Mechanism of hole carrier generation and nature of pseudogap in doped La214

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Abstract

The generation of hole carriers in HTS is considered in the framework of model [1]. According to this model the hole conductivity starts up at the dopant concentration exceeding the percolation threshold for chain of negative-U centers (NUS). The conductivity (and superconductivity) takes place in the band formed by the oxygen pπ-orbitals hybridized with the pair orbitals of NUS. It is shown that the inclusion of two-particle hybridization results in the temperature dependences of hole carrier concentration n(T)$\propto$T and resistivity R(T)$\propto$T. As far as the mechanism of superconducting gap suppression in HTS is the occupation of pair level with electrons, the superconducting gap (pseudogap) in small nonpercolative clusters containing short chains of NUS has to open at T above T$_c$ because of the large relative fluctuations of the number of particles between pπ-band and pair level in small clusters.

Key words: negative-U center; percolation; hole carriers; pseudogap

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Here we consider the process of the generation of hole carriers, the features of the transport and optical properties in the framework of the proposed model of HTS electronic spectrum [1] as well as the nature of pseudogap. Let there is an infinite cluster including a quantity of NUS together with the nearest oxygen ions. The two-particle hybridization of the pair states with the O2$p_{x,y}\pi$ states of oxygen ions surrounding NUS results in the broadening both of the pair states and of the O2$p_{x,y}\pi$ ones. The pair level broadening can be expressed [2], [3] as $\Gamma \sim \pi(DV)^2kT$, where V is the constant of hybridization, D is the density of states at the top of O2p band. The broadening of band states is $\gamma \sim \Gamma/DE_0$, where E_0 is the energy width of statistic distribution of pair states over sites. This broadening smoothes the features of the band state density and results in its independence on energy over the interaction range. The occupation of pair level results from transitions of electrons from $\pi p_{x,y}$ oxygen orbitals to the NUS and accompanied by the generation of hole carriers in the oxygen band. We call the phase where the additional hole carriers appear through this mechanism as -U phase. The electron occupancy of NUS η as well as the hole concentration n in -U phase are determined by the balance of rates of electron pair transitions from oxygen $p_{x,y}\pi$ subband to pair level and back. If N is NUS concentration so $n = 2N\eta$. The rate of electron transitions from pair level to singlet orbitals is proportional to $N\eta\Gamma \sim \eta T$. The rate of reverse process is determined by the frequency of electron-electron scattering and proportional to $\gamma^2(1-\eta) \propto T^2(1-\eta)$. Therefore

$$n = 2NT/(T_0 + T), \tag{1}$$

where T_0 is temperature-independent value. Thus $n \propto T$ at low temperature and tends to $2N$ at high temperature according to experiment.

As it follows from the above consideration the hole carrier distribution turns out to be nondegenerated owing to the interaction with NUS. Taking into account the nondegeneracy of carrier distribution (absence of the Pauly blocking) and their high concentration ($10^{21} - 10^{22}$ cm^{-3}) the electron-electron scattering (more precisely to say hole-hole scattering in this

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case) is likely to provide the dominant contribution to the relaxation processes in HTS. As far as the interaction of two holes in the system with NUS corresponds to the effective attraction, it will not be conventional Coulomb scattering. The main mechanism of carrier relaxation in HTS is likely to be similar to that assumed for the metals and alloys with strong electron-phonon coupling [4]. In these materials the electrons in a layer $\sim k\Theta_D$ at the Fermi surface (Θ_D is Debye temperature) are attracted due to virtual phonon exchange. This electron-electron interaction enhanced by phonon-mediation effects far exceeds the screened Coulomb repulsion. Therefore in the metals with strong electron-phonon interaction the dominant channel of the electron-electron scattering will be determined by the virtual phonon exchange. The dominant relaxation process in HTS is the electron-electron scattering as well and the main channel of this scattering is the interaction of hole pairs on NUS. This process may be considered as an exchange by virtual bosons (exitons) with energy W. As far as $W \sim 0.1 - 1$ eV (in contrast to the exchange by virtual phonon with energy $E \sim k\Theta_D < 0.03$ eV) the temperature range, where the scattering processes with exchange of virtual bosons are dominant, expands to $T \sim 10^3$ K [4].

The temperature dependence $\rho(T)$ in such a model may be obtained from the Drude formula $\rho = m^*\nu/ne^2$ (here m^* is the effective mass of holes, ν - the rate of hole-hole scattering). For $W \gg E$ the amplitude of scattering doesn't depend on the particle energy. Assuming that density of states is energy-independent ν will be determined only by the hole concentration and statistical factor in scattering cross-section (i.e. the phase volume available for occupation with scattered particles). The latter is proportional to $E_1 + E_2$ (here E_1 and E_2 are the energies of scattering holes measured from the top of valence band). Thus

$$\nu \propto n(E_1 + E_2). \qquad (2)$$

For dc-conductivity $E_1 \sim E_2 \sim \Gamma \propto T$ and $\nu \propto nT$, so that $\rho(T) \propto T$.

The dominant contribution of electron-electron scattering into the scattering process also has an effect upon both of frequency and temperature dependencies of optical conductivity σ_{opt}:

$$\sigma_{opt} = \frac{e^2 n}{m^*} \frac{\nu_{opt}}{\omega^2 + \nu_{opt}{}^2}. \qquad (3)$$

here ω is the photon frequency, ν_{opt} - the rate of optical relaxation. For the electron-electron scattering (at $n = 10^{21} - 10^{22}$ cm^{-3}) the collision frequency is $\sim 10^{14} - 10^{15}$ s^{-1}. Thus $\nu_{opt} \gg \omega$ for IR region and the formula for optical conductivity becomes more simple:

$$\sigma_{opt}(\omega, T) = e^2 n/m^* \nu_{opt}. \qquad (4)$$

For optical relaxation we have $E_1 \sim \omega, E_2 \sim \gamma \propto T$. From where $\sigma_{opt} \propto \omega^{-1}$ (for $\omega \gg \Gamma$) and $\sigma_{opt} \propto T^{-1}$ (for $\omega < \Gamma$)in a good agreement with the data of various experiments.

The proposed model allows to give an alternate interpretation of the experiments on the pseudogap observation in under- and optimally- doped HTS [5],[6]. As it follows from experiment the pseudogap has the same symmetry and about the same value as the superconducting gap but it vanishes at $T^* > T_c$ (T^* decrease with x down to T_c).

We believe that the observed pseudogap is nothing but just the same superconducting gap opening at $T > T_c$ because of the large fluctuations of the number of particles between valence band and pair level in the short chains of NUS. The point is that in HTS the mechanism of the superconducting gap suppression is the occupation of pair level with electrons. Therefore the decrease of pair level occupation by fluctuation may result in turning on superconductivity in such chains at $T^* > T_c$ (first-order phase transition [7]). At small x the great bulk of NUS are grouped on short chains where large relative fluctuations of the number of particles are possible. With x the increasing part of NUS belong to the infinite percolation cluster. Therefore T^* decrease with x down to T_c, unless all NUS are integrated in infinite percolation cluster.

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