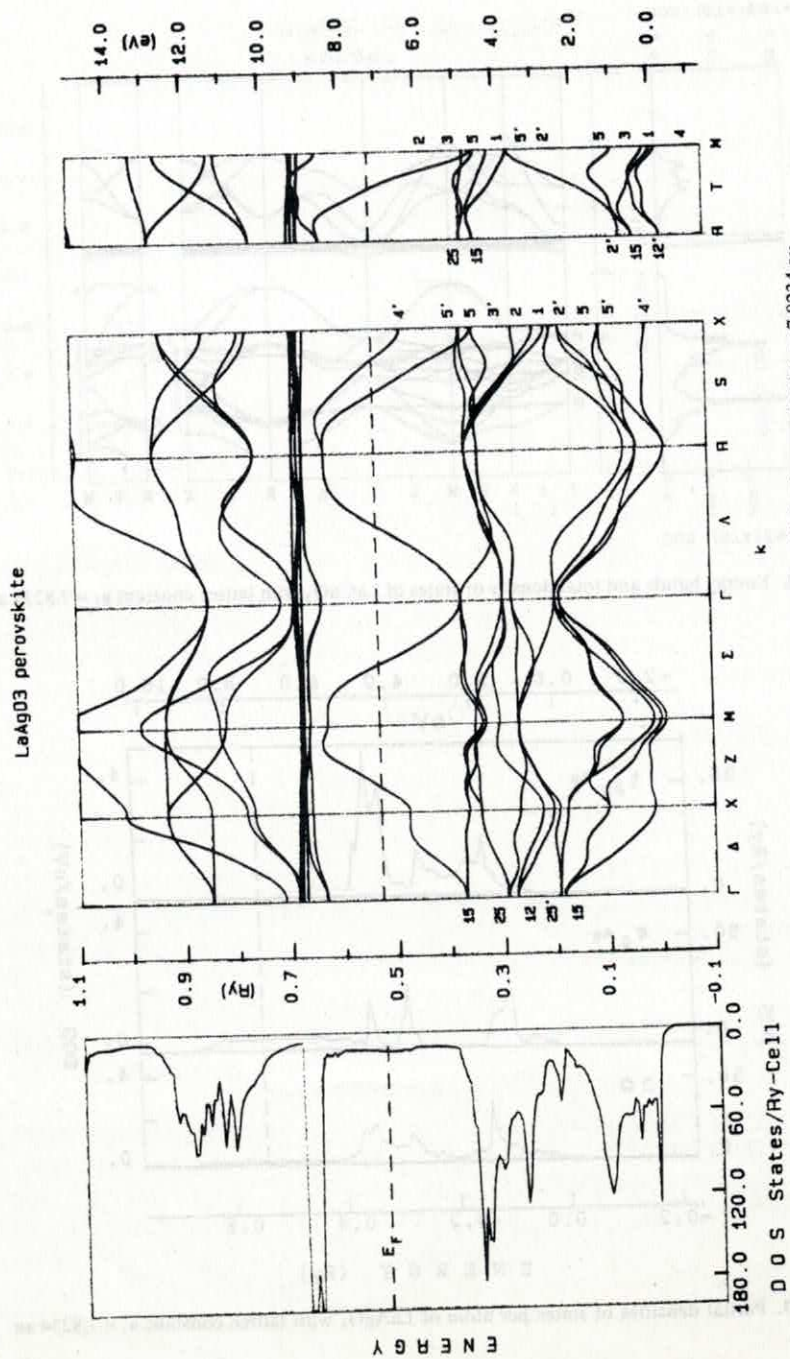


Fig. 1. Energy bands and total density of states of LaAgO₃ with lattice constant $a_1 = 7.8234$ au.

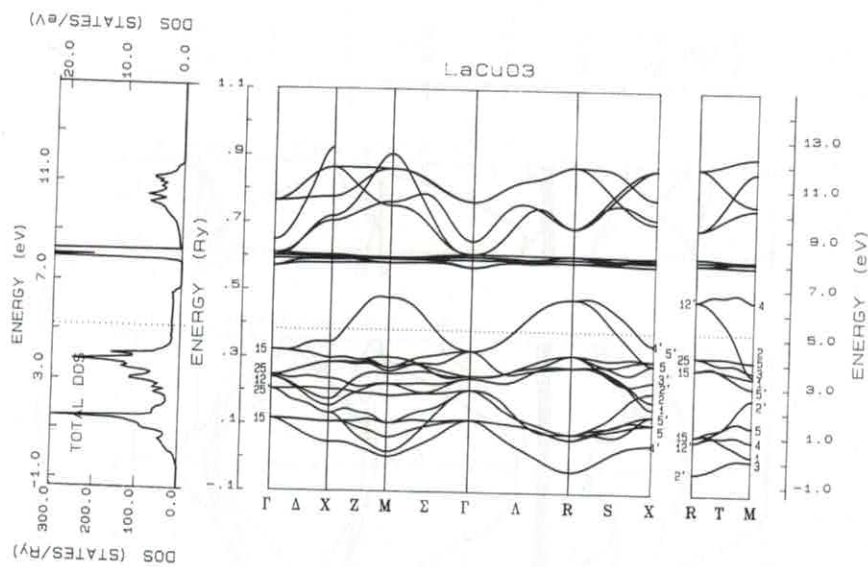


Fig. 2. Energy bands and total density of states of LaCuO₃ with lattice constant $a_1 = 7.8234$ au.

