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CVM STUDY OF CHARGE TRANSFER IN $YBa_2Cu_3O_{6+X}$ MATERIAL

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Abstract

The number of positive holes transferred from the CuO_x basal planes to the superconducting CuO_2 planes of $YBa_2Cu_3O_{6+x}$ material was calculated as a function of oxygen content x, by the use of numerical cluster variation method (CVM). The calculations were performed for the set of three different temperatures and for the different values of the parameter ξ_l which represents the ratio of the number m of divalent oxygen ions in the chain fragment and the total number l of oxygen ions in the chain fragment. The obtained hole count versus x dependence showed no plateau behavior for low temperatures (t=0.25 and t=0.35) while for t=0.45 indication of plateau behavior is present.

Introduction

The high T_c superconductor $YBa_2Cu_3O_{6+x}$ is well known for its characteristic two plateaus in T_c (critical temperature of superconducting transition) versus x dependence [1]. While the origin of lower 60K plateau is still unclear, the existence of the plateau at 93K is associated with an optimal doping of the superconducting CuO_2 planes [2]. Though, it is believed that the plateau at 60K is related to the degree of oxygen ordering in CuO_x planes [3], which act as a reservoir of holes from where they are transferred to the CuO_2 planes. The dependence of number of holes transferred from CuO_x planes on x is expected to exhibit behavior similar to that of $T_c(x)$. Doping of CuO_2 planes with holes through the increase of the oxygen content is related to the valence change of Cu(1) ions (Cu ions in the basal planes). In the parent $YBa_2Cu_3O_6$ compound all the Cu ions in the basal planes are monovalent being surrounded by only two apical oxygen atoms. With increase of oxygen content the chain fragments (sequences of Cu and oxygen ions aligned along *b* crystallographic axes) are formed, and can be characterized by its length l and by its charge. The general form of the chain fragment of length l can be written as $Cu_{l+1}^{+2}O_m^{-2}O_{l-m}^{-}$ .Since the neutral chain fragment includes only one divalent oxygen ion it follows that the chain having m divalent oxygen ions must have transferred $m-1$ holes [4]. The optimal value of the parameter $\xi_l=m/l$, governing for the charge transfer is estimated to be $\xi_{l(opt)} \approx 0.7$ for long chains ($l>>1$). It is not expected that this value differs much for the short chains. Thus the optimal chain configurations have been established to be $Cu_3^{2+}O^{2-}O^{-}$ for $l=2$, $Cu_4^{2+}O_2^{2-}O^{-}$ for $l=3$, and $Cu_5^{2+}O^{2-}O^{-}$ for $l=4$. For the longer chains this rule can be generalized as: $m=nint(l(m/l)_{opt})$ (*nint* is the nearest integer). Applying this rule to estimate the number of holes transferred from the chains of different lengths the total amount of holes transferred from the CuO_x planes can be calculated.

Results and Discussion

The number of holes n_h transferred from the basal planes to the CuO_2 planes is given by the following formula [5]:

$$n_h = \sum_{n=1}^{\infty} \left[l \, \mathrm{int}(\xi_l l) - 1 \right] p(l) \ , \qquad (1)$$

where *p(l)* is the probability of finding a chain of length *l* in the system, and it is determined by the expression [6]:

$$p(l) = \frac{(l_{av} - 1)^{l-1}{}_{av}}{l^{l}_{av}} \ , \qquad (2)$$

where l_{av} is the average chain length.

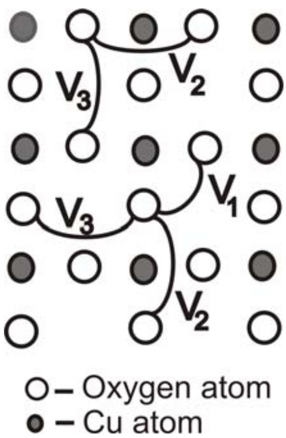

Fig. 1. Basal plane lattice with ASYNNNI model interactions

In order to calculate the hole count n_h we have employed the numerical cluster variation method and the well known ASYNNNI model which describes the thermodynamics of oxygen ordering in terms of two dimensional Ising model with asymmetric interactions of next nearest neighbors (Fig. 1). For the values of model interactions we used those obtained, from the first principles calculations, by Sterne and Wille [7]. The hole count was calculated for different values of ξ_l ranging from *0.1* to *1.0*. The calculated values of hole count are shown at figure 2. as a function of oxygen content *x* and for three different temperatures 0$t=k_BT/V_1$. It can be seen that for $t=0.25$ and for $t=0.35$ no indications of possible plateau existence in the range of stability of OrthoII phase is present, but only a kink occurs for the value of *x* for which the onset of the plateau could be expected. For $t=0.45$ the $n_h(x)$ function exhibits a close to plateau behavior for some values of parameter ξ_l .

