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A TWO-DIMENSIONAL STRUCTURE FACTOR CALCULATION FOR THE Cu-1 PLANE IN $YBa_2Cu_3O_6$

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The anisotropic radial distribution function and two-dimensional (2D) structure factor was calculated for the Cu-1 plane in $YBa_2Cu_3O_{6+x}$ when $x \approx 0$, based on data generated by a molecular dynamics simulation. The results indicate a stable square lattice and support the validity of layered two-dimensional screened Coulomb potential used in the simulation.

1. Introduction

Atomistic simulations are widely used to study the structure of perovskite-type oxides, including high temperature superconducting materials. Typically, interatomic forces are modeled by pair potentials of the Buckingham type,[1–4]

$$V_{ij}(r) = Z_i Z_j \frac{e^2}{r} + A_{ij} e^{-r/\rho} - C_{ij} \frac{1}{r^6} \tag{1}$$

including, occasionally, three-body interactions to fix bond angles.

Such techniques reproduce crystal structure accurately and are highly successful in approaching problems like defect properties or oxygen diffusion mechanisms.[4] However, since the potentials employed are not microscopically-based and depend on adjustable parameters *for each type of bond*, they are of limited use studying the interactions within high-T_c materials. Some theories of superconductivity, especially those which ascribe a significant role to Coulomb interactions, have implications for the form of forces. They might be tested indirectly by studying whether they lead to a microscopically-based explanation of material structure.

2. MD Simulation

High-T_c materials are notable for their layered nature, thus it might be possible to improve our interionic potentials by departing from the commonly used

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isotropic three-dimensional Coulomb-based potentials. Malozovsky and Fan have proposed[5,6] an extension of the Vissher–Falicov potential[7] for materials consisting of two-dimensional layers of charges, by accounting for the exchange-correlation effects in cuprates with the Hubbard approximation, which means conventional methods like the random-phase approximation are no longer adequate. As the Malozovsky–Fan potential is closely connected to their Coulomb-based approach to superconductivity,[8] there would be much interest in seeing if it helps predict material structure as well.

We have conducted a molecular dynamics simulation of the Cu-1 plane in $YBa_2Cu_3O_{6+x}$ when $x \approx 0$, taking account of the Cu ions' interactions with one another and with modulating layers of Ba and O above and below. Experimentally, this is a square lattice of Cu ions, which is an appropriately simple system to test if a stable lattice can be formed without additional attractive terms like the $-Cr^{-6}$ in Eq. (1). The Malozovsky–Fan effective Coulomb potential is

$$\tilde{V} = \frac{e^2 Z_i Z_j}{\kappa} \left(\frac{1}{r} - \tilde{v}_{\mathrm{el}} \right) , \tag{2}$$

where κ is the dielectric constant. $\tilde{v}_{\mathrm{el}}$ arises from electron exchange-correlation interactions:

$$\tilde{v}_{\mathrm{el}}(\mathbf{r}_i - \mathbf{r}_j) = \int_0^\infty dk J_0(k|\rho_i - \rho_j|) \Bigg[e^{-k|z_i - z_j|} - \Phi(z) \frac{\sinh ck}{\sqrt{A^2(k) - 1}} \times \left(A(k) - \sqrt{A^2(k) - 1} \right)^{|z_i - z_j|/c} \Bigg] , \tag{3}$$

in which $A(k) = |\cosh ck + (\eta(k)/k a_{\mathrm{B}}^*) \sinh ck|$, $\eta(k) = 2\Pi(k)/(1 - \alpha P(k))$, $P(k) = \Pi(k)/\sqrt{1 + k^2/k_{\mathrm{F}}^2}$, $\Pi(k) = 1 - \mathrm{Re}\sqrt{1 - 4k_{\mathrm{F}}^2/k^2}$ and $\Phi(z) = -\cos \pi(z_i - z_j)/c$ when $\alpha P(k) > 1$ and $\Phi(z) = 1$ otherwise. $a_{\mathrm{B}}^* = \kappa/e^2 m^*$ is the effective Bohr radius; k_{F} is the Fermi wave vector with the convention $\hbar = 1$; and $\alpha = 1/a_{\mathrm{B}}^* k_{\mathrm{F}}$ is the interelectronic coupling constant. The most significant adjustable parameters for the simulation are the dielectric constant κ and the effective mass m^*. Typically, $\kappa \sim 5$–15 and $m/m_e^* \sim 1$–5; the existence of a stable lattice is not sensitive to these parameter values.

