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The new metal–insulator transitions and nanoscale phase separation in doped cuprates

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ABSTRACT

We use the theory of extrinsic and intrinsic polarons to examine the new mechanisms of metal-insulating transitions (MITs) and nanoscale phase separation in hole-doped cuprates and propose a unified description of these interrelated phenomena. We argue that the relevant charge carriers in these polar materials are extrinsic (impurity-bound) and intrinsic large polarons. We show that the strong carrier-defect-phonon and carrier-phonon interactions together with the charge inhomogeneities are responsible for the carrier localization, the ordering of polaronic carriers and formation of their superlattices, the new MITs and nanoscale phase separation, which are accompanied by the stripe formation in the lightly to the slightly underdoped cuprates. We demonstrate that in doped cuprates $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{7-\delta}$ the static (insulating) and dynamic (metallic) stripes coexist in the doping range $x \simeq 0.03$–0.13. Our results are in quantitative agreement with experimental findings in these high-T_c materials.

1. Introduction

The doped cuprates are inhomogeneous systems (where the dopants and charge carriers are distributed inhomogeneously) and the underdoped cuprates are more inhomogeneous than overdoped ones [1–4]. In such inhomogeneous materials, the phenomena of carrier localization and

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metal–insulator transitions (MITs) are very complicated by many factors, such as dopant-driven and carrier-driven inhomogeneities, carrier-dopant (defect)-lattice and carrier-lattice interactions, specific types of charge ordering, which usually were ignored in the existing theoretical approaches to the problem of carrier localization, MITs and high-T_c superconductivity in doped cuprates. In particular, the strong electron correlation (i.e. on-site Coulomb repulsion) causes the carrier localization and Mott-type MIT in undoped cuprates, which are charge-transfer (CT)-type Mott–Hubbard (MH) insulators [5–8], but it is not obvious which processes will dominate in doped cuprates. The insulating and metallic states of doped cuprates are essentially different from those of ordinary metals and undoped cuprates. Because the electronic structure of the cuprates are changed dramatically with doping and the low-energy electronic structure of the doped cuprates is quite different from the high-energy electronic structure of the CT-type MH insulators. In doped cuprates, the electronic inhomogeneity and charge ordering play an important role in nanoscale phase separation in real space [1–3,9–13], which is intimately related to carrier localization and MITs in these materials. So far, the analyses of the carrier localization and MITs and their relation to nanoscale phase separation in inhomogeneous doped cuprates are still inconclusive and the mechanisms of these electronic processes are not well understood yet. In this work, we study the relevant mechanisms of MITs and nanoscale phase separation in inhomogeneous hole-doped cuprates. In Section 2, we discuss the relevant mechanisms of carrier localization and segregation in doped cuprates. The ordering of polaronic carriers with the formation of different superlattices in these materials are considered in Section 3. In Section 4, we present the new criterions for MITs, which are used to study the relevant MITs and nanoscale phase separation in inhomogeneous hole-doped cuprates. The theoretical predictions are compared with experimental results for MITs and stripe formation in various doped cuprates. Our obtained results are summarized in Section 5.

2. Carrier localization and segregation

Hole doping of the cuprates produces first quasi-free holes having the mass m_b in the oxygen valence band. In polar cuprates, these hole carriers interacting both lattice vibrations and with lattice defects (e.g. dopants or impurities) are self-trapped either near the defects (defect-assisted extrinsic self-trapping) or in a defect-free deformable lattice (phonon-assisted intrinsic self-trapping). Therefore, the ground states of such hole carriers are their self-trapped (i.e. localized extrinsic and intrinsic polaronic) states lying in the CT gap of the cuprates [14]. A large ionicity of the cuprates $\eta = \varepsilon_\infty/\varepsilon_0 \ll 1$ (where ε_∞ and ε_0 are the high-frequency and static dielectric constants, respectively) enhances the polar electron–phonon interaction and the tendency to polaron formation. Actually, the relevant charge carriers in hole-doped cuprates are large polarons [14–17] and the strong electron–phonon interactions are responsible for enhancement of the polaron mass $m_p = (2.0–3.0)m_b$ [15,18] (where $m_b \simeq m_e$ is the free electron mass). The formation of nearly small Frölich polaron [19] might be also relevant. According to Ref. [14], the ground state energies or binding energies E_{ep} of extrinsic polarons would increase rapidly with decreasing ε_∞ from 5 to 3 or with increasing η from 0 to 0.12 and are equal to $E_{ep} \simeq (0.11–0.18)$ eV (for $\varepsilon_\infty = 3.5–4.5$ and $\eta = 0.12$) and $E_{ep} \simeq (0.086–0.14)$ eV (for $\varepsilon_\infty = 4$ and $\eta = 0–0.12$). Whereas the binding energies E_p of intrinsic polarons would decrease noticeably with increasing η from 0 to 0.12 (i.e. $E_p \simeq (0.085–0.065)$ eV for $\varepsilon_\infty = 4$ and $\eta = 0–0.12$), but E_p increases from 0.054 eV to 0.09 eV with decreasing ε_∞ from 4.5 to 3.5 at $\eta = 0.10$. We believe that the carrier-defect-phonon and carrier-phonon interactions together with the charge inhomogeneities play an important role in hole-doped cuprates and are responsible for the carrier localization and segregation, which may manifest themselves via local (nanoscale) phase separation in real space and stripe formation (i.e. the polaronic carriers form metallic domains separated by insulating domains [14,20]). In these materials, the inhomogeneous spatial distribution of polaronic carriers leads to their segregation into carrier-rich and carrier-poor regions. Perhaps the carrier-defect-phonon and carrier-phonon interactions give rise to charge aggregation in carrier-rich metallic regions together with charge depletion in spatially separated carrier-poor regions with no mobile carriers. In general, the local charge inhomogeneity and the competition between the kinetic energy and the aligning interactions produce nanoscale self-organized structures called stripes.