Conclusion

The number of holes transferred from the CuO_x planes was calculated as a function of oxygen content x for different temperatures and for different values of parameter ξ_l . The choice of parameter ξ_l has no much influence on the shape of the n_h versus *x* curve accept that its higher values bring in holes to the CuO_2 planes for lower values of *x*. At low temperatures no plateau is present in the hole count which is due the fact that at low temperatures long oxygen chains dominate at $x=0.5$ and that additional oxygen atoms tend to form chains thus producing holes, which is not the case at higher temperatures when additional oxygen can exist as isolated, creating no holes and producing a plateau in n_h versus *x* dependence.

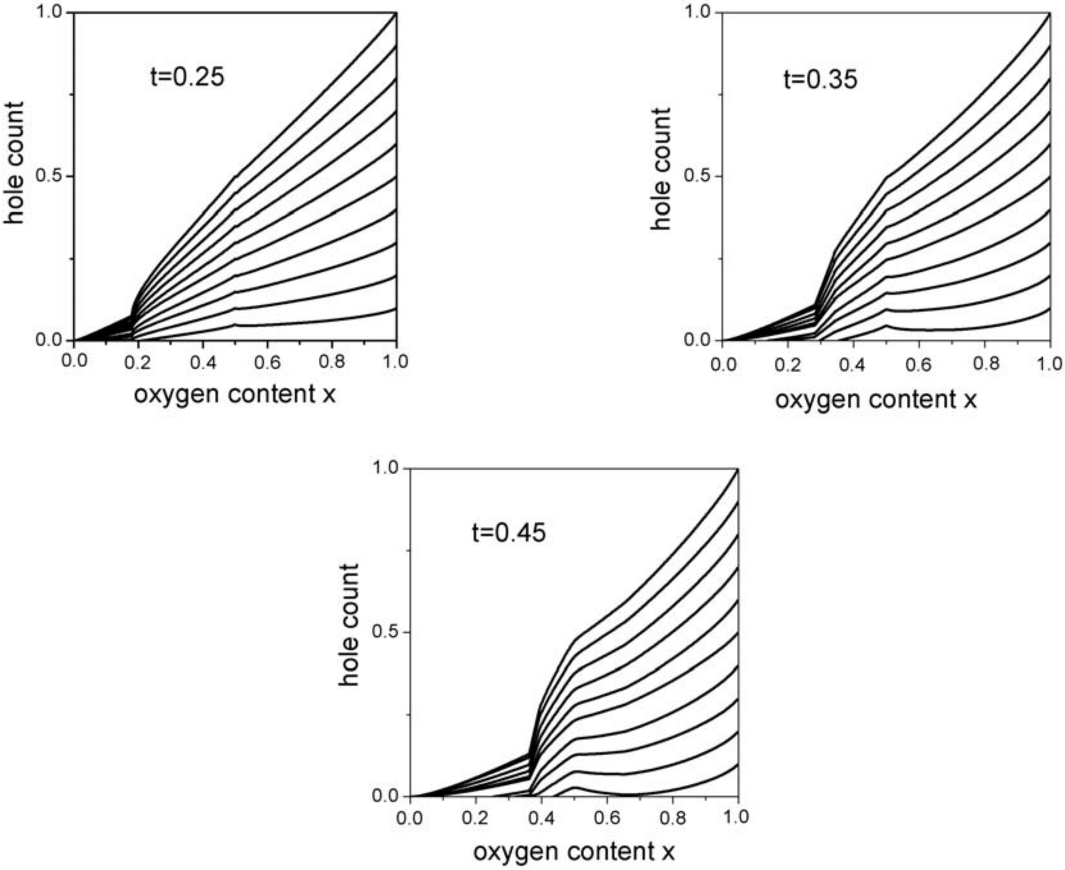

Fig. 2. Hole count as a function of oxygen content x for three different temperatures. For each temperature $n_h(x)$ is shown for ten different values of parameter ξ_l from *0.1*(lowest curve) to *1.0* (highest curve), with step of *0.1*.

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