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Nano-scale intrinsic inhomogeneity in the cuprates

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Abstract

The possibility that nano-scale electronic inhomogeneity is intrinsic in the high-temperature superconducting cuprates has been suspected from many experiments, and recent STM observations enhanced this view. However, the subject is still highly controversial, particularly with respect to its relevance to the mechanism of superconductivity. We present recent results of inelastic neutron scattering measurement that support the intrinsic nature of inhomogeneity and discuss its implications.
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1. Introduction

It has already been 20 years since the discovery of high-temperature superconductivity (HTSC) [1], but its mechanism is still unclear and highly controversial. The prevailing view on the mechanism of HTSC has been that it is a purely electronic phenomenon that occurs in a two-dimensional periodic lattice plane of CuO_2 [2]. Early reports on experimental observation of lattice distortion or inhomogeneity [3] have been disregarded by many as irrelevant side effects due to extrinsic disorder. On the other hand, it is now widely agreed that the superconductivity in the underdoped pseudo-gap phase is inhomogeneous because of the competition against the antiferromagnetic (AFM) phase or charge ordered (CO) phase [4]. Recent results of careful STM studies gave more direct evidence of electronic inhomogeneity [5–7] as well as local charge ordering [8]. However, since STM is a surface-sensitive probe, it is possible that the bulk state is different from the surface. Also, a recent study suggests that the electronic inhomogeneity is related to pair breaking by oxygen interstitial impurities [9]. Thus, the question whether the inhomogeneity is an intrinsic property of HTSC or not remains unanswered.

In this paper, we focus on this question in light of some new data on the dispersion of the Cu–O bond-stretching phonons by inelastic neutron scattering. In our view, the strong propensity toward charge localization and inhomogeneity is an integral part of the HTSC phenomenon in the cuprates, as has been advocated for a long time by Müller [10]. While we need more data and theoretical development to confirm this point and clarify its relevance to the HTSC mechanism, the field is finally changing from early denial toward a wider, quiet acquiescence of intrinsic inhomogeneity in the cuprates.

2. Unusual nature of phonon dispersion in the cuprates

Phonon dispersion in the cuprates has been carefully studied by inelastic neutron scattering [11–14]. While most phonon modes are not strongly affected by charge doping, the in-plane Cu–O bond-stretching modes, particularly the half-breathing mode at $\boldsymbol{q} = (\pi, 0)$ in the units of $1/a$, or $(0.5, 0)$ in the units of $2\pi/a$, where a is the in-plane lattice constant, show strong doping dependence [11,12]. This mode is noteworthy for its strong phonon-induced charge transfer, which can be spin dependent and induce spin–phonon interaction [15]. Even though the softening of the half-breathing mode can be largely accounted for by

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the LDA calculation [16], Hubbard model [17] and the t–J model [18–20], this mode deserves further careful attention.

The dispersion of the $\boldsymbol{q} = (\Delta, 0)$ in-plane Cu–O bond-stretching mode of the fully doped sample shows a strong discontinuity at $(\pi/2, 0)$ or $(0.25, 0)$, both in LSCO [13] and in YBCO [21], suggesting the importance of this wave vector. This could be related to either the $4a$ stripes [21] or $2a$ periodicity [13]. In addition, the dispersion appears to be split around this wave vector into two branches, an upper branch that connects to $\boldsymbol{q} = (0, 0)$ and the lower branch that connects to $\boldsymbol{q} = (\pi, 0)$.

Now when the doping level is increased, the softening around $\boldsymbol{q} = (\pi, 0)$ is expected to change smoothly up to the optimum doping [18,20]. However for YBCO, the dependence of softening on charge density is unusual [22]. In particular, the energy at the zone boundary is not linearly dependent on charge density, but is nearly constant, as shown in Fig. 1 [23]. What changes is its intensity, which grows with doping (Fig. 2 [23]). This growth occurs at the expense of the intensity at the energy range corresponding to the phonon energy of the undoped sample. The phonon dispersion was determined by the inelastic neutron scattering measurements made with the MAPS spectrometer at the ISIS facility of the Rutherford-Appleton Laboratory, UK. The simplest way to explain this behavior is to assume that there are only two states of the phonon, softened and unsoftened, and doping changes only the relative intensity, thus the volume fraction, of each mode. While these two regions could represent the completely undoped and optimally doped states, other possibilities involving spin correlations exist, as discussed below. The splitting of this mode in YBCO was explained in terms of the interaction with the apical mode [21]. However, the mixing with the apical mode is weak [14], and it is difficult to believe that it

