PHYSICAL REVIEW B **76**, 020507(R) (2007)

# Superconducting gap variations induced by structural supermodulation in $Bi_2Sr_2CaCu_2O_8$

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(Received 27 April 2007; published 20 July 2007)

We discuss the possibility that the strain field introduced by the structural supermodulation in Bi-2212 and certain other cuprate materials may modulate the superconducting pairing interaction. We calculate the amplitude of this effect, visible in scanning tunneling spectroscopy experiments, and thereby relate a change in the local superconducting gap with the change in the local dopant displacements induced by the supermodulation. In principle, since this modulation is periodic, sufficiently accurate x-ray measurements or *ab initio* calculations should enable one to determine which atomic displacements enhance pairing and therefore $T_c$.

DOI: 10.1103/PhysRevB.76.020507 PACS number(s): 74.72.Hs, 74.81.−g, 74.62.Bf, 74.20.−z

In the twenty years since the discovery of the high-$T_c$ cuprates, an intense theoretical and experimental effort has not reached a consensus on the origin of the phenomenon, although much has been learned. Progress has been slow due both to the complexity of the materials, and the difficulty of the theoretical problem of strong electronic correlations. One advantage researchers in the high-$T_c$ field have is a set of new experimental tools which provide *local* information on the electronic state. Chief among these new methods is scanning tunneling spectroscopy (STS), which is providing fascinating new insights and forcing new ways of thinking about the high-$T_c$ problem by yielding an unprecedented level of detail.[1–5] Traditionally, such atomic scale information has been considered irrelevant to the phenomenon of superconductivity, since rapid oscillations of pair wave functions on length scales smaller than the coherence length $\xi$ are integrated out in the conventional pairing theory, where it is assumed that $\xi \gg a$, with $a$ the lattice spacing. In the cuprate superconductors, on the other hand, $\xi$ is much smaller than in conventional materials, approaching $a$ itself, and it is conceivable that a new type of approach accounting for atomic scale physics will be required to solve this problem.

This possibility was highlighted recently when McElroy *et al.*[6] discovered the positive correlation of the positions of dopant atoms in superconducting Bi-2212 with the local energy gap. It was argued that these atoms were in fact interstitial O atoms,[6] probably located between the BiO and SrO layers.[7] Subsequently, Nunner *et al.*[8] showed that a good fit to several independent measured STS correlations could be understood if one assumed that the dopants, in addition to delivering holes to the $CuO_2$ plane and inducing a screened Coulomb potential, also modulate the local pair interactions. The idea is that each dopant distorts the lattice around it in such a way as to modify the effective electronic structure, characterized by hopping integrals $t, t', \ldots$, exchange constants $J$, electron-phonon couplings $\lambda$, resulting in a modified local pairing interaction between electrons as well.[9,10] Phenomenological fits to the data of McElroy *et al.*[6] then led to the conclusion that a substantial modulation of the pair interaction on an atomic scale is present in the effective low-energy Hamiltonian of the disordered $Bi_2Sr_2CaCu_2O_8$ (BSCCO) material.[8,11–13]

More recently, Slezak *et al.*[14] performed an extensive STS study of the supermodulation (SM) in BSCCO. From these local measurements it was found that the gap is modulated with the SM phase $\phi^{SM}$ with an amplitude of order 10% of its average value in near-optimally doped samples, providing a remarkable direct quantitative link between atomic displacements in the unit cell and the local superconducting gap $\Delta$. In other words, the SM induces a pair-density wave in Bi-2212.

In this work we extend the model of Ref. 8 to include effects of the SM strain field. In a similar spirit, we assume that the local atomic displacements caused by the SM generate an additional, sinusoidal modulation of the pairing interaction $g$, which we refer to as a $g$ wave. The supermodulation presumably originates from a mismatch between the insulating layers and the preferred bond lengths of perovskite crystal. It can be characterized by a wave vector $q_{SM}$, has a wavelength of approximately $\lambda_{SM}=2\pi/q_{SM}\approx 26$ Å $\approx 4.8$ unit cells, runs along the $a$ axis, and leads to displacements of the atomic positions of up to 0.4 Å. It is believed that one of the main effects of the SM is to modulate the distance between the apical oxygen and the $CuO_2$ plane.[15–17] For simplicity, we neglect the periodic changes in other terms in the Hamiltonian, such as the electron hopping. We will show that the amplitude of this $g$ wave can in principle be determined by comparison with experiment, given the assumptions already specified. In this case, one should be able to relate the change in the pair potential $\delta g$ to the atomic displacements caused by the SM, information which should be available with sufficiently precise x-ray data, or from *ab initio* calculations. The philosophy here is similar to that of Nunner *et al.*,[8] but the measurement of changes in the local gap caused by the supermodulation has the advantage that the associated periodic displacements should be easier to determine empirically than in the case of the random O dopants. As discussed below, current x-ray data on Bi-2212 are not yet able to answer this question, but there appears to be no fundamental obstacle to improving the precision so as to be able to achieve this goal; they may then be able to remove any remaining ambiguity as to the microscopic origin of the modulated pairing in this material.

