Band spectrum transformation and T_c variation in the $La_{2-x}Sr_xCuO_y$ system in the underdoped and overdoped regimes

M. V. Elizarova* and V. E. Gasumyants
Department of Semiconductor Physics and Nanoelectronics, St. Petersburg State Technical University, 29 Polytekhnicheskaya, St. Petersburg, 195251, Russia
(Received 6 March 2000)

The results on the resistivity and thermopower temperature dependences for the $La_{2-x}Sr_xCuO_y$ ($x=0.05-0.30$) system are presented. The experimental data together with the thermopower results of other authors have been analyzed within a phenomenological narrow-band model. This model was shown to be applicable to the $La_{2-x}Sr_xCuO_y$ system that gives a strong support for a narrow peak of the density-of-states in the vicinity of the Fermi level to exist in the band spectrum of high-T_c superconductors. Within the narrow-band model we have determined the main band spectrum parameters (the band filling degree, the effective bandwidth, and the degree of the charge carriers localization) and traced their variation with an increasing Sr content in the $La_{2-x}Sr_xCuO_y$ system. These parameters were shown to change in a different way in the underdoped regime and the overdoped one that points to a distinction between those two regimes. Nevertheless we have observed that the critical temperature value correlates with the total effective bandwidth so that the maximal T_c at the optimal doping level corresponds to a minimum of the bandwidth. Based on the results obtained we discuss the genesis of the conduction band in the underdoped regime as well as a mechanism of its transformation in the overdoped regime. The possible reasons for the modification of the superconducting properties of the $La_{2-x}Sr_xCuO_y$ system with increasing Sr content, both in the underdoped regime and the overdoped one are also considered.

I. INTRODUCTION

Despite numerous studies there is still no clear understanding of all the processes accompanying the crossover from the underdoped regime to the overdoped one in high-T_c superconductors (HTCS's). To study this question the $La_{2-x}Sr_xCuO_y$ system is a very promising object due to a possibility to go throughout both those regimes by a gradual Sr doping while well-investigated Y-based HTSC's have a limited and hardly realized overdoped region.

It is well known that $La_{2-x}Sr_xCuO_y$ demonstrates a nonmonotonic dependence of the critical temperature T_c on the doping level. With increasing Sr content the T_c value rises in the underdoped regime ($0.05 \leqslant x \leqslant 0.15$) reaching a maximum at the optimal doping level and then falls in the overdoped regime ($x > 0.15$).[1–3] At present, there is no consensus on the physical reason for the superconductivity to appear under Sr doping in the underdoped regime, as well as for the superconductivity suppression in the overdoped one. The first question is related to the problem of the proximity of the insulating and superconducting states in the HTSC's. It is not clear what mechanism plays the main role in an insulator-superconductor transition, how the band structure changes under doping and what the properties and main parameters of the band responsible for both superconducting and normal-state properties of those compounds are. As for the overdoped regime, several approaches have been proposed to explain the observed drop of T_c in $La_{2-x}Sr_xCuO_y$ such as a phase instability,[4] a perturbation of the periodic potential in the CuO_2 sheets because of the oxygen vacancies formation,[5] a decrease of the effective magnetic interactions caused by hole doping.[6] However, this question remains still open and calls for further investigations.

Considering different HTCS's systems, it is necessary to note that in the last few years many authors have assumed the existence of a narrow peak in the density-of-states (DOS) function of HTCS's materials to be responsible for their normal-state[7–12] and superconducting[13–17] properties. Different microscopic models were discussed to clarify possible reasons for this narrow peak formation such as the presence of the Van Hove singularity,[18] the formation of a narrow ''impurity band'' in the Mott-Hubbard gap,[19–23] and models based on an assumption of the charge transfer by quasiparticles with a large effective mass.[11,24,25] In particular, studying the $La_{2-x}Sr_xCuO_y$ system Mamedov *et al.*[26] and Bok and Bouvier[27] argue that T_c depends nonmonotonically on the Sr content because the Fermi level passes through a DOS peak when the doping level increases. In addition, Rietveld *et al.*[28] studying the doping dependence of the chemical potential have concluded that their results can be best explained assuming that an increasing Sr content results in the doping of a narrow band lying near the middle of the gap. However, quantitative estimations of parameters of this peak or band and the comparison of their variation under doping with changing superconducting properties are still absent.

We have earlier proposed a phenomenological narrow-band model allowing us to describe the temperature dependences of the transport coefficients (the resistivity, thermopower, Hall coefficient), to determine some band spectrum parameters, to trace their variation under different deviations from stoichiometry, and to observe a correlation between the parameters of the charge-carrier system in the normal state and the T_c value.[29] As shown in our previous publications,[29–32] this model can be successfully employed

TABLE I. Lattice parameters and oxygen content of $La_{2-x}Sr_xCuO_y$.

x	a, Å	b, Å	c, Å	y
0.00	5.396	5.356	13.144	4.03
0.05	5.371	5.369	13.219	4.02
0.10	5.350	5.350	13.220	4.01
0.15	5.340	5.340	13.237	3.99
0.20	5.335	5.335	13.246	3.95
0.25	5.330	5.330	13.260	3.93
0.30	5.331	5.331	13.261	3.90

to study the doping effect in the Y- and Bi-based HTCS's. In this paper we show the applicability of our approach to the case of La-based HTCS's and use it to discuss the band genesis and band spectrum transformation in $La_{2-x}Sr_xCuO_y$ in comparison with changing superconducting properties in both underdoped and overdoped regimes.

