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# ORDER-DISORDER TRANSITIONS IN AN ASYMMETRIC NEXT-TO-NEAREST NEIGHBOURS ISING-TYPE MODEL

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The distribution of Cu–O chains with respect to their length and orientation in YBCO–123 is studied by means of numerical simulations of the ASYNNNI model. It is found that the formation of Cu–O chains can be either anisotropic or isotropic, depending on the temperature and concentration. A suitable order parameter is introduced to study transitions between the isotropic and anisotropic phases of the model.

The topic of oxygen ordering in the basal Cu–O plane of $YBa_2Cu_3O_{6+x}$ (where $0 < x \leq 1$) has been studied in considerable detail [1]. From the theoretical point of view, the temperature-concentration phase diagram is well explained by the two-dimensional asymmetric next-to-nearest neighbours Ising model (the ASYNNNI model) [1]. In particular, the model contains as ground states two ordered orthorhombic structures consisting of Cu-O chains. Ortho I occurs (at appropriate temperatures) for $x$ close to 1 (50% O concentration) and Ortho II for $x$ close to 0.5 (25% O concentration). The Ortho I structure is shown for a 10 by 10 lattice in Fig. 1: in this structure, all the O sites in the Cu–O chains are occupied. The Ortho II phase is similar, except that all the O sites in alternate Cu–O chains are vacant.

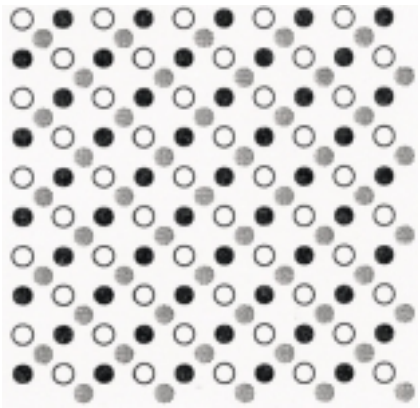

Fig. 1. The Ortho I structure in the basal plane of YBCO–123 for a $10 \times 10$ lattice

The orthorhombic structures are anisotropic in the sense that the Cu–O chains are all oriented in one direction (in Fig. 1, to the right). One can ask whether there are also isotropic structures which contain chains that are oriented in both possible directions. The purpose of

this paper is to use the ASYNNNI model to study this question and, in particular, to study transitions between the isotropic and anisotropic structures.

In the ASYNNNI model, only the interactions of an oxygen ion with its nearest-neighbour oxygen ions ($V_{NN} = V_1$) and its next-to-nearest neighbour oxygen ions are taken into account. For the latter there are two types of interaction: $V_2$ (or $V_3$), according to whether a Cu atom is (is not) present in the NNN bond (see Fig. 1). The Hamiltonian is

$$H = V_1 \sum_{NN} n_i n_j + V_2 \sum_{NNN} n_i n_j + V_3 \sum_{NNN}{}' n_i n_j, \tag{1}$$

where $n_i = 1$ if site $i$ is occupied by an oxygen ion, otherwise $n_i = 0$. The site contribution to $H$ has been omitted in Eq. (1) because it is irrelevant to the study of oxygen mobility in the context of the model. We have used the potentials [2] $V_1 = 0.190\text{eV}$, $V_2 = -0.136\text{eV}$, $V_3 = 0.054\text{eV}$. (Other values of these potentials are given in the literature; however, our results are not particularly sensitive to the precise values.)

We have used Monte Carlo simulations of the ASYNNNI model to study the isotropy of the ground state configurations for a large number of points in the temperature-concentration plane. For this purpose it is necessary to identify a suitable «order parameter» to distinguish between the isotropic and anisotropic phases of the model (see below). In this paper we present some preliminary results on the behaviour of this order parameter, more details are published elsewhere.

In our Monte Carlo simulations of the canonical ensemble, we have used the Metropolis algorithm. All simulations were on a lattice 64 by 64. A detailed analysis was performed of the Cu–O chains in the equilibrium configurations obtained from the numerical simulation. For this purpose, histograms revealing the frequency of formation of chains of particular lengths and orientations (either «left» or «right») were produced from large samples of equilibrium configurations. The analysis of such histograms led to the formulation of a quantity which depends on the Cu–O chain pattern and exhibits a dramatic change for certain values of the temperature and concentration, and can thus serve as an order parameter for studying the isotropy of the model.

