Physica C: Superconductivity and its applications 532 (2017) 13–16

Contents lists available at ScienceDirect

Physica C: Superconductivity and its applications

journal homepage: www.elsevier.com/locate/physc

Effect of surface charge and s-wave component on (001) surface and bulk states of $YBa_2Cu_3O_{7-\delta}$

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ARTICLE INFO

Article history:
Received 26 October 2016
Revised 16 November 2016
Accepted 21 November 2016
Available online 22 November 2016

Keywords:
YBCO superconductor
Surface charge effect
Sub-dominant effect

ABSTRACT

The local densities of the (001) surface and bulk states (LDOS) of thin $YBa_2Cu_3O_{7-\delta}$ films were studied based on the self–consistent tight binding model. The CuO-chain and CuO_2-plane layers were considered to be a coupling between bands, and then the input surface charge density and the s-wave sub-dominant component were included in the material. In the calculation process, the surface and bulk states were determined, for comparison. It was found that the size of the superconducting gap of a plane layer at the surface increased with an increasing input of the surface charge density, but the LDOS in the bulk were not affected much by this change. When the s-wave component was included in the material, it affected several peaks in the LDOS. This caused some peaks to split while some other peaks became sharper.

1. Introduction

In 1911, a new state of material, called superconductivity, was observed by the Dutch physicist Prof. Heike Kamerlingh Onnes, at a very low critical temperature (4.2 K) [1–4]. After that, much research has been focused on how to understand the physics and increase the critical working temperature of this material. Fortunately, a conventional superconductor that can be explained by the BCS theory [5,6] was observed at 203 K [7]. Among many types of superconductor, yttrium barium copper oxide (YBCO) is one of the most important high temperature superconductors that gives rise to exiting novel physics and practical applications. For example, the physics of the main gap, subgap feature, and zero-biased conductance peak (ZBCP) that provide supporting evidence for $d_{x^2-y^2}$ symmetry of the order parameter in this material [8–12], and satellite peaks that are used to characterize and specify the properties of this material [13–17]. It has been used in devices, for instance, to produce a part of a high speed train and in magnetic resonance imaging (MRI). This indicates why we are interested in theoretical studies of this material.

In addition, considering Fig. 1 for an illustration of YBCO, a coupling between the CuO chain and the CuO_2 plane, including plane–plane coupling, is one of the most interesting recent research topics in both experimental and theoretical works [18–23]. This coupling can cause, for example, a split in the ZBCP of the (110) surface states of a YBCO superconductor [24], and in organic superconductors [25]. However, the broken time-reversal symmetries of the surface states and the sub-dominant of the order parameter can also cause the ZBCP to split even if there is no coupling between the bands (see Ref. [24] and references therein for ZBCP splitting and non-splitting scenarios, including Ref. [26] for the existence of zero-energy surface bound states that are believed to be responsible for the ZBCP) [24,27–29]. The sub-dominant of the order parameter refers to the s-wave component, and it was observed as about 15–20% of the main order parameter [30–32]. Other than that, some work shows an interesting result related to the effect of this coupling on the Fermi energy and the density of states with and without the Ca-doping concentration [33]. Thus, this indicates how a coupling scenario between bands and the sub-dominant of the order parameter have crucial effects in this material.

Another interesting feature is that this material exhibits a polar behavior [33]. Experimentally, when the YBCO sample is prepared with the production process, it is too complicated to obtain surface states that are clean enough. This brings about a charge density that occurs at the surface, and this leads to a polar behavior in the material [22,34]. Another reason for the exhibition of the polar character is that in this material there is no natural cleavage of the plane layer. Thus, the surface charge density effect is also interesting in this material.

