



Phase diagram of oxygen ordering in $\text{YBa}_2\text{Cu}_3\text{O}_{6+2c}$. The three-atom interactions

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Abstract

A cluster variation method (CVM) has been used to calculate the phase diagram of oxygen ordering in $\text{YBa}_2\text{Cu}_3\text{O}_{6+2c}$ in terms of two dimensional Ising model that, besides of repulsive nearest-neighbor (NN) interaction $V_1 > 0$ and two types of next-to-nearest neighbor (NNN) pair interactions $V_2 < 0$ and $V_3 > 0$, includes additional three-atom effective interaction V_{th} coupling two NNN oxygen atoms already bounded by V_2 (through Cu(1) ion) with the third O atom that is connected with one of these two by the repulsive NNN Coulomb interaction $V_3 > 0$. Phase diagrams were calculated for several different sets of interaction constants V_1 , V_2 , V_3 , and V_{th} together with the corresponding phase diagrams obtained for $V_{\text{th}} = 0$. The arrangement of main orthorhombic structures in (c, T) space and the nature of the phase transition curves between them is found to be in a very good agreement with those of the corresponding phase diagrams of the well-known ASYNNNI model, which had already proven itself as accurately reproducing the number of experimental findings on the structural phase diagram of $\text{YBa}_2\text{Cu}_3\text{O}_{6+2c}$. On the other hand, unlike to the predictions of the ASYNNNI model ($V_{\text{th}} = 0$), it is shown that inclusion of three-atom interaction V_{th} results in significant increase of the number of isolated basal plane oxygen ions which are generally considered as not giving rise to the charge transfer process and the onset of superconductivity. The importance of obtained oxygen superstructures of low temperature oxygen ordering and its possible impact on existence of plateaus in $T_c(c)$ dependence has been discussed.

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1. Introduction

One of the most interesting characteristics of the $\text{YBa}_2\text{Cu}_3\text{O}_{6+2c}$ superconducting compound is

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its well-known two-plateaus behavior of T_c versus c dependence [1–3]. The two plateaus of $T_c(c)$, at 60 K and 90 K, are commonly associated with two different orthorhombic structural phases, known as ortho-I (OI) and ortho-II (OII), whose existence is connected with symmetry breaking $a \neq b$ along a and b crystallographic axes of the system. The basic feature of orthorhombic structural phases is that oxygen atoms are ordered into CuO chains, in the direction of b -crystallographic axes, due to the attractive superexchange interaction between two oxygen atoms mediated by Cu(1) ion. While in tetragonal structural phase ($a = b$) material is not a superconductor, the transition from antiferromagnetic to superconducting behavior coincides with Tetra-to-Orthorhombic structural phase transition at nearly $c \approx 0.2$. It is the CuO chains which are generally seen as necessary background for the onset of superconductivity in $\text{YBa}_2\text{Cu}_3\text{O}_{6+2c}$ in the way that they act as generator of electronic holes which are then in part transferred to CuO_2 layers where superconductivity is taking place (the CuO_2 layers are located between Y and Ba ions along the direction of c -crystallographic axes).

The ground states of OI and OII structural phases are basically associated with different alteration schemes of α columns of oxygen sites in the basal plane. In OI phase oxygens equally populate all α columns while in OII phase (also known as “the cell doubled” phase) α_1 columns are more populated than α_2 (Fig. 1(a)). At nonzero temperatures, along both α_1 and α_2 columns CuO chains of various lengths alternate with empty chain fragments (sequences of vacant oxygen sites) resulting in different average chain lengths l_{av} . Almost all mechanisms of charge transfer that have been proposed so far were based on the assumption that Cu(1) ions normally exist as Cu^+ when the basal plane is free of oxygens ($c = 0$) for they are bounded by two oxygen atoms along c -axis (as, for example, in Refs. [4–6,9]). When an isolated oxygen atom is embedded in the basal plane, it then takes two electrons from two nearest neighboring Cu(1) ions, due to its well-defined tendency to two fold electro-negativity, transferring them from Cu^+ into Cu^{2+} . Therefore, the existence of isolated oxygen atoms does not violate local electric balance

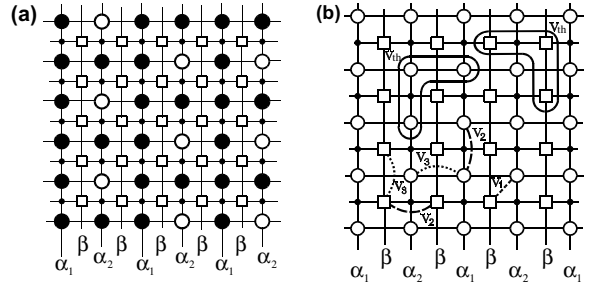


Fig. 1. The basal plane lattice of $\text{YBa}_2\text{Cu}_3\text{O}_{6+2c}$. (a) Fragmented chain structure at $c = 0.375$. Large black circles denote oxygen atoms on α_1 and α_2 columns, while open circles and squares denote unoccupied oxygen sites on α_2 and β sublattices, respectively; small black circles denote Cu(1) ions, (b) The NN interaction ($V_1 > 0$), the NNN interactions ($V_2 < 0$ and $V_3 > 0$), and the three-atom interaction V_{th} of the Hamiltonian (1).

implying that there is no need for transfer of additional negative charge from the rest of the system to take place. On the other hand, when l oxygen atoms are linked in a CuO chain they could have taken only $l + 1$ electrons from as many of Cu(1) ions participating in such chain, while the remainder of $l - 1$ electrons are believed to must have been transferred from other parts of the system (mainly from CuO_2 sheets). Within such a simple scenario the amount of transferred electronic holes should be proportional to fraction of four-fold coordinated Cu(1) ions, but theoretical calculations of this quantity showed no two plateaus when it was considered as a function of oxygen content c [6]. Another approach to the problem was grounded on proposition that not only isolated oxygen ions were to produce no charge transfer, but that there might be a certain critical chain length l_{cr} so that chains with $l \leq l_{cr}$ do not in fact give rise to hole creation as well [7]. On the other hand, in study of Gawiec et al. [8] it was proposed that in a chain of length l only $m < l$ of oxygen ions exist as O^{2-} , while the remainder $l - m$ ions are O^- , implying in this way that chain of length l must have transferred only $m - 1$ electronic holes. In this approach, all of $l - 1$ four-fold coordinated and the two 3-fold coordinated Cu(1) ions were assumed to reside as Cu^{2+} , while the ratio m/l was estimated to be nearly equal to 0.7 at least for the case of long chains [8].

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