Calculation of positron annihilation in High T_c copper oxides.

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LMTO calculations have been done in order to obtain electronic and positronic states in YBaCuO compounds. The annihilation rates have been calculated including the enhancement effects. Folded momentum density spectra are calculated and used for prediction of Fermi surface signals. The influence of lattice defects on the spectra is studied by the comparison between experimental and calculated positron lifetimes.

The calculations show that positrons in YBaCuO compounds are good probes of Cu-O chain related electronic states [1, 2]. Therefore clear Fermi Surface (FS) signals related to these states should be seen. Experimentally these FS structures have escaped observation for long time in YBa2Cu3O7-δ (1:2:3) [3]. A possible explanation of the difficulty to observe a clear Fermi surface (FS) signal in 1:2:3 is that in less oxygenated samples the Cu-O chains give smaller signals than in an ideal pure sample (δ = 0). The presence of oxygen defects would explain the observed complex temperature dependences of the lifetime and that calculated lifetimes are smaller than the experimental ones [7].

The YBa2Cu4O8 (1:2:4) superconductor may be a better candidate since the oxygen content is stable [4] and it forms twin-free crystals. Therefore, we have studied the 1:2:4 structure in order to determine the amplitudes of the positron annihilation signal.

Self-consistent calculations of the electronic structure have been performed using the LMTO (Linear Muffin Tin Orbitals) method. The positron potential is taken as the inverse of the electron Coulomb potential. The positron is assumed to be thermalized when annihilating and its wave function is then calculated only at k = 0. Then the positron wave function calculation is carried out using the LMTO method. The annihilation rates are calculated using the electronic and positronic states and an enhancement factor proposed by Jarlborg and Singh which take in account the screening around the positron impurity [8]. In 1:2:4 as in 1:2:3, we find that the positron in mostly distributed in the layers containing the Cu-O chains. The calculated lifetimes in (ps) are 156 for 1:2:3 (if δ = 0) and 183 for 1:2:4. If \[ N(t) = N(0) \sum I_i \exp(-\mu_i t) \] is the number of positrons remaining at time t, then the experimental lifetime known as bulk lifetime is calculated as \[ 1/\tau = \sum I_i \mu_i. \] The experimental values using Poosit [7] for 1:2:3 and 1:2:4 are respectively 170 ± 5 and 198 ± 5. These results were confirmed by the MaxEnt method [6]. The details of the experimental setup can be found in reference [7]. The different τ in the two compounds can be understood by the fact that more open space exists in the 1:2:4 (chain layers). In 1:2:3, when δ increases, the lifetime increases reaching a calculated value of 200 (ps) and an experimental one of 215 ± 5 (ps) for δ = 1. This is explained by the positron tendency to localize in the oxygen-deficient zones [8].
The 1:2:4 FS is composed of 4 sheets: 2 barrels for the two-dimensional Cu-O planes and 2 ridges for the one-dimensional Cu-O chains. The 1:2:3 FS is also composed of 4 sheets: 2 barrels, only one ridge and a small area hole pocket around the S point. In Figure 1, we show the LCW Momentum Density in the folded k-space for the 1:2:4 without (a) and with (b) positron wavefunction and enhancement effects (the signal is convoluted with experimental resolution ~ 0.5 (mrad) in 1(b)). Figure 1(a) gives essentially the electronic occupation as a function of the Bloch wave vector. The non-homogeneity of the positron distribution destroys the Cu-O plane FS modulation in figure 1(b). The Cu-O ridge signal is larger almost by a factor 2 with respect to 1:2:3 and should allow for an experimental detection.

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References


Figure 1: LCW Momentum Density (a) without and (b) with-positron effects.