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Photoelectron escape depth and inelastic secondaries in high-temperature superconductors

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We calculate the photoelectron escape depth in the high-temperature superconductor Bi2212 by use of electron energy-loss spectroscopy data. We find that the escape depth is only 3 Å for photon energies typically used in angle-resolved photoemission measurements. We then use this to estimate the number of inelastic secondaries, and find this to be quite small near the Fermi energy. This implies that the large background seen near the Fermi energy in photoemission measurements is of some other origin. [S0163-1829(99)08017-0]

Angle-resolved photoemission spectroscopy (ARPES) has become one of the key tools used to unravel the mystery surrounding the origin of high-temperature superconductivity in the layered copper oxides.[1] The surface sensitivity of this probe is well known, but to date, no estimate has been made of the photoelectron escape depth. A related question is the origin of the large ‘‘background’’ present in ARPES spectra near the Fermi energy, which needs to be understood before a truly quantitative understanding of the data is possible. In this paper, we make use of electron energy-loss spectroscopy (EELS) data to calculate both the photoelectron escape depth and the resulting inelastic secondaries. We find that for photon energies typically used in ARPES experiments, the escape depth is low (3 Å) implying that the electrons are coming from the top CuO layer. We then calculate the secondary emission and find that it is very small near the Fermi energy, in agreement with earlier estimates by Liu, Anderson, and Allen.[2] This implies that the large background is not due to secondaries.

To calcuate the escape depth and secondaries, we need to know the electron loss spectrum. Fortunately, in the system most studied by ARPES, Bi2212, this has been done some time ago by Nucker *et al.*[3] They determined the quantity $\mathrm{Im}[-(1/\epsilon)]$ where ϵ is the dielectric function. To aid in our numerical calculations, we use a simple analytic form to model these data. We represent the data by a sum of three terms:[4]

$$\mathrm{Im}\left(-\frac{1}{\epsilon}\right)=\sum_i c_i \frac{\omega\Gamma_i\omega_i^2}{(\omega^2-\omega_i^2)^2+\omega^2\Gamma_i^2} \tag{1}$$

with $c_i^{-1}=(6.1,2.1,2.9)$, $\omega_i=(1.1,18.5,32.8)$, and $\Gamma_i=(0.7,13.6,17.0)$ (eV units for ω_i and Γ_i). The result is plotted in Fig. 1. The sharp peak at about 1 eV is the plasmon associated with the near Fermi energy band. The broad double peaked structure is plasmons associated with the main CuO valence bands, and is similar to what is seen in Cu metal.[5]

The inverse differential path length is given by[5]

$$\lambda^{-1}(E,E')=\frac{1}{\pi a_0 E}\ln\left(\frac{1+\sqrt{E'/E}}{1-\sqrt{E'/E}}\right)\mathrm{Im}\left(-\frac{1}{\epsilon(E-E')}\right), \tag{2}$$

where a_0 is the Bohr radius. The inverse escape depth is then

$$\lambda_{tot}^{-1}(E)=\int_0^E dE'\lambda^{-1}(E,E'). \tag{3}$$

In Fig. 2 we plot the escape depth. From the above equations, we expect minima near twice the plasmon energy, and this is indeed what we find, with a sharp local minimum at about 2 eV, and a much broader global minimum at about 50

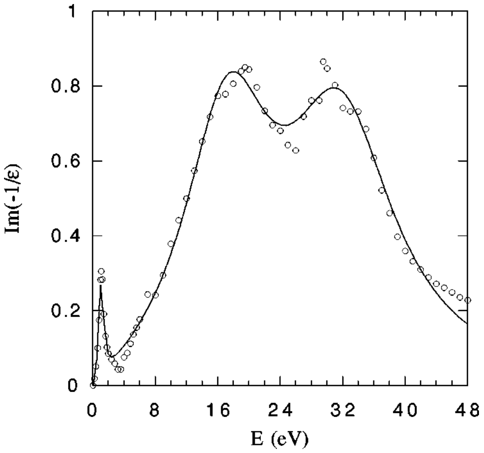

FIG. 1. Plot of the imaginary part of the inverse dielectric function for Bi2212. The circles are data of Ref. 3, the solid line the model of Eq. (1).

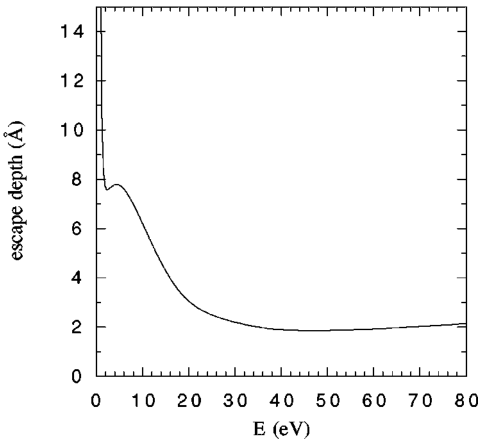

FIG. 2. Plot of the photoelectron escape depth obtained from Fig. 1.

eV. We note that for the photon energies typically used in ARPES experiments (19–22 eV), the escape depth is quite short (3 Å).

We now turn to the calculation of inelastic secondaries, due to primary photoelectrons which lose energy as they transport out of the crystal. The contribution to the photocurrent is[5]

$$B(E)=\int_E^\infty dE'\lambda_{tot}(E)\lambda^{-1}(E',E)I(E'), \tag{4}$$

where $I(E)$ is the measured photocurrent. In Fig. 3, we plot this for a spectrum at the $(\pi,0)$ point for a $T_c=87$ K overdoped Bi2212 sample. We compare this to the phenomenological Shirley background often used for estimating secondaries which is of the form[2]

$$B(E)=c_{Sh}\int_E^\infty dE'F(E'), \tag{5}$$

where $F(E)$ is the primary spectrum $[I(E)-B(E)]$. Fitting to the high binding-energy tail, we find $c_{Sh}=0.065$, close to the value obtained by Liu *et al.*,[2] and a factor of 25–60 times smaller than estimates which attribute the flat background of the near Fermi energy band to secondaries. We note the close match of the phenomenological Shirley background to the exact result, and thus confirm the earlier conclusions of Liu *et al.*[2] That is, the flat background cannot be due to secondaries, but is of some other origin.

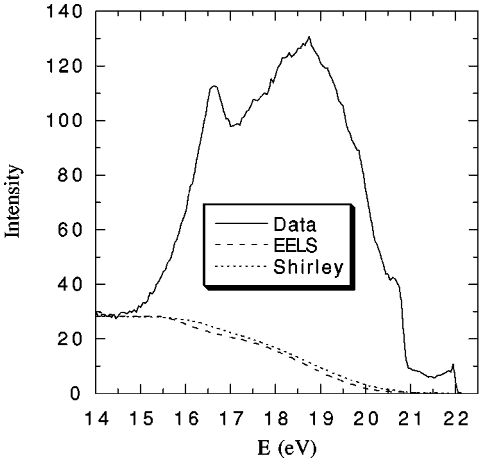

FIG. 3. Main valence band spectrum at the $(\pi,0)$ point for a $T_c=87$ K overdoped Bi2212 sample (22 eV photons). The dashed line is the calculated secondary emission. The dotted line is the secondaries estimated from a phenomenological Shirley background.

In conclusion, we have calculated the photoelectron escape depth and the resulting secondary emission for the high-temperature cuprate superconductor Bi2212 using EELS data. The result is that the escape depth is short (3 Å) for typical photon energies, and that the resulting secondary emission is too weak to account for the flat background associated with the near Fermi energy emission. This background is therefore of some other origin, which we hope to explore in a future paper.

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