Positron-annihilation studies on the Bi-Sr-Ca-Cu-O superconductor

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The results of positron-lifetime measurements as a function of temperature, across T_c, and as a function of heat treatment are presented. The lifetime in Bi-Sr-Ca-Cu-O does not show any variation with temperature in the range of 10 to 300 K, a result that is in contrast with other cuprate superconductors. The absence of lifetime variation across T_c is understood in terms of the calculated positron-density distribution, which indicates that the maximum of the positron density is in the region between the Bi-O layers with no significant density in the superconducting CuO_2 layers. Positron-lifetime measurements as a function of heat treatment indicate a decrease in lifetime as the annealing temperature is lowered from 800 °C to 100 °C. The decrease in lifetime, which is correlated with the increase in the weight of the sample, is explained in terms of the intercalation of the excess oxygen in the region between the Bi-O layers, which is the region probed by the positron.

I. INTRODUCTION

Since the discovery[1–3] of superconductivity in the Bi-Sr-Ca-Cu-O system, extensive studies[4] have been made on a variety of physical properties such as the structure, electronic structure, transport properties, thermodynamic properties, etc. The structure[5,6] consists of perovskite-like CuO_2 layers, separated by a Ca layer, and this group of layers is sandwiched between Sr-O and Bi-O layers. The perovskitelike CuO_2 layer is similar to those seen in other cuprate superconductors and is thought to be responsible for superconductivity in these systems. The Bi-O layer is considered to play an important role in the doping of holes in the CuO_2 layers. Electron band-structure calculations[7] indicate that the Bi-O band acts as a metallic reservoir which allows an increase in the number of holes in the CuO_2 layer. In addition to the Bi-O layer, the doping may also arise due to variations in the cationic and oxygen stoichiometry.[8] There have been several studies[9–12] on the influence of oxygen stoichiometry on the superconducting properties of the Bi-Sr-Ca-Cu-O system. In this system, there is a reversible increase in T_c with the decrease in oxygen content, a behavior which is opposite to that observed in the Y-Ba-Cu-O system. The details of the mechanism by which the oxygen stoichiometry affects the superconducting properties of Bi-Sr-Ca-Cu-O have attracted considerable attention.[13]

Since the advent of high-temperature superconductors, there have been several positron-annihilation studies on these materials, in particular on the temperature dependence of positron-annihilation parameters across T_c. Experiments have been carried out in the hole doped cuprate superconductors Y-Ba-Cu-O,[14–19] La-Sr-Cu-O,[20] Tl-Ba-Ca-Cu-O,[21,22] Y-Ba-Cu-O (Y 1:2:4:8),[23] in the electron doped superconductor Nd-Ce-Cu-O,[24] and in the copperless superconductor Ba-K-Bi-O.[25] In the hole doped superconductors large changes in the annihilation parameters have been observed at temperatures below T_c. However, both an increase and a decrease in annihilation parameters have been observed in the various systems and even in the same system of Y-Ba-Cu-O. This has generated a considerable interest in understanding the underlying reason for the temperature variation of annihilation parameters in the high-temperature superconductors and several theoretical model shave been proposed.[26–28] It has been recently shown[29,30] that the nature of change of annihilation parameters below T_c is related to the disposition of the positron-density distribution with respect to the CuO_2 layers and that the variation of annihilation parameters in the superconducting state is indicative of local charge transfer in the vicinity of the CuO_2 layers. In this paper, we report the results of the temperature dependence of annihilation parameters in the Bi-Sr-Ca-Cu-O system and analyze the results in terms of the calculated positron-density distribution.

Positron-annihilation spectroscopy has been shown[31,32] to be sensitive to the oxygen stoichiometry in the Y-Ba-Cu-O system. The annihilation characteristics, viz., the positron lifetime and the Doppler broadened line-shape parameter are observed to increase as the oxygen stoichiometry changes from the orthorhombic $YBa_2Cu_3O_7$ to the tetragonal $YBa_2Cu_3O_6$. This arises because, in the Y-Ba-Cu-O system, the positrons probe the basal plane containing the Cu-O chains[33] and the depletion of oxygen atoms takes place from the Cu-O chains. In this paper, we report the results of positron-lifetime measurements in heat-treated Bi-Sr-Ca-Cu-O. We analyze these results in terms of the theoretically calculated positron-density distribution and show that the variation in lifetime is correlated with the changes in the oxygen stoichiometry.