In the following, we use the conventional $d$-wave BCS Hamiltonian defined on a two-dimensional (2D) square lattice,

 

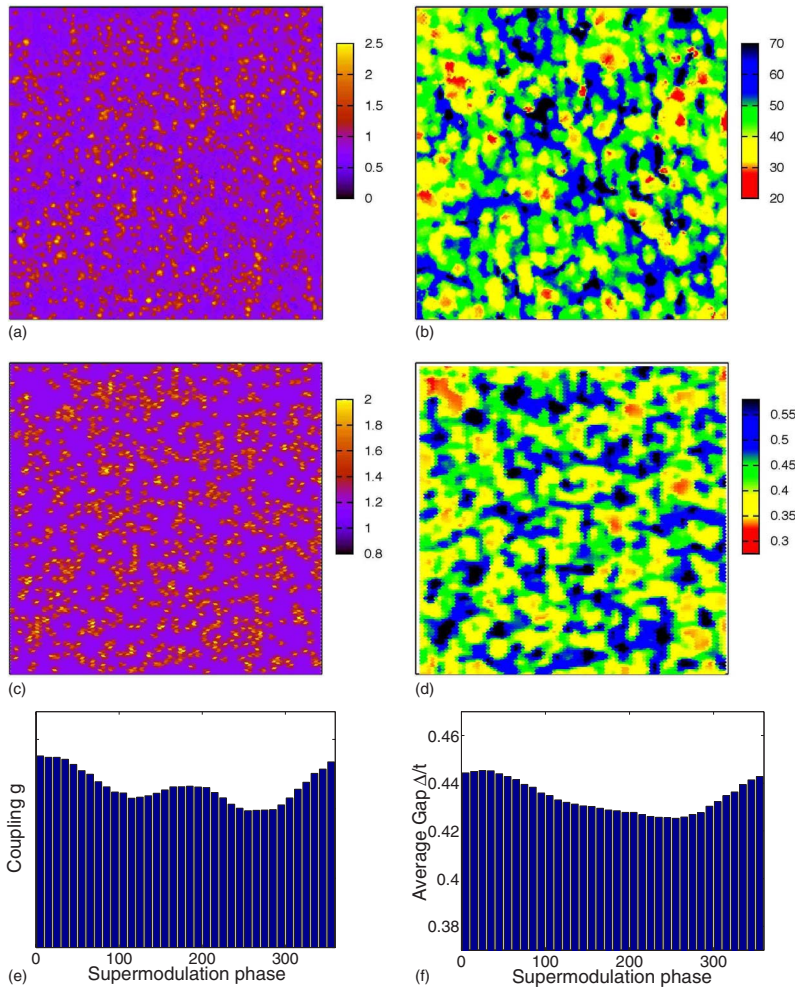


FIG. 1. (Color online) (a) Experimental $dI/dV$ map (arb. units) at −960 meV of an optimally doped BSCCO sample (Ref. 6). (b) Experimental gap map (meV) in the same region as (a) at $T=4$ K. (c) The theoretical impurity potential extracted from (a) assuming a distance from the $CuO_2$ plane $r_z=0.5$ and $\lambda=0.5$. (d) The gap map resulting from using (c) as the pairing potential in the BdG equations with $\delta g_{imp}=1.5t$. (e) and (f) display the $g$ histogram and $\Delta$ histogram vs $\phi^{SM}$, respectively. The model results [(c)–(f)] are for $\delta g_{SM}=0.0$.