II. SAMPLES AND EXPERIMENTAL DETAILS

The resistivity and thermopower measurements were performed for a series of $La_{2-x}Sr_xCuO_y$ ceramic samples ($x=0.05-0.30$). The samples were prepared by the standard solid-state powder processing technique. The high-purity powders of the respective oxides (La_2O_3, SrO, CuO) were mixed in the required proportions and ground. The mixtures were calcined at 970 °C for 20 h, reground, then pressed into pellets and sintered at 990 °C for 20 h. Finally, the pellets were heated in flowing oxygen at 450 °C for 10 h and furnace cooled down to room temperature. All the samples were subjected to x-ray powder diffraction analysis, which showed that they were of single-phase with an accuracy of 1–2 %. The lattice parameters are shown in Table I. At low Sr content the sample structure is orthorhombic. With increasing doping level the orthorhombic distortion measured at room temperature decreases and becomes negligible at $x>0.05$ in agreement with data of Refs. 33–35. The oxygen content of all the samples was determined by iodometric titration to an accuracy of ± 0.01 and also presented in Table I. The observed decrease in the y value with increasing Sr content is in agreement with the published data.[35] Note, that in the overdoped regime the oxygen content decreases with x stronger compared to the underdoped one.

The resistivity and thermopower were measured for all the samples in the temperature range of $T=T_c-300$ K. The resistivity was measured by the standard four-probe method. The thermopower was measured relative to copper electrodes, its absolute value was calculated by correcting for the thermopower of copper. The temperature difference between the two ends of the sample was kept around 1–2 K throughout the measuring procedure and measured by a copper-constantan thermocouple mounted inside the copper electrodes.

As noted above, the aim of this paper is to check the applicability of the narrow-band model to the $La_{2-x}Sr_xCuO_y$ system as well as to reveal the main tendencies of the band spectrum transformation with increasing Sr content. We have earlier shown the thermopower to be the most informative transport coefficient for the quantitative analysis in the framework of this model.[29,30] For this reason, in order to obtain reliable and more detailed information for further analysis, in addition to our data we will use the experimental results on the thermopower available in publications of other authors[5,36,37] who have also used the standard ceramic techniques of sample preparation with some differences in annealing regimes.

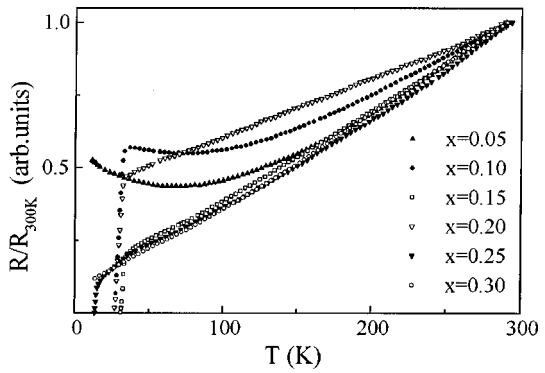

FIG. 1. The normalized resistance vs temperature for $La_{2-x}Sr_xCuO_y$.

III. RESULTS AND THIER ANALYSIS WHITHIN THE NARROW-BAND MODEL

For the undoped sample the resistivity demonstrates the typical semiconducting behavior increasing strongly as temperature decreases and the absolute value of the thermopower is big ($S\approx 200-250\ \mu$V/K). The temperature dependences of the normalized resistance for samples with $x=0.05-0.3$ are shown in Fig. 1. As one can see increasing doping results in the transformation of the resistivity from an insulatorlike to a metal-like behavior. Note, that contrary to the underdoped region in the overdoped one the $\rho(T)$ dependence retains to be linear for the samples with a low T_c value and even for nonsuperconducting $La_{1.7}Sr_{0.3}CuO_y$.

The critical temperature value as a function of the Sr content is shown in Fig. 2 together with data of Refs. 5,36,37. It is seen that our data are in agreement with those obtained for $La_{2-x}Sr_xCuO_y$ by other authors. The critical temperature has a maximum at $x=0.15$, the superconductivity arises at $x>0.05$ and vanishes at $x>0.25$. A disagreement between the T_c values obtained by different authors is obviously

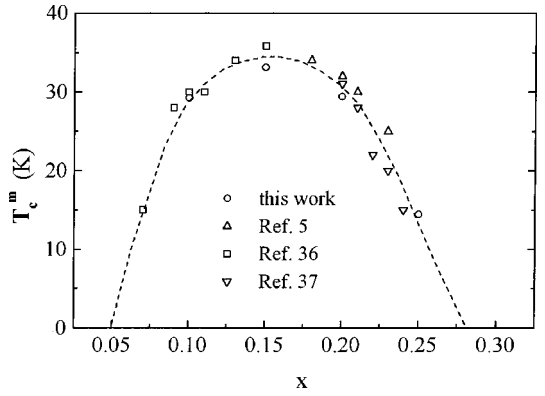

FIG. 2. The critical temperature vs Sr content in $La_{2-x}Sr_xCuO_y$.

