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The effect of doping with Zn and Ni on the $\text{YBa}_2\text{Cu}_3\text{O}_7$ electron subsystem

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Abstract. The electron structure, Stoner parameters, and exchange-enhanced local contributions to the spin susceptibility have been calculated for pure, Zn-doped, and Ni-doped $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO7) within the local density approximation, using a self-consistent T -scattering matrix method. It has been found that the Zn impurity causes a breaking of p-d covalence bonds in its vicinity, and gives rise to an island of reduced spin susceptibility and density of states at the Fermi level. This leads to the destruction of spin fluctuations near the impurity. The influence of Ni doping on the YBCO7 electron subsystem is much smaller than that of Zn doping. On the basis of the present results and the spin-fluctuation model, the effects of Zn and Ni doping on the critical temperature and NMR spectra of YBCO7 have been explained.

1. Introduction

Upon Zn and Ni doping of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ (YBCO), impurities substitute for the copper atoms Cu_2 located in the CuO_2 planes [1]. The doping induces no noticeable changes in the crystal lattice [2]. The Zn impurities sharply suppress the critical temperature T_c of YBCO ($dT_c/dy > 10$ K/at.% for $\text{YBa}_2(\text{Cu}_{1-y}\text{Zn}_y)_3\text{O}_7$). The effect of Ni doping on T_c is less than half that of Zn doping [1]. Thus the dopants are accurately inserted directly into the key subsystem of the material, and their effects on the superconductivity are essentially different. This picture suggests that the Zn and Ni impurities could be excellent probes for parameters controlling high- T_c superconductivity. This idea has motivated a number of investigations of the effect of Zn and Ni doping on the normal and superconducting properties of YBCO. Many investigations have been devoted to studying the effect of doping on the magnetic excitations in YBCO. This is perhaps due to the neutron scattering experiment [3] in which a gap in the spin excitations for superconducting YBCO has been found, as well as to a successful development of the model of spin-fluctuation-induced superconductivity (SFIS) [4–6].

The neutron scattering study [7], and measurements of Knight shifts ^{63}K , and the spin-lattice relaxation time $^{63}\text{T}_1$ [8, 9] have shown that Zn doping of YBCO leads to the disappearance of the gap mentioned above, whereas Ni doping causes no noticeable change in the spin excitations. Ishida *et al* [8] have found a strong temperature dependence of $1/({}^{63}\text{T}_1T)$ for the normal state of $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO7). This has been associated with antiferromagnetic (AF) spin fluctuations. The authors of [8] have also shown that the Zn doping suppresses this dependence much more strongly than the Ni doping.

Starting from the SFIS model, Ishida *et al* [8] have explained their results as follows: the nonmagnetic Zn impurities in YBCO destroy the local magnetic order around themselves, and hence weaken the pairing potential, and suppress T_c . The Ni impurities are expected to be magnetic; therefore they do not produce the above effect. Monthoux and Pines [5] have carried out a strong-coupling calculation of the effect of doping on T_c for YBCO for the model spin-fluctuation-induced interaction. A consideration of the Zn impurity in YBCO as a potential scatterer has led to considerable underestimation of the effect. To take into account the destruction of the magnetic correlation in the vicinity of Zn, Monthoux and Pines [5] used a simple phenomenological model, and have obtained a reasonable result, though the effect was overestimated.

