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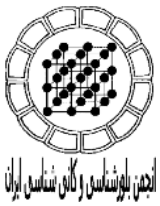

استفاده از دینامیک گلوبر در روش مونت کارلو برای آنسامبل بزرگ بندادی به منظور بررسی انتقال فاز ساختاری در سیستم ابررسانای گرم $YBCO_x$ (0<x<1)

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(دریافت مقاله ۸۶/۱۲/۲۰ ، نسخه نهایی ۸۷/۹/۲۲)

چکیده: در این مقاله انتقال ساختاری چارگوشی به راستگوشه در سیستم $YBa_2Cu_3O_{6+x}$ (۰≤x≤۱) به وسیله دینامیک گلوبر در شبیه‌سازی مونت کارلو بررسی شده است. در این شبیه‌سازی، فرآیند مرتب‌سازی اکسیژن در YBCO بر پایه مدل آیزینگ *ASYNNNI* بوده و همچنین تاثیر پتانسیل شیمیایی بر پخش اکسیژن در داخل صفحات لایه‌ای Cu-O ابررسانای YBCO نیز مطالعه شده است. برای مجموعه خاصی از پتانسیل‌های برهم‌کنش و دما نمودارهای فراوانی اکسیژن جذب شده بر حسب پتانسیل شیمیایی رسم شده و فاز ساختاری منظم بلند برد راستگوشه (ارتوI) و فازهای ابرساختاری کوتاه برد راستگوشه II و راستگوشه III به صورت موضعی مشاهده گردیده‌اند که نتایج مربوط به فاز ابر ساختاری کوتاه برد راستگوشه II در توافق کلی با داده‌های پراکندگی نوترون است.

واژه‌های کلیدی: *انتقال فاز ساختاری – دینامیک گلوبر – YBCO.*

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GCMC Glauber dynamics study for structural transitions in $YBCO_x$ (0<x<1), HT_c system

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Abstract: We have chosen an Ising ASYNNNI (ASYmmetric Next Nearest Neighbor Interaction) model under a grand canonical regime to investigate structural phase transition from a high symmetric tetragonal (Tet) to a low symmetric orthorhombic in $YBa_2Cu_3O_{6+x}$, 0<x<1, HT_c system. Ordering process for absorbed oxygens from an external gas bath into the basal plane of the layered system is studied by Monte Carlo Glauber dynamics which focuses on the effect of chemical potential in the bath on the oxygen diffusion inside the basal plain, as well. It is predicted short range super-lattice phases called orthorhombic II and III (OII, OIII) and also a long range orthorhombic I (OI) phase, corresponding to the oxygen stoichiometry, x, and temperature. It is consistent with literatures and confirmed by our ND studies (ILL, France) too.

Keywords: *Phase transition- Gluaber dynamic-YBCO*

Introduction

YBCOx has a layered Provoskite structure, which the Copper Oxide planes are separated by Barium Oxide and Yttrium layers. Structural behavior of the sample is strongly depends on the stochiometric index, x, which it is related to the oxygen concentration in the basal CuO plane (between BaO layers) [1]. Oxygen ordering occurs in the 2-D basal plane lattice such that the incoming oxygens accommodates between two adjacent Cu atoms to make …Cu-O-Cu… chains in any of two possible normal directions (along with the primitive vectors a & b) in the plane [2]. This system is an ideal model for studying a planar ordering phenomena and formation a long range parallel chain structures is a vital aspect for superconductivity in YBCOx [3, 4].

Despite of existing articles [5, 6], in here by using a Monte Carlo Glauber dynamics for a grand canonical ensemble, we have studied the oxygen-ordering process and it is shown the possibility of phase transition from a tweed like structure (randomized chain's length and directions, so called "Tet" phase for x<0.4), to one of the ordered structures with parallel and relatively long chains, so called "orthorhombic" phases. Depending on the temperature and the oxygen content in the basal plane the orthorhombic are known as OI, OII and OIII [3, 7, 8, 9], Fig. 1.

The computation method

A Monte Carlo approach with a "generalized ASYNNNI" Ising model has been employed. In this regard, for calculating the total energy of each configuration in the basal plane, four asymmetric next nearest neighbor interactions (v_1, v_2, v_3 & v4) between the oxygen ions inside the Cu square net matrix have been taken to account, Fig. 2, [10]. The essential assumption in this model is that the aforementioned interactions are independent of temperature (T) and x.

