

## Density of states in $\text{La}_2\text{CuO}_{4+y}$

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We describe the excess holes in the  $\text{CuO}_2$  sheets of  $\text{La}_2\text{CuO}_{4+y}$  as a two-dimensional hole gas in a quantum well in the presence of negatively charged impurities. We calculate the density of states with a multiple-scattering approach. We discuss the broadening of the impurity band with increasing  $y$ , which corresponds to an increasing hole concentration. The spectral density, which describes for vanishing hole concentration the Fourier transform of the squared wave function, is evaluated. We compare our results with recent measurements of  $\text{La}_2\text{CuO}_{4+y}$  with  $y < 0.007$ .

### I. INTRODUCTION

The electronic properties of superconducting  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  and  $\text{La}_2\text{CuO}_{4+y}$  are theoretically not well understood.<sup>1</sup> However, it is widely believed that the transport properties are determined by two-dimensional  $\text{CuO}_2$  sheets.  $\text{La}_2\text{CuO}_4$  ( $x=0$ ) is an antiferromagnetic insulator in which the magnetic order is destroyed by a few percentage of holes. For a review, see Ref. 2.

Holes are created in  $\text{La}_2\text{CuO}_4$  by doping with Sr ( $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ ) or by annealing in  $\text{O}_2$  ( $\text{La}_2\text{CuO}_{4+y}$ ). Superconductivity is only present if the hole density is larger than a critical hole density  $N_{3s}$ . For the phase diagram of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ , see Ref. 3. With increasing hole concentration, an insulator-metal transition takes place at a certain hole concentration. In the insulating phase the resistivity is strongly temperature dependent.<sup>4,5</sup> Recent experiments on the temperature-dependent conductivity<sup>5</sup> and the frequency-dependent dielectric constant<sup>6</sup> of  $\text{La}_2\text{CuO}_{4+y}$  with  $0.001 < y < 0.007$  have been interpreted as an insulator-metal transition in a two-dimensional semiconductor. At the three-dimensional hole concentration  $N_3 = 7 \times 10^{19} \text{ cm}^{-3}$  ( $y \sim 0.007$ ) the static in-plane dielectric constant was increased by a factor 4 compared to the static (extrapolated) dielectric constant at zero doping:  $\epsilon \sim 30$ .<sup>6</sup> The static out-plane dielectric constant was nearly independent on the doping concentration and gave evidence for the two-dimensional character of the transport. The critical three-dimensional hole concentration  $N_{3c}$  was estimated as  $N_{3c} > 7 \times 10^{19} \text{ cm}^{-3}$ .<sup>6</sup> Previous measurements<sup>7</sup> of the frequency-dependent dielectric constant of lightly doped  $\text{La}_2\text{CuO}_4$  have been discussed in Ref. 6 and the interpretation given in Ref. 7 has been criticized. For  $N_{3c} < N_3 < N_{3s}$ ,  $\text{La}_2\text{CuO}_{4+y}$  is expected to exhibit metallic properties. Superconductivity is only found for  $N_3 > N_{3s}$ . However, for  $y > 0.01$ , the samples become inhomogeneous in oxygen content<sup>6</sup> and one has to use  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  to study the large doping regime.<sup>3,4,8</sup> Therefore, experimental data for  $N_{3s}$  are not available for

$\text{La}_2\text{CuO}_{4+y}$ . The experimental results<sup>3,4</sup> found for  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  indicate  $N_{3c} \sim N_{3s}$  with  $N_{3s} \sim 5 \times 10^{20} \text{ cm}^{-3}$  ( $x \sim 0.05$ ). The possibility of a transition from an insulator to a superconductor for zero temperature was discussed in Ref. 9 for thin films made of  $\text{DyBa}_2\text{Cu}_3\text{O}_7$ . More experimental work is needed to determine  $N_{3c}$  and  $N_{3s}$ .