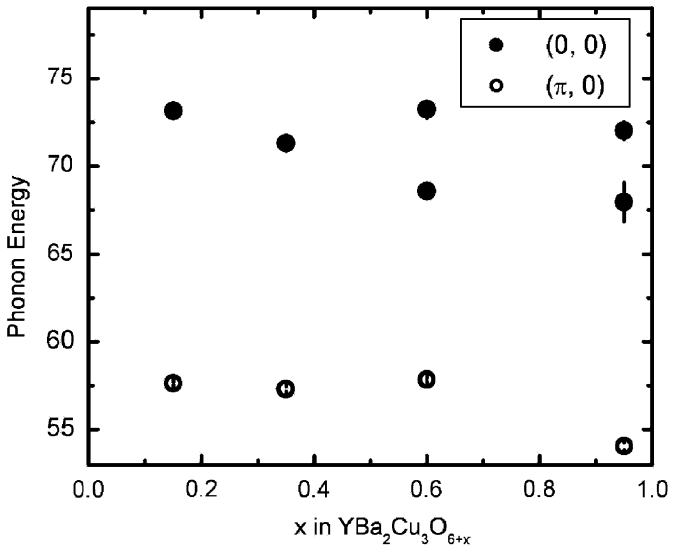

Fig. 1. Charge density dependence of the phonon energy of the Cu–O bond-stretching LO mode at $(0, 0)$ and $(\pi, 0)$ in $YBa_2Cu_3O_{6+x}$ at $T = 10$ K [23]. Momentum q is in the unit of $2\theta/a$, where a is the in-plane tetragonal lattice constant. The split at high values of x is due to orthorhombic lattice distortion. Note that the energy is nearly independent of x.

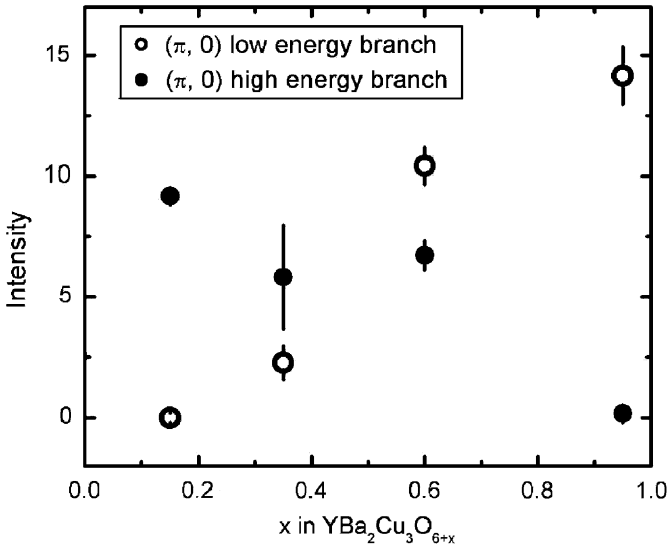

Fig. 2. Doping dependence of the inelastic neutron scattering intensity, $S(Q, \omega)$, of the Cu–O bond-stretching LO phonon mode at $(\pi, 0)$ in $YBa_2Cu_3O_{6+x}$ at $T = 10$ K, for the high-energy branch (~72 meV) and lower energy branch (~57 meV) [23]. The shift in the spectral weight from the higher energy branch to the lower one is apparent.

will fully explain this phenomenon, as discussed in detail elsewhere.

Another interesting observation is that at elevated temperatures above 200 K, we observed a new mode in the $YBa_2Cu_3O_{6.6}$ (YBCO6.6) sample. In this sample, the Cu–O bond-stretching mode disperses from 72 meV at the zone center to 58 meV at the zone boundary. The measurement was made with the HB-3 spectrometer of HFIR, Oak Ridge National Laboratory. Above about 200 K a dispersionless mode appeared at 65 meV, of which intensity is about one-fourth of the low-temperature mode (Fig. 3 [23]). A possibility is that this represents a local mode around a trapped charge, such as a polaron.

3. Polaronic bound state

Owing to advances in the angle-resolved photo-electron spectroscopy (ARPES) measurement, we now have a good understanding of the Fermi surface in the cuprates [24]. While details vary from one system to the other, the most conspicuous common feature of the electronic dispersion in the cuprates is its strong and distinct anisotropy. The branch toward $\boldsymbol{q} = (\pi, \pi)$ (nodal direction) is strongly dispersing (small effective mass), while there is a van-Hove singularity (saddle-point) at $\boldsymbol{q} = (\pi, 0)$ (anti-nodal direction), where the effective mass is quite large. According to STM observations, while the anti-nodal particles are strongly spatially inhomogeneous, the nodal particles do not see inhomogeneity at all. This is partly because of the large difference in their effective mass, but also suggestive of the nature of disorder.

The undoped cuprate has a large charge transfer gap with some dispersion [25,26]. When it is lightly doped,

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