Therefore, in this work, we are interested in the theoretical study of the effect of the input surface charge density and sub-dominant of the order parameter on the LDOS of $YBa_2Cu_3O_{7-\delta}$ material. The approach we used was the self-consistent tight binding

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http://dx.doi.org/10.1016/j.physc.2016.11.009
0921-4534/

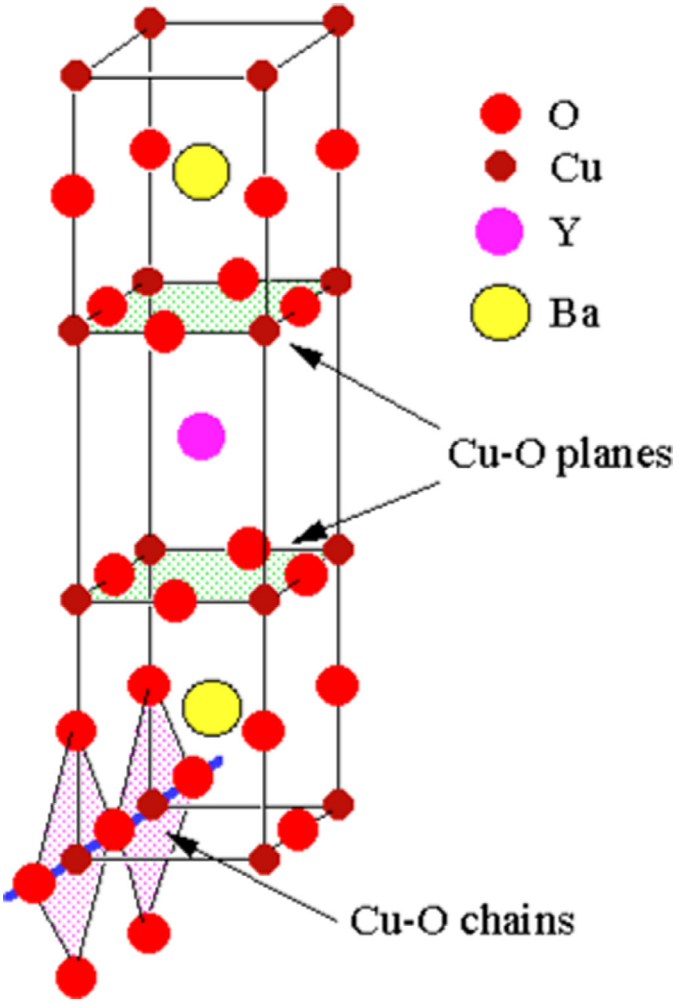

Fig. 1. Schematic illustration of CuO_2 plane and CuO chain of $YBa_2Cu_3O_{7-\delta}$ superconductor. This leads to the coupling scenario between chain and plane layers or plane and plane layers.

model under coupling between bands, calculating the LDOS at the surface and bulk states for comparison, as explained in Section 2. The main area of interest was to focus on the LDOS at the surface and the bulk states with and without an input surface charge and s-wave component of the order parameter, as expressed in Section 3. In this section, we compared, point by point, the LDOS within particular parameters. Finally, we finish with the conclusion as illustrated in Section 4.

2. Model and formalism

An illustration of the chain–plane and plane–plane coupling occurring in $YBa_2Cu_3O_{7-\delta}$, a high temperature superconductor, is expressed in Fig. 1. In this system, one can express the Hamiltonian as:

$$\hat{H} = \hat{H}_p + \hat{H}_c + \hat{H}_\perp \tag{1}$$

where $\hat{H}_p$ is the Hamiltonian for the isolated plane, $\hat{H}_c$ is the Hamiltonian for the isolated chains, and $\hat{H}_\perp$ is the single-electron hopping term that couples the two layers (plane–plane or plane–chain coupling). The plane Hamiltonian is given by:

$$\hat{H}_p = \sum_{ij\sigma} t_{p,ij}\hat{c}^\dagger_{p\sigma}(\vec{r}_i)\hat{c}_{p\sigma}(\vec{r}_j) + \sum_{ij}[\Delta_{ij}\hat{c}^\dagger_{p\uparrow}(\vec{r}_i)\hat{c}^\dagger_{p\downarrow}(\vec{r}_j) + \Delta^*_{ij}\hat{c}_{p\downarrow}(\vec{r}_j)\hat{c}_{p\uparrow}(\vec{r}_i)], \tag{2}$$

Table 1
Parameters for tight binding model of YBCO [33].