$$\hat{H}=\sum_{\langle ij\rangle\sigma} t_{ij}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma}+\sum_{i\sigma}(V_i-\mu)\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}+\sum_{\langle ij\rangle}(\Delta_{ij}\hat{c}^{\dagger}_{i\uparrow}\hat{c}^{\dagger}_{j\downarrow}+\text{H.c.}), \tag{1}$$

where in the first term we include nearest $t$ and next-nearest $t'=-0.3t$ neighbor hopping. We set the chemical potential $\mu=-t$ in order to model the Fermi surface of BSCCO near optimal doping, and $\Sigma_{\langle ij\rangle}$ denotes summation over neighboring lattice sites $i$ and $j$. Disorder of the usual screened Coulomb type is included in the impurity potential $V_i=V_0 f_i$ where $f_i=\Sigma_s \exp(-r_{is}/\lambda)/r_{is}$, where $r_{is}$ is the distance from a defect $s$ to the lattice site $i$ in the plane. Distance (energy) is measured in units of $\sqrt{2}a(t)$, where $a$ is the Cu-Cu distance, and the calculations are done at $T=0$. Note that the particular form of $f_i$ is merely a convenient way to vary the range of the impurity potential landscape through the parameter $\lambda$. The $d$-wave order parameter $\Delta_{ij}=g_{ij}\langle\hat{c}_{i\uparrow}\hat{c}_{j\downarrow}-\hat{c}_{j\downarrow}\hat{c}_{i\uparrow}\rangle/2$ is determined self-consistently via

$$\Delta_{ij}=\frac{g_{ij}}{2}\sum_n [u_n(i)v_n(j)+v_n(i)u_n(j)]\tanh\left(\frac{E_n}{2T}\right). \tag{2}$$

Here, $\{E_n,u_n,v_n\}$ is the eigensystem resulting from diagonalization of the Bogoliubov–de Gennes (BdG) equations associated with Eq. (1). The pairing interaction $g_{ij}$ is assumed to vary in space relative to its homogeneous value $g_0$ as

$$g_{ij}=g_0+\delta g_{imp}(f_i+f_j)/2+\delta g_{SM}\cos(\phi_i^{SM}), \tag{3}$$

where $\delta g_{imp}$ and $\delta g_{SM}$ are the amplitudes of the dopant and $g$-wave modulation, respectively, and $i,j$ are nearest neighbors. In the homogeneous case $g_{ij}=g_0$ we choose $g_0=1.16t$ giving $\Delta_{ij}=0.1t$. In the inhomogeneous case we make sure to adjust $g_0$, in order to maintain the same average gap as in the corresponding homogeneous system. The third ($g$-wave) term in Eq. (3) is taken to vary sinusoidally with the SM phase $\phi_i^{SM}$, a phase variable associated with the structural supermodulation as determined in Ref. 14. In the following, we use the experimentally determined $\phi_i^{SM}$ as input in Eq. (3), and ignore for simplicity the conventional potential ($\tau_3$ channel) associated with each dopant, and consider disorder only in the pair ($\tau_1$) channel. The goal will be to adjust the amplitude $\delta g_{SM}$ to obtain better quantitative agreement with the experiments of Ref. 14.

That a nonzero value of $\delta g_{SM}$ is required is illustrated in Fig. 1 which shows results obtained with $\delta g_{SM}=0$.[12] The input to the theory is, in a field of view (FOV) of 49 nm $\times$49 nm, the measured conductance at −960 meV (a), known to track the positions of the dopant oxygens. The corresponding gap map obtained by McElroy *et al.*[6] is shown in (b). In Fig. 1(c) we display the impurity potential generated by assuming that each of these dopants provides a po-