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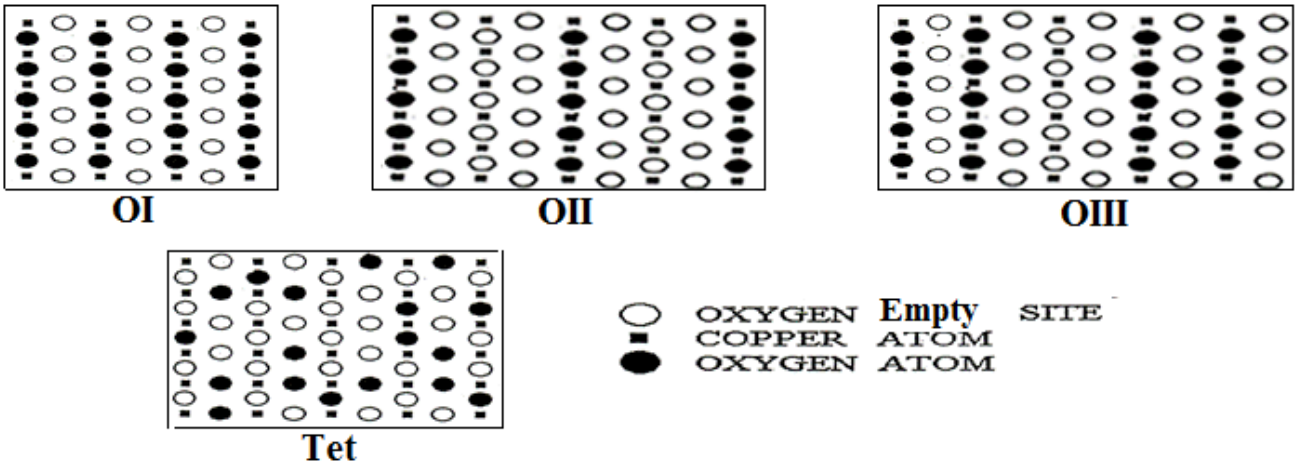

Fig. 1. OI: in high oxygen concentrations (x>0.75) is the long range and stable phase [7], the long range ordered OII & OIII phases has not been observed even at low temperatures. OII with every other parallel chains and OIII, with 2 filled chains separated with an empty one.

In the grand canonical ensemble frame, the Hamiltonian (H) for each configuration of the oxygens in the lattice can be written as:

$$H(\Phi)-\mu N=-V_1\sum_{\langle r,r'\rangle}^{nn}\sigma(r)\sigma(r')-V_2\sum_{\langle r,r'\rangle}^{nnnCu}\sigma(r)\sigma(r')$$

$$-V_3\sum_{\langle r,r'\rangle}^{nnn}\sigma(r)\sigma(r')-V_4\sum_{\langle r,r'\rangle}^{nnnn}\sigma(r)\sigma(r')-\mu\sum_{\langle r\rangle}\sigma(r)$$

Where, σ(r) = 1 or 0, is the site occupation number, and the summations run over oxygen pairs (r, r') [3] also:

nn: the nearest neighbor interactions knowing as v_1

nnnCu: next nearest neighbor interactions with a Cu bridge knowing as v_2

nnn: next nearest neighbor interactions without Cu bridge knowing as v_3

nnnn: next next nearest neighbor interactions without Cu bridge knowing as v_4 [11]

The chemical potential, μ, is related to the oxygen pressure in the external gas bath that it surrounds the lattice [12], and the interaction parameters are defined as [3]: (k_B is the Boltzman constant)

V_1 = 5430 k_B, V_2 = -0.36 V_1, V_3 = 0.12 V_1, V_4 = 0.02 v_1

The Glauber dynamics simulates a grand canonical ensemble such that, the lattice is surrounded by an external virtual lattice full of oxygens (as the gas bath with chemical potential, μ).