Thus the authors of [5, 8] have provided a description of the effect of Zn and Ni doping on T_c and on the NMR spectra which is in agreement with the model of SFIS. However, it is not difficult to find another explanation of the results considered. Thus, the temperature dependence of $1/T_1T$ can originate from the temperature diffusion of the density of electron states near the Fermi level E_F , and the residual density of states at E_F observed below T_c [8] can be caused by extrinsic nonsuperconducting phases induced by the Zn impurity. The size of such inclusions can be more than the superconducting correlation length ξ , but less than is needed for x-ray or neutron diffraction effects (like in the ortho-II phase of YBCO; see [10]). Thus they cannot be detected by means of x-ray or neutron measurements, but can produce a residual density of states at E_F , where the main phase is in the superconducting state. Thus, for a more reliable interpretation of these NMR measurements, it is very important to find any additional parameters controlling spin excitations in YBCO, and to study the effect of doping on them. On the other hand, the substitution of Zn or Ni for Cu in YBCO must induce a modification of the chemical binding, whose energy substantially exceeds the AF spin-fluctuation energy. Therefore it is quite reasonable to consider the effect of doping on the spin excitations, taking into account the chemical binding modification that occurs upon this doping. Szunyogh *et al* [11, 12] calculated the average effects of Zn and Ni doping on the YBCO electron structure. These are useful in the study of long-range processes at high impurity concentrations. But when considering pairing and related phenomena in copper oxides, local effects are very important, since $\xi \sim 10 \text{ \AA}$. Szunyogh *et al* [11, 12] used a model potential for the impurity. Their calculation and tight-binding calculation [13] have led to the opposite conclusion about the Ni impurity spin state in YBCO7. So, the question of the Ni spin state in YBCO has remained open.

Thus, the Zn and Ni impurities could be more effectively used as a tool for clarifying the mechanism of high- T_c superconductivity. The present work is an attempt to realize this by means of the density functional theory within the local density approximation (LDA). In this work the effect of the Zn and Ni impurities on the local characteristics of the chemical binding and electron structure has been investigated. The local parameters of the electron subsystem which:

- (i) strongly depend on the features of the chemical binding;
- (ii) control the spin excitations;
- (iii) control the Knight shift and spin–lattice relaxation;
- (iv) are closely coupled with the SFIS model parameters; and
- (v) are obtainable within the LDA have been selected.

The change in these parameters upon doping has been determined versus the distance to the impurity. A self-consistent description of the influence of the Zn and Ni impurities on the electron structure, chemical binding, AF spin fluctuations, NMR spectra, and superconductivity has been given.

2. The computational method

The results of the present paper have been obtained with the multiple-scattering self-consistent-field method in the ‘lattice site–angular moment’ representation for the T -matrix in the muffin-tin (MT) approximation for the potential. In this approach, the equations for the T -matrix are as follows [14]:

$$\sum_{n_1 L_1} \{ \delta_{LL_1}^{n n_1} t_{n_1}^{-1} - g_{LL_1}^{n n_1} \} T_{L'L}^{n'n} = \delta_{nn'}^{LL'} \quad (1)$$

where n denotes the lattice site number, $L = l, m$ are angular moments, t_{nl} are the single-site scattering matrix elements, $g_{LL_1}^{n n_1}$ denote the free-electron Green’s function matrix elements, and $T_{LL'}^{n n'}$ are scattering path matrix elements. The effect of oxygen vacancy disordering is taken into account by means of the average t -matrix approximation version named ATA2 given by Bansil [15]. The exchange and correlation potentials are determined within the LDA [16]. The solution of equation (1) is used to determine the local density $N_l^n(E)$ of electron states, the components $N_m^n(E)$ of their expansion in lattice harmonics, and the valence charge density $\rho(\mathbf{r})$. The computational details have been described in [17, 18].

To reduce the effects of the finite number of scattering atoms, the atom whose local electron structure is determined is placed at the centre of the cluster. Hence, the equations (1) are solved for a set of clusters. In the present calculation of the YBCO7 electron structure, the smallest cluster, centred around Y, contains 43 atoms, and the biggest one, centred around Cu2, contains 48 atoms.