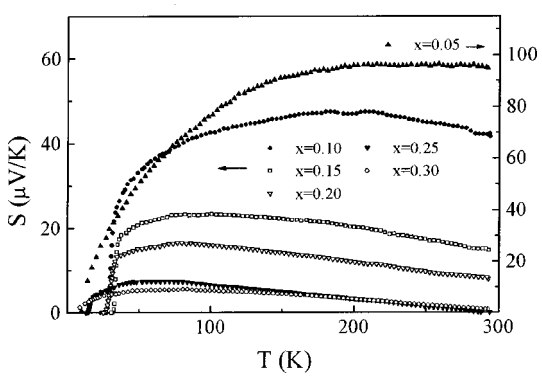

FIG. 3. The thermopower vs temperature for $La_{2-x}Sr_xCuO_y$.

caused by different oxygen content that results from the used oxidizing regime. Since our aim is to study the main peculiarities of the band spectrum transformation in the underdoped and overdoped regimes on the basis of the analysis of the normal-state transport properties we do not consider an anomalous suppression of superconductivity in a local region around $x \approx 0.12$.[36] Note, that Kumagai *et al.*[36] indicated that they did not find any anomalous behavior in the normal state including the thermopower data.

The temperature dependences of the thermopower for samples with $x = 0.05-0.30$ are shown in Fig. 3. The specific features of the thermopower behavior can be summarized as follows. At low doping level (when the absolute value of the thermopower is big) the $S(T)$ curves look to be typical for all the HTCS's systems. At high temperatures, the thermopower increases slightly as temperature decreases, then has a broad maximum and finally falls down. With increasing Sr content the absolute value of the thermopower decreases and a maximum of the $S(T)$ curves shifts downwards lower temperatures. For $x \geqslant 0.15$ the thermopower increases almost linearly with decreasing temperature becoming qualitatively analogous to that for most HTCS's systems, excluding the Y-based one. Note, that all the peculiarities of the $S(T)$ dependences and their modification under doping are in agreement with those obtained in Refs. 5,36,37. The value of the thermopower at room temperature $S_{300\,K}$ as a function of Sr content obtained both by us and in Refs. 5,36,37 is shown in Fig. 4. Comparing the data of different authors allows one

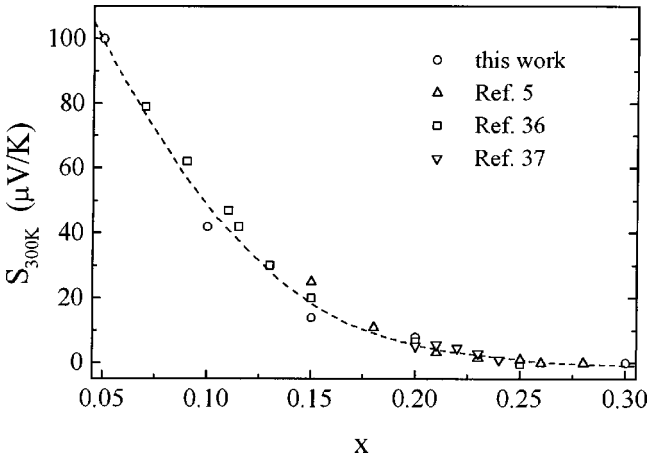

FIG. 4. The thermopower value at room temperature as a function of the Sr content in $La_{2-x}Sr_xCuO_y$.

to clearly recognize the doping effect on the thermopower value. Increasing Sr content results in a decrease of the thermopower from about 100 μV/K for $x = 0.05$ down to a very small value for $x > 0.2$. It is necessary to note, that the $S_{300\,K}$ value falls rapidly for $x < (0.15-0.20)$, i.e., in the underdoped regime, and changes insignificantly with further increase of the Sr content in the overdoped regime.

Both our results and data of Refs. 5,36,37 have been analyzed within the narrow-band model described in details elsewhere.[29] Our model is based on an assumption that the band structure of HTCS's contains a narrow density-of-states peak located near the Fermi level E_F. Two possible scenarios of the peak formation are the Van Hove singularity in the DOS function[12] and states transfer resulting in the midgap bandlike states appearance.[22,23,38] We have earlier shown that in this case it is the narrowness of this peak that mainly determines the peculiarities of the electron transport in the normal state.[29] This allows us to use the simplest approximation for the DOS $D(E)$ and differential conductivity $\sigma(E)$, functions in the form of rectangles of different width. If so, one can obtain the analytical expressions for the temperature dependences of the chemical potential μ and the transport coefficients, which can be used for quantitative comparison of the experimental results and calculated data. In doing so, the three model parameters can be determined. These are the band filling with electrons F, which is equal to the ratio of the number of electrons to the total number of states in the band; the total effective bandwidth W_D, and the ''conductivity'' effective bandwidth W_σ. Note, that the variation of the ratio W_σ/W_D with changing sample composition characterizes the variation of the degree of the charge carriers localization.[29] Within this approach, the thermopower can be described as

