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A Positron Trapping Model in High T_c Superconducting Materials*

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Abstract According to simple physical picture and competition mechanism of positron trapping in defects, a trap-annihilation model have been given. Furthermore, the characteristics of positron trapping in high T_c superconducting materials are discussed by this model. It may be used for discussing non-equilibrium defects in materials.

Keywords positron annihilation, high T_c superconductor, trap-annihilation model
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In many defected systems, the lifetime for multi-component spectra can be treated according to the trapping model reported by West et al[1,2]. However, the analysis of experimental data is sometimes difficult due to the effect of time resolution of spectrometers. All positrons are trapped, and annihilated in the saturated traps, i.e. high concentration traps. In this case, the trapping model is not applicable. In this paper, a simple physical picture, a definition of positron trap and some basic assumptions are introduced; a trap-annihilation model is proposed based on the competition mechanism. The characteristics of positron trapping in high T_c superconducting samples, taken as a good example, are also discussed according to our model.

1 Theoretical Model

1.1 Definition and classification

Positron traps denote the non-perfect regions of the crystals, such as vacancies, dislocations, grain boundaries, interfaces and surfaces. There are no atoms or more loose atomic arrangements on those regions, therefore, the positrons can be attracted to traps in a negative electrostatic potential.

Based on their positron potentials, positron traps can be classified into two categories: shallow traps and deep traps. The positrons in the shallow traps have the possibility to escape from the traps. The deep traps, on the other hand, do not release positrons. Fig. 1 shows the physical picture of positron traps. E_s and E_d represent the positron potential for a shallow trap and a deep trap, respectively.

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In addition, positron traps can also be classified as saturated traps and nonsaturated traps according to their concentration. The former is for high concentration traps which may trap and annihilate all positrons and for which the positron annihilation parameter does not change as its concentration increases further. The latter is for low concentration that partly annihilates the positrons.

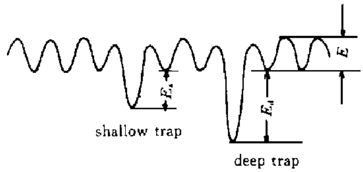

Fig. 1 Physical picture of positron traps

1.2 The distribution of positron in traps

The characteristic parameter of annihilation, F is a linear function of the positron state

$$F=\sum_j F_j N_j \Big/ \sum_j N_j=\sum_j P_j F_j \tag{1}$$

Where, F_j, N_j and P_j are the positron annihilation parameter, the number of positron and the probability of positron trapping in trap j, respectively.

In order to deal with the problem of positron trapping, a critical total concentration C_0 is introduced, which is defined as follows

$$C=\sum_i C_i \qquad C_0=\sum_i C_{i0} \tag{2}$$

Where, C is total effective concentration for all traps; C_i and C_{i0} are the real concentration for trap i and its critical concentration respectively.

According to the definition of positron traps, if $C_i < C_{i0}$ then trap i is a nonsaturated trap; conversely, if $C_i \geqslant C_{i0}$ then trap i is a saturated trap. However, the lifetime spectra can be analyzed by the trapping model reported by West et al[1,2] only in the case of nonsaturated traps. Thus we suggest that the probability of positron annihilation in saturated traps may be written as Maxwell-Boltzmann (M-B) distribution for which we get

$$P_i= A_i \exp(-E_i/kT) \qquad P_j/P_i= N_j/N_i= A_{ij}\exp(-E_{ij}/kT) \tag{3}$$

Where, $A_{ij}= A_j/A_i$ is a proportional coefficient, $E_{ij}= E_j-E_i$, E_i and E_j are the positron potentials in trap i and trap j, respectively.

2 Positron Trapping in High T_c Superconductor

2.1 Positron traps in high T_c superconducting samples

Compared to that of simple metals, the crystal structure of high T_c superconducting samples is complicated and anisotropic, and they contain more defects than simple metals, for instance, the oxygen vacancy, Cu(1)-O chain, the Cu(2)-O plane. The boundaries of superconducting phase are also involved in defects which have direct effects on superconductivity.