To obtain the effect of doping on $N_l^n(E)$ in the vicinity of the impurity, the following approximation has been proposed. It is assumed that the influence of the impurity on the electron states involves a finite space region. In the cluster centred around the impurity, the subcluster including a perturbation region is selected. In this way, the matrix of the coefficients in (1) decomposes into a block matrix. So, if equation (1) is rewritten as $\mathbf{AT} = \mathbf{b}$, then it can be represented in the form

$$\begin{aligned} A_{11}T_1 + A_{12}T_2 &= \mathbf{b} \\ A_{21}T_1 + A_{22}T_2 &= 0. \end{aligned} \quad (2)$$

Here the perturbation affects only the A_{11} -block. The other blocks corresponds to the scattering of the self-consistent nonperturbed system. Then, to calculate the electron states in the subcluster, equation (2) can be reduced to the form

$$(A_{11} - A_{12}A_{22}^{-1}A_{21})T_1 = \mathbf{b}. \quad (3)$$

It is important that the A_{22} -matrix has to be inverted just once per energy point. Furthermore, an iterative process for the self-consistent calculation is produced with equation (3). The dimension is equal to the A_{11} -matrix dimension. In the present case the system (3) contains only 61 equations.

In order to determine the Stoner parameter S_n , in this work the method developed by Gunnarsson [19] has been employed.

3. Results and discussion

In the present work, the self-consistent calculation of the YBCO7 electron structure has been carried out. Then, $N_l^n(E)$ and $\rho(\mathbf{r})$ have been self-consistently computed for the Zn and Ni impurities, for the neighbouring oxygen atoms O*, and for the nearest copper atoms Cu* lying in the same plane. Figures 1 and 2 show the density of d states obtained for the

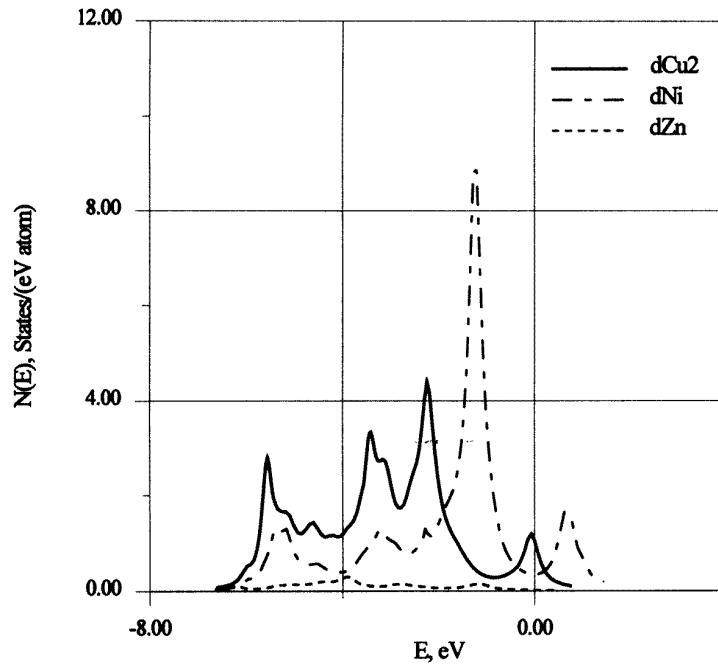


Figure 1. The local density of electron states at Cu2 and at the impurities for pure and doped $\text{YBa}_2\text{Cu}_3\text{O}_7$.

impurity site (IS) for Cu2 and Cu*, as well as the density of p states for O2 and O*. The point at which $E = 0$ corresponds to E_F .

The calculation results for the pure YBCO7 are in agreement with various band calculations. The $N_l^n(E)$ peaks situated near the Fermi level E_F are the most important details for the following consideration. They correspond to the antibonding part of the split $d_{x^2-y^2}$ Cu2-p_x O2 subband, and are a clear manifestation of the well-known covalence p-d binding in the CuO₂ planes. The relative position of this peak and E_F coincides with that given in [20, 21]; however, the peak shape is sharper in the present calculation. This difference could be caused by a cluster effect in the present method.