$$S = -\frac{k_B}{e}\left\{\frac{W_\sigma^*}{\sinh W_\sigma^*}\left[\exp(-\mu^*)+\cosh W_\sigma^* - \frac{1}{W_\sigma^*}(\cosh\mu^*+\cosh W_\sigma^*) \times \ln\frac{\exp(\mu^*)+\exp(W_\sigma^*)}{\exp(\mu^*)+\exp(-W_\sigma^*)}\right]-\mu^*\right\}, \quad (1)$$

where

$$\mu^* \equiv \mu/k_BT = \ln\frac{\sinh(FW_D^*)}{\sinh[(1-F)W_D^*]}, \quad (2)$$

k_B is the Boltzmann constant, e is the electron charge, $W_D^* \equiv W_D/2k_BT$, and $W_\sigma^* \equiv W_\sigma/2k_BT$. These formulas are derived for the case of a symmetric band. Our previous results showed such an assumption to be justified for the $YBa_2Cu_3O_y$ system (see Refs. 29,31,32). On the other hand, to explain the $S(T)$ dependences for the Bi-2212 and Bi-2223 samples we have involved the assumption about a slight asymmetry of the conduction band. As mentioned above, the $S(T)$ dependences for the $La_{2-x}Sr_xCuO_y$ system are analogous, in their main peculiarities, to those for the Bi-based HTCS's. This fact suggests the conduction band in this case also to be asymmetric. For this reason, to achieve the best agreement of the experimental and calculated results

we have used an asymmetric narrow-band model. It is shown in Refs. 29,30 that the simplest method to take the asymmetry into account is the introduction of some distance bW_D (where b is the asymmetry parameter) between the centers of rectangles approximating the DOS and differential conductivity functions. In this case μ^* calculated by formula (2) should be replaced by $\mu^* - bW_D/k_BT$ and formula (1) remains valid. It should be stressed, that formula (2) gives a possibility to calculate the exact value of S (in units of μV/K) so that it can be used for the quantitative analysis of the experimental $S(T)$ data allowing to determine the values of the band spectrum parameters for samples of different composition.

Thus to describe quantitatively the temperature dependences of the thermopower for the $La_{2-x}Sr_xCuO_y$ system it is necessary to use the asymmetric narrow-band model containing four fitting parameters. If so, before analyzing the concentration dependences of these parameters the question on uniqueness of determination of their values from the experimental data analysis has to be investigated. In the framework of the symmetric narrow-band model all the three parameters (F, W_D, W_σ) can be determined uniquely because each of them affects different peculiarities of the $S(T)$ curve.[29] The introduction of an additional asymmetry parameter (b) can generally lead to a broadening of the possible region of the variation of all the parameters values giving a possibility to fit reasonably the experimental data. For this reason, we have preliminarily studied the influence of the possible range of b values on the accuracy of determination of other parameters.

First, we have observed that the degree of the band asymmetry is very small and the b value can be varied in a narrow region $[b = -(0.01-0.04)]$. Further, one can suppose that a tendency in b variation with doping level is attributed to the nature of the band transformation under increasing Sr content. Taking this into account, we have tried to fit the experimental data for three different types of b variation with x. Those are a gradual rise of the band asymmetry (increasing asymmetry degree), the fixed b value for all the samples (unchanged asymmetry degree), and the fixed bW_D value [a fixed shift between the centers of rectangles approximating the $\sigma(E)$ and $D(E)$ functions]. The first approach was observed not to allow to fit the experimental data for all the samples well. The second and the third ones give reasonable fitting results. To demonstrate this we present in Fig. 5 the best-fitted curves for several samples (both ours and measured in Refs. 5,36) calculated for the cases of fixed either b or bW_D values. As one can see, the fitting results look to be reasonable for a temperature range from $T = 300$ K temperature down to at least $T = 70-100$ K. At lower temperatures there is a discrepancy between the experimental data and calculated curves. This is due to the fact that expressions we use are derived in the framework of the assumption that the Fermi smearing is comparable with the bandwidth W_D. At $T < 100$ K this condition ($W_D \cong k_BT$) is obviously violated, so that the model becomes far too rough and calculations give an error. Note, that as compared to the $YBa_2Cu_3O_y$ system, in $La_{2-x}Sr_xCuO_y$ violation of the $W_D \cong k_BT$ condition leads to a more essential discrepancy of the experimental and calculated results because the temperature of the superconducting transition in $La_{2-x}Sr_xCuO_y$ is lower than in $YBa_2Cu_3O_y$, whereas the value of the bandwidth is close to that for $YBa_2Cu_3O_y$ as it will be shown below.