II. EXPERIMENTAL DETAILS

$Bi_2Sr_2CaCu_2O_{8+d}$ (Bi 2:2:1:2) samples were prepared by the solid-state reaction of appropriate amounts of Bi_2O_3, CuO, $SrCO_3$, and $CaCO_3$ in air. The details of the processing conditions can be found in Ref. 3. X-ray diffraction pattern could be indexed to the Bi 2:2:1:2 phase with trace amounts of unreacted CuO and Bi_2O_3. Resistivity measurements showed the sample to be superconducting with a T_c of 80 K.

Positron-lifetime measurements were carried out using a fast-fast coincidence spectrometer having a resolution function made up of a sum of two Gaussians having full width at half maximum (FWHM) of 285 ps (80%) and 425 ps (20%). For the measurements of positron lifetime as a function of temperature, a pair of Bi 2:2:1:2 pellets, sandwiching a 15-μCi ^{22}NaCl source deposited on 1.0-mg/cm^2 Al foil, was mounted on the cold head of a closed cycle helium refrigerator. The temperature could be adjusted between 300 and 10 K with a stability of ± 0.1 K. The lifetime spectra measured at various temperatures were analyzed using the PATFIT program,[34] taking into account the annihilation in the source foil. The source correction in the present experiments was $\tau = 190$ ps at 7% which was calculated as previously described.[14]

In addition to measurements as a function of temperature, experiments were also carried out on heat-treated Bi 2:2:1:2 samples to study the influence of oxygen stoichiometry. In these experiments, Bi 2:2:1:2 samples were heated in air for one hour and quenched to liquid-nitrogen temperature before positron-lifetime measurements were carried out at room temperature. The annealing temperature was varied from 800 °C to 100 °C on the same set of samples. To estimate the change in oxygen stoichiometry resulting from the heat treatment, the weight of the sample was measured after each heat treatment. The weight of the samples before the heat treatment was 190.7 mg.

III. RESULTS AND DISCUSSIONS

Results of the positron-lifetime studies as a function of temperature across T_c, and as a function of heat treatment and measured at room temperature are presented in Secs. III A and III C, respectively. These results are discussed in terms of the theoretically calculated positron-density distribution and lifetimes, presented in Secs. III B and III C.

A. Temperature dependence of positron lifetime

The lifetime spectra measured at various temperatures were best fitted to two exponential components after taking into account the annihilation in the source foil. The variation of the lifetime parameters τ_1 and τ_2 and the intensity of the first component, I_1, are shown in Fig. 1. It is seen that all the lifetime parameters are independent of temperature. The lifetime component $\tau_2 \simeq 360$ ps, with $I_2 = 15\%$, can be attributed[35] to the annihilation from the pores and surfaces of the sintered sample, whereas the lifetime component $\tau_1 \simeq 220$ ps can be associated with the