Parameter	Value
t_p	105 meV
t'	−0.277
t''	0.234
t'''	−0.042
t_c	500 meV
$t_{\perp p}$	61 meV
$t_{\perp c}$	$1.1t_{\perp p}$

where $\hat{c}^\dagger_{p\sigma}(\vec{r}_i)$ and $\hat{c}_{p\sigma}(\vec{r}_i)$ are the creation and annihilation operators for an electron in the plane on site i with spin σ and position $\vec{r}_i = (x_i, y_i)$, $t_{p,\,ij}$ refers to the hopping matrix elements in the plane layer, and Δ_{ij} is the superconducting pair energies that only exist in the plane layer. For the chain layer, the Hamiltonian is:

$$\hat{H}_c = \sum_{ij\sigma} t_{c,ij}\hat{c}^\dagger_{c\sigma}(\vec{r}_i)\hat{c}_{c\sigma}(\vec{r}_j), \tag{3}$$

where $t_{c,\,ij}$ refers to the hopping matrix elements in the chain layer. In this layer, there is no superconducting order parameter, but superconductivity can be induced by the proximity effect. When we take a square tight-binding lattice with hopping up to the third-nearest neighbor in the plane and the first-nearest neighbor in the chain, one can obtain the dispersions for the plane, $\xi_p(k)$, and chain, $\xi_c(k)$, layers:

$$\begin{aligned}\xi_p(k) = {} & -2t_p[\cos(k_x) + \cos(k_y) + 2t'\cos(k_x)\cos(k_y) \\ & + t''(\cos(2k_x) + \cos(2k_y)) \\ & + 2t'''(\cos(2k_x)\cos(k_y) + \cos(2k_y)\cos(k_x))] - \mu_p,\end{aligned} \tag{4}$$

$$\xi_c(k) = -2t_c\cos(k_y) - \mu_c, \tag{5}$$

where t_pt', t_pt'', t_pt''' refer to the hopping amplitude to the first, second, and third nearest neighbors, respectively, in the plane layer. $\mu_{p(c)}$ is the chemical potential of the plane (chain) layer.

The Hamiltonian describing the interlayer hopping, plane–plane, or plane–chain, is:

$$H_\perp = t_{\perp p,c}\sum_{i\sigma}[\hat{c}^\dagger_{1\sigma}(\vec{r}_i)\hat{c}_{2\sigma}(\vec{r}_i) + \hat{c}^\dagger_{2\sigma}(\vec{r}_i)\hat{c}_{1\sigma}(\vec{r}_i)], \tag{6}$$

where subscripts 1 and 2 refer to the two different layers and $t_{\perp p,\,c}$ is the hopping matrix elements between the plane–plane and the plane–chain layers, respectively. The model parameters used in this work are shown in Table 1. The order parameter for the superconductivity is represented by a $d_{x^2-y^2} + g_s$ wave, where g_s is the s-wave component. In the calculation, the order parameter for layer i of the plane is given by:

$$\Delta_{ip}(k) = \frac{\Delta_{i0}}{2}[\cos(k_x) - \cos(k_y)] + g_{is}, \tag{7}$$

where Δ_{i0} is the maximum gap.

Finally, the density of state of layer i that is pronounced as the local density of states, LDOS, can be obtained using:

$$\rho_i(\omega) = \frac{1}{N_k}\sum_k A_i(k,\omega), \tag{8}$$

where N_k is the number of k points, and:

$$\begin{aligned}A_i(k,\omega) = {} & \sum_{\alpha=1}^{2N}\left[|\psi_{\alpha,k}(i,\uparrow)|^2\delta\left(\omega - \xi_{\alpha,k}\right)\right. \\ & \left. + |\psi_{\alpha,k}(i,\downarrow)|^2\delta\left(\omega + \xi_{\alpha,k}\right)\right]\end{aligned} \tag{9}$$