Possible superconductivity at the surface of a contact of insulating La_2CuO_4

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An excess electric charge can be induced by a field or a Schottky contact at the surface of a substance such as insulating La_2CuO_4. It may be possible to observe a superconductivity in a two-dimensional system produced in this manner.

We know quite well that the compounds $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{7-\delta}$ can exist in either a superconducting or insulating (antiferromagnetic) state. The transition between these two states is controlled by the strontium concentration x or the oxygen concentration δ. According to the standard theoretical interpretation, La_2CuO_4 of stoichiometric composition, containing one conduction electron per unit cell, should be a Mott-Hubbard antiferromagnetic insulator.

The experimental data basically confirm this interpretation. The metallic behavior and the superconductivity arise only upon a change in the concentration of electrons, achieved by doping with strontium or by using a nonstoichiometric oxygen concentration. There is also the possibility that a crystalline disorder produced in this

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manner also plays a role in the superconductivity: suppressing it or, on the contrary, promoting it, suppressing the Hubbard gap and the antiferromagnetism.

In order to eliminate a side effect of the disorder, we suggest studying the superconductivity in a two-dimensional system of electrons which is induced at the surface of an insulating La_2CuO_4 single crystal or a crystal of a similar compound, by means of an external electric field at a low temperature. This effect might be implemented in structures such as a field-effect transistor or a Schottky contact. The surface of the contact should be parallel to the CuO_2 layers.

The superconductivity which arises at a contact through the Bose condensation of bipolarons in a self-consistent surface level was studied previously by Kirova and the present authors.[1] If a bipolar superconductivity occurs in these substances, the conclusions reached in Ref. 1 would be completely applicable to them. In the present letter we wish to discuss those effects which do not depend on the nature of the high-temperature superconductivity and which are related exclusively to the two-dimensional nature of the copper oxides. We assume that the CuO_2 layers are coupled only weakly to each other and that the superconductivity, like antiferromagnetism, can occur independently in each layer.

The distribution of the electric potential φ in La_2CuO_4 is described by a discrete Poisson equation with the boundary conditions

$$\epsilon_L(\varphi_{m+1}-2\varphi_m+\varphi_{m-1}) = -4\pi e d n_m,\ m = 1,2,\ldots;$$

$$\epsilon_L(\varphi_0-\varphi_1) = -\epsilon_D E_D d + 4\pi e d n_0;\ \varphi_\infty = 0. \tag{1}$$

Here e is the charge of a hole, ϵ_D and E_D are the dielectric constant and electric field in the insulating interlayer, ϵ_L is the dielectric constant of the La_2CuO_4 crystal, d is the distance between the CuO_2 layers, and φ_m and n_m are the electric potential and excess concentration of holes in the mth layer of CuO_2. In the approximation of independent layers, n_m is determined unambiguously by the value of φ_m, by virtue of the constancy of the electrochemical potential, i.e., $n_m = n(\varphi_m)$. The layer indices $m = 0, 1,\ldots$ are counted from the surface of the contact.

We first consider the case in which the bulk phase of La_2CuO_4 is not superconducting but does have a metallic state density ν; i.e., the residual doping suppresses the gap in the spectrum. In this case we have $n(\varphi) = -e\varphi\nu$. Equations (1) have the solution

$$\varphi_m = \varphi_0 \exp(-mk),\ k = \operatorname{arcch}(\eta+1),$$

$$\varphi_0 = -\epsilon_D E_D d/[\eta + (\eta(\eta+2))^{1/2}]\,\epsilon_L,\ \eta = 2\pi d\nu e^2/\epsilon_L. \tag{2}$$

with $\nu = 2$ (eV·molecule)$^{-1}$, $d = 13$ Å, and $\epsilon_L = 10$, we find $\eta = 17$ and $k = 3.5$. The electric field is thus screened by essentially a single CuO_2 layer, with the index $m = 0$. The excess hole concentration at this layer is $n_0 \approx \epsilon_D E_D/4\pi e$. If we use SiO_2, with the typical parameter values[2] $E_D = 6\times10^6$ V/cm and $\epsilon_D = 4$ as the insulating layer, we have $n_0 = 1.3\times10^{13}$ cm^{-2}, which corresponds to 2% of a hole per unit cell. This figure is slightly lower than the experimental value of the critical strontium

concentration x_c, i.e., the concentration required for the appearance of superconductivity ($x_c = 6\%$ according to the data of Ref. 3). However, the absorbed values of x_c may be determined by not only the electron concentration but also percolation effects and the suppression of superconductivity by impurity scattering. Accordingly, there is the possibility in principle of a superconductivity at small values of n_0 also, at least with a sufficiently low transition temperature. In addition, there are insulating films with far larger values of $\epsilon_D E_D$ (see Table 7 of the review by Mach and Muller[4]).

We now consider a pure insulator or La_2CuO_4 with a gap $2\Delta = 2e\varphi_c$ in its spectrum. In this case, ignoring the residual carrier concentration in the volume, we find

$$n(\varphi) = 0, \ |\varphi| < \varphi_c; \quad n(\varphi) = e\nu' \ (|\varphi| - \varphi_c), \ |\varphi| > \varphi_c. \tag{3}$$

The behavior described by (3) was found under the natural assumption that at large values of Δ the carriers have a quadratic dispersion law $\Delta + p^2/2M$. By virtue of the two-dimensional nature of the model, the state density $\nu' = M/2\pi$ is constant. The ratio ν'/ν may be either small or larger, at small and large values of Δ/t, respectively, where t is the jumping integral in the CuO_2 plane.