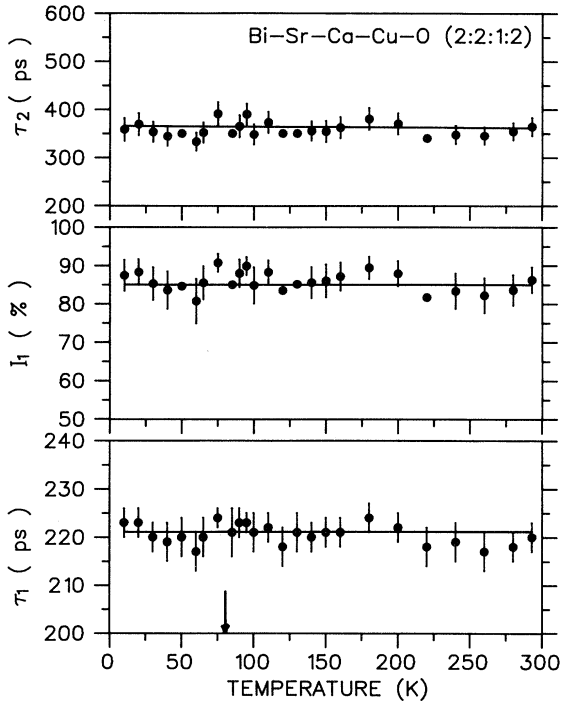

FIG. 1. Variation of lifetime parameters τ_1, τ_2 and the intensity of the first component, I_1, as a function of temperature in Bi 2:2:1:2. The arrow refers to the T_c of the sample.

annihilation in the bulk of the sample. Using the lifetime components, τ_1, τ_2, and I_1, the average lifetime $\bar{\tau}$ and lifetime in the bulk τ_B, were evaluated using the two state trapping model equations:[35]

$$\bar{\tau} = (\tau_1 I_1 + \tau_2 I_2) \tag{1}$$

and

$$\tau_B = (I_1/\tau_1 + I_2/\tau_2)^{-1} . \tag{2}$$

The lifetimes $\bar{\tau}$ and τ_B are found to be 240 and 233 ps, respectively, and independent of temperature.

In addition to the lifetime results reported above, we have also carried out positron-lifetime measurements on two mixed phase samples containing 40% Bi 2:2:1:2 and 60% Bi 2:2:2:3, and 10% Bi 2:2:1:2 and 90% Bi 2:2:2:3, respectively. Even in these mixed phase samples, the positron lifetime was found to be independent of temperature as in the pure Bi 2:2:1:2 system. Further, we have also carried out the measurement of the Doppler broadened line-shape parameters, which are also observed to be temperature independent.

The lack of variation of lifetime with temperature in the Bi 2:2:1:2 system is in distinct contrast to the other hole doped superconductors. For example, in La-Sr-Cu-O,[20] and in Tl-Ba-Ca-Cu-O (Tl 2:2:2:3),[21,22] an increase in lifetime has been observed below T_c, whereas in Y-Ba-Cu-O (Y 1:2:3) (Refs. 14, 15, 17, and 29) and Y-Ba-Cu-O (Y 1:2:4:8),[23] a decrease in lifetime has been observed in the superconducting state. The different temperature

dependencies (i.e., both an increase and decrease) seen in these cuprate superconductors have been correlated[29,30] with the nature of the positron-density distribution with respect to the CuO_2 layers. Consequently, we try to understand the lack of temperature variation in the Bi 2:2:1:2 system in terms of the calculated positron-density distribution.

B. Calculation of positron-density distribution and lifetimes

The calculation of positron-density distribution and lifetime in the Bi-Sr-Ca-Cu-O system has been carried out following the method discussed in Refs. 30 and 33. The lattice parameters of the tetragonal unit cell were taken to be $a=3.814$ Å and $c=30.52$ Å with the atomic positions as given in Ref. 5. The positron potential is calculated[30,33] as a sum of the Hartree electrostatic potential due to electrons and ions and the electron-positron correlation potential[36] in the local-density approximation. The Hartree potential and the electron density were obtained from the results of the self-consistent orthogonalized linear combination of atomic orbitals (OLCAO) band-structure calculations.[37,38] The positron wave function was obtained by solving the Schrödinger equation in real space under periodic boundary conditions using the numerical relaxation method.[39] The resulting positron-density distributions in the (010) and (110) planes are shown in Fig. 2. From this figure it is seen that the maximum of the positron density is in the region between the Bi-O layers. The positron density at the CuO_2 layer is at the minimum contour level of 0.0001 e^+/a.u.^{3} The calculated positron density is seen to be in good agreement with those obtained using the linearized augmented plane wave (LAPW) method[40] and in qualitative agreement with the calculations using superimposed atomic potentials and electron densities.[41]