For small doping densities the transport properties of semiconductors are determined by shallow impurities. The experimental results<sup>5,6</sup> on  $\text{La}_2\text{CuO}_{4+y}$  are in a doping regime ( $N_3 < N_{3c}$ ) where overlapping effects between shallow impurity states could be important. Impurity states for  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  have also been discussed within the  $t-J$  model.<sup>10</sup>

Impurity bands for low doping have been proposed from an analysis of photoemission studies of the high- $T_c$  material  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ , see Fig. 9 of Ref. 11. For large doping, a band-tail description is more adequate. High-energy electron-energy-loss spectroscopy<sup>12</sup> and photoemission spectroscopy<sup>13</sup> of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  and other high- $T_c$  material<sup>11,14</sup> suggest such a behavior. However, the Fermi-liquid picture, which is behind the concept of shallow impurity states (where the binding energies scale with the effective rydberg), which we use in our calculations, has been criticized by Anderson.<sup>15</sup> For the high- $T_c$  materials, the concept of impurity bands in the framework of a spin-polaron theory was recently discussed by Mott.<sup>16</sup> However, he did not specify the dimensionality of the impurity band. A polaron picture for  $\text{La}_2\text{CuO}_{4+y}$  was discussed in Refs. 7 and 17.

A direct proof of the two-dimensional transport in the normal state ( $T > T_c = 90 \text{ K}$ ) of superconducting copper-oxide films ( $\text{GaBa}_2\text{Cu}_3\text{O}_7$ ) came from magnetoresistance measurements.<sup>18</sup> It was found that only the magnetic field perpendicular to the  $\text{CuO}_2$  planes contributed to the magnetoresistance. From the experimental results in the insulating phase<sup>6</sup> and the normal phase,<sup>18</sup> we conclude that a model with confinement in one dimension must be used to describe the electronic properties of the copper oxides.

We have studied the electronic density of states and impurity bands in two-dimensional semiconductors.<sup>19</sup> The experimental results<sup>5,6,18</sup> motivated us to apply our theoretical results to  $\text{La}_2\text{CuO}_{4+y}$ . The paper is organized as follows. In Sec. II we describe the model. The results are presented and discussed in Sec. III. The conclusion is in Sec. IV.

## II. MODEL AND THEORY

The excess oxygen in  $\text{La}_2\text{CuO}_{4+y}$  gives rise to holes and negatively charged impurities. We assume that the charged acceptor occupies lattice sites in planes which are between the  $\text{CuO}_2$  planes. The distance between  $\text{CuO}_2$  planes is  $d_{\text{CuO}_2} = 6 \text{ \AA}$ . An upper bound of  $3 \text{ \AA}$  for the charge distribution (half-width) of the holes perpendicular to the  $\text{CuO}_2$  sheets was determined in experiment.<sup>6</sup> From this experimental information we propose the following model: The holes are confined in a quantum well of width  $L$  and the impurities are located at the edge of the quantum well, see Fig. 1. The model is described as a two-dimensional hole gas in the presence of negatively charged impurities. For low-impurity concentrations, the charged impurities give rise to bound states and if the impurity concentration increases, the overlapping effects between bound states become important and result in an impurity band and eventually in a merging of the impurity band with the valence band.

We calculate the density of states (DOS) of the disordered two-dimensional hole gas by using the fifth Klauder approximation.<sup>20</sup> Exchange and correlation are neglected and the valence-band edge of the free-hole gas is at energy  $E = 0$ . The DOS is given as the sum over the wave vectors of the imaginary part of the Green function (the spectral density). In this paper we use  $\hbar/2\pi = 1$ . The results are presented in units of the effective Rydberg ( $1 \text{ Ry}^* = me^4/2\epsilon_L^2$ ).  $m$  is the hole mass and  $\epsilon_L$  is the dielectric constant of the host material and they define the effective Bohr radius in the system  $a^* = \epsilon_L/me^2$ . Our numerical results are for  $\text{La}_2\text{CuO}_{4+y}$  with  $m = 2m_e$  and  $\epsilon_L = 31.0$  ( $a^* = 8.2 \text{ \AA}$ ,  $1 \text{ Ry}^* = 28.3 \text{ meV}$ ).<sup>6</sup>  $m_e$  is the

electron mass in vacuum.

For the calculation we need, as an input, the Fourier transforms of the hole-impurity interaction potential  $V_{ei}(\mathbf{q}, z_i)$ .  $\mathbf{q}$  is a two-dimensional wave vector.  $z_i$  is the distance of the impurity plane from the quantum-well edge. For the two-dimensional system,  $V_{ei}(\mathbf{q}, z_i)$  is written as<sup>21</sup>

$$V_{ei}(\mathbf{q}, z_i) = -\frac{2\pi e^2}{\epsilon_L q} F_I(\mathbf{q}, z_i). \quad (1)$$

The form factor  $F_I(\mathbf{q}, z_i)$  for a quantum well with infinite barriers describes the finite confinement effects and was calculated in Ref. 22. For Eq. (1) we assumed that the charged acceptors can be described as point charges.