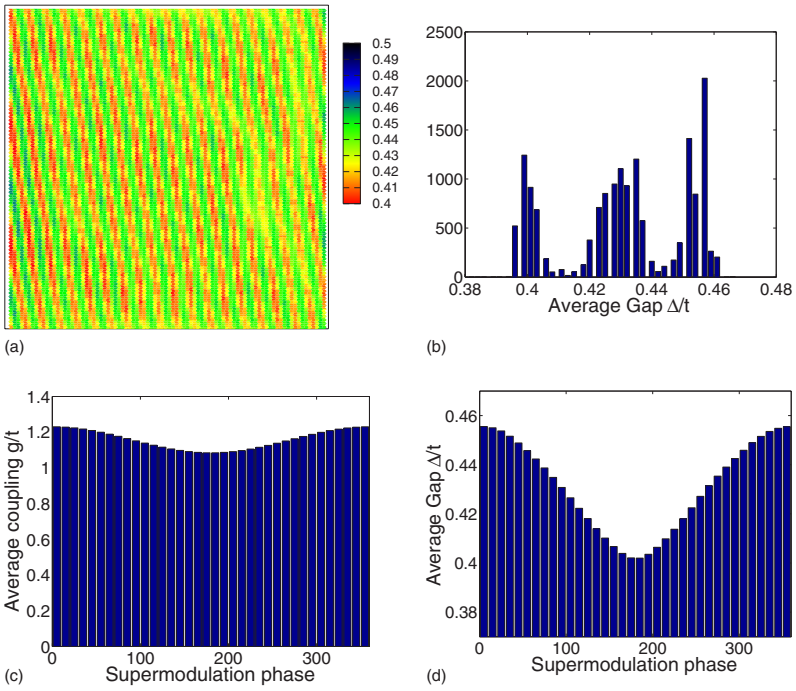


FIG. 2. (Color online) For clarity we show here the self-consistent results for the superconducting gap $\Delta$ resulting from a pure $g$ wave ( $\delta g_{imp}=0$ and $\delta g_{SM}=0.08t$): (a) real-space gap map, (b) conventional gap histogram, (c) $g$ histogram vs $\phi^{SM}$, and (d) $\Delta$ histogram vs $\phi^{SM}$.

tential centered on the bright spot positions of (a) which decays as a screened exponential *in the pairing channel*, as described above. The similarity to (a) is manifest. The experimental FOV is modeled as a $90\times90$ lattice system rotated 45° with respect to the 3.83 Å Cu-Cu bonds. Therefore our system consists of $2\times90\times90$ sites and is aligned with the experimental FOV. The gap map computed from the coherence peak-to-peak distance in the theoretical local density of states (LDOS) using (c) as input pair potential $\delta g_{imp}$ is shown Fig. 1(d). Gap maps reasonably consistent with experiment are found for $\delta g_{imp}\sim1.5t$.

Although various correlations among O positions and the LDOS $\rho(E)$ are successfully reproduced by the Nunner *et al.*[8] approach, one deficiency appears upon closer examination of the gap maps Figs. 1(b) and 1(d). The experimental result [Fig. 1(b)] contain nearly vertical linear striated modulations visible to the eye, which match the corresponding scanning tunneling microscope (STM) topograph and are therefore caused by the SM. These are not obviously manifest in the theoretical gap map presented in Fig. 1(d). In fact, weak correlations of the dopant positions with the supermodulation phase are indeed present in the data, as seen in Figs. 1(e) and 1(f) and lead, for the disorder parameters which reproduced the gap-map statistics, to a small net modulation of the gap with $\phi^{SM}$.

In Fig. 1(e), it is seen that the experimental dopant distribution is correlated with $\phi^{SM}$ at 0 and 180°, leading to a peak in the coupling $g$ vs $\phi^{SM}$ at these phases in our model. Figure 1(f) shows a histogram of the gap in Fig. 1(d) vs SM phase $\phi^{SM}$. Because of the effective smearing of the order parameter response over scales of order the coherence length $\xi\sim\lambda_{SM}$, the 180° peak is partially wiped out and a resulting weak 360°-periodic modulation of 4–5 % of $\Delta$ vs $\phi^{SM}$ remains, qualitatively similar to the experiments.[14] Increasing the phenomenological amplitude of the dopant potential leads to overall fluctuations of the gap amplitude which are much too large compared to experiment. Therefore in order to generate a 10% variation of $\Delta$ vs $\phi^{SM}$, and maintain quantitative agreement with the spatial extent and overall amplitude of the gap variations evident from the experimental gap maps, we need to include a nonzero $\delta g_{SM}$. This is fully consistent with the notion[8] that the reason the oxygens modulate the pairing is due to local distortions of the lattice, and the SM should produce similar effects on its own. Hence in the following we investigate the possibility that a $g$ wave is present in the system in addition to the dopant $\tau_1$ disorder.

In Fig. 2, we first show the effects of a pure $g$ wave without $\tau_1$ disorder, i.e., $\delta g_{imp}=0$. From Fig. 2(a), which displays the gap in real space, it is seen that the SM agrees well to that observed in the corresponding experimental FOV by Slezak *et al.*[14] as it should per construction. The gap histogram is shown in Fig. 2(b) and in Fig. 2(c) [Fig. 2(d)] we show the histograms for the input $g$ wave (self-consistent $\Delta$) vs SM phase $\phi^{SM}$, both of which trivially exhibit a sinusoidal dependence. Figure 3 displays typical results when including both $\delta g_{imp}$ and $\delta g_{SM}$ into the simulation. Here, we used the same disorder parameters as in Andersen *et al.*[12] to obtain the gap maps [Figs. 1(c) and 1(d)], but with $\delta g_{SM}=0.06t$ (a) and $\delta g_{SM}=0.14t$ (b). In both these plots the striated gap modulations are evident. For the parameters used in Fig. 3(a), we show in Figs. 3(c) and 3(d) the $g$ histogram and $\Delta$ histogram, respectively. As seen, the oscillation of $g$ vs $\phi^{SM}$ of roughly sinusoidal form is still found, with amplitude close to the input $\delta g_{SM}$. The gap response has a corresponding amplitude of about 10% of its average value in agreement with the measurements by Slezak *et al.*[14] Therefore within the modulated pairing scenario, an experimental gap modulation amplitude of approximately 10%, is caused by a SM-induced $g$ wave of similar size relative to the background pairing strength $g_0$. Note that after including the SM phase, it is Fig. 3(a) that should be compared to the experimental gap map in Fig. 1(b).