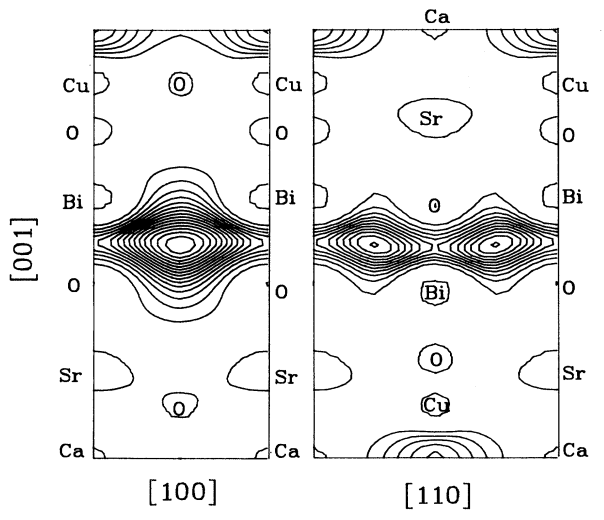

FIG. 2. Contour plot of the positron-density distribution in the (010) and (110) planes of Bi 2:2:1:2. The maximum of the positron density is in the region between the Bi-O layers. The minimum contour level is at 0.0001 e^+/a.u.^{3} and the contour increments are at 0.005 e^+/a.u.^{3}

With the calculated positron density and the electron density from the OLCAO band-structure calculations, the annihilation rate from the valence (λ_v) and the core (λ_c) are evaluated using the formula[30,33]

$$\lambda_v = \int |\psi_+(\mathbf{r})|^2 [2+134 n_v(\mathbf{r})] d\mathbf{r} \tag{3}$$

and

$$\lambda_c = 16\pi \int |\psi_+(\mathbf{r})|^2 n_c(\mathbf{r}) d\mathbf{r} , \tag{4}$$

where $|\psi_+(\mathbf{r})|^2$ is the positron density, $n_v(\mathbf{r})$ and $n_c(\mathbf{r})$ refer to the valence and core electron densities, and the factor $2+134n_v(\mathbf{r})$ takes into account the enhancement of valence electron density around the positron. The electrons from the 6*s* and 6*p* orbitals of Bi, 4*s* orbitals of Ca, 4*p* and 5*s* orbitals of Sr, 3*d* and 4*s* orbitals of Cu, and 2*s* and 2*p* orbitals of O were treated as valence electrons and the annihilation rate was calculated using Eq. (3), taking into account the enhancement of electron density around the positron. The electrons in the remaining inner orbitals were treated as core electrons and the annihilation rate was calculated in the independent particle approximation using Eq. (4). The valence and the core annihilation rates were evaluated to be 4.2370 and 0.1441 ns^{-1}, respectively, leading to the calculated lifetime of 228 ps. This is seen to be in very good agreement with the experimental bulk lifetime of 233 ps.

As mentioned earlier, the temperature dependence of positron-annihilation parameters in the various high-temperature superconductors has been shown[29,30] to be dependent on the disposition of the positron-density distribution with respect to the CuO_2 plane. The annihilation from the apical oxygen atom and the CuO_2 plane are important[30] in determining the temperature dependence of positron-annihilation parameters in the superconducting state. In those systems in which a decrease in annihilation parameters is observed, as in undoped Y-Ba-Cu-O,[29] there is a dominant contribution to the annihilation from the apical oxygen atom. In systems such as Tl 2:2:2:3,[21,22] wherein an increase in annihilation parameters is observed below T_c, the annihilation is dominated by the CuO_2 plane, in particular the planar oxygen atoms. With this correlation, the different temperature dependencies seen in the various high-temperature superconductors have been consistently explained[29,30] in terms of a charge transfer from the CuO_2 plane to the apical oxygen atom.