The two-dimensional impurity density  $N_i$ , which is active in scattering, is related to the two-dimensional hole density  $N$  in our model by

$$N_i = 2N. \quad (2a)$$

The factor 2 comes from the fact that impurities are located on both sides of the  $\text{CuO}_2$  planes, see Fig. 1. In principle, one also has to sum over the impurity layers which are further away from the considered  $\text{CuO}_2$  plane. However, because of the larger separation, the bound states due to these remote impurity layers are weakly bound and would slightly modify the valence-band edge. We emphasize that, in a bulk sample, the condition of charge neutrality is fulfilled with Eq. (2a) due to the superlattice structure.

The three-dimensional hole concentration  $N_3$  is defined by

$$N_3 = N/d_{\text{CuO}_2}. \quad (2b)$$

We use the notation of Ref. 6 and refer in our numerical results to  $N_3$ . In terms of the quantum-well parameters, we study a system with  $L = d_{\text{CuO}_2}$  and  $L/a^* = 0.71$ . Impurities (density  $N_i$ ) are located at the edges of the quantum well ( $z_i = 0$  and  $L$ ) to simulate interstitial impurities.<sup>23</sup> This corresponds to a quantum well with impurities at  $z_i = L$  and an impurity density  $2N_i$ , see Fig. 1.

## III. RESULTS

### A. Density of states

In Fig. 2 we show the DOS versus energy ( $E$ ) for five different doping concentrations. Also indicated is the Fermi energy  $\epsilon_F$  at temperature zero, assuming that the spin degeneracy is lifted. We conclude from Fig. 2 that, in the experimental available doping range ( $8 \times 10^{18} \text{ cm}^{-3} < N_3 < 7 \times 10^{19} \text{ cm}^{-3}$ ), the impurity band in  $\text{La}_2\text{CuO}_{4+y}$  is very broad. For the width  $\Gamma$  of the impurity band, we find

$$\Gamma = (1.8 \text{ Ry}^*) [N_3 / 10^{19} \text{ cm}^{-3}]^{1/2}.$$

For  $N_3 = 3 \times 10^{19} \text{ cm}^{-3}$  the impurity band has already merged with the valence band. The critical density  $N_{3c}$ , where the impurity band merges with the conduction band, is about  $N_{3c} \sim 2 \times 10^{19} \text{ cm}^{-3}$ .

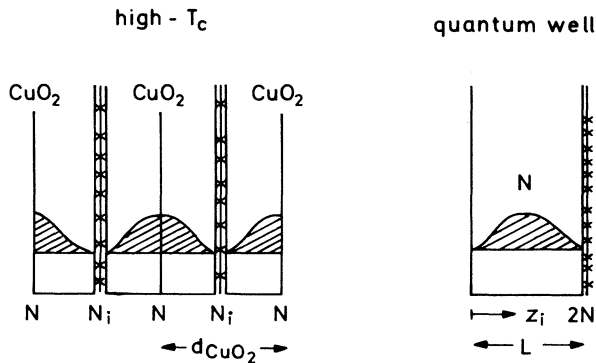


FIG. 1. We show schematically the model for the high- $T_c$  superconductor ( $\text{CuO}_2$  planes and acceptors) together with the quantum-well model.

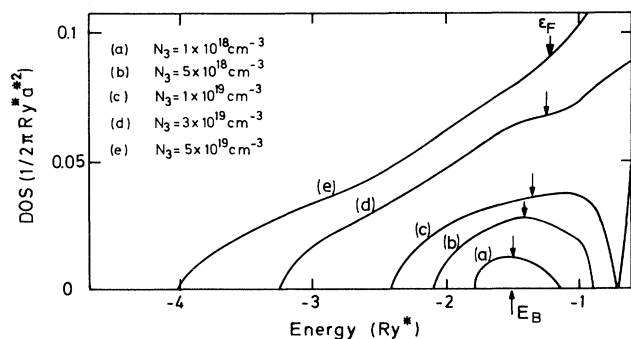


FIG. 2. Density of states (DOS) vs energy  $E$  for various hole concentrations and impurities located at the edge of the quantum well. The Fermi energies  $\epsilon_F$  are indicated by arrows.

