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IMPACT OF OXYGEN DISORDER ON T_C SUPRESSION IN Zn DOPED$REBa_2Cu_3O_{6+x}$ SUPEROCNDUCTORS

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ABSTRACT

Conducting properties of $REBa_2Cu_3O_{6+x}$(RE123) type high T_c superconductors (RE=Y, 4f elements) are highly sensitive to the oxygen order in the oxygen deficient CuO_x planes which can be disrupted by doping with different metals,thus leading to a change of the superconducting transition temperature T_c. In this article we shall employ a simple theoretical model of charge transfer to studyhow $T_c(x)$ dependence is affected by the increase of oxygen disorder in the CuO_x planes, which is displayed in reduced average CuO chain length, l_{av}. The results indicate that though the increased oxygen disorder can produce significant decrease in T_c, it cannot be the only factor responsible forT_c reduction in Zn doped RE123 superconductors.

INTRODUCTION

Copper substitution by metal ions in $REBa_2Cu_3O_{6+x}$ high-T_c superconductors was widely used to study superconductivity in these materials,no matter which copper site is substituted Cu1 in CuO_x planes or Cu2 in the superconducting CuO_2 planes [1,2]. It is of special interest to study influence of nonmagnetic Zn ions substitution for copper ions at Cu2 site. Though the mechanism of superconductivity suppression due to Zn doping is not fully understood yet, it is believed that the main cause is the pair breaking which occurs due to dipoles formation which actas a strong scattering centers for charge carriers [1,3].It was also observed that Zn doping produces oxygen depletion of the CuO_x planes followed by increased oxygen disorder in these planes, thoughthe sample generally remains orthorhombic [3]. Increased oxygen disorder implies that length of CuO chains (sequences of Cu and O ions aligned along one of the crystallographic axes) formed in the CuO_x plains is decreased. Since charge carriers can be transferred only out of those CuO chains whose length, l, is equal to or greater than some critical length, l_{cr}, (usually assumed to be 3 or 4 oxygen ions) this chain length reduction is followed by a decrease in

charge carriers concentration in the superconducting CuO_2planes, which consequently leads toaT_c suppression.
Therefore we find it interesting to investigate how reduction of the average CuOchain length, l_{av}, is reflected upon the superconducting transition temperature dependence on oxygen concentration, $T_c(x)$.

THEORETICAL MODEL

In order to study thermodynamics of oxygen ordering in the CuO_x planes of RE123 superconductor we have used the well-known ASYNNNI model (Asymmetric Next Nearest Neighbor Ising model) [4]defined by the Ising Hamiltonian, which includes repulsive nearest neighbor interaction $V_1>0$ between oxygen ions, and two types of next-to-nearest neighbor interactions: attractive interaction,$V_2<0$, which is mediated by copper atoms and direct repulsiveinteraction, $V_3>0$. Since the attractive V_2 interaction is the main factor governing formation of CuO chains, in what follows we will assume that oxygen disordering in the CuO_x planes caused by the Zn doping is due to reduced strength of this interaction. WeakerV_2 interaction will lead to the formation of shorter CuO chains and the overall average chain length will be reduced. Concentration of positive holes transferred out to the CuO_2 planes can be calculated by the use of the simple charge transfer model [5] where the number of holes in one CuO_2 plane per one Cu ion (doping), p, is given by the following expression:

$$p = \frac{\mu}{2}\left[x_1\left(1-\frac{1}{l_{av,1}}\right)^{l_{cr}-1} + x_2\left(1-\frac{1}{l_{av,2}}\right)^{l_{cr}-1}\right] \qquad (1)$$

where $l_{av,1}$ and $l_{av,2}$ (x_1 and x_2) are average chain lengths (oxygen concentrations) on two non-equivalent sublattices of the CuO_x plain lattice, which are distinguishable in the Ortho II structural phase, and μ is the proportionality coefficient, $\mu\approx0.19$ [5].

RESULTS AND DISCUSSION

In order to calculate quantities necessary to evaluate doping p, we have employed Cluster Variation Method (CVM) simulations of the ASYNNNI model in a 4,5-point clusters approximation. For values of the interaction parameters we chose those obtained from the first principle calculations (LMTO values): V_1=6.9mRy, V_2= –2.4mRy, V_3=1.1mRy [6]. The CVM simulations were performed at constant oxygen equilibrium temperature T_{eq}=450K=const., which is the best representative of the room temperature in experiments at which most of the samples are equilibrated.