Figure 1 demonstrates the essential difference obtained for the densities of d electron states of Cu2, Zn, and Ni in YBCO7. The majority of the d Zn states in Zn-doped YBCO7 lie deeper than the d Cu2-p O subband (in the figure, its tail is just seen). Therefore, the substitution of Zn for Cu2 violates the p-d hybridization, and causes the breaking of the covalence bonds between the IS d states and the neighbouring oxygen-atom p states. This manifests itself in a drastic decrease in the $N_p^{O^*}(E)$ peak near E_F . These changes cause a sharp fall in $N_d^{IS}(0)$ and $N_p^{O^*}(0)$. Moreover, some decrease in $N_d^{Cu^*}(0)$ takes place (see figure 2).

The present calculation shows that the d Ni states in Ni-doped YBCO7 exhibit a strong energetic overlapping with the d Cu2-p O2 subband. In addition, the d wavefunction of Ni is more extended than that of Cu. Therefore the d Ni-p O* binding is stronger than the d Cu2-p O2 binding. That causes a large subband splitting, and the $N_p^{O^*}(E)$ and $N_d^{Ni}(E)$ peaks corresponding to the rising of the antibonding $d_{x^2-y^2}$ Ni-p_x O* states to above E_F . The $N_p^{O^*}(E)$ peak reflecting the d Cu*-p O* binding appears too, though its intensity decreases.

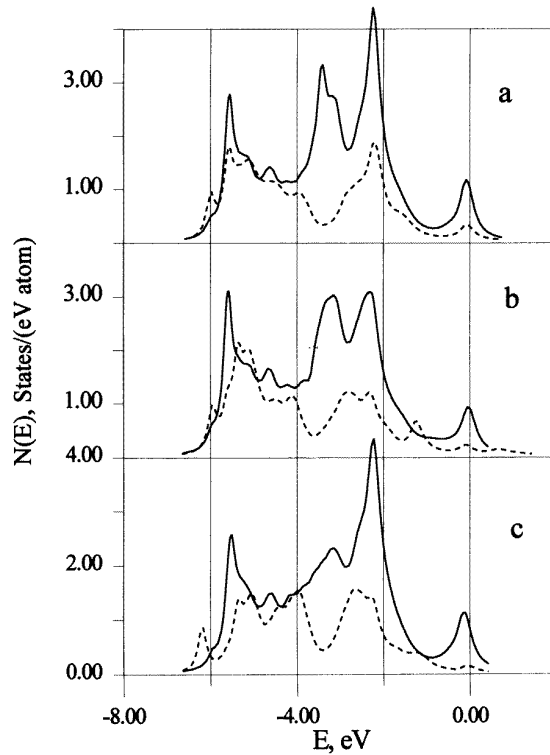


Figure 2. The local density of states at the Cu atoms (solid line) and O atoms (dashed line): (a) Cu₂ and O₂ in pure YBa₂Cu₃O₇; (b) Cu* and O* in Ni-doped YBa₂Cu₃O₇; and (c) Cu* and O* in Zn-doped YBa₂Cu₃O₇.

As a result, for YBCO7 doped with Ni one can see in figures 2 and 3 two highly energetic peaks. These chemical binding modifications lead to the decrease of $N_d^{IS}(0)$, $N_p^{O^*}(0)$, and $N_d^{Cu^*}(0)$.

An atomic substitution naturally leads to a change in the crystal potential. In figure 3 the radial dependences of the self-consistent MT-potential variation $\delta V(r)$ near the impurity site upon Zn and Ni doping are shown. The variation near the nucleus originates from the difference in the atomic number, and has a Coulomb-like character, and the difference between the Zn and Ni cases is just as regards the sign. With the increase of the radius, the role of the electron contribution in the potential grows, and a noticeable difference in the magnitude of $\delta V(r)$ appears. As a result, the substitution of Zn for the Cu₂ atom in YBCO7 induces more perturbation of the potential than does the substitution of Ni.