It is a characteristic feature of our model with  $N_i = 2N$  that the Fermi energy is located near the center of the impurity band. Mott<sup>16</sup> argued that the Fermi energy is lying in the lower Hubbard band due to a finite compensation  $K_0$ . Our argument is based on the superlattice structure of the high- $T_c$  material.

If we take our value for  $N_{3c} \sim 2 \times 10^{19} \text{ cm}^{-3}$  as the actual one and if we compare this value with the experimental result<sup>6(b)</sup>  $N_{3c} > 7 \times 10^{19} \text{ cm}^{-3}$ , we conclude that the mobility edge is located in the valence band and that the Fermi energy crosses the mobility edge in the band-tail regime. We mention that  $N_c$  (or  $N_{3c}$ ) defines a Mott criterion:  $N_{ic}^{1/2} a^* = 0.13$ .<sup>19</sup> However, the underlying physics is quite different from the one in the original argument of Mott.<sup>24</sup> In two dimensions a Coulomb impurity always has a finite binding energy even in the screened case<sup>21,25</sup> and  $N_c$  is determined by the vanishing of the gap between the impurity band and the valence band. In contrast, the derivation of Mott<sup>24</sup> for the critical concentration uses the vanishing of the binding energy due to screening when the electron density increases.

A weakly screened electron-impurity interaction potential is used in our calculations. This is justified by the insulating behavior of the samples found in the experiments. We use a fixed hole density  $N = 1.0 \times 10^9 \text{ cm}^{-2}$  (which corresponds to  $N_3 = 1.7 \times 10^{16} \text{ cm}^{-3}$ ) for the screening function in order to reduce screening effects.<sup>19</sup>

The binding energy  $E_B$  of a single impurity at the edge of the quantum well is about  $1.5 \text{ Ry}^*$ , see Fig. 2. We then conclude that confining effects are important for a quantitative understanding of bound states in  $\text{La}_2\text{CuO}_{4+y}$ . With the effective Rydberg in  $\text{La}_2\text{CuO}_{4+y}$ , we get for the binding energy of a single impurity  $E_B = 42 \text{ meV}$ , which is in good agreement with experimental results.<sup>5,6</sup>

The total number of states per unit area in the impurity band for spin degeneracy equal to 1 is given by the impurity density  $N_i = 2N$ . The three-dimensional DOS is written as  $\rho_3(\epsilon_F) = \rho(\epsilon_F) / d_{\text{CuO}_2}$ . We estimate the width of the impurity band (as half-ellipse) via  $N_i \sim \pi \rho(\epsilon_F) \Gamma / 4$ . The small DOS  $\rho_3(\epsilon_F) \sim 10^{21} / \text{eV cm}^3$  at the Fermi energy for  $N_3 = 1.5 \times 10^{19} \text{ cm}^{-3}$  found in experiment<sup>6</sup> indicates

that the impurity band must be very broad:  $\Gamma = 38 \text{ meV} \sim 1.4 \text{ Ry}^*$ .

### B. Spectral density

Recently, we have studied the spectral density  $A(k, E)$  versus the impurity density for impurities located in the center of the quantum well<sup>26</sup> and versus  $z_i$  for fixed impurity density.<sup>27</sup> We have shown that, for vanishing impurity density, the spectral density is given by the Fourier transform of the squared wave function of the bound state. The studies of the spectral density versus impurity concentration provide information about overlapping effects.

In Fig. 3 we show  $A(k, E = \epsilon_F)$  versus wave number for four different doping concentrations. The normalized spectral density depends on the doping concentration. The increasing width at half maximum of the normalized spectral density with increasing hole density as shown in Fig. 3 indicates the importance of overlapping effects.