The high T_c superconducting sample contains many traps of positron. In order to easily analyze the lifetime spectra measured, a "quasi-trap" concept is introduced and defined as follows

$$E_0=\sum_i E_i/N=\sum_j E_{sj}/N+\sum_k E_{dk}/N \tag{4}$$

$$F_0=\sum_i F_i P_i=\sum_i F_i \Big/ \Big(1+\sum_j P_i/P_j\Big) \tag{5}$$

Where, E_i is the positron potential of trap i, E_0, F_0 are the positron potential and characteristic parameter of "quasi-trap", respectively. E_{sj} and E_{dk} are the positron potentials for shallow trap j and deep trap k, and the other symbols have the same meaning as in formula (1). Analysis of formulas (4) and (5) shows that the "quasi-trap" concept may solve the annihilation characteristics for many traps in high T_c superconducting samples. It means that a "quasi-trap" is analyzed, the other traps are regarded as background. Taking the positron potential of the "quasi-trap" as a standard, the traps can be classified into shallow traps ($E_i < E_0$) and deep traps ($E_i > E_0$).

2.2 Variation of positron annihilation parameter with the positron potential

When a high T_c superconducting system with many defects transiting from one state to another state, some shallow traps and deep traps are produced or eliminated. Taking the positron potential of the "quasi-trap" as a standard, the positron annihilation parameter increases when a deep trap is produced; conversely, it decreases when a shallow trap is produced. Similarly, the positron annihilation parameter decreases when a deep trap is eliminated; conversely, it increases when a shallow trap is eliminated. High T_c superconducting samples contain many kinds of defects, i.e. many shallow traps and deep traps, thus variation of positron annihilation parameter with trap parameters (such as trap concentration, trap potential) may be discussed as follows.

(1) For the saturated traps, the probability of positron annihilation may be written as M-B distributions. Replacing $F_i = \tau_i$ in formula (5), then, for M-B distribution, we get

$$\tau_0 = \sum_i \tau_i \Big/ \Big[1 + \sum_j \exp(E_{ij}/kT) / A_{ij} \Big] \tag{6}$$

Where τ_0 is a lifetime of "quasi-trap", which represents a mean lifetime in many saturated traps. τ_i is the lifetime of trap i. According to the results of formula (6), the mean lifetime depends on the positron potential of trap i and its lifetime, independent of its real concentration.

(2) For the nonsaturated traps, positron annihilation obeys the trapping model reported by West et al[1], we may get[2]

$$\tau = \sum_i \Big(1 + \sum_j K^{ij} / k\lambda_j\Big) \Big/ \Big(\lambda_i + \sum_j K_{ij}\Big) \tag{7}$$

Where, λ_j is the annihilation rate of positron in trap j; K_{ij} is the time-independent transition rate; τ is the mean lifetime of positron in nonsaturated traps.

(3) In other case, positrons annihilate both in nonsaturated traps and in saturated traps. If they are independent of each other, then the mean lifetime of positron may be written as follows

$$\tau = P_a \tau_a + P_b \tau_0 \tag{8}$$

Where P_a, P_b are the probability of positron annihilation in nonsaturated and saturated traps; τ, τ_0 are the "mean" lifetimes of positron in nonsaturated and saturated traps respectively.

In fact, based on the competition mechanism of positron trapping in traps, replacing $\lambda^* = 1/\tau_0$ in formula (6), then for M-B distribution, we get

$$\lambda^* = 1/\tau_0 = \sum_i \Big[1 + \sum_j \exp(E_{ij}/kT) / A_{ij} \Big] / \tau_i \tag{9}$$

Thus, the real mean lifetime of positron may be written as

$$\tau = \sum_i \left(1 + \sum_j K_j^* / k\lambda_j^* \right) \Big/ \left(\lambda^* + \sum_j K_j^* \right) \tag{10}$$

Where, λ^* is the annihilation rate of positron in saturated traps; K_j, λ_j^* are the transition rate and annihilation rate in nonsaturated trap j respectively. The mean lifetime of positron can be given by the analyses of formulas (9) and (10); the results in high T_c superconducting samples are shown in Fig. 2. Curves d_k and curves s_j are the changes of positron annihilation parameter (τ) due to the introduction of deep trap d and shallow trap s, respectively. Generally, $\tau_s \leqslant \tau_0 \leqslant \tau_d$, where τ_s and τ_d are the shortest (about 100 ps) and the longest (about 500 ps) lifetimes of all traps in high T_c superconducting sample. The mean lifetime measured has somewhat dispersion from τ_0 due to a limit of the competition mechanism. Similiar results can be given if the probablity of positron annihilation in saturated traps is written as Fermi-Diric (F-D) distribution.

