Why $T_c$ of LSCO is so low but $T^*$ is so high?

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Abstract. We propose the microstructural model of $La_{2-x}Sr_xCuO_4$ which supposes simultaneous coexistence in $CuO_2$ plane of nanodomains with various types of doped hole ordering. The model is based on earlier proposed mechanism of negative-U centers (NUC) formation in HTSC under doping. In accordance with proposed mechanism such nanodomain structure in underdoped (overdoped) sample results in simultaneous coexistence of superconducting and insulating (normal metal) nanodomains. Bulk superconductivity arises thanks to the Josephson links between superconducting microdomains, whose $T_c$, $T^*$ and $T^\nu$ are defined by number NUC’s involved in the given nanodomain. In the framework of the presented model we have calculated $La_{2-x}Sr_xCuO_4$ phase diagram, which was found to be in the remarkable agreement with the experimental one.

1. Introduction

$La_{2-x}Sr_xCuO_4$ is the most studied high-$T_c$ superconducting compound whose phase diagram exhibits many well-reproducible features. However, most of them have no satisfactory explanation up to now. In particular it concerns of 1) the reason of low temperatures of superconducting transition at simultaneous existence of diamagnetic regions up to 70 K [1], and 2) the reason of wide temperature interval (up to 120 K) of anomalous Nernst effect [2].

Earlier we proposed [3,4] the mechanism of NUC formation in HTSC under doping. The model is based on the assumption of rigid localization of doped holes in the vicinity of Sr dopants. According to the model [3,4] the NUC’s in $La_{2-x}Sr_xCuO_4$ are formed on pairs of neighboring $Cu$-ions in the $CuO_2$ plane if the doped holes are localized on four oxygen ions around two neighboring $Cu$ sites (Figure 1). We distinguish four different types of mutual arrangement of two doped holes, which determine the local properties of the crystal for $x<0.25$. Simple estimation shows that the doped hole localized on oxygen ion is able to reduce the charge-transfer gap $\Delta_t$ for the four nearest $Cu$ ions by $\sim$1.6-1.8 eV. If two localized doped holes are spaced $3a$ or $a\sqrt{5}$, where $a$ is the lattice constant in $CuO_2$ plane (Figure 1a,c), they reduce the charge-transfer gap $\Delta_t$ for the interior pair of nearest $Cu$ ions to the extent that it is possible two-electron transition to this pair of $Cu$ ions from neighboring oxygen ions while single-electron transitions are still impossible. These arrangements correspond to the formation of NUC on the interior pair of nearest $Cu$ ions. It is important that in the intermediate case, when the doped holes are spaced $a\sqrt{8}$ (Figure 2b), no pairs of the nearest $Cu$ ions can emerge, each having a nearby doped hole, i.e. a NUC is not formed. If doped holes are spaced $2a$ (Figure 1d), then for the inner $Cu$ ion the gap $\Delta_t$ vanishes for single-electron transitions too. This last case corresponds to that of ordinary metal.
Figure 1. (a-d) - the types of arrangement of two nearest localized doped holes in \( \text{CuO}_2 \) plane. (a, c) if the doped holes are spaced \( 3a \) or \( a \sqrt{5} \) the NUC (shaded ellipse) is formed on the interior pair of nearest Cu ions; (b) if the doped holes are at a distance \( l = a \sqrt{8} \), no pairs of the nearest Cu ions can emerge each having the doped hole in the neighborhood, i.e. a NUC is not formed; (d) if doped holes are spaced \( 2a \), then for the inner Cu ion the gap \( \Delta_v \) vanishes for single-electron transitions too. This case corresponds to the ordinary metal; e) Thin curve shows the boundary of nanodomain including percolation cluster of NUC’s formed by doped holes spaced \( l = \sqrt{5} \) apart. Solid circles are the projections of dopant ions (Sr) onto the \( \text{CuO}_2 \) plane. Open circles and rectangles are the localization regions of doped holes and additional hole pairs around NUC’s, correspondingly.

Thus doped carriers in our model are localized, and they are responsible for the formation of NUC’s. These NUC’s act as pair acceptors and generate additional holes. Pair hybridization of valence band states with NUC’s determines the behavior of high-\( T_c \) superconductors. In such system the electron pairing responsible for high-\( T_c \) superconductivity emerges because of strong renormalization of the effective electron-electron interaction when scattering with intermediate virtual bound states of NUC’s is taken into account [5-8].

The proposed mechanism of the interaction between electrons from valence band and pair states is effective if the NUC’s form percolation clusters. In \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) such clusters can be formed along broken lines with segments (connecting doped holes) whose length is \( l_{\text{com}} = 3 \) or \( l_{\text{com}} = \sqrt{5} \) (in units of \( a \)). In general case there is no reason to expect the presence of large clusters with properties totally determined by one of the types of arrangement shown in figure 1(a-d). In addition the sizes of such clusters in \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) are confined by doped holes localized around some Cu sites in \( \text{CuO}_2 \) plane because they prevent these Cu sites to form NUC’s. (Unlike \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \), in single-plane \( \text{Ta}_2\text{Ba}_2\text{CuO}_6-x, \text{HgBa}_2\text{CuO}_4+\delta \) and two-plane HTSC compounds the doped holes are localized out of \( \text{CuO}_2 \) plane). Therefore, it should be expected that only small nanodomains including of some segments of broken lines \( l_{\text{com}} = 3, \sqrt{5} \) in length will be formed in \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \). Their sizes and quantity will grow at approach to commensurable concentration \( x = 1/9 \) and \( 1/5 \), accordingly. The existence of such nanodomains with a given \( l_{\text{com}} \) is possible in the concentration range satisfying the condition \( 0.593/l_{\text{com}}^2 < x \leq 1/l_{\text{com}}^2 \). This range is bounded above by \( x_{\text{com}} = 1/l_{\text{com}} \) value; at higher concentrations, the existence of physically significant domains with given \( l_{\text{com}} \) violates the condition of mean concentration constancy. Nanodomains with a given \( l_{\text{com}} \) distance remain intact up to some \( x = x_p \) value, which corresponds to the two-dimensional percolation threshold \( x_p = 0.593 \) at a random distribution of doped holes. That is the percolation cluster serves as a carcass of a given nanodomain (figure 1e).