For vanishing impurity density the spectral density describes the wave function  $\Psi(k)$  in the  $\mathbf{k}$  space:  $A(k, E) \propto |\Psi(k)|^2$ . In the limit of isolated impurities, the  $1s$  bound state in an ideally ( $L = 0$ ) two-dimensional system ( $z_i = L/2 = 0$ ) is described by  $\Psi(r) \propto \exp(-r/\alpha)$  and

$$|\Psi(k)|^2 \propto 1/(1+k^2\alpha^2)^3$$

with  $\alpha = a^*/2$ .<sup>26</sup> In this case the binding energy is  $E_B = 4 \text{ Ry}^*$  and the expectation values  $\langle r^n \rangle$  are given by  $\langle r \rangle = a^*/2$  and  $\langle r^2 \rangle = a^{*2}/4$ . For  $N_3 = 5 \times 10^{17} \text{ cm}^{-3}$ , the spectral density found numerically and shown in Fig. 3 can be fitted by

$$|\Psi(k)|^2 \propto 1/(1+k^2\alpha^2)^3$$

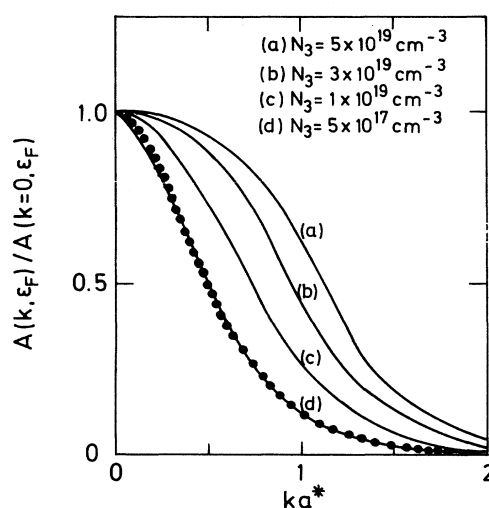


FIG. 3. Spectral density  $A(k, E = \epsilon_F) / A(k = 0, E = \epsilon_F)$  vs wave number  $k$  for various hole concentrations. The dotted line represents  $1/(1+k^2\alpha^2)^3$  with  $\alpha = 1.0a^*$ , see text.

with  $\alpha = 1.0a^*$ , see the dotted line in Fig. 3. We conclude that  $\langle r \rangle = \alpha \sim 8.2 \text{ \AA}$ . This is in agreement with estimates for the orbit  $a_0$  in the  $\text{CuO}_2$  plane from experiment:  $a_0 = 8 \pm 2 \text{ \AA}$ .<sup>6</sup> The larger value of  $\langle r \rangle = a^*$  compared with  $\langle r \rangle = a^*/2$  for the ideal two-dimensional system is due to the larger binding energy for the ideal two-dimensional system.

In order to get a better understanding of how overlapping effects change the spectral density, we study  $A(k, E)$  for  $E \sim -\frac{4}{9} \text{ Ry}^*$ , the energy of the  $2p_{\pm}$  bound state. The spectral density versus wave number for  $E = -0.4 \text{ Ry}^*$  is shown in Fig. 4. With increasing impurity density the spectral density changes dramatically due to overlapping effects. The  $2p_{\pm}$  bound state for the ideal two-dimensional system is written<sup>26</sup> as

$$|\Psi(k)|^2 \propto (ka^*)^2 / (1 + k^2\beta^2)^5$$

with  $\beta = 3a^*/2$ ,  $\langle r \rangle = 3a^*$ ,  $\langle r^2 \rangle = 81a^{*2}/8$ , and the binding energy is  $E_B = (4 \text{ Ry}^*)/9$ . The dotted line in Fig. 4 represents

$$|\psi(k)|^2 \propto 42(ka^*)^2 / (1 + k^2\beta^2)^5$$

where  $\beta = 1.85a^*$ . We conclude that, for  $N_3 = 5 \times 10^{17} \text{ cm}^{-3}$ , the spectral density for  $E = -0.4 \text{ Ry}^*$  can be interpreted as a  $2p_{\pm}$  state.