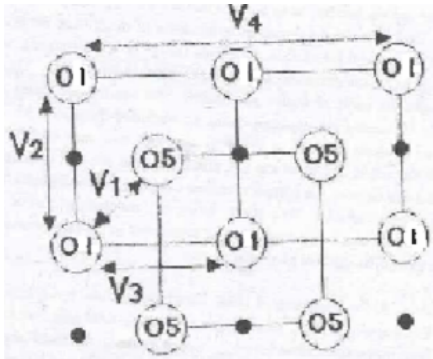

Fig. 2. Schematic presentation of the O-O interactions in the basal plane. Solid dots show the Cu lattice matrix and O1 & O5 are the possible oxygen sites.

Now for producing a typical configuration, two procedures can be occurred next; i- transferring oxygen from the bath to random sites in the lattice, if the site energy (calculated from v_i s interactions) are less than the μ value of the bath, ii- oxygen ordering inside the lattice by interchanging between a randomized chosen pair (in arbitrary distances) of an occupied & a vacant sites. In the both cases a Metropolise algorithm has been used to make decision for producing final configuration (with corresponding probability) or no. Each replacement or filling an empty site is a distinguished new configuration and calls a Monte Carlo step, McS, and the algorithm works based on an energetic comparison between two successive McSs, now if the energy difference, ΔE, is

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negative the new McS is accepted certainly, otherwise the new McS would be accepted with a probability of $P=\exp(-\Delta E/k_bT)$. The procedure is repeated until the fluctuation in total energy of the system (the above mentioned Hamiltonian) being negligible. Therefore with an adjustable (pre given) external chemical potential in the bath, the oxygen concentration changes gradually during the ordering process. This is in contrast with the conventional canonical dynamics in literatures that they increase the oxygen concentration step by step and then at each step allows the system relaxed only through a series of nearest neighbor jumps to available vacant sites [12]. On the other hand, in the Glauber dynamic because the full & vacant interchanges occurs at arbitrary distances, so the volume of calculations reduced substantially, and also to rationalize the computation time, the initial configuration has been chosen with a pre determined concentration (not an empty lattice).

Briefly; after choosing a random pair of full & vacant sites in each McS, the total configuration energies after and before interchanging is calculated, now if their difference, ΔE, is smaller than zero the swapping occurs surely, but if $\Delta E \geq 0$, it still can happen just with a probability as:

$$P = \exp(-\frac{\Delta E}{k_B T})$$

In principle the chosen initial configuration should not have any effect on the final results.

A random number, C, is called in the range of $0 \leq C \leq 1$ and if $C \leq P$, the transition is accepted and a new configuration is produced, but if C>P, it won't be done and the initial configuration will be considered as a new one. This procedure can be repeated for a large number of McSs.

Results and discussion

For a 100x100 lattice with 5000 available sits Fig.s 3 a-b show the variation of "oxygen density in the basal plan" versus chemical potential of the bath at temperatures 540 and 380°K. It is clear that for $\mu < 20000$, the density oscillate about its asymptotic value, 0.5 (corresponding to x = 1), which indicates formation of the OI long range phase with parallel O-Cu-O chains, but for $\mu > 20000$, the very high and unrealistic external chemical potential forces the system to be oxygen overloaded, whereas all available O1 & O5 sites are being occupied now.

In Fig.3- a, the plateau around density 0.43 can be attributed to a high density short range super structure in vicinity of the OI phase, but in Fig.3- b in addition, there are two other plateaus around densities of 0.25 and 0.37 (corresponding to x= 0.5 & 0.75) that they would be indications for the OII and OIII short range superstructures. It seems that the OIII phase are more stable than OII and it is because in the former the number of particles are higher and therefore the interactions are more efficient for ordering procedure.

In principle superstructures always appear as a short range order areas and it is because of the role of entropy and also availability of many empty sites for incoming oxygen ions.