For considering the effect of potential variation on the electron states in solids, the scattering phase shifts $\delta_l^n(E)$ are suitable characteristics. Figure 4 shows the energetic dependence of the d phase shifts for the Cu₂, Zn, and Ni self-consistent MT potentials in YBCO7. Upon the substitution of Ni for Cu₂, the region of the resonance scattering is shifted towards E_F by about 1.5 eV. The substitution of Zn gives an opposite and much stronger effect. As a result, the resonance d Zn scattering goes into the bound-state region. This distinction causes the difference that is obtained in $N_d^n(E)$. However, the most important contribution to the potential impurity effect on the superconducting coupling is given by the scattering near E_F . Figure 4 shows that in that region the d scattering is

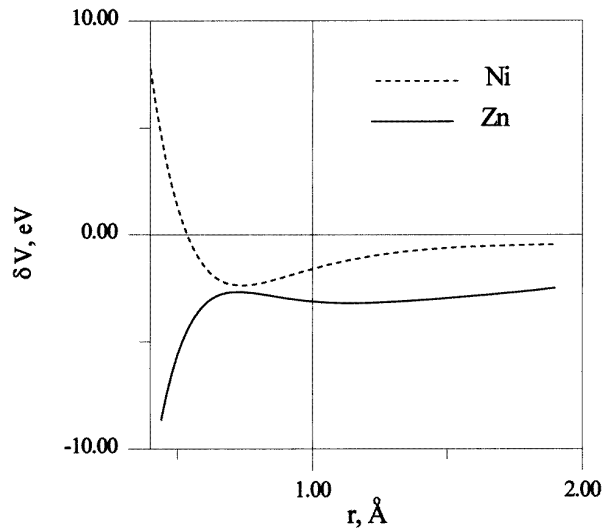


Figure 3. The variation of the impurity site potential in $\text{YBa}_2\text{Cu}_3\text{O}_7$ with the substitution of Ni and Zn for Cu2.

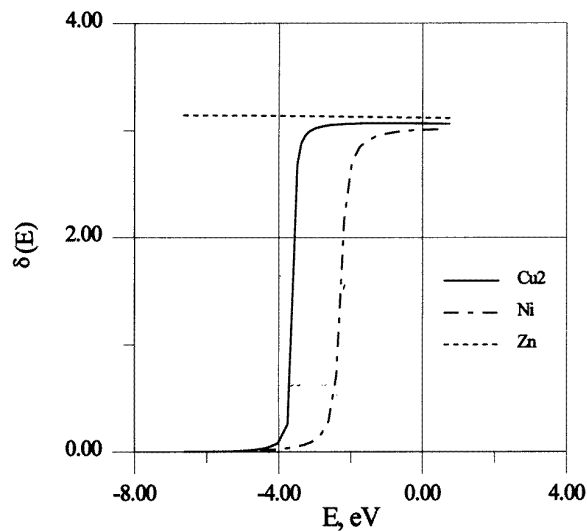


Figure 4. The energetic dependence of the phase shifts for Cu2 and the impurities in $\text{YBa}_2\text{Cu}_3\text{O}_7$.

weak ($\delta_d^{\text{IS}}(E) \approx \pi$) for both the Cu2 atom and the impurities. Moreover, the magnitudes of the variations of $\delta_d(E)$ caused by the Zn and Ni substitutions are nearly equal. Thus, the present results suggest that the difference between the effects of Zn and Ni doping on T_c of YBCO7 is not connected with the impurity potential scattering. For the Zn doping, this conclusion is in complete agreement with the results of Monthoux and Pines [5].

The spin state of the atoms in copper oxides is a very important characteristic to consider when investigating high-temperature superconductivity within current models (especially

within the SFIS model). Therefore it is important to know what the spin is at the Zn and Ni impurities in YBCO7.