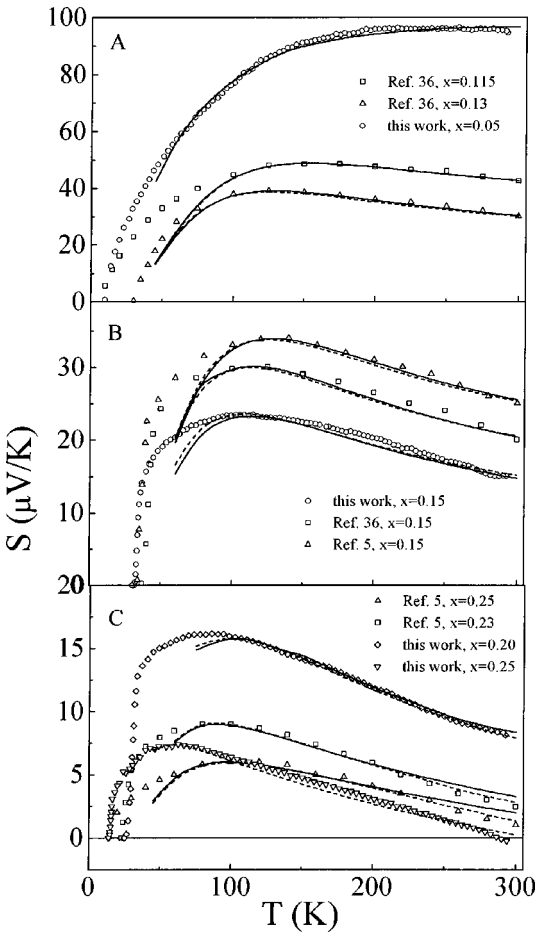

FIG. 5. The experimental and calculated $S(T)$ dependences for $La_{2-x}Sr_xCuO_y$. Different symbols present the experimental data, lines are the best-fitted curves calculated within the narrow-band model in case of fixed bW_D (solid lines) or fixed b (dashed lines) values with increasing Sr content.

Figure 5 shows that in the underdoped regime ($x < 0.15$) both used types of varying asymmetry degree give good fitting results. In the overdoped regime ($x > 0.20$) the case of fixed b value is more preferable. This result means, taking into account variation of the bandwidth with Sr content presented below, that the difference between the $D(E)$ and $\sigma(E)$ rectangles centers characterizing the band asymmetry, remains constant or even decreases in the underdoped regime, but increases in the overdoped one. This suggests the nature of the band transformation in those two regimes to be rather different, that will be discussed hereafter. In addition, we have performed the calculations for each sample, using the whole possible range of the b variation. The calculation results have shown that the values of the main band spectrum parameters (F, W_D, W_σ) vary quite insignificantly for each sample that makes it possible to reveal reliably the tendencies in their variation throughout the whole range of doping. The concentration dependences of the band filling and the bandwidth are shown in Figs. 6 and 7, respectively, with an error of their determination resulted from the possible range of the b variation. As for the W_σ value, we have noted above that the variation of the W_σ/W_D ratio is more informative

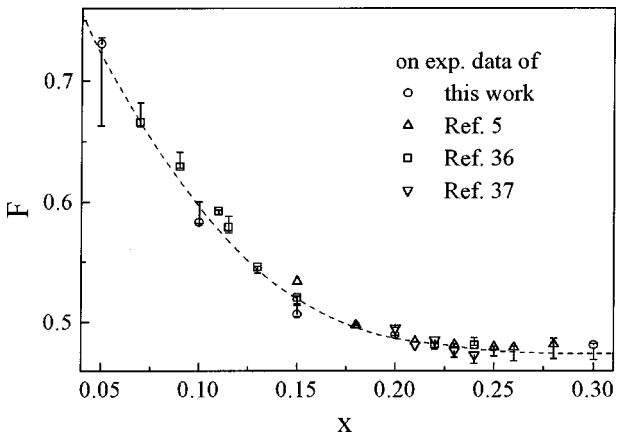

FIG. 6. The band filling as a function of the Sr content in $La_{2-x}Sr_xCuO_y$.

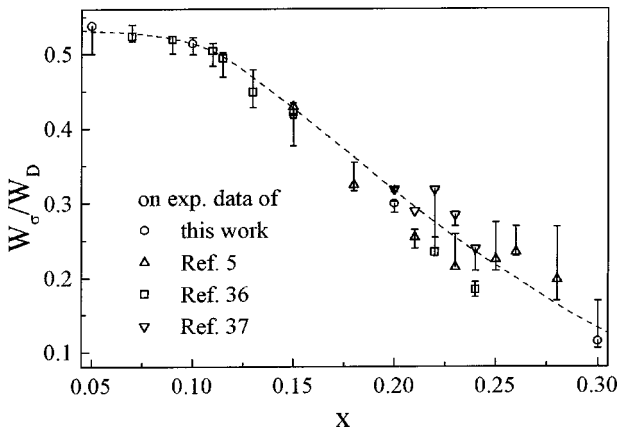

FIG. 8. The W_σ/W_D ratio as a function of the Sr content in $La_{2-x}Sr_xCuO_y$.

because it characterizes the changing degree of the charge carrier localization. For this reason Fig. 8 shows the W_σ/W_D value as a function of the Sr content. The results presented in Figs. 6–8 allow one to conclude that applying the asymmetric narrow-band model to the analysis of the thermopower of $La_{2-x}Sr_xCuO_y$ we can determine the main band spectrum parameters with a good accuracy and, therefore, can use these data to discuss the band transformation with Sr content.