In the Bi 2:2:1:2 system, it is seen from Fig. 2 that the positron density is mainly located in the region between the Bi-O planes and the positron density in the CuO_2 plane is a factor of 750 less than the maximum between the Bi-O planes. In addition to the small positron density in the superconducting CuO_2 plane, the positron density is also seen to be small at the apical oxygen atom [see the (110) projection in Fig. 2]. We emphasize this since the apical oxygen atom is known[42] to play an important role in the charge transfer between the CuO_2 layer and the surrounding polarizable medium. A calculation[30] of the partial annihilation rate from the apical oxygen atom, by evaluating the overlap of the positron density with the

OLCAO electron density in a spherical volume characterized by the ionic radii of the oxygen atom, yields a value of 0.1102 ns^{-1}. This corresponds to only[43] 2.5% of the total annihilation rate (4.3811 ns^{-1}). Thus the small positron density at the CuO_2 plane and a negligible overlap with the apical oxygen atom can account for the insensitivity of the positron-annihilation parameters to the superconducting transition in the Bi 2:2:1:2 system.

C. Studies on heat-treated Bi-Sr-Ca-Cu-O

The heat treatment of high-temperature superconductors is known to have a large effect on its superconducting properties.[4] In contrast to the Y-Ba-Cu-O system, the annealing of Bi-Sr-Ca-Cu-O in oxygen atmosphere results in a reduction of T_c. The extra oxygen is believed[5] to go into the region between the Bi-O layers. The increase in the oxygen coordination around the Bi ion leads to an incrase in the effective valence of Bi ion towards 3+. This results in the reduction of the effective valence of Cu, viz., the hole concentration in the CuO_2 layer leading to the suppression of T_c.[13] Since the positron density is mainly in the region of the Bi-O layer (cf. Fig. 2), the positron-annihilation parameters must be sensitive to the intercalation of the oxygen atom due to heat treatment. With this motivation, positron-lifetime measurements have been measured at room temperature on Bi 2:2:1:2 samples annealed in air at various temperatures in the range of 800–100 °C.

The variation of lifetimes τ_1, τ_2, and the intensity of the first component, I_1, as a function of annealing temperature are shown in Fig. 3. The significant feature of this figure is the decrease in the lifetime component τ_1 from 210 ps at 800 °C to 195 ps at 100 °C. This variation in lifetime with annealing temperature was reversible in that on heat treating again at 800 °C, the original lifetime values were recovered. The bulk lifetime as evaluated using Eq. (2) is plotted as a function of the annealing temperature in Fig. 4. In the top panel of this figure we plotted the measured weight of the sample as a function of annealing temperatures after each heat treatment. The increase in the weight of the sample at lower temperatures is consistent with the earlier measurements[10,11] and arises due to the uptake of oxygen. In the present experiments, the increase in weight of the sample from 191.4 mg at 800 °C to 192.7 mg corresponds to an increase of

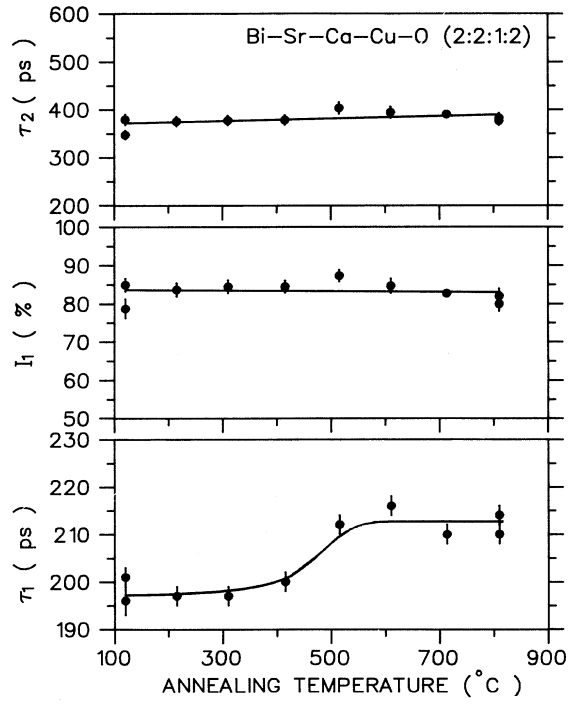

FIG. 3. Variation of lifetime parameters τ_1, τ_2 and I_1 measured at room temperature as a function of annealing temperature.

