Extrinsic (Bi)Polaronic Metal-Insulator Transition in Doped High-T_c Oxides

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Abstract

The possiblity of the extrinsic Mott transition and (bi)polaronic metal-insulator transition (MIT) in doped high-T_c oxides is studied within the continuum model of extrinsic carrier self-trapping, the extrinsic Hubbard and (bi)polaronic band models using the variational method and tight-binding approximations. The proper criterions for Mott's and extrinsic (bi)polaronic MIT's are obtained. It is shown that the anysotropy of the dielectric and (bi)polaronic properties of doped high-T_c oxides is responsible for the smooth MIT, stripe formation and suppression of high-T_c superconductivity.

Key words: Doped high-T_c oxides; Mott transition-extrinsic (bi)polaronic MIT

1. Introduction

As is well know the ground states of doped carriers in many solids are their self-trapped (in a deformable lattice or near impurity) states. Such self-trapped (i.e. intrinsic or extrinsic (bi)polaronic) states are discovered in different doped systems, such as alkali halides, oxides (including also high-T_c oxides) and semiconductors [1]. The formation of intrinsic and extrinsic (bi)polaronic states and bands in the energy gaps of insulators and semiconductors leads to many important phenomena (e.g. defect formation, luminescence, metal-insulator transitions, superconductivity, etc.) [1, 2]. For instance, the Mott insulators, charge-transfer (CT) insulators (high-T_c oxides are the same) show the metallic behaviour as doping level increases. The origin and nature of the metal-insulator transitions (MIT's) in doped high-T_c oxides is still poorly understood, although much theoretical effort has been devoted to examining this question. So far, the (bi)polaronic effects characteristic for any polar solids are not included in the existing models of the MIT's (see also [3]). In this paper we consider the extrinsic (bi)polaronic mechanism for the MIT in doped high-T_c oxides.

2. Formation of (bi)polaronic states and bands

In oxide high-T_c superconductors the doped carriers (holes or electrons) are trapped first by impurity (or defect) potentials and are localized near the substitional ions or defects (e.g. vacancies in $YBa_2Cu_3O_{7-x}$). The ground state energies of interacting one carrier-impurity-phonon and two carrier-impurity-phonon systems can be calculated within the continuum model of extrinsic carrier self-trapping [4]. As it is well known, the doped carriers in polar compounds interact with acoustic and optical phonon fields as well as with the short- and long-range defect fields. Then the ground state energies of large-radius one- and two-carrier imputity centers will be determined in the continuum model and adiabatic approximation from the following relations [2]

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$$E_1 = \frac{B}{27g_s^2}[2 - 9g_s g_l - 2(1 - 3g_s g_l)^{3/2}] \quad (1)$$

and

$$E_2 = \frac{2B}{27G_s^2}[2 - 9G_s G_l - 2(1 - 3G_s G_l)^{3/2}], \quad (2)$$

where $B = 3\pi\hbar^2/2m^* a_0^2, g_s = g_{sL}(1+b_S), g_l = g_{lL}(1-\eta+\eta b_l), G_s = gsL(2+b_s), G_l = g_{lL}(1-2\eta+\eta b_l), g_{sL} = E_d^2/2Ka_0^3B$, $g_{lL} = e^2/\varepsilon_\infty a_0 B$, $b_s = 2^{5/2}[(E_{\alpha D}/E_\alpha) - (KV_{sD}/E_\alpha^2)]$, $b_l = 2^{3/2}Z$, $\eta = \varepsilon_\infty/\varepsilon_0$, m^* is the effective mass of a carrier, a_0 is the lattice constant, K is an elastic constant, E_α and $E_{\alpha D}$ are the deformation potentials of a carrier and a defect, respectively, V_{sD} is the short-range defect potential.

The stable one- and two-carrier extrinsic self-trapped states are formed at $E_1 - 2E_2 > 0$ and $E_1 - 2E_2 < 0$, respectively. At low doping level the shallow (for $b_s < 0$) or nearly deep (for $b_s > 0$) localized one- and two-carrier impurity states are formed in the CT gap of high-T_c oxides. When $b_s < 0$ the (bipolaronic effects near the impurity ion (i.e. Sr^{2+} in $La_{2-x}Sr_xCuO_4$) or defect (e.g., oxygen vacancies in other copper oxides) are suppressed by the short-range repulsive defect potetial and the hydrogenic impurity states are formed. While, at $b_s > 0$ the formation of large (bi)polarons bound to impurities or defects becomes possible in some doped high-T_c oxides with small-radius impurities (e.g. Ca^{2+}, Th^{4+}). The extended states of such (bi)polarons form extrinsic (bi)polaronic bands with increasing doping in the underdoped regime.

3. The criterions for extrinsic Mott transition and (bi)polaronic metal-insulator transitions

For $b_s < 0$ the proper criterion for extrinsic Mott transition is determined from the relation $W = U \simeq 0.86E_I$ [2], where $W = 2ZJ$ is the bandwidth of the impurity band, U is the Coulomb repulsive energy between two carriers on the impurity center, $E_I = e^2/2\varepsilon a_H$, ε is the effective dielectric constant, a_H is the Bohr radius of the hydrogenic impurity centers, z is the coordination number, $J = \hbar^2/2m^* a_I^2$ is the transfer energy of tight-binding theory, a_I is the lattice constant of the impurity superlattice. When $n = 1/a_I^3$ and $z = 6$ the criterion for extrinsic Mott transition has the form $n_c^{1/3} a_H \simeq 0.27$. But the MIT in doped high-T_c oxides is not described by this criterion [2]. In doped polar compounds the extrinsic (bi)polaronic MIT seems to be realized at $b_s > 0$. At some doping level the large-radius extrinsic bipolaron would dissociate into two extrinsic polarons and then the MIT occurs at the overlapping of half-filled extrinsic polaronic band with the valence or conduction band. Such a MIT driven by the carrier localization takes place if the kinetic energy of extrinsic polarons is smaller than their binding energy E_{bI}. Therefore, the criterion of the extrinsic (bi)polaronic MIT can be determined as $ZJ = E_{bI}$ or $Z\hbar^2/2m_{IP}^* a_I^2 = E_{bI}$ from which at $z = 6$ we obtain $n_c = (m_{IP}^* E_{bI}/3\hbar^2)^{3/2}$, where m_{IP} is the effective mass of an extrinsic polaron. At $m_{IP}^* = 2m_e$ and $E_{bI} \simeq 0.09eV$ [2] we find $n_c \simeq 7 \cdot 10^{20} cm^{-3}$ and $x_c = n_c/n_a \simeq 0.07$, where $n_a \simeq 10^{22} cm^{-3}$ is the density of the lattice atoms. We believe that the dielectric anisotropy and the anisotropy of (bi)polaronic effects are responsible for the smooth MIT, stripe formation and suppression of T_c in doping range $x = 0.07 - 0.15$.

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