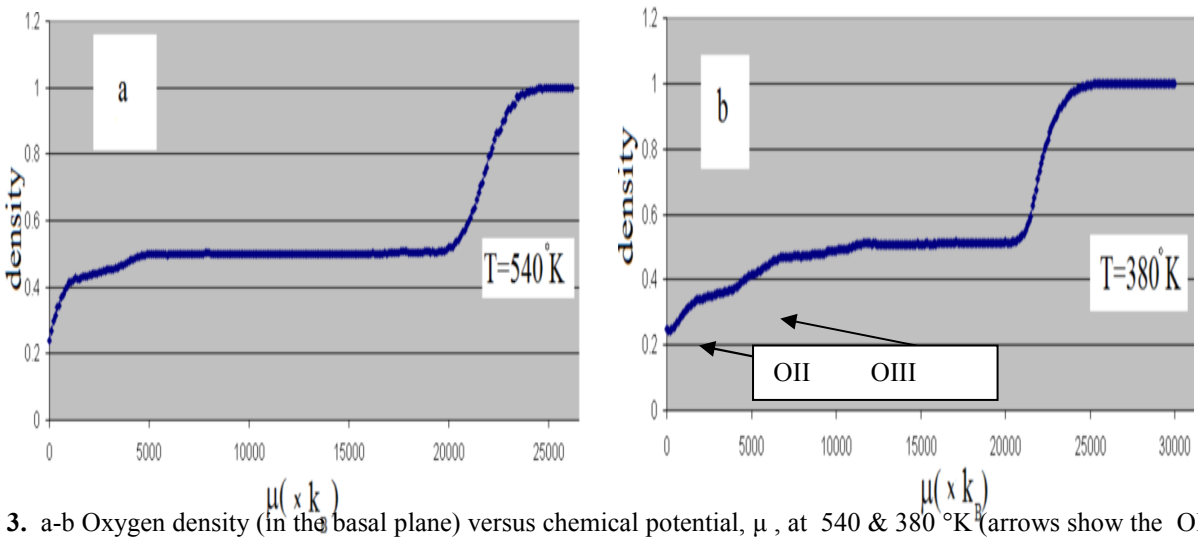

Fig. 3. a-b Oxygen density (in the basal plane) versus chemical potential, μ , at 540 & 380 °K (arrows show the OII & OIII plateaus.

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In Figs.4 the simulated long range OI phases and short range superstructures; OII and OIII are shown. The short range superstructure result for OII phase is in consistence with our neutron diffraction (ND) data. In Fig.5 the pattern shows the ND from a $YBCO_{x=0.4}$ sample at room temperature after Reitveld method refinement with two inserted Tet and OII models (below 200°C we expect a cross over region between Tet and OII [13]).

According to the OII model the peak around 4.6 Å (d space) would be indexed as (102) supperlattice pick, and it is clear that the pick is wide and week that indicates there is no a long range OII order area. Fig 6 shows the growth of the superlattice peak with increasing oxygen stoichiometry [14], unfortunately because of some technical shortages we were not able to perform experiments up to higher value of oxygen uptakes (higher oxygen pressures).

Conclusions

We have used a Monte Carlo Glauber dynamic under a grand canonical regime to investigate structural phase transition in $YBCO_x$ system. The system was surrounded by an external oxygen bath with adjustable chemical potential (proportional to its pressure) and our simulations indicate formation of a long range order OI phase at high oxygen content ($x \approx 1.0$) and also OII & OIII superstructures around moderate oxygen contents ($x \approx 0.5$ and $x \approx 0.75$).

Although there is not ample experimental data in this regards, these results are in general agreement with our ND data from a sample in a Tet+OII cross over region.

