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A Monte Carlo study on distribution of CuO chains in $YBa_2Cu_3O_{6+2c}$

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Abstract

Distribution of CuO chains in $YBa_2Cu_3O_{6+2c}$, with respect to different chain lengths, has been studied in terms of the two dimensional asymmetric next-nearest-neighbor Ising (ASYNNNI) model, for the case of orthorhombic-I structural phase. If $p(l)$ stands for the fraction of CuO chains of length l (l equals to number of oxygen atoms that are linked in the chain), the results obtained show that $p(l)$ decreases monotonically with l, very accurately fitting to $p(l) = AB^l$, as at very low temperatures so at a very high temperatures as well (ranking from ≈300 K to 1800 K), and at all values of oxygen concentration c. Both parameters A and B were found to depend on (c, T) only through a single quantity—the average length $l_{av}(c, T)$ of CuO chains in the system. The expressions for $A(l_{av}) = A(l_{av}(c, T))$ and $B(l_{av}) = B(l_{av}(c, T))$, that were derived out of extensive Monte Carlo (MC) numerical simulations on the chain probability distribution $p(l)$ and independently obtained values of l_{av} were found to be very accurately fulfilled at all calculated points of (c, T) space. The particular behavior of $p(l)$ dependance has been assigned to $1d$ Ising model type of oxygen atom fluctuations along cooper mediated $V_2 < 0$ bonds (i.e., along b crystallographic axes). The importance of knowing the exact form of $p(l)$, for evaluation of the number of transferred electronic holes from CuO chains to superconducting CuO_2 layers, has been discussed together with its possible impact on the two-plateaus shape of $T_c(c)$ dependance.

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Keywords: CuO chains; Distribution of CuO chains; Oxygen ordering

1. Introduction

It is very well known by now that vanishing of semiconducting antiferromagnetic state and the onset of superconducting hole-doped state in high T_c superconductor $YBa_2Cu_3O_{6+2c}$ coincides with

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symmetry breaking in the basal CuO_{2c} planes accompanied with growth of the CuO chains along b-crystallographic axes [1–5]. Various superconducting orthorhombic structural phases, characterized by different alternation schemes of CuO chains and Cu-vacancy chains along *a*-crystallographic axes, are associated with different superconducting states of the system resulting in a well known two-plateaus like behavior of $T_c(c)$ dependance [2,3].

The common feature of all superconducting orthorhombic superstructures is that CuO chains (''full segments'') of various lengths alternate with ''empty'' Cu-vacancy segments along *b*-crystallographic axes [6,7]. Full chains may have different lengths ranking from $l = 1$ (isolated oxygen atoms) to lengths with tens, and even hundreds, of oxygen atoms which is particularly the case near stoichiometries $c = 0.25$ (OII structural phase) and $c = 0.50$ (OI structure) [6]. Ability of a full chain to act as a hole dopant is generally believed to depend on its length in the way that, for example, either the chains of the length l, having the composition $Cu^{2+}_{l+1}O^{2-}_{m}O^{-}_{l-1}$ are proposed to must have transferred $m-1$ holes to CuO_2 layers [8,9], or that there might be a certain critical chain length l_{cr} so that chains with $l < l_{cr}$ do not actually contribute to the charge transfer and, thus, to the onset of superconductivity [10–12]. However, whatever a mechanism for charge transfer from chains with given l might be, an issue of what is the fraction of basal plane oxygen atoms, which are involved in chains of this particular length, poses itself as inevitable step for the purpose of accurate counting of the number of transferred electronic holes as a function of oxygen content c. If $p(l)$ denotes the probability for a CuO chain to have the length l then the fraction of variable amount of oxygens in $YBa_2Cu_3O_{6+2c}$, participating in such chains, is proportional to $lp(l)$.

On the other hand, very little (even, perhaps nothing) has been done so far on clarifying the actual form of $p(l)$ dependance. Only chain lengths averaged on the macroscopic scale were possible to be determined in experiments with NQR (Nuclear Quadrupolle Resonance) on samples $YBa_2Cu_3O_{6+2c}$ slightly doped with Gd, since the electric field gradient at the cooper nuclei depends on the valence state of the ion itself and on the charge and local configuration of surrounding atoms [10–14]. Theoretically, the average chain length l_{av} has been determined in numerous studies (as it was made, for example, in Refs. [5–7] and [15]) through the fraction $f(c, T)$ of 3-fold coordinated Cu(1) ions, characterizing the number of chain ends in the system, via simple expression $l_{av} = 2c/f(c, T)$.

The problem of the distribution $p(l)$ with respect to different chain lengths is analyzed in this study. In the Section 2 the theoretical model, that is used as input for obtaining results of numerical Monte Carlo calculations, that are shown in the Section 3, is briefly presented, while the discussions of the results obtained, together with some conclusions, are exposed in the Section 4.

2. The model Hamiltonian

The most widely used theoretical model to describe the thermodynamics of oxygen ordering in $YBa_2Cu_3O_{6+2c}$ is the ASYNNNI model originally proposed by de Fontaine and Wille [16,17] which, besides of the fact that stabilizes the two major orthorhombic structural phases (the so-called orthorhombic I (OI), and orthorhombic II (OII)) as its ground states, also provides a reasonable good agreement of the general topology of the phase diagram with experimental findings. The Hamiltonian of the model is given by (see Fig. 1)

$$H = V_1 \sum_{\mathrm{NN}} \sigma_i \sigma_j + V_2 \sum_{\mathrm{NNN'}} \sigma_i \sigma_j + V_3 \sum_{\mathrm{NNN}} \sigma_i \sigma_j, \qquad (1)$$

where NN denotes that summation runs over all nearest neighbor pairs of oxygen sites in the basal plane, while NNN and NNN′ stand for next-to-nearest neighbor sites corresponding to the direct repulsive O–O interactions $V_3 > 0$ and to the attractive $V_2 < 0$ interactions with Cu(1) ion in-between, respectively. In our numerical calculations based on the Monte Carlo method the values of interaction constants obtained by Linear–Muffin–Tin Orbital method (LMTO) of Sterne and Wille [18] were used as input parameters. However, as it will become evident throughout the subsequent sections, the derived form of the