The larger spectral density at small wave numbers

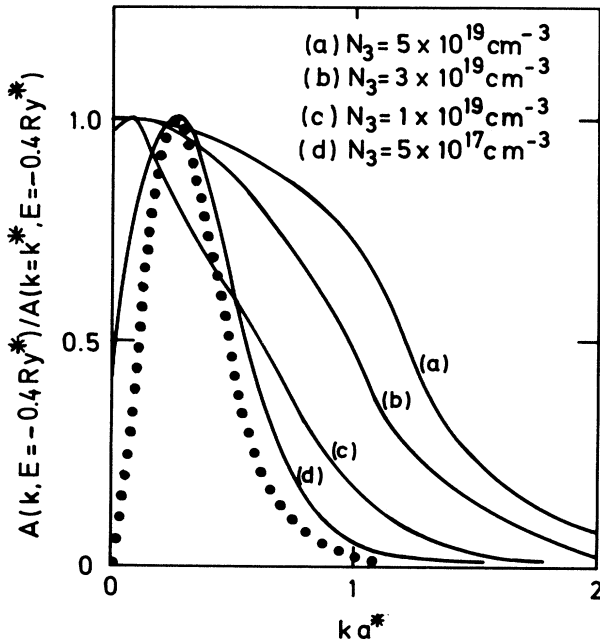


FIG. 4. Spectral density  $A(k, E = -0.4 \text{ Ry}^*) / A(k = k^*, E = -0.4 \text{ Ry}^*)$  vs wave number  $k$  for various hole concentrations.  $k^*$  is the wave number where  $A(k, E = -0.4 \text{ Ry}^*)$  has a maximum. The dotted line represents  $42(ka^*)^2 / (1 + k^2\beta^2)^5$  with  $\beta = 1.85a^*$ , see text.

( $ka^* < 0.2$ ) in the numerical result for  $N_3 = 5 \times 10^{17} \text{ cm}^{-3}$  is presumably due to hybridization effects with the  $2s$  state with  $E_B \sim 0.35 \text{ Ry}^*$ . The spectral density of the  $2s$  bound state for an ideal two-dimensional system is finite for vanishing wave number, see Table I in Ref. 26. For  $N_3 > 1 \times 10^{19} \text{ cm}^{-3}$ , hybridization effects (overlapping effects) of the  $2p_{\pm}$  with the  $2s$  state and the  $1s$  state have dramatically changed the spectral density. With increasing impurity density, strong hybridization of all the states ( $1s, 2s, 2p_{\pm}, \dots$ ) occur and for  $N_3 = 5 \times 10^{19} \text{ cm}^{-3}$  the spectral density for  $E = \epsilon_F = -1.2 \text{ Ry}^*$  (Fig. 3) and  $E = -0.4 \text{ Ry}^*$  (Fig. 4) are very similar.

### C. Discussion

In our model for the impurities, we assume that the acceptors can be described as positively charged point charges. The exact nature of the acceptor is not yet established.<sup>23</sup> For the calculations we used a very simple model (a quantum-well model with infinite barriers) with one band (the valence band) and with parabolic dispersion. Therefore, our model cannot compete with more refined band-structure calculations<sup>28</sup> where, however, disorder effects have been neglected. It is well known that a better model should include a second  $3d$  copper band, for a review see Ref. 11. The charge-transfer gap between the  $2p$  O band and the  $3d$  Cu band is about  $2 \text{ eV} \sim 71 \text{ Ry}^*$ , see Ref. 29. We do not expect that the  $3d$  Cu band seriously influences the impurity band near the  $2p$  O band edge.

The high- $T_c$  materials are *naturally* layered systems and should be described as superlattices. Superlattice effects are neglected in our model. We believe that these effects could change the binding energies of the bound state but the qualitative features of our model are probably correct.

It is shown in Fig. 2 that the Fermi energy moves slightly to higher energies with increasing hole densities. In the photoemission experiments<sup>11,14</sup> it was found that the Fermi energy is in the gap, in agreement with our calculation, and moves only slightly with doping. Exchange and correlation [ $\Sigma_{xc}(k_F, \epsilon_F)$ ] have been neglected in our calculation, but it is well known<sup>21</sup> that these effects shift the valence-band edge to negative energies. This shift increases with doping. The numerical calculation done for silicon metal-oxide-semiconductor structures<sup>30</sup> can be written as

$$\Sigma_{xc}(k_F, \epsilon_F) = E_{ex} + E_c$$

with

$$E_{ex} = -(0.71 \text{ Ry}^*)(Na^*)^{0.428}$$

and  $E_c = -0.12 \text{ Ry}^*$ .<sup>19</sup> For  $N_3 = 5 \times 10^{19} \text{ cm}^{-3}$  we get

$$\Sigma_{xc}(k_F, \epsilon_F) = -0.26 \text{ Ry}^* .$$

The real Fermi energy for  $N_3 = 5 \times 10^{19} \text{ cm}^{-3}$  would be located at

$$\epsilon_F = -1.2 \text{ Ry}^* - 0.26 \text{ Ry}^* = -1.46 \text{ Ry}^* .$$

The small increase of the Fermi energy as seen in Fig. 2 is

compensated by exchange and correlation and we expect that, the Fermi energy does not change very much with doping. We would like to mention that the calculation in Ref. 30 was done for free electrons. We expect that, for localized holes the effects of exchange and correlation are smaller than for free holes.