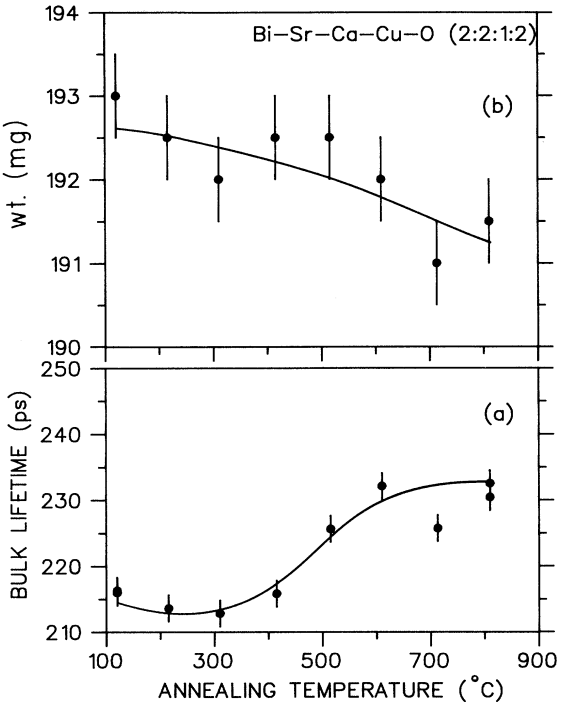

FIG. 4. (a) Variation of bulk lifetime obtained at room temperatures as a function of annealing temperature in Bi 2:2:1:2. (b) Variation of sample weight as a function of annealing temperature. The lifetimes were calculated from the data shown in Fig. 3.

TABLE I. Calculated positron lifetimes in the Bi-Sr-Ca-Cu-O system, having various oxygen stoichiometries.

System	λ_v (ns^{-1})	λ_c (ns^{-1})	τ_{calc}[a] (ps)
$Bi_2Sr_2CaCu_2O_8$	4.0582	0.5201	218.4
$Bi_2Sr_2CaCu_2O_9$	4.7423	0.6636	184.9
$Bi_2Sr_2CaCu_2O_{10}$	5.5037	0.8456	157.5

[a]The $\tau_{calc}=(\lambda_v+\lambda_c)^{-1}$, where λ_v and λ_c are the positron-annihilation rates from valence and core electrons evaluated using the superimposed atomic electron densities according to Eqs. (3) and (4), respectively.