The d Zn states fall out of the d Cu–p O subband; hence one can confidently conclude that stable spin polarization at the Zn impurity in YBCO7 is absent. An estimation of the Ni impurity spin state is a more difficult task. It is well known that atoms in Ni metal have uncompensated spins; this is successfully reproduced within the LDA [22]. The Ni oxide is magnetic as well, but there are reasons for supposing that in this compound electron correlations play a noticeable role in forming the spin state [23]. Therefore, it is important to understand whether the LDA is applicable for a description of the Ni impurity spin state in YBCO7.

Various experiments (for instance [24]) show that the Cu2 atoms in the CuO₂ planes provide conditions just for weak electron correlation effects (Pines [5] calls this system a nearly antiferromagnetic Fermi liquid). How does the Ni impurity change the picture? Ni has a d function that is more extended than that of Cu. Therefore, the usual Ni–O distance is longer than the Cu–O one: the Ni–O bond length in NiO is about 2.08 Å. When a Ni atom occupies a Cu2 site in YBCO7, the Ni–O2 distance can become as short as 1.93 Å. This enhances the p–d covalence binding (see above), and increases the p–d hopping integral. Besides which, the d-electron density on Ni is smaller than that on Cu, and, hence, the electron–electron repulsion U at the Ni is expected to be weaker than that at Cu2. All of these differences suggest that electron correlation effects near the Ni impurity in YBCO7 are weaker than in the unperturbed CuO₂ plane. Hence the LDA is applicable for considering the Ni impurity spin state in YBCO7. Thus it is reasonable to compare the character of the d Ni states in the Ni metal and YBCO7.

An important YBCO crystal structure feature is that the Madelung potential magnitude at the Cu2 site is comparatively low [25]. Hence, in contrast to the case for Ni metal, the main peaks of $N_d^{\text{Ni}}(E)$ in Ni-doped YBCO7 are situated below E_F . On the other hand, as has been noted above, the antibonding peak of the d Ni–p O* subband lies above E_F . As a result, $N_d^{\text{Ni}}(0)$ is comparatively small (see figure 1), which prevents the appearance of a local spin at the Ni impurity. For such a system, the Stoner parameter obtained within the LDA is applicable for estimating the tendency towards spin polarization of the Ni impurity.

Initially, Stoner [26] introduced S as a characteristic of the instability towards ferromagnetism. However, later studies show that S characterizes a local spin splitting. The expression for S obtained by Gunnarsson within the LDA [19] contains parameters which do not control any long-range interaction, but do control the local spin polarization. Heine and Samson [27] found conditions of the local spin polarization directly connected with S . Moreover the authors of [28] have clearly shown that the Stoner parameter has to be identified with the Hund's-rule exchange. Thus S is a characteristic of the spin splitting of atoms in solids.

On this basis, one can estimate the tendency of an impurity to exhibit spin polarization by comparing the S -values of different atoms in the compound. To this end, the Stoner parameters S_n have been computed for Cu, Zn, and Ni in YBCO7. The results are: $S_{\text{Cu2}} = 0.768$, $S_{\text{Zn}} = 0.007$, and $S_{\text{Ni}} = 0.238$. Since the value of S_{Ni} is much smaller than that of S_{Cu2} , one can conclude that the Ni impurity in YBCO7 is nonmagnetic.

To check additionally the correctness of that estimation, a self-consistent calculation of the electron structure and the Stoner parameter for the 43-atom Ni-metal cluster was carried out. It has been found that $S = 1.36$. So, the test shows that the Stoner criterion is realized within the present approach, because the Ni atom in metal has a magnetic moment which is approximately equal to $0.61\mu_B$ [22].

So, a number of distinctions between the effects of doping with Zn and Ni on the local

characteristics of the YBCO7 electron structure have been found. The following ones are believed to be related to high-temperature superconductivity:

- (i) the d Zn states lie deeper than the d Cu2-p O2 subband, while the latter and the d Ni states exhibit a strong energetic overlapping;
- (ii) the Zn doping causes the breaking of the covalence p-d bonds near the impurity, while the Ni doping induces only a modest modification; and
- (iii) the doping leads to a decrease in the density of the IS states at E_F by factors of 67 for Zn and 3 for Ni.

