Electron density in Infinite-layer *p*- and *n*-type superconductors

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Maps of the electron density of infinite-layer *p*- and *n*-type superconductors are calculated and plotted. The greatest differences between these two types of superconductors are found in the (0,0,0.5) plane. It might be possible to raise the T_c by replacing the trivalent rare-earth ion by a tetravalent ion (e.g., Pr^{4+} or Tb^{4+}). © *1995 American Institute of Physics.*

The correlation which exists between the number of closely spaced copper–oxygen planes and the superconducting transition temperature T_c has raised the hope that it would be possible to synthesize infinite-layer superconductors. To some extent, this hope has already been realized. These superconductors can have either a *p*-type or an *n*-type conductivity. An example of the former is the superconductor $Sr_{0.7}Ca_{0.3}CuO_2$, with $T_c = 110$ K (Ref. 1). An example of the latter, according to Ikeda *et al.*,[2] is $Sr_{1-x}Nd_xCuO_2$, which has the record-high transition temperature for *n*-type superconductors: $T_c = 44$ K. The superconducting transition temperature is independent of the Nd concentration (between $x = 0.05$ and $x = 0.10$).

Data on the electron density in $Sr_{1-x}Ca_xCuO_2$ were discussed in Ref. 3. A calculation was carried out for individual tetragonal cells of $CaCuO_2$ ($a = 3.86$ Å and $c = 3.20$ Å) and $SrCuO_2$ ($a = 3.926$ Å and $c = 3.432$ Å). In particular, a map was presented for the (001) plane. It can be concluded from that map that there is a strong Cu–O coupling. A map presented for the (010) plane indicates that the distribution of the electron density along the *c* direction is two-dimensional. A map presented for the (110) diagonal plane reveals a very low electron density near a Ca site.

We have found a self-consistent distribution of the electron density through nonempirical calculations by a modified Thomas–Fermi method.[4] This method has been used previously to study the high-T_c superconductors $YBa_2Cu_3O_{6+x}$ (Ref. 5) and La_2CuO_4 (Ref. 6).

In the present study we calculated the distribution of the electron density for "quadruple" cells, for both *p*-type and *n*-type superconductors, i.e., for $Sr_3Ca(CuO_2)_4$ ($a = 7.814$ Å, $c = 3.363$ Å, with $n = 64$ electrons) and for $Sr_3Nd(CuO_2)_4$ ($a = 7.90$ Å, $c = 3.39$ Å, $n = 65$). The structure and its parameters are shown in Fig. 1. The actual composition of the *n*-type superconductor is approximately $Sr_9Nd(CuO_2)_{10}$. Because of the complexity of the calculations, we used an $Sr_3Nd(CuO_2)_4$ cell, in which the neodymium concentration is higher. However, we do not believe that the distribution of the

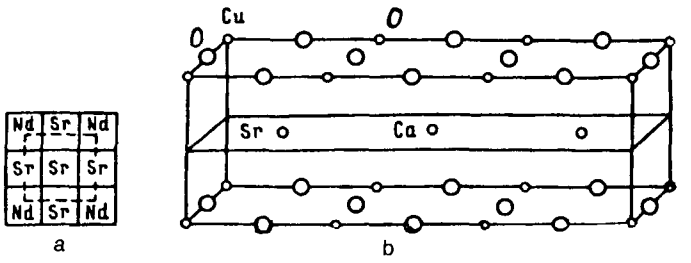

FIG. 1. a—One model of the $Sr_3Nd(CuO_2)_4$ crystal, with the cell used in the calculations shown; b—structure of the $Sr_2Ca(CuO_2)_3$ cell.

electron density changes significantly near Nd or its nearest neighbors. "Triple" cells are accordingly shown on the maps of the electron density.

The maps of the electron density in the (001) and (010) planes, for both $Sr_3Ca(CuO_2)_4$ and $Sr_3Nd(CuO_2)_4$, are very similar to the results shown for these planes in Ref. 3. We will accordingly not reproduce them here. The neodymium ion at a distance ~ 1.5 Å from these planes has an extremely slight effect (causing some decrease in the electron density at the center of the map). The sharpest difference between the two types

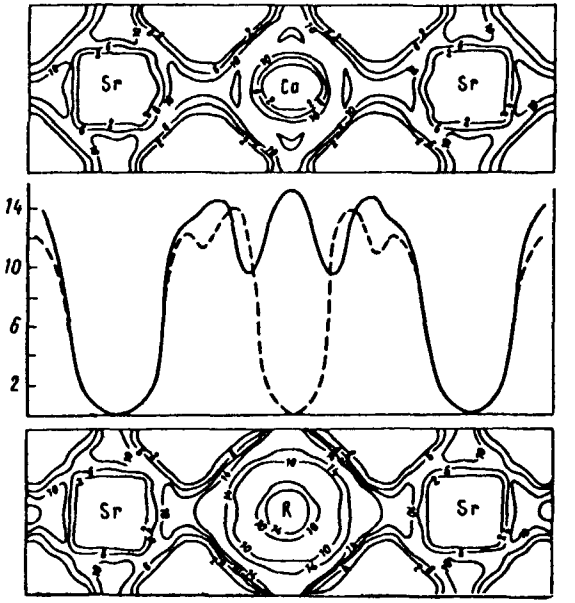

FIG. 2. Comparison of the electron densities in the (0,0,0.5) plane of $Sr_3Ca(CuO_2)_4$ (at the top) and of $Sr_3Nd(CuO_2)_4$ (bottom). Curves of the variation of the electron density along the longitudinal axes of the maps are compared at the middle of this figure. Solid curve—$Sr_3Ca(CuO_2)_4$; dashed curve—$Sr_3Nd(CuO_2)_4$. The electron density is given in units of the number of electrons per cell.

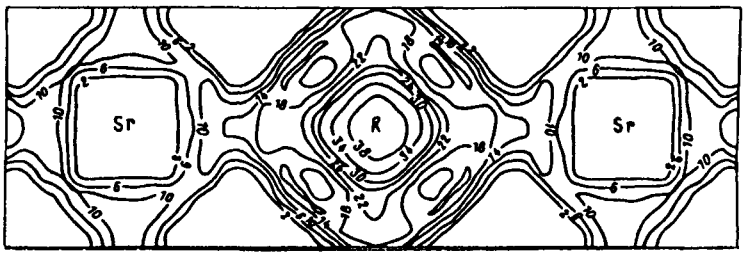

FIG. 3. Map of the of the (0,0,0.5) electron density for $Sr_3RE^{4+}(CuO_2)_4$.

of superconductors can be seen in Fig. 2, at the top of which there is a map of the (0,0,0.5) plane, which lies between the basal planes of the p-type superconductor; the same plane of the n-type superconductor is shown at the bottom. At the middle of the figure, curves of the electron density along the longitudinal axes of the maps are compared. We see that the electron density of the p-type superconductor varies in regular way from zero near the core of the strontium and calcium ions to ~ 14 e/cell in the intermediate region.

This regularity is disrupted in the n-type superconductors near the central ion, where the electron density reaches a maximum. Obviously, this maximum density stems from the trivalent nature of the rare-earth ion. If the nature of the n-type superconductivity with the record-high T_c is determined by the elevated electron density near the central rare-earth atom, one might suggest that a further increase in this density would raise the superconducting transition temperature even further.

Figure 3 shows a map of the distribution of the electron density in the (0,0,0.5) plane in the case in which there is a tetravalent rare-earth atom at the center of the cell. The best possibility for synthesizing a superconductor of this type is to replace the Nd^{3+} by praseodymium or terbium.

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