The solution of Eqs. (1) with function (3) depends on the potential difference (V) which is applied to the gate which controls the surface carrier concentration. Under the condition $V < V_c = \varphi_c(1 + \epsilon_L l_D/\epsilon_D l_L)$, the La_2CuO_4 crystal behaves as an insulator and does not screen out an electric field: $n_m = 0$ for all m. Here l_L is the thickness of the La_2CuO_4 crystal, and l_D is the thickness of the insulating layer. When a threshold voltage $V = V_c$, corresponding to $|\varphi_0| = \varphi_c$, is reached, the charge flows to the CuO_2 layer with index $m = 0$ and partially screens the electric field, so the potential $|\varphi_1|$ would not exceed φ_c. When the next threshold voltage is reached, charge also flows to the $m = 1$ layer, etc. The La_2CuO_4 volume breaks up into two domains: the metallic domain, which we were discussing above, and an insulating domain, across which the potential difference must not exceed φ_c. The estimates above show that in the case $\nu' > \nu$ the metallic domain consists of a single layer, for which we can use the same estimate of the excess charge density.

In two-dimensional semiconducting structures, a large fraction of the charge induced by the electric field is usually bound in surface states which are formed by ruptured valence bonds. In the layered compounds which we are discussing here, there should be few capture centers, since all of the valence bonds are complete within a single layer, and the layers are independent of each other from the chemical standpoint. Their surface, in contrast with the surfaces of three-dimensional semiconductors, should therefore not contain capture centers.

A metallization of a surface layer of CuO_2 can be observed from the change in the capacitance C of a capacitor connected between the contacts of the gate. At $V < V_c$ we have $C = \epsilon_D\epsilon_L/4\pi(\epsilon_D l_L + \epsilon_L l_D)$. If there is a substantial screening by intrinsic carriers, the length l_L should be replaced by the corresponding screening length. In the case $V \gg V_c$, nearly all of the applied voltage will drop across the insulating layer, so we will have $C = \epsilon_D/4\pi l_D$.

A manifestation of a surface conductivity can be observed in resistance measurements, if the current density in the CuO_2 monolayer does not exceed the critical

current density j_c. Taking $j_c = 10^5$ A/cm^2, as an estimate, we find that the measurement current should be limited to $j_c ld \approx l \cdot 10$ mA/cm, where l is the length of the contact. This quantity is quite large, so a superconductivity could be observed in resistance measurements.

A surface charge can also be induced by a Schottky contact. A necessary condition for charge flow is that the contact potential difference, which arises during the deposition of the metal on the La_2CuO_4 surface, be greater than φ_c. In this case the electric field is not limited by breakdown of the insulating layer. However, the surface concentration of electrons can be adjusted only by choosing a different metal.

The experiment proposed here might be used to test the charge symmetry of the properties of La_2CuO_4, which has been assumed in all single-band models, in contrast with the models which emphasize the role played by unfilled p orbitals of oxygen.[5] Under actual experimental conditions, however, one would have to allow for the effects of the residual majority carriers. When an inversion electron layer is produced in a typical p-type material, a depleted barrier layer is formed.

The effect discussed here might also be used to fabricate superconducting electronic instruments which could be controlled by an electric field. For technical purposes, there it would not be necessary to work with pure La_2CuO_4. One might create a doping level such that the material is not superconducting in the absence of an electric field, while a small change in the hole concentration induced by an applied field would cause the surface layer of the material to go superconducting.

We conclude with a list of the specific properties of the new materials which, in combination, make a surface superconductivity look feasible: the independence of the elementary layers, the absence of ruptured valence bonds at the surface, and the strong dependence of T_c on the carrier concentration.

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Translated by Dave Parsons

Feasibility of the extreme Field Effect as seen 2 decades ago,
V. Yakovenko 1988, unpublished.
Achievable concentrations of electrons at the surface of the CuO_2 plane for different gate dielectrics. x=15% was most wanted.

Dielectrics	**E_D 10^6V/cm**	**ε_D**	**$\varepsilon_D E_D$ 10^7V/cm**	**$n=\varepsilon_D E_D/4\pi e$ 10^{13} cm^{-2}**	**$x=n(3.8A)^2$ in % - 10^{-2}**
SiO_2	**6**	**4- 10**	**2.4 - 6**	**1.3 – 3.3**	**1.9 – 4.8**
Al_2O_3	**5**	**8 - 9**	**4 – 4.5**	**2.2 - 2.5**	**3.2 – 3.6**
Y_2O_3	**5**	**9 - 13**	**4.5 – 6.5**	**2.5 – 3.6**	**3.6 – 5.2**
HfO_2	**50**	**15**	**75**	**41.4**	**60**
$PbTiO_3$	**0.5**	**30 - 200**	**1.5 – 10**	**0.83 – 5.5**	**1.2 – 7.9**

Notice the promising case of HfO_2 gate. Exotic in mid-80's, it became a working material today, in epoch of high-K and 32 nm.