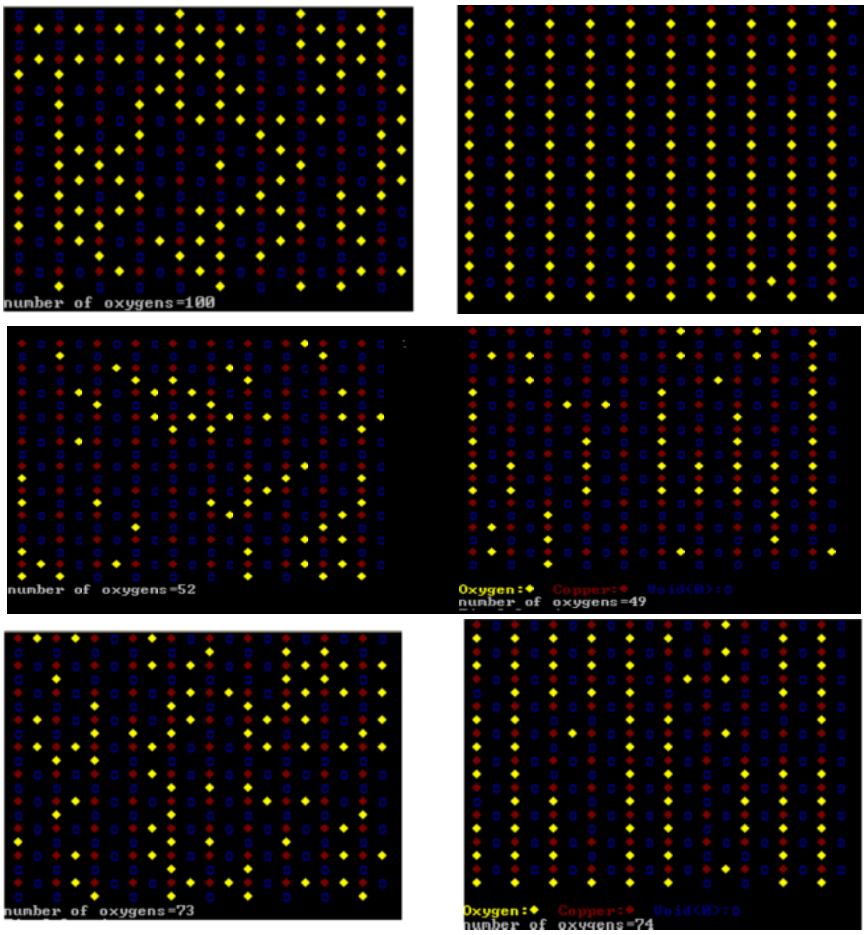

Fig. 4. a) T = 540 °K & density = 0.5 the initial disordered (**left**) and the final ordered configurations for OI (**right**) after 2500 McSs (gray points are the Cu lattice and white points are oxygens). **B)** T = 380°K & density: 0.25 the initial disordered (**left**) and the final short range ordered configurations for OII (**right**) after 8500 McSs. **C)** T = 380 °K & density: 35% - the initial disordered (**left**) and the final short range ordered configurations for OIII (**right**) after 5000 McSs.

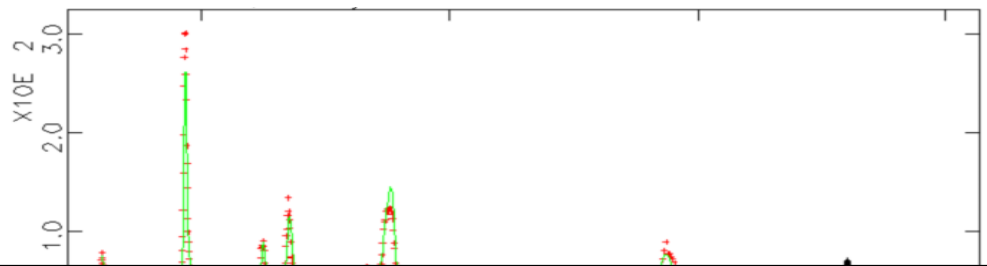

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Fig. 5. Neutron diffraction of a sample with x ~ 0.4 at 300°C. A double phase (Tet & OII) Rietveld refinement shows the volume fraction of the OII phase is about 40 %. The solid line shows the superlattice (102) reflection (D1A, ILL France).

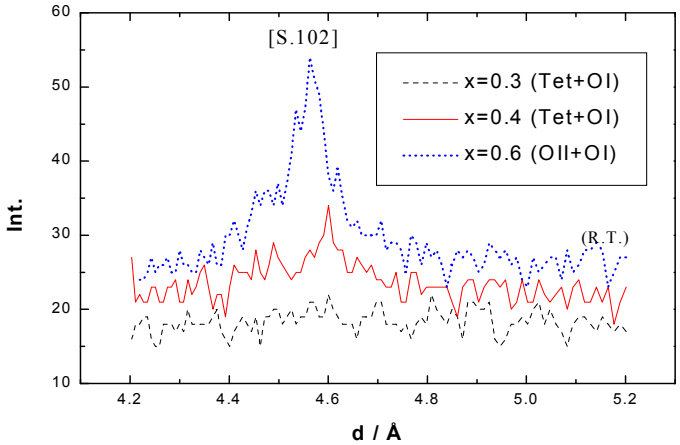

Fig. 6. Growing of the superlattice (102) peak with oxygen uptaking (powder ND data)

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