Specifically, we define an order parameter

$$\Delta = |N_L - N_R|/N, \tag{2}$$

where $N_L$ ($N_R$) is the number of oxygen ions in chains oriented to the left (right), and $N$ is total number of oxygen ions. It is clear that for the Ortho I and Ortho II structures, either $N_R = N$ and $N_L = 0$ (as in Fig. 1) or $N_L = N$ and $N_R = 0$; in either case $\Delta = 1$.

Typical results for the temperature and concentration dependence of this order parameter are shown in Figs. 2 and 3. In Fig. 2 the temperature is fixed

at 0.05 eV and the order parameter is plotted for values of the concentration parameter between 0.2 and 1.4. (Note that in YBCO–123 $x \leq 1$; however, it is also of interest to study the ASYNNNI model for $x > 1$.) The first feature to notice in Fig. 2 is the lack of symmetry of the order parameter about $x = 1$: thus the order parameter (2) for the ground state does not possess the particle-hole symmetry of the Hamiltonian in Eq. (1).

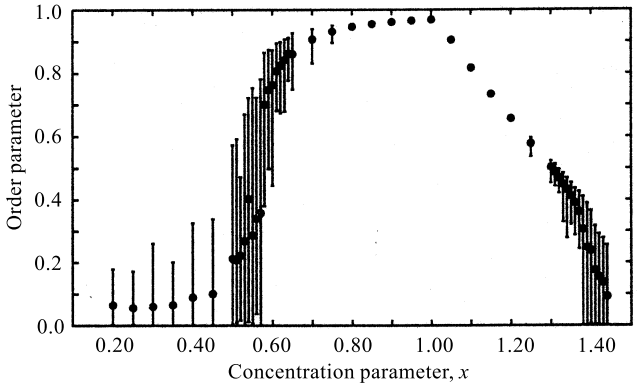


Fig. 2. Variation of the order parameter defined in Eq. (2) with concentration parameter for a temperature $T = 0.05$ eV

We also see that in Fig. 2 $\Delta \approx 1$ for $x = 1.0$: the structure corresponds to the Ortho I phase. The structure at the left-hand edge of the «plateau» in Fig. 2 (at $x \approx 0.6$) corresponds mainly to the Ortho II phase. We remark that for lower values of $T$ the plateau in Fig. 2 broadens: the right-hand edge remains at $x = 1$, but the value of $x$ at the left-hand edge decreases. Conversely, for higher values of $T$ the plateau becomes narrower. The order parameter in Fig. 2 decreases to half its maximum value at $x_c = 0.55$ and $x_c = 1.28$. To clarify the behaviour of the model at these two points, many additional simulations were performed with a much smaller step in $x$ and significantly increased number of Monte Carlo steps. The statistical analysis of the results clearly shows a dramatic increase of the variance, which is typical for the behaviour of any statistical system near a critical point, and is a direct consequence of what is often referred to as «critical slowing down» or «critical increase of the relaxation time».

Similar remarks apply to Fig. 3 where $\Delta$ is plotted as a function of temperature for fixed $x = 0.80$. The results indicate a critical temperature $T_c \approx 0.10$ eV for the transition from anisotropic to isotropic orientation of Cu–O chains at this concentration. We remark that the decrease in $\Delta$ for the lower temperatures ($T \lesssim 0.02$ eV) in Fig. 3 is associated with inhomogeneous configurations of the model which occur at these temperatures [3]. The critical values ($x_c$, $T_c$) obtained

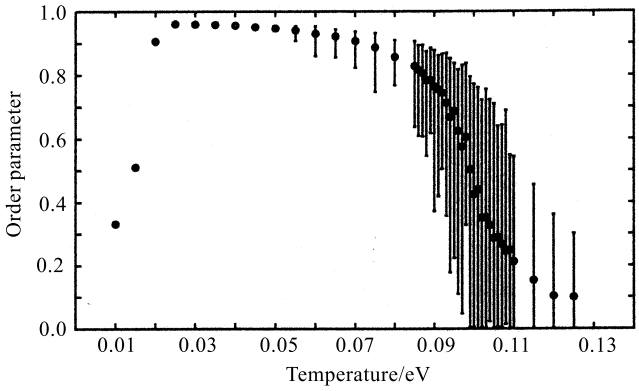


Fig. 3. Variation of the order parameter with temperature for a concentration parameter $x = 0.80$

from analysis of the order parameter can be used to determine a phase diagram for the isotropic and anisotropic phases of the model [4].

REFERENCES

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