Let us first point to the values of the band spectrum parameters, which are characteristic of the $La_{2-x}Sr_xCuO_y$ system as a whole and the main tendencies in their changes under doping. The effective bandwidth changes in a range of 90–170 meV depending on the Sr content that is of the same order as in undoped and slightly doped samples of the Y-based (Refs. 29,31,32) and Bi-based[30] HTCS's. At the same time, it is necessary to note that contrary to the last two systems the W_D value in $La_{2-x}Sr_xCuO_y$ changes nonmonotonically with increasing doping level, decreasing in the underdoped regime and increasing in the overdoped one. As a result, the W_D value has a minimum at $x \approx 0.15$, i.e., at the optimal doping level corresponding to a maximum of the $T_c(x)$ dependence. The band filling F drops rapidly with increasing doping in the underdoped regime (at $x = 0.05-0.18$, from $F \approx 0.7$ to the value about 0.5), but throughout the entire overdoped region F remains almost constant. Let us note that our data on the band filling change under doping are in a good agreement with the results of Rietveld *et al.*[28] who have observed that the chemical potential in $La_{2-x}Sr_xCuO_y$ shifts continuously as a function of Sr content. They have concluded that both the ''impurity model'' assuming that doping creates the states in the Mott-Hubbard gap while the chemical potential remains more or less unchanged near the middle of the gap and the ''semiconducting model'' assigning the increase of the $D(E_F)$ value and a strong shift of the chemical potential from the middle of the gap to the top of the valence band under doping cannot explain their experimental results on the photoelectron spectra. In the framework of our approach the observed $F(x)$ dependence can be easily explained as shown in the next section.

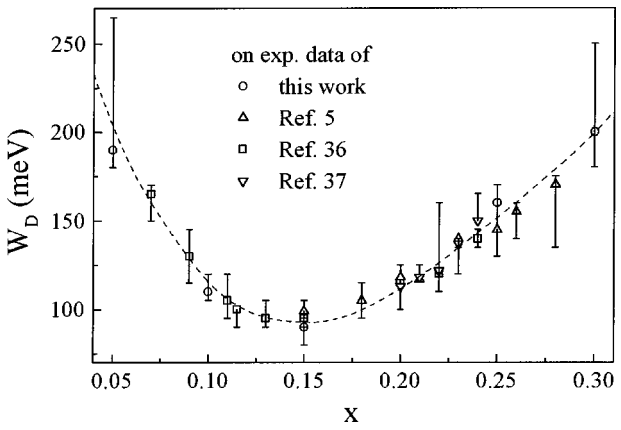

FIG. 7. The effective bandwidth as a function of the Sr content in $La_{2-x}Sr_xCuO_y$.

Our calculations also show that the W_σ/W_D ratio decreases gradually with increasing Sr content, but to a different extent before and after the optimal doping (see Fig. 8). In the underdoped regime it changes insignificantly (from 0.53 to 0.42 as x runs from 0.05 to 0.15) being almost unchanged for $x = 0.05-0.11$, whereas in the overdoped one the W_σ/W_D ratio falls rapidly (from 0.42 to 0.11 at $x = 0.15-0.30$). In the framework of our model this means that the degree of the charge carrier localization changes insignificantly in the first region of doping and increases strongly in the second one. Thus all the parameters characterizing the properties of the charge-carrier system in $La_{2-x}Sr_xCuO_y$ change with increasing Sr content to a different extent (or even to a different way in the case of the bandwidth), before and after the optimal doping level. This clearly indicates that the band spectrum transformation in the underdoped and overdoped regimes is caused by different reasons pointing to a distinction between those two regimes. Below we discuss the possible reasons for the observed band spectrum transformation throughout the whole doping range.

IV. DISCUSSION

A. Underdoped regime

Let us first discuss the possible mechanism of the conduction band genesis. As shown analytically and by the quantum Monte Carlo technique (see Refs. 22,38–40) doping of a Mott insulator initiates an appearance of bandlike states in the Mott-Hubbard (MH) gap resulting in the formation of a

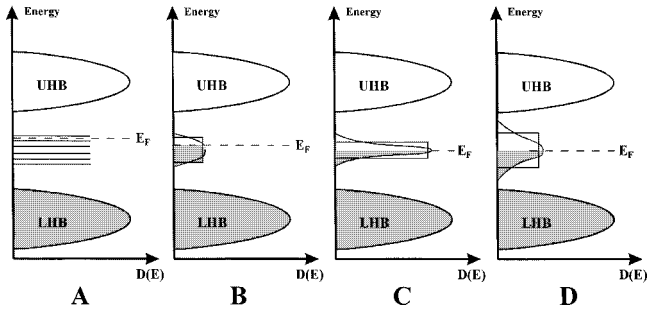

FIG. 9. Schematic picture of the band structure transformation with increasing Sr content in the $La_{2-x}Sr_xCuO_y$ system. (a) Low doping ($x<0.05$), (b) intermediate doping, (c) near-optimal doping, (d) high doping.

narrow peak in the DOS function. We believe that our experimental data on the transport properties of $La_{2-x}Sr_xCuO_y$ and the results on the band spectrum transformation obtained within the narrow-band model can be interpreted in the framework of the ''midgap scenario.''