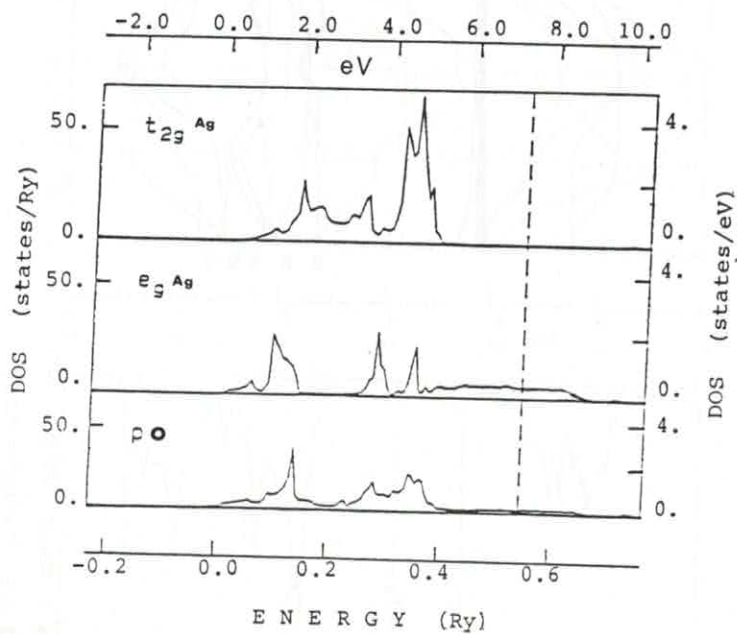


Fig. 3. Partial densities of states per atom of LaAgO₃ with lattice constant $a_1 = 7.8234$ au.

Table I. Fermi Energy E_F (Ry), Total Densities of States (states/Ry) $N(E_F)$, Component DOS Inside Muffin-Tin Spheres, and Contributions to η (eV/A²) from the La, M, and Three O Sites in LaMO₃, M = Cu, Ag for the Lattice Constants a_1 and a_2

	LaCuO ₃ (a_1)	LaAgO ₃ (a_1)	LaAgO ₃ (a_2)
E_F	0.382	0.525	0.505
$N(E_F)$	19.37	13.64	13.87
$N_{La}(E_F)$	0.17	0.16	0.14
$N_M(E_F)$	7.86	5.34	5.37
$N_O(E_F)$	9.98	7.03	7.17
η_{La}	0.00	0.00	0.00
η_M	0.894	1.109	1.104
η_O	1.433	2.156	2.125

element. We calculated η for each site, using the rigid muffin-tin approximation (RMTA). Table I shows for LaCuO₃ and LaAgO₃ the DOS at E_F along with a comparison of the values of η for the sites of La, Cu (or Ag), and the sum of the three O, for the lattice constants a_1 and a_2 . We see that although $N(E_F)$ is less for LaAgO₃ than for LaCuO₃, the η parameter is larger for both O and Ag in LaAgO₃ than for O and Cu in LaCuO₃. The increase of η by $\sim 50\%$ for O and by 25% for Ag is due to a dramatic increase of the matrix element $\langle I^2 \rangle$ in LaAgO₃. This comes from an enhanced $p-d$ scattering in LaAgO₃. In both compounds, La does not contribute to η . It should be stressed that these values of η are probably a lower bound because, in materials with free-electron-like bands near E_F , the RMTA underestimates η [9]. The results for η presented in Table I are similar to those found in La₂CuO₄. It was argued [1] that a $T_c \approx 40$ K could be understood in terms of an electron-phonon interaction mechanism, if the lattice stiffness F is relatively small.

4. CONCLUSIONS

This work suggests that the substitution of Cu by Ag in the cubic perovskite introduces a widening of the occupied energy bands and an increase of the electron-phonon interaction. Due to the striking resemblance of the band structures, it appears that the cubic perovskite is a good model on which to base studies of the electronic properties of the more complicated perovskite-like structures. On the basis of this model and the assumption that the electron-phonon interaction is a valid mechanism for superconductivity in these materials, it appears likely that substitution of Cu by Ag may enhance the transition temperature.

ACKNOWLEDGMENTS

We wish to thank Dr. W. E. Pickett for useful discussions and acknowledge partial support from the U.S. Office of Naval Research, and the Research Center of Crete, Greece.

REFERENCES

1. W. E. Pickett, H. Krakauer, D. A. Papaconstantopoulos, and L. L. Boyer, *Phys. Rev. B* **35**, 7252 (1987).
2. D. A. Papaconstantopoulos and L. L. Boyer, *Workshop on Novel Mechanisms of Superconductivity*, S. A. Wolf and V. Z. Kresin, eds. (Plenum Press, New York, 1987).
3. L. Hedin and B. I. Lundqvist, *J. Phys. C* **4**, 2064 (1971).
4. L. L. Boyer, *Phys. Rev. B* **19**, 2824 (1979).
5. G. Lehman and M. Taut, *Phys. Status Solidi. B* **54**, 469 (1972).
6. K. Pavlides, Private communication.
7. N. C. Bacalis, K. Blathras, P. Thomaidis, and D. A. Papaconstantopoulos, *Phys. Rev. B* **32** 4849 (1985).
8. G. D. Gaspari and B. L. Gyorffy, *Phys. Rev. Lett.* **28**, 801 (1972).
9. A. D. Zdetsis, E. N. Economou and D. A. Papaconstantopoulos, *Phys. Rev. B* **24**, 3115 (1981).