Effect of Magnetic Ion Ni-doping for Cu in the CuO_2 Plane on Electronic Structure and Superconductivity on Y123 Cuprate

Shixun Cao [a,1], Pinglin Li [a], Guixin Cao [a] and Jincang Zhang [a]

[a] *Department of Physics, Shanghai University, Shangda Road 99, Shanghai 200436, P. R. China*

Abstract

The YBa_2Cu_{3-x} $Ni_xO_{7-\delta}$ with $x = 0 \sim 0.4$ have been studied using positron annihilation technique. The changes of positron annihilation parameters with the Ni substitution concentration x are given. From the change of electronic density n_e and T_c, it would prove that the localized carriers (electron and hole) in Cu-O chain and CuO_2 planes have enormous influence on superconductivity by affecting charge transfer between the reservior layer and CuO_2 planes.

Key words: High-T_c superconductor; Electron Structure; Positron annihilation; Ni-substitution

For Y123 system, many studies on ion substitution, especially the Cu site substitution have been taken because the importance of CuO_2 plane in high-T_c superconductivity. Ni is one of the Cu site dopants for which there are substantial evidence of substitution in the CuO_2 planes. Many researchers believe that Ni depress superconductivity mainly through magnetic pair breaking effect. Recently, some results proved that the primary effect of Ni doping on the conducting carriers of Y123 is to increase their elastic scattering rate and weaken the coupling between electrons and phonons[1,2]. As an effective probe of electron density, Positron Annihilation Technique (PAT) has been used in the study of high T_c superconductors to elucidate the nature of both the normal and superconducting states. In this paper, $YBa_2Cu_{3-x}Ni_xO_{7-\delta}$ with $x = 0.0 \sim 0.4$ have been studied by using PAT, which indicated that superconductivity is highly related with the local electronic structure of CuO_2 planes and the charge transfer between reservoir layers and conducting layers.

Samples of $YBa_2Cu_{3-x}Ni_xO_{7-\delta}$ ($x = 0 \sim 0.4$) were prepared by solid-state reaction method. All samples were confirmed to be single phase by X-ray diffraction measurement. The resistivity *vs* temperature was conducted by the standard DC four-probe method. ρ(T) measurement shows the unsubstituted sample has a superconducting transition temperature T_c of 91.5 K. As x increases, the value of ρ(T) increases monotonically at normal state. The curve of ρ(T) shows an significant upturn at low temperatures when $x \geq 0.2$.

The positron lifetime spectra were measured at room temperature (20 ± 0.5^oC) by using the ORTEC-100U fast-fast coincidence lifetime spectrometer. Two pieces of identical samples were sandwiched together with a $10\mu C^{22}Na$ positron source deposited on a thin Mylar foil (about $1.2 mg/cm^2$). Each spectrum contain more than 1×10^6 counts. After subtracting background and source contributions, the lifetime spectra were analyzed in two-lifetime components by POSITRONFIT-EXTENDED program with the best fit ($\chi^2 \leq 1.2$).

Fig.1 gives the positron annihilation parameters as functions of x. The shorter lifetime τ_1 ranges from 180 to 200ps, coinciding with the results for YBCO in other papers[3]. With the increase of doping level, τ_1 has an increase of about 5ps before $x = 0.05$, following a quick decrease until a minimum at $x = 0.2$, then increases gradually. The change of longer lifetime parameter τ_2 is similar to that of τ_1. Typically, for Y123 system, the lifetime according to bulk annihilation is about 159ps, trapping state annihilation for single oxygen vacancy

[1] Corresponding author. FAX number: +86-21-66134080. E-mail address: sxcao@mail.shu.edu.cn

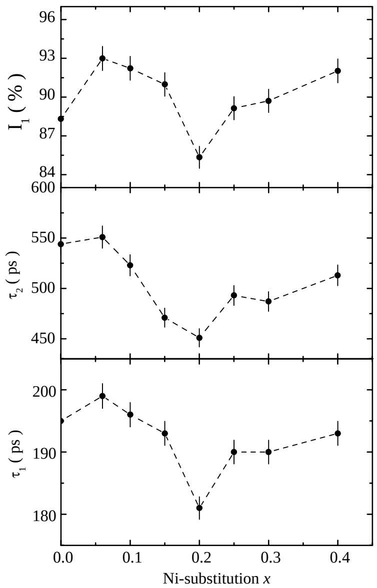

Fig. 1. Positron annihilation parameters as functions of x.

is about 170ps; for ion vacancies, it is always more than 200ps[4]. For our samples, τ_1 is about 180∼200ps, far more larger than that of bulk annihilation, so it may related with both the bulk annihilation and point defects trapping state annihilation. Our τ_2 is about 450∼550ps, may be related with microvoid trapping state annihilation.

In the CuO_2 planes, Ni ions act as acceptors, make it possible for oxygen vacancies to exist near the dopant sites, where potential well is formed and easy to trap positrons. So the positron distribution in the CuO_2 plane region may detect the dopant sites, contributing to the change of τ_1. On the other hand, there is significant lattice distortion for Ni substituted sample, this may contribute to the change of electron density distribution n_e, so to the change of positron lifetime. The cooperation and competition between these two factors may result in the change of our experimental results.

One characteristics of the $\tau_1(x)$ curve is that $\tau_1(x)$ has a minimum at $x = 0.2$, where the corresponding sample begin to show a clear $\rho(T)$ upturn. This gives us some hint of possible relation between the positron annihilation parameter and superconductivity. Fig.2 shows the change of the calculated local electron density n_e with x. n_e has a maximum value near $x = 0.2$. This is different with the results of Fe substitution and oxygen deficient YBCO systems, which gives the decreasing results of n_e[5,6]. This suggest that there exist two different kinds of mechanisms. A Hall study by Clayhold *et* al.[7] reported that Ni substitution affect the hole density in CuO_2 planes of $YBa_2Cu_{3-x}Ni_xO_7$,

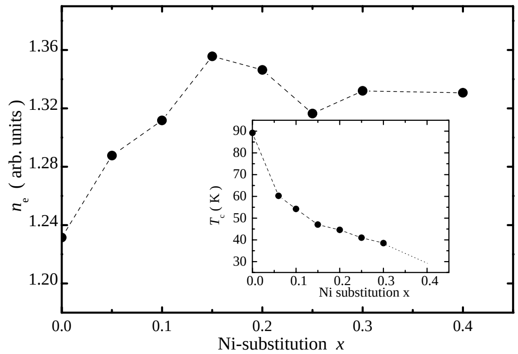

Fig. 2. Local electron density as function of x. The inset is the change of T_c with x.

consisting with our τ_1 result. This implies that for Ni substitution, with the increase of x, more electrons are localized around the dopant site, resulting in the decrease of hole density. The charge transfer may be one of the important factors. The increase of τ_1 at larger doping region reflect the weakening of electron localization. In the small doping region, where T_c decreases quickly with the increase of x, τ_1 decreases almost monotonically. For larger doping concentration, τ_1 has a small increase. From the variations of n_e and T_c at small doping level and the appearance of high electron density at larger doping concentration, it would prove that the localized carriers (electron and hole) in Cu-O chain and CuO_2 planes have enormous influence on superconductivity by affecting charge transfer between the reservoir layer and CuO_2 planes.

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