As mentioned the undoped sample La_2CuO_y is semiconducting. The analysis of the resistivity and thermopower data for this sample indicates that the conduction process corresponds to the variable-range-hopping mechanism although it is hard to distinguish whether the hopping is three or two dimensional. Consequently, at low Sr concentration ($x \leqslant 0.05$) there are impurity levels introduced into the gap which are, probably, only partially overlapped [see Fig. 9(a)]. Thus at such a low doping level the new midgap band is not completely formed so that we cannot apply the narrow-band model to describe the experimental results. Based on our results it is hard to determine the exact Sr concentration at which these midgap states transform into the conduction band. However, the $\rho(T)$ transformation allows us to conclude that the band formation (a crossover from the localized states to the bandlike states) takes place at the Sr concentration of $x \approx 0.05$. In addition, results of our calculations for the sample with $x=0.05$ are in a reasonable agreement with the experimental $S(T)$ curve [see Fig. 5(a)]. These two facts give a good reason to conclude the new ''midgap'' conduction band to be already formed at the Sr concentration of $x=0.05$ that makes the narrow-band model valid. Note that this conclusion is in agreement with the results of Ref. 23 where an impurity band is proposed to be formed at x about 0.06.

For low doping the Fermi level is located in the upper half of an impurity band ($F \approx 0.6-0.7$) where states are still localized, even if partially. As a result, the resistivity for samples with $x=0.05-0.10$ demonstrates a semiconductor-like behavior at low temperatures (see Fig. 1), and the thermopower value is big (see Fig. 4). An increasing doping results in a transition from separated midgap states appeared in the MH gap to the new midgap impurity band. In addition, the Fermi level shifts to the middle of the band (a strong decrease of the F value). Both these effects lead to a transition to the metal-like behavior of the resistivity and a decrease of the $S_{300\,K}$ value. It is necessary to note, that since the F value is equal to the ratio of the total number of electrons to the total number of states in the band, its fast drop with an increasing Sr content in the underdoped regime can be interpreted as an introduction of states into the band on the background of increasing hole number due to the Sr impurity effect. It is important that this effect may be caused not by a direct impact of Sr but by a states transfer from the Hubbard bands. Thus, the ''midgap'' band cannot be called an ''impurity'' band in its usual meaning.

Moreover, in the region of low and intermediate doping ($x \leqslant 0.15$) our calculations show a narrowing of the conduction band (see Fig. 6) that can be also interpreted as a result of the appearance of additional states in the midgap band resulting in the further DOS peak rising. Note, that the observed decrease of the W_D value with increasing number of states looks to be reasonable because in the framework of our approach we estimate an *effective* bandwidth using the simplest approximation for the DOS function. If the midgap states appear in the MH gap forming a narrow band, an increasing doping level leads to a rise of the DOS peak in the middle of that band that corresponds to a narrowing of the effective bandwidth estimated within a rectangular approximation of the DOS function. Thus, at intermediate doping ($0.05 < x \leqslant 0.15$) the narrow conduction band is already formed in the MH gap and increasing doping results in a rise of the DOS peak [see Figs. 9(b) and 9(c)]. At the same time, in this region the Fermi level is located close to the middle of the band. As a result, the $D(E_F)$ value increases with increasing the Sr content that can initiate a T_c increase.

As mentioned in the previous section the degree of the states localization changes insignificantly in the underdoped region. To interpret this fact let us comment some structural aspects of the Sr doping effect in the $La_{2-x}Sr_xCuO_y$ system. It was found that OT transition itself is unrelated to the disappearance of superconductivity, but introducing non-native Sr cations distorts the orthorhombical structure and results in a gradual change of the CuO_6 octahedra tilt.[35] At the same time at $x<0.15$ the number of oxygen vacancies rises very slightly.[35] This means that in the underdoped regime the lattice disordering is mainly caused by the Sr impurity, and the lattice compensates its disturbance without significant loss of oxygen. If so, one can expect a relatively slight increase of the states localization that agrees with the results of our calculations. Thus, the main peculiarity of the band spectrum transformation in the underdoped regime is the formation of the new midgap narrow band. This band develops in the middle of the MH gap and increasing Sr content leads to a rise of the DOS peak, in particular, to an increase of the $D(E_F)$ value. The last effect can be considered as the main reason for the rise of the T_c value.

B. Overdoped regime

At a near optimal Sr content the midgap DOS peak has a maximal magnitude, the Fermi level is located in the middle of this peak and, therefore, the $D(E_F)$ value is peaked [see Fig. 9(c)]. This corresponds to the highest T_c value. When the doping level increases further, the Fermi level is pinned in the middle of the midgap band (the band filling F remains to be about 0.5 in the overdoped region—see Fig. 7). This results in the unchanged slope of the $\rho(T)$ dependences for $x \geqslant 0.15$ so that the resistivity retains a metal-like behavior for all the overdoped samples (see Fig. 1). Note, that our calculations show that at $x>0.15$ the band filling with elec-

trons is just below 0.5, while the thermopower value is still positive. However, as shown in our previous publications on Bi-based HTSC's,[30] the positive sign of the charge carriers in the case of $F<\frac{1}{2}$ and, correspondingly, a positive value of the thermopower in the normal state can be explained due to an asymmetry of the conduction band.