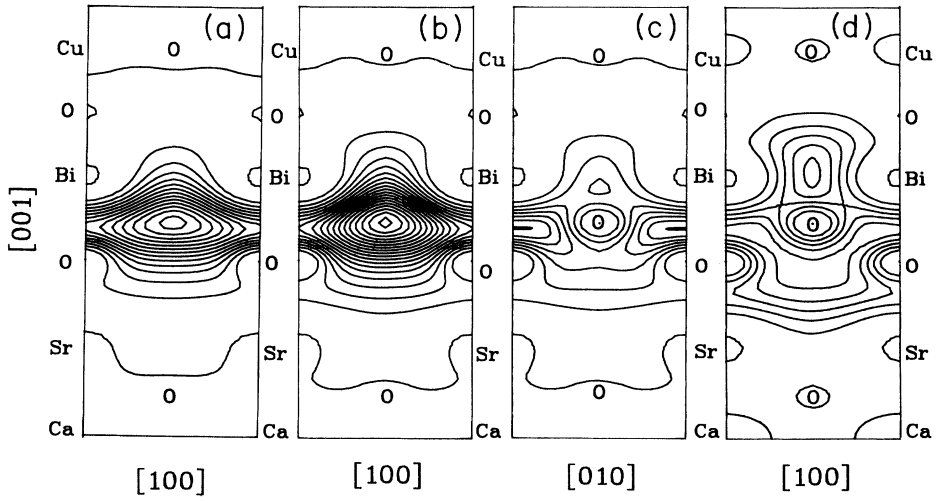

FIG. 5. Contour plots of the positron density in (a) (010) plane of $Bi_2Sr_2CaCu_2O_8$, (b) (010) plane of $Bi_2Sr_2CaCu_2O_9$, (c) (100) plane of $Bi_2Sr_2CaCu_2O_9$, and (d) (010) plane of $Bi_2Sr_2CaCu_2O_{10}$. The extra oxygen atoms have been located at the $(0,\frac{1}{2},\frac{1}{4})$ position for $Bi_2Sr_2CaCu_2O_9$ and at both $(0,\frac{1}{2},\frac{1}{4})$ and $(\frac{1}{2},0,\frac{1}{4})$ positions for $Bi_2Sr_2CaCu_2O_{10}$. The contour levels are the same as in Fig. 2. Notice that even in the presence of the extra oxygen atoms, the positron density is maximum in the region between the Bi-O layers.

0.38 oxygen atoms per formula unit. Thus the decrease in lifetime on lowering the annealing temperature is correlated with the increase in the oxygen content.

In the $Bi_2Sr_2CaCu_2O_8$ structure, the extra oxygen atoms can be located at the $(0,\frac{1}{2},\frac{1}{4})$ and $(\frac{1}{2},0,\frac{1}{4})$ positions [O(4) site in the notation of Ref. 5] in between the Bi-O layers. Half occupancy of these sites would lead to nine oxygen atoms per formula unit where as complete occupancy would lead to ten oxygen atoms per formula unit. With this structural information, positron-density distribution has been calculated for the O_8, O_9, and O_{10} structures with the positron potential obtained as a superposition of atomic potentials[44] and the correlation potential in the local-density approximation obtained using the superposed atomic electron densities.[44] The calculations have been carried out as discussed in Sec. III B and the resulting positron-density distributions are shown in Fig. 5.

In the $Bi_2Sr_2CaCu_2O_8$ structure, the positron-density distribution as obtained using the superimposed atomic potentials and electron densities[44] is shown in Fig. 5(a). This is seen to be qualitatively similar, in that the positron density is mainly in the region between the Bi-O planes, to the results obtained using the potentials and electron density from the rigorous OLCAO band-structure calculations (cf. Fig. 2). This indicates that in the Bi 2:2:1:2 system, the location of the positron density in the region between the Bi-O layers arises primarily due to the large interlayer separation (3.186 Å) and is insensitive to the details of the positron potential. With the addition of the extra oxygen atom at the $(0,\frac{1}{2},\frac{1}{4})$ position, the maximum of the positron density is still in the region between the Bi-O layers for the O_9 structure [cf. Fig. 5(b)]. The positron density in the region of the extra oxygen atom for the O_9 structure is seen clearly in the (100) projection as shown in Fig. 5(c). The positron distribution for the O_{10} structure with the oxygen atoms at both $(0,\frac{1}{2},\frac{1}{4})$ and $(\frac{1}{2},0,\frac{1}{4})$ positions is shown in Fig. 5(d).

Using the calculated positron density and the superposed atomic electron density,[44] the annihilation rates with the valence (λ_v) and core (λ_c) have been calculated using Eqs. (3) and (4), respectively. The calculated valence and core annihilation rates and the lifetimes in the various Bi-Sr-Ca-Cu-O systems are shown in Table I. It is seen that the lifetime progressively decreases with the intercalation of oxygen atom in the Bi-O layer. It is noted that the lifetime decreases by 33.5 ps when the oxygen stoichiometry increases from O_8 to O_9. In our experiments, a decrease in bulk lifetime of 15 ps is observed (cf. Fig. 4) when the oxygen stoichiometry increases by 0.38. This scales very well with the calculated decrease in lifetime with the oxygen content.

IV. SUMMARY AND CONCLUSIONS

In the Bi-Sr-Ca-Cu-O system, the positron density is mainly confined to the region between the Bi-O layers. The lack of positron density in the superconducting CuO_2 layer and at the apical oxygen atom accounts for the temperature independence of lifetime across T_c. However, the presence of the positron density in the region of the Bi-O layer makes the positron technique sensitive to probe the intercalation of oxygen atoms between the Bi-O layers.

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