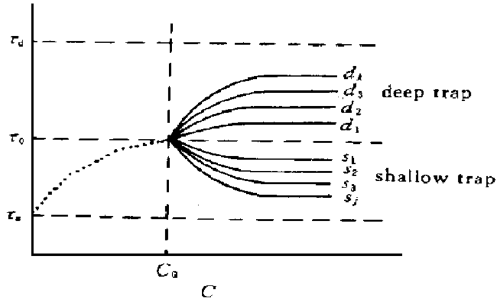

Fig. 2 Mean positron lifetime as a function of trap concentration in high T_c superconducting samples

2.3 Experimental test

The defects of high T_c superconducting samples were investigated by many authors[3-5] using PAT. Manuel et al[3] suggested that the large dispersion of the experimental results around T_c mainly come from the sintered sample, the temperature, the treatment, the homogeneity and the presence of eventual second phase. According to the trap-annihilation model, the number, the kind and the distribution of defects in high T_c superconducting samples are somewhat different. It implies that a lot of traps exist in the samples.

The positron annihilation parameter as a function of temperature has been widely investigated[3-5]. For instance, an increase and a decrease of lineshape S-parameter around T_c in $YBa_2Cu_3O_{7-\delta}$ were reported by Ishibashi et al[4]; and the anomalies of lifetime were reported by Teng et al[5] as well. According to analysis of Fig. 2, the introduction of a deeper trap results in an increase of the positron annihilation parameter, and the introduction of a more shallow trap results in a decrease of the positron annihilation parameter. The kind, depth and concentration of many traps will produce a sudden change as soon as the superconducting transition takes place in the samples. Therefore, τ_0, τ_1, τ_2, and their relative intensities I_1, I_2 from each group are different. In fact, these values do not represent the characteristic parameter of a trap, but the "mean lifetime" for some traps. Thus, different data were reported[3-5].

3 Conclusion

(1) A trap-annihilation model is proposed based on the competition mechanism for positron trapping in defects.

(2) The characteristics of positron annihilation in traps for high T_c superconductor are discussed by this model. The large dispersion of the experimental data around T_c can be explained.

(3) The model may be used to study non-equilibrium defects in other materials.

References

1 West R N. Positron studies of condensed matter. Adv Phys, 1973, 22 263~ 383
2 Hautojarvi P. Positrons in Solids. New York: Springer-Verlag Berlin Heidelberg, 1979. 89
3 Manuel A A. Positron annihilation in high-T_c superconductor: present status. J Phys Condens Mater I (SA), 1989, 107~ 117
4 Ishibashi S, Yamaguchi A, Suzuki Y, et al. Study of superconductors with high transition temperature by positron annihilation. Jap J Appl Phys, 1987, 26 (L): 688~ 689
5 Teng M, Shen D, Chen L, et al. Abnormal behavior of positrons annihilating in the ceramic superconductor YBaCuO in the transition temperature region. Phys Lett A, 1987, 124 363~ 366

高温超导体中的一个正电子陷阱湮没模型

吴奕初* 朱梓英

摘 要 从简单的正电子物理图像出发,引入正电子在陷阱中湮没竞争机制,提出了一个新的陷阱湮没模型,并采用这个模型分析了多陷阱的高温超导材料中的正电子湮没特征,此模型可用于探索非平衡缺陷问题的普遍情况.

关键词 正电子湮没,高温超导材料,陷阱湮没模型
分类号 O 571.33, TM 26

。简 讯。

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(芊 子)

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