Resonant Inelastic X-ray Scattering Study of La_2CuO_4

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Introduction

To elucidate the many-body physics of strongly correlated electron systems, it is important to understand their electronic excitations. In particular, resonant inelastic x-ray scattering (RIXS) provides a bulk-sensitive, element-specific, and momentum-resolving spectroscopic tool for measuring particle-hole pair excitations [1-4]. In our study, we focus on the insulating member (x = 0) of the superconducting copper oxide family, $La_{2-x}Sr_xCuO_4$. For the so-called Mott insulator, La_2CuO_4, optical studies have revealed a charge-transfer gap of ~2 eV. We have studied the momentum dependence of this charge- transfer gap excitation at finite **q**-positions by using the RIXS technique and observed quite a large dispersion of ~1 eV. In addition, a second higher-energy excitation has also been observed.

Methods and Materials

The experiment was carried out at the Complex Materials Consortium Collaborative Access Team (CMC-CAT) beamline 9-ID with a double-bounce Si(111) monochromator and a secondary Si(333) channel-cut monochromator. A spherical, diced Ge(733) analyzer was used to obtain an overall energy resolution of ~0.4 eV full width at half maximum (FWHM). The polarization of the incident x-ray was kept fixed along the c-direction. A single crystal sample of La_2CuO_4, grown with the floating-zone method, was used in our experiments. In our measurements, the incident photon energy was fixed at E_i = 8991 eV, while the final photon energy was varied to produce spectra as a function of energy transferred to the electron system.

Results

We have measured the energy spectra at the high-symmetry **q**-positions as shown in Fig. 1, where momentum transfer is denoted in the tetragonal notation of the copper-oxygen plane (a = b = 3.85 Å). As shown in Fig. 1, we can observe two peaks, both of which show clear dispersion as **q** is varied. Analysis of the low-energy peak along the (0 0) to (π 0) direction yields a bandwidth of ~1 eV. We have also measured the momentum dependence along the c-direction, which is perpendicular to the copper-oxide plane, as shown in top two scans of Fig. 1. The dispersionless behavior along the c-direction suggests that these excitations are effectively 2-D. The line shape and/or width change at the (π π) position is quite dramatic, with one of the peaks losing most of its spectral weight around (π π).

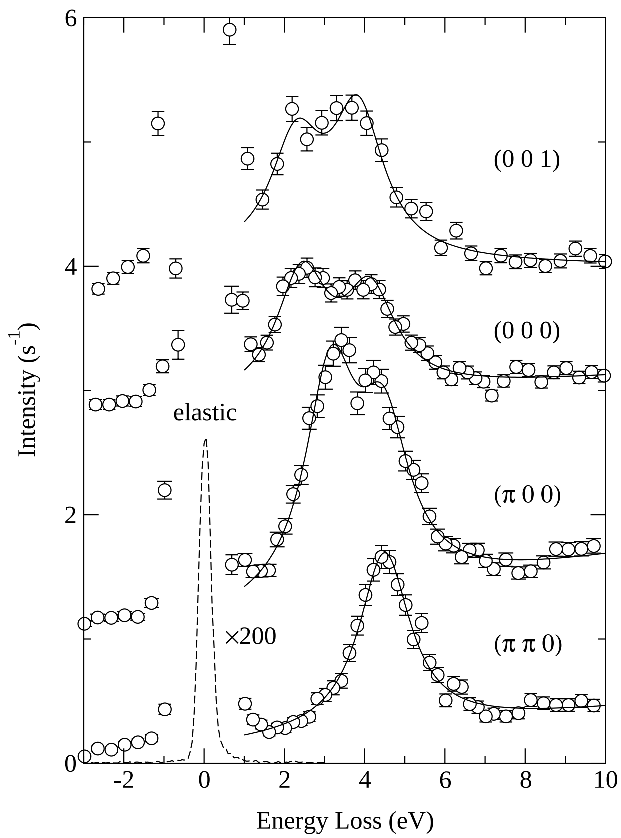

FIG. 1. Inelastic scattering spectra for a fixed momentum transfer as noted. A representative scan through an elastic line is plotted to show the instrumental resolution of the experiment. Each spectrum is offset vertically for clarity, and solid lines are fits to double Lorentzian line shape.

Discussion

The observed bandwidth of the low-energy excitation is much larger than the typical single particle dispersion observed with photoemission techniques [5]. In addition, it is well known that the localized holes in the insulating copper oxide plane have a spin-half degree of freedom, with strong antiferromagnetic correlations. This suggests that the electrons and holes created by the x-rays prefer forming a bound exciton mode, since these excitons can propagate without disrupting the antiferromagnetic order of the copper oxide plane. However, understanding the detailed properties of these excitons both theoretically and experimentally is still open [6]. Future work is planned to study the doping dependence of these features as carriers are added and a metallic phase is induced. It will be particularly interesting to observe any changes in the spectra upon entering this metallic phase and to look for the background state for high-temperature superconductivity.

Acknowledgments

Work was performed at Brookhaven National Laboratory through the support of the U.S. Department of Energy (DOE), Division of Materials Science, under Contract No. DE-AC02-98CH10886. Use of the APS was supported by the DOE Office of Science, Office of Basic Energy Sciences, under Contract No. W-31-109-ENG-38. We also thank CMC-CAT for its support.

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