These results can easily be connected with both the parameters of the SFIS model [5, 6] and the characteristics measured in NMR experiments. So, a key characteristic of the SFIS model is the spin-spin correlation function, which is proportional to the experimentally obtained spin susceptibility χ_0 . The latter may be expressed in terms of the local susceptibilities χ_n . Taking into account exchange enhancement, one can write

$$\chi_0 = \sum_n \chi_n = \sum_{n,l} \frac{2\mu_B^2 N_l^n(0)}{1 - S_n} \quad (4)$$

where the first summation is taken over atoms in the cell. In this work, the χ_n have been computed for Cu2, O2, and IS, as well as for O* and Cu* near the Zn and Ni impurities.

Another important parameter controlling AF spin fluctuations is the effective magnetic interaction J_{ij} between electrons with antiparallel spins located at neighbouring sites. The Hubbard-like models give a very clear expression for this: $J_{ij} \sim t_{ij}^2/U$, where t_{ij} is the intersite hopping integral. U is the unscreened intrasite Coulomb repulsion. It is known that the effect of chemical binding on U is negligible. This is actually a characteristic which depends only on the atomic number. Hence the two substitutions considered induce the same perturbations of U . In the present case, t_{ij} is proportional to the covalence splitting magnitude of the $d_{x^2-y^2}$ Cu2-p_x O2 subband. For the NMR measurements, the Knight shift $K_n \propto \chi_n$, and, neglecting the electron-electron interaction, $1/T_1T \propto [N_d^n(0)]^2$ (the Korringa rule)

So, we have selected the local characteristics which control AF spin fluctuations, are directly connected with the parameters of the SFIS model, manifest themselves in NMR experiments, and have been obtained in the present calculations. They are $N_l^n(0)$, χ_n , and the magnitude of the $d_{x^2-y^2}$ -p_x splitting. For the following considerations, it is useful to introduce the parameters

$$D\chi = \chi_{n^*}/\chi_n \quad DN = N_l^{n^*}(0)/N_l^n(0)$$

where n denotes Cu2 and O2 atoms, and n^* denotes Zn, Ni, O*, and Cu* atoms; $l = p$ for oxygen and $l = d$ in the other cases. These parameters describe a suppression of the characteristics considered at the n^* -site upon the doping. They are shown in figure 5 as functions of the distance to the impurity. The points 0.0, 0.5, 1.0 on the x -axis correspond to the positions of the impurity, O*, and Cu* atoms respectively.

The $N_l^{Cu^*}(0)$ suppression effect can be compared with the experimental data. Ishida *et al* [8] succeeded in separating the contributions to $1/T_1T$ of the Cu sites away from and near to the impurity, i.e., in fact, of the Cu2 and Cu* sites for both normal and superconducting states. Using the result of [8], neglecting the spin-fluctuation effect at high temperature ($T = 300$ K), and applying the Korringa rule, we have estimated the experimental ratios $N_d^{Cu^*}(0)/N_d^{Cu2}(0)$. These are equal to 0.88 and 1.0 for the Zn and Ni doping respectively. The corresponding calculated ratios are 0.86 and 0.92, which is in reasonable agreement with the experimental data.