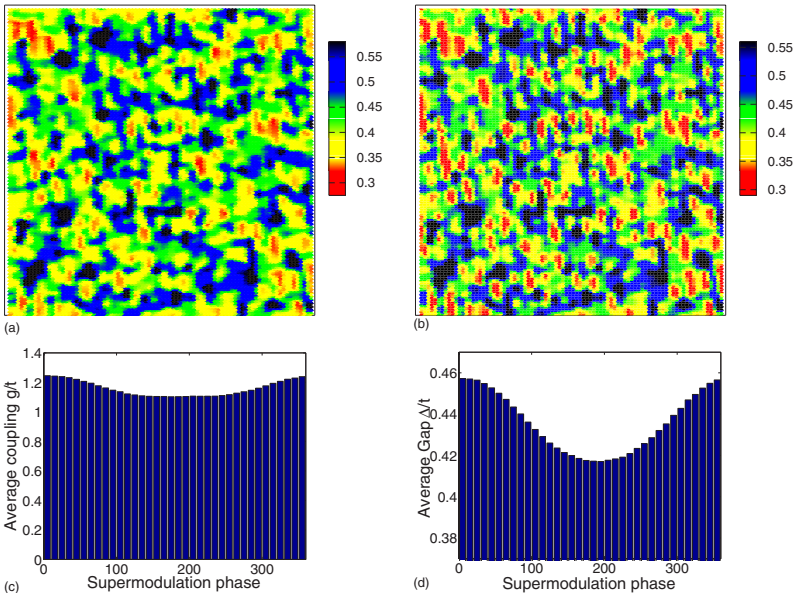


FIG. 3. (Color online) (a), (b) Real-space gap maps for $\delta g_{imp}=1.5t$, and $\delta g_{SM}=0.06t$ (a) and $\delta g_{SM}=0.14t$ (b). For the parameters in (a) we show (c) the $g$ histogram vs $\phi^{SM}$, and in (d) the $\Delta$ histogram vs $\phi^{SM}$.

We would now like to extract which type of atomic displacements are present in the SM and associated with the enhanced pairing at 0 and 360° SM phase. In principle, this information should be available from careful x-ray diffraction data, but this is complicated by the existence of deviations of this system from stoichiometry, both through Bi/Sr substitutions and oxygen interstitials, which together determine the incommensurability of the true system. Early x-ray analysis[18–21] suggested a weak correlation of the interstitial oxygen position with the SM, but as remarked above this correlation does not appear to be the most significant one present in the STM gap maps.

More recently, progress in the analysis of incommensurate systems[22,23] has been made, and new short-range ordered structures have been identified,[24] but the various studies disagree at essential points,[14] and it does not appear to be possible with present data to identify the actual displacements of atoms near the SM maximum or minimum with sufficient precision to eventually draw conclusions regarding the microscopic origin of the pairing modulations. There does appear to be a statistically significant correlation of the $z$ coordinate of the apical oxygen relative to the $CuO_2$ plane with the SM phase,[25] but it anticorrelates with the local gap. This behavior is the opposite of that which might be expected on the basis of the analysis by Pavarini *et al.*,[26] who pointed out an empirical correlation between apical O coordinate $z$ and $T_c$. This may point to the primacy of other atomic displacements, or suggest that $T_c$ itself is less related to in-plane pairing strength and more to interlayer couplings. In any case, our analysis should provide incentive for a repeated assault on the x-ray analysis of this compound, with the hope of eventually providing direct local information on the origin of the pairing.

The authors are grateful to J. C. Davis for advice and encouragement at all stages of this work. Calculations were performed at the University of Florida High-Performance Computing Center (http://hpc.ufl.edu).

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