2. Phase diagram of \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \)

As follows from our reasoning \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) must be treated as a set of two-dimensional nanodomains where doped holes can form percolation clusters with \( l_{\text{com}} = 3, \sqrt{5} \) (NUC chains), \( l_{\text{com}} = 2 \) (conventional metal) and \( l_{\text{com}} = \sqrt{8} \) (insulator). The boundaries of regions of the existence of percolation broken lines with segment lengths \( l_{\text{com}} \) are shown in figure 2a. The percolation regions for domains with \( l_{\text{com}} = 3 \)
and \( \sqrt{5} \), that is for NUC clusters, are indicated by thick lines. The experimental phase diagram \( T_c(x) \) for \( La_{2-x}Sr_xCuO_4 \) is shown in figure 2b. The coincidence of the regions of superconductivity in the experimental phase diagram with intervals of percolation for \( l_{\text{com}} = \sqrt{5} \) and 3 proves the conclusion that the fragments in question, which include pairs of neighboring Cu ions in \( CuO_2 \) plane, are responsible for superconductivity in \( La_{2-x}Sr_xCuO_4 \).

![Figure 2](image2.png)

Note that the “dip” in \( T_c(x) \) in the range \( 0.11 < x < 0.12 \), caused by the absence of percolation over the chains of NUC’s, is superimposed on the region of existence (as \( x \to 1/8 \)) of \( \sqrt{6} \times \sqrt{6} \) lattice of doped holes corresponding to the insulating phase. In our recent work [10] we have shown that just this feature makes it possible to observe in this region a static incommensurable magnetic texture which imitates static stripe modulation with an incommensurability parameter \( \delta = x \).

The temperature of superconducting transition \( T_c \) of nanodomains with \( l_{\text{com}} = 3 \) and \( \sqrt{5} \) is depressed relatively infinite domain by fluctuations [11]. The matter is that the potential of superconducting pairing depends on occupancy of pair level and the superconductivity turns on if the occupancy is less than some critical value. Therefore in small clusters (containing small number of NUC’s) the thermal fluctuations of pair level occupancy may turn on (turn off) the superconductivity at \( T > T_{c\infty} \) \( (T < T_{c\infty}) \), where \( T_{c\infty} \) is \( T_c \) for infinite cluster. There are two temperatures \( T_c \) and \( T^* \) \( (T_c < T_c < T^*) \) for each size of cluster (and, consequently, for each doping level) so that in the range \( T_c < T < T^* \) cluster “fluctuates” between superconducting and normal states.

Figure 3. The dependence of the temperatures \( T^* \) and \( T_c \) on the number of NUC in cluster - \( N_U \) [11]. The inset shows the same dependence for \( N_U < 50 \).
We have calculated $T_c$ and $T^*$ in dependence on number of NUC’s in cluster (figure 3 [11]). In the framework of model these temperatures arise as two roots of the same equation. As it follows from figure 4 for optimally doped $La_{2-x}Sr_xCuO_4$ with $T_c=40K$ the average size of clusters which define $T_c$ includes no more than 5 NUC (or 10 Cu sites). Actually in morphology and properties optimally doped and underdoped $La_{2-x}Sr_xCuO_4$ is similar to underdoped $YBa_2Cu_3O_{6+\delta}$ with $\delta<0.65$.

At the same time $T^*$ goes up with decreasing of NUC number in cluster, i.e. small nanoclusters may became superconducting due to fluctuation of NUC occupancy starting from $T^*>T_c$. The lifetime of such fluctuations increases with temperature lowering. Starting from certain temperature $T^*$ the fluctuations lifetime becomes to be large enough for the superconducting nanoclusters to form big cluster by means of Josephson coupling. In such long-life superconducting clusters the giant Nernst effect and anomalous diamagnetism gets to be observed.

Conclusion
In conclusion we propose the microstructural model of $La_{2-x}Sr_xCuO_4$, which supposes simultaneous coexistence in CuO$_2$ plane of nanodomains with various type of doped hole ordering. With regard to the proposed mechanism such fragmentation in underdoped (overdoped) sample results in simultaneous coexistence of superconducting and insulating (normal metal) nanodomains. Bulk superconductivity arises thanks to the Josephson links between superconducting microdomains, whose $T_c$, $T^*$ and $T^*$ are defined by number NUC’s involved in the given microdomain. In the framework of the presented model we have calculated $La_{2-x}Sr_xCuO_4$ phase diagram which was found to be in the remarkable agreement with experimental one.

Acknowledgements
This work supported by RFBR (grant 08-02-00881) and Russian Federal Agency for Science and Innovations (contract 02.552.12.7003).

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