To explain the suppression of superconductivity in the overdoped region we propose the following interpretation of the data obtained. We have earlier shown that in the case of doped Y- and Bi-based HTSC's the suppression of superconductivity correlates with a broadening of the conduction band in the underdoped regime.[29–32] In its turn, this band broadening is caused by a gradual increase of the lattice disordering induced by increasing doping level according to the Anderson localization mechanism. As a result, increasing doping in Y- and Bi-based HTSC's leads, in addition to the band broadening, to a rise of the number of states localized at the band edges. As described in the previous section increasing Sr content in the $La_{2-x}Sr_xCuO_y$ system in the overdoped region leads to an analogous transformation of the conduction band (see Figs. 7, 8). On the other hand, at $x>0.15$ the lattice disordering degree was found to rise much stronger compared to the underdoped region. Indeed, Radaelli *et al.*[35] have observed that in the case of overdoped $La_{2-x}Sr_xCuO_y$ on the background of the structural distortions (occurring mostly in the oxygen environment nearest to a substituted La site[41]) at $x>0.15$ the process of the oxygen vacancies formation in the CuO_2 planes is enhanced.[33] Note, that our data on the oxygen content give support to this conclusion (see Table I). Furthermore, Muradyan *et al.*[42] reported that in the overdoped region the Sr distribution at La positions becomes nonuniform and the oxygen vacancies are stimulated to appear in the areas of a higher Sr content leading to an additional disordering in the lattice as a whole. Thus the comparison of the structural changes and the band transformation in the overdoped regime with those for the underdoped one in the case of Y- and Bi-based HTSC's gives a good reason to conclude that the observed broadening of the conduction band accompanied by a localization of states is caused by a gradual rise of the lattice disordering with increasing Sr content. As a result of such a transformation of the midgap narrow band the $D(E_F)$ value decreases with x in the overdoped regime that leads to the suppression of superconductivity. Note, that our schematic picture of the midgap band transformation in the overdoped regime is in agreement with a model of Liang[23] who argued that at a high Sr content the central narrow band destroys because of increasing disordering [see Fig. 9(d)].

At last, let us discuss some details of the band spectrum transformation in the overdoped region. As mentioned above at $x>0.18$ the variation of the band filling is very slight, whereas the localization degree rises in this range of doping much stronger than in the region of low and intermediate doping. Since the band filling F is equal to the ratio of the number of electrons to the total number of states in the band, a very slight variation of the F value with increasing Sr content on the background of the decrease of electrons number can be explained by decreasing the number of states in the midgap band. This means that in the overdoped regime the states are transferred from the narrow band and, therefore, a strong reconstruction of the band spectrum takes place. Other evidence for states to escape from the midgap band is a rise of the band asymmetry degree in the region of a high Sr content. In this connection we would like to note that some authors analyzing the transport properties of $La_{2-x}Sr_xCuO_y$ have also pointed to a possibility of such a states transfer in the overdoped regime.[21,23] Thus our results show that the main reason for the suppression of superconductivity in the overdoped regime is likely to be a strong modification of the band spectrum leading to a collapse of the midgap narrow band which is responsible for the superconductivity in $La_{2-x}Sr_xCuO_y$.

V. CONCLUSIONS

The foregoing analysis of the experimental data on the resistivity and thermopower in the normal state in the $La_{2-x}Sr_xCuO_y$ system within the narrow-band model in comparison with varying superconducting properties allows us to draw the following conclusions.

(1) The transport properties of the $La_{2-x}Sr_xCuO_y$ system can be reasonably described in the framework of the phenomenological model based on the assumption that the band structure of high-T_c materials contains a sharp density-of-states peak near the Fermi level.

(2) The main band spectrum parameters change in the $La_{2-x}Sr_xCuO_y$ system with increasing Sr content in a different way in the underdoped and overdoped regimes. The band filling drops sharply at low Sr content and changes insignificantly at $x>0.15$, while the degree of the charge-carrier localization increases stronger in the overdoped regime. The effective bandwidth decreases in the underdoped region and increases in the overdoped one demonstrating a minimum at the optimal doping level.

(3) The results obtained give support to the ''midgap'' scenario of the conduction band formation in the underdoped regime. The optimization of the superconducting properties of the $La_{2-x}Sr_xCuO_y$ system with increasing Sr content is caused by a rise of the narrow DOS peak in the Mott-Hubbard gap in which the Fermi level is pinned. The maximum of the T_c value corresponds to a maximum of the density-of-states function at the Fermi level.

(4) The most likely reason for the superconductivity suppression in the overdoped regime in $La_{2-x}Sr_xCuO_y$ is a modification of the band structure. An increasing Sr content results in the broadening of the conduction band and the localization of states caused by general disordering in the lattice, as well as in a states transfer from the midgap band responsible for the superconductivity that leads to the collapse of this band.

ACKNOWLEDGMENTS

We wish to thank Dr. I. B. Patrina for preparing the $La_{2-x}Sr_xCuO_y$ samples and determination of the oxygen content as well as Dr. S. N. Lykov and Dr. E. V. Vladimirskaya for fruitful discussions and useful comments.

*Electronic address: marina@twonet.stu.neva.ru

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