The details of the simulation and the qualitative results it produces are given elsewhere[9]; here we present figures for a typical anisotropic radial distribution function and structure factor, which shows quantitatively that a stable square lattice is obtained. The anisotropic radial distribution function is

$$g(\mathbf{r}) = \frac{A}{N^2} \left\langle \sum_{i \neq j} \delta(\mathbf{r} - \mathbf{r_{ij}}) \right\rangle , \tag{4}$$

where A is the area and N the number of ions. The positional data for $g(\mathbf{r})$, displayed in Fig. 1, was generated through a MD simulation at $T = 500$ K, where some defects have begun to appear in the lattice structure. Overall, however, the lattice retains its shape.

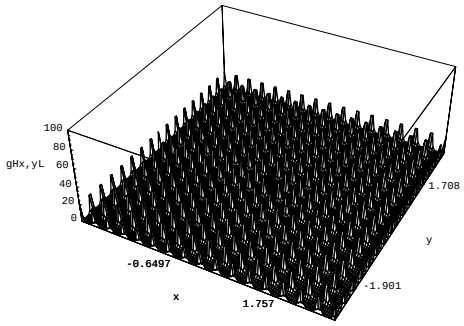
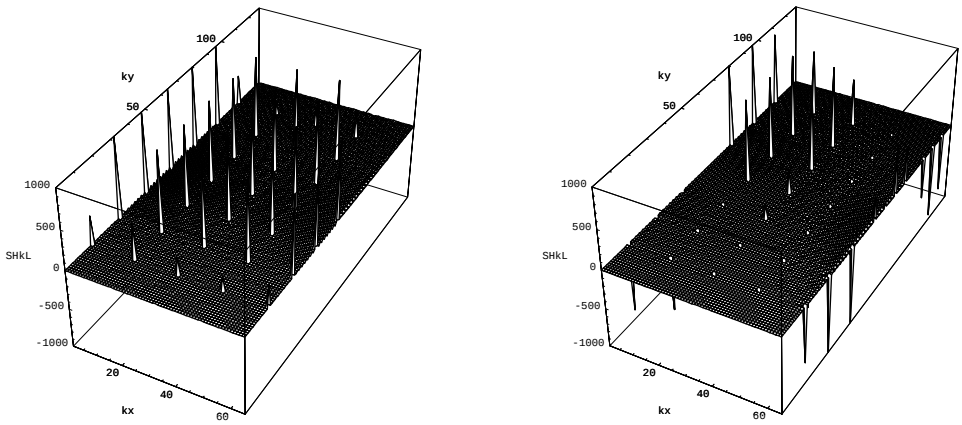


Fig. 1. Radial distribution function $g(\mathbf{r})$ for ions in Cu-1 plane; $T = 500$ K. The lattice constant is $\sim$0.385 nm.



(a) (b)

Fig. 2. Anisotropic structure factor $S(\mathbf{k})$; $T = 500$ K. Real part on the left, imaginary part on the right.

Figure 2 shows the real and imaginary parts of the structure factor

$$S(\mathbf{k}) = 1 + \frac{N}{A} \int g(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r} \,. \tag{5}$$

Clearly, a stable square lattice is obtained. This is due to the in-plane Malozovsky–Fan potential having an attractive part, similar to a Lennard–Jones potential.

3. Discussion

Our layered two-dimendsional Coulomb potential reproduces the experimental square lattice without bond-specific adjustable parameters. This, is, of course, a simplified model which has its limitations. Firstly, the square (as opposed to a triangular) lattice arises from the symmetry of the overall unit cell, which is imposed

on the Cu-1 plane in the MD simulation through interactions with modulating Ba and O layers. Secondly, Eq. (3) is anisotropic in the z direction but isotropic within the charge layers. This means this simple approximation is not sufficient to reproduce the Cu-O chain structures at $x \approx 1$. More detailed consideration of Friedel oscillations and correlation effects should improve the potential.

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