We have studied the spectral density. Due to the increasing hybridization of the  $1s$  state when the doping density increases (see Fig. 3), we expect that  $\langle r^2 \rangle$  for the  $1s$  state increases with increasing doping. This is because the excited bound states ( $2s, 2s, 2p_{\pm}$ ) have larger  $\langle r^2 \rangle$  than the  $1s$  state. Therefore, we expect that the polarizability also increases with increasing doping as found in experiment.<sup>6</sup>

For a more detailed analysis of the polarizability, one needs to calculate the dielectric function which is more involved. Our conclusion is based on the spectral density and the density of states and a direct comparison with the measurements<sup>5,6</sup> cannot be made. In the photoemission experiments the DOS is directly determined. The sensitivity of this method is not yet sufficient to get very detailed information on the DOS in the low-doping regime. However, we would like to mention that the density of states at the Fermi level is an important parameter for high- $T_c$  materials. A discussion on the importance of the density of states and the spectral density for theories of the high- $T_c$  materials can be found in Ref. 31.

For  $N_3 < 1 \times 10^{18} \text{ cm}^{-3}$ , the normalized spectral density is nearly independent of the doping concentration. This result indicates that the width of the impurity band (see Fig. 2) is determined by Coulomb potentials with locally different strengths and these give rise to locally different binding energies. Overlapping effects of wave functions are expected to change the spectral density. Therefore, we believe that overlapping effects are not yet very important for densities  $N_3 < 1 \times 10^{18} \text{ cm}^{-3}$ . We conclude that the width of the impurity band for  $N_3 > 1 \times 10^{19} \text{ cm}^{-3}$  is determined by overlapping effects and Coulomb potentials with locally different strengths.

The DOS of the free- (0) hole gas in two dimensions for  $m = 2m_e$  is

$$\rho^0(\varepsilon_F) = 8.4 \times 10^{14} / \text{eV cm}^2 .$$

We find

$$\rho_3^0(\varepsilon_F) = 1.4 \times 10^{22} / \text{eV cm}^3 .$$

From Fig. 2 we estimate  $\rho(\varepsilon_F) \sim \rho^0(\varepsilon_F) / 20$  for  $N_3 = 1.5 \times 10^{19} \text{ cm}^{-3}$  and we get

$$\rho_3(\varepsilon_F) \sim 0.7 \times 10^{21} / \text{eV cm}^3 ,$$

which is in reasonable agreement with the estimate from experiment [Ref. 6(b)]:

$$\rho_3(\varepsilon_F) \sim 10^{21} / \text{eV cm}^3 .$$

This agreement between theory and experiment for the DOS at the Fermi energy for  $N_3 = 1.5 \times 10^{19} \text{ cm}^{-3}$  supports our argument that the impurity band is very broad for  $N_3 = 1.5 \times 10^{19} \text{ cm}^{-3}$ .

From the magnetic-field dependence of the binding energy, one gets information about the extension of the wave functions of bound states. The analysis performed in Ref. 6(b) with theoretical expressions from Ref. 32 gave localization lengths which are about 10 times larger than estimated from the polarizability at zero field. This discrepancy might be due to the large width of the impurity band, see Fig. 2, and the application of the isolated impurity limit might be inadequate.

#### IV. CONCLUSION

We conclude from our calculations that, in high- $T_c$  materials, impurity bands (with large band width) are present for small hole densities. At large hole densities the impurity band has merged with the valence band. We believe that our work indicates that, in high- $T_c$  materials with small doping densities, disorder is an important quantity for a correct description of the density of states at the Fermi energy: The Fermi energy is located in the gap due to the renormalization of the valence band because of disorder.

Our theoretical results (the existence of an impurity band for small doping density, the density of states at the Fermi energy, the weak dependence of the Fermi energy on the doping density, and the location of the Fermi energy in the gap) are consistent with experimental results on high- $T_c$  material for the temperature-dependent conductivity,<sup>5</sup> the frequency-dependent dielectric constant,<sup>6</sup> the photoemission spectroscopy,<sup>11</sup> and the high-electron electron-energy-loss spectroscopy.<sup>12</sup>

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