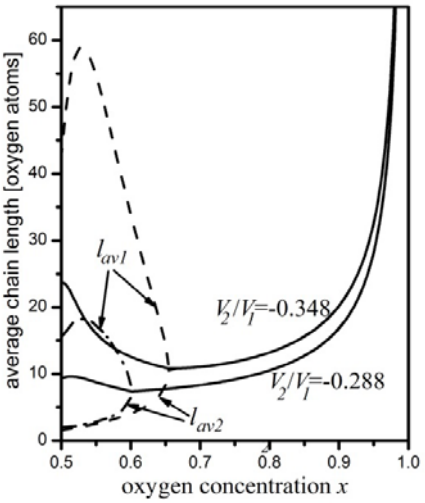

Figure 1. l_{av} as a function of x for two values of V_2 interaction.

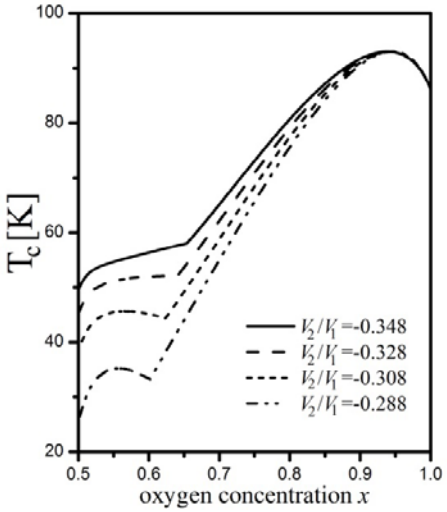

Figure 2. T_c as a function of x for different values of V_2 interaction.

The quantities of interest have been calculated for LMTO values of V_1 and V_3 interactions, and for four different values of V_2 interaction, one of them being the LMTO value and the other three values were chosen to have somewhat lower intensities so that oxygen disorder was increased.In the figure 1 we presented$l_{av}(x)$ dependences, calculated for two different V_2 values. One can observe thatreduced intensity of V_2 interaction produces shorter CuO chains, which is particularlyemphasized in the region of ortho II phase, where two different chain lattices can be distinguished.With further x increase,V_2interaction has less and less influence on the length of CuO chains, sincefulfilling of lattice with oxygen atomsnecessarily leads to formation of longer CuOchains.

Employing expression (1) and the well-knownempirical relation between T_c and doping p [7]:

$$T_c(p) = T_{c,max}[1 - 82.6(p - 0.16)^2] \quad (2)$$

we were able to calculate T_c as a function of x, and this dependence obtained for four different V_2 values and for l_{cr}=4 is shown in the figure 2. One can observe that$T_c$significantly decreases with V_2interaction intensity reduction, this decrease being the most pronounced in the OII phase. However$T_c$is not so drastically reduced in the OI structural phase where the main T_c reduction due to Zn doping occurs. One can also observe that two lower$T_c(x)$ curves display a minimum at x=$x_{OII/OI}$, where transition from orthoII to orthoI structural phase occurs. Appearance of this minimum can be understood if one observe (figure 1) that in the region $x\in(0.5,x_{OII/OI})l_{av1}$ decreases,

implicating that the number of CuO chain with $l \geq l_{cr}$ which can transfer holes to the CuO_2 planes is decreased. This decrease cannot be compensated by the increase of average chain length on α_2 lattice where initially many CuO chains with $l \leq l_{cr}$ existed. Therefore T_c is reduced and minimum in $T_c(x)$ dependence is formed at $x_{OII/OI}$ when two sublattices become equivalent and l_{av}, as well as T_c, starts to increase. Though for $V_2/V_1 = -0.348$ $l_{av1}(x)$ and $l_{av2}(x)$ behave in the same way as in the $V_2/V_1 = -0.288$ case, decrease of l_{av1} does not produce chains with $l \leq l_{cr}$, since l_{av1} was initially much larger then l_{av1} for $V_2/V_1 = -0.288$. On the other hand chains with $l \geq l_{cr}$ are formed on the α_2 sublattice as x increases, and therefore T_c is enhanced in the region $x \in (0.5, x_{OII/OI})$ and no minimum exists.

CONCLUSION

CVM simulations of the ASYNNNI model were performed to investigate how the $T_c(x)$ dependence behaves with the increase of oxygen disorder in the chain planes of the RE123 superconductor, which is manifested in the reduction of the average chain length. Since T_c suppression observed in our simulations was not as drastic as the experimentally observed one in Zn doped RE123 samples[3] we conclude that oxygen disorder due to Zn doping can be only partially responsible for the experimentally observed T_c suppression. In order to make more precise estimation on the contribution of Zn doping induced oxygen disorder to the T_c reduction, experimental results on the average chain length in Zn doped RE123 samples are desirable.

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