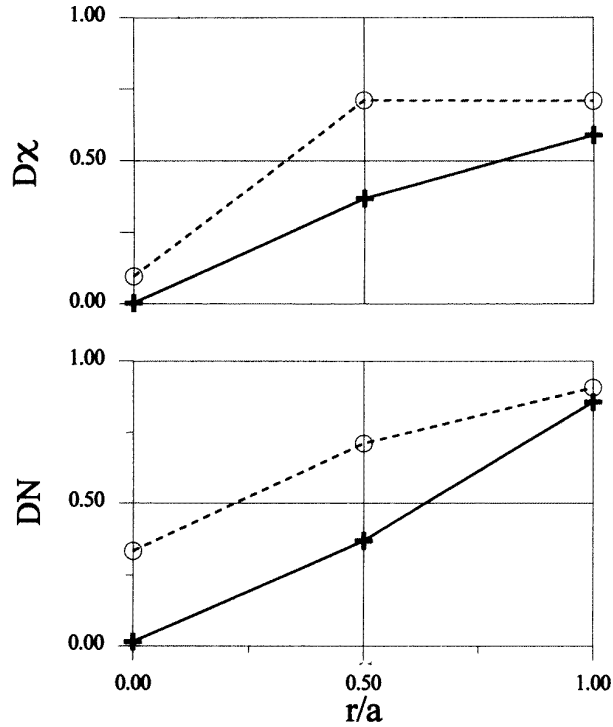


Figure 5. The parameters for the suppression of $N_l^n(0)$ and χ_n versus the distance to the impurity for Zn-doped (solid line) and Ni-doped (dashed line) YBa₂Cu₃O₇.

Figure 5 shows that the Zn doping of YBCO7 suppresses $N_l^n(0)$ and χ_n at the surrounding atoms much more than the Ni doping. Moreover, in contrast to the Ni effect, the Zn impurity induces a breaking of p-d covalence bonds in its vicinity. This leads to a sharp decrease in J_{ij} . This undoubtedly indicates that the Zn impurity destroys AF spin fluctuations around itself much more strongly than the Ni. Thus we have found an expected distinction between the effects of Zn and Ni doping on AF spin fluctuations in YBCO7. However, this is not caused by different spin states at the impurities [8, 5]. The present results show that for YBCO7 the spontaneous spin polarization is absent at both Zn and Ni. The main difference between the effects of doping on the spin fluctuations originates from the different effective magnetic interactions and local spin susceptibilities in the vicinity of the impurity.

So, we have obtained a close correlation between the effects of doping on the calculated parameters associated with AF spin fluctuation, and measured T_c . This seems to be strong evidence in favour of a spin-fluctuation-induced superconductivity mechanism in copper oxides [4–6].

The present study gives some results enabling a correction to be made of the approximation used in [5]. To take into account a destruction of the spin-fluctuation around Zn in YBCO7, Monthoux and Pines [5] expressed the spin-spin correlation function just in terms of r and ξ . This means that the origin of the spin fluctuation suppression is strongly localized at Zn, and has a $\delta(r)$ -like shape. The present results show that this origin (the fall in χ_n , and the breaking of the covalence bonds) involves a comparatively

large area, including the impurity and the surrounding O* and Cu* atoms. Monthoux and Pines [5] assumed that Ni in YBCO7 does not involve AF spin fluctuations in its vicinity. The present results show that this impurity must cause a noticeable suppression of spin fluctuations, though this effect is much smaller than in the Zn doping case.

In summary, self-consistent calculations of the YBCO7 electron structure and local exchange-enhanced spin susceptibility have been carried out. The changes in these characteristics upon Zn and Ni doping have been calculated. The results give the following picture of the effect of doping on the YBCO7 properties. Because d Zn states in YBCO7 lie deeper than the d Cu2-p O2 subband, the Zn doping causes a breaking of the p-d covalence bonds in the vicinity of the impurity and, hence, a sharp decrease in the effective magnetic interaction between neighbouring atoms. In addition, the Zn impurities form around themselves islands of reduced densities of states at the Fermi level, and reduced local spin susceptibilities. As a result, in doped YBCO7, AF spin fluctuations are destroyed around the Zn impurities. According to the SFIS model, this leads to a decrease in the pairing potential, and to a suppression of T_c . Since d Ni states in YBCO7 strongly overlap the d Cu2-p O2 subband energetically, the Ni doping causes only a modest modification of the electron subsystem in the vicinity of the impurity, with some decrease in the density of states at E_F . This is a possible reason for the comparatively weak effect of Ni doping on T_c for YBCO7.

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