

Imaging the impact on cuprate superconductivity of varying the interatomic distances within individual crystal unit cells

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Many theoretical models of high-temperature superconductivity focus only on the doping dependence of the CuO₂-plane electronic structure. However, such models are manifestly insufficient to explain the strong variations in superconducting critical temperature, T_c , among cuprates that have identical hole density but are crystallographically different outside of the CuO₂ plane. A key challenge, therefore, has been to identify a predominant out-of-plane influence controlling the superconductivity, with much attention focusing on the distance d_A between the apical oxygen and the planar copper atom. Here we report direct determination of how variations in interatomic distances within individual crystal-line unit cells affect the superconducting energy-gap maximum Δ of Bi₂Sr₂CaCu₂O_{8+ δ} . In this material, quasiperiodic variations of unit cell geometry occur in the form of a bulk crystalline “supermodulation.” Within each supermodulation period, we find $\approx 9 \pm 1\%$ cosinusoidal variation in local Δ that is anticorrelated with the associated d_A variations. Furthermore, we show that phenomenological consistency would exist between these effects and the random Δ variations found near dopant atoms if the primary effect of the interstitial dopant atom is to displace the apical oxygen so as to diminish d_A or tilt the CuO₅ pyramid. Thus, we reveal a strong, nonrandom out-of-plane effect on cuprate superconductivity at atomic scale.

apical oxygen | dopant atoms | out-of-plane influence | superconducting energy gap | supermodulation

The superconductive copper oxide materials exist in a variety of complex crystal forms (1). Introduction of $\approx 16\%$ holes into the insulating CuO₂ crystal plane by chemical doping generates superconductors with the highest critical temperature, T_c , known. However, the maximum T_c varies widely between crystals sharing the same basic in-plane electronic structure, by up to a factor of 10 at the same hole density in monolayer cuprates (1). These variations obviously cannot be due to the doping-dependence of CuO₂ in-plane electronic structure, and it has long been hypothesized (2) that there must be a key out-of-plane influence that controls the basic electronic structure of cuprates. Identification of such an out-of-plane influence may be pivotal to finding a route to higher- T_c cuprate superconductors.

Much attention has been focused on the “apical” oxygen atom as a primary candidate for the cause of such out-of-plane effects. This atom is positioned at the apex of the CuO₅ pyramid (Fig. 1A), the key chemical unit within the unit cell of bi- and trilayer cuprates (monolayer cuprates contain an analogous CuO₆ octahedron). Hybridization of the p_z orbital on the apical oxygen and the out-of-plane Cu $d_{3z^2-r^2}$ orbital should be quite strong (3). The importance of the apical oxygen location is supported empiri-

cally by experiments involving chemical substitution of cations at adjacent sites (4, 5), which result in dramatic effects on T_c . Because the substituted cations have the same valence but different radii, their primary effect is a geometrical displacement of the apical oxygen atom. Similarly, the effects of hydrostatic pressure (6–8)—although their microscopic interpretation is not always clear—generate large changes in T_c in response to distortion of the crystal geometry. Taken together, these experiments imply that distortion of the CuO₅ pyramidal geometry might be the source for the dramatic out-of-plane effects on maximum T_c .

Changes in interatomic distances within the unit cell should, in theory, have major effects on both the underlying electronic structure and the superconducting state (2, 9). For example, based on calculation of Madelung (electrostatic) site potentials, Ohta *et al.* (2) argue that the geometry of the pyramidal unit—in particular the displacement of the apical oxygen d_A (Fig. 1A)—determines the relative energy levels of key electronic orbitals of the apical and in-plane O atoms and the Cu atoms. These energy-level shifts affect hole propagation through the stability of the Zhang–Rice singlet state (10), such that the state of the apical oxygen atom is directly correlated with T_c . Further, Pavarini *et al.* (9) derive a relationship between d_A and T_c by considering translationally invariant changes in unit cell geometry on the in-plane hopping rates t along (1, 0) and t' along (1, 1). Finally, Nunner *et al.* (11) have proposed that such geometrical distortions of the unit cell may locally alter the electron-pairing interactions. Until now, however, no direct test of such theories has been possible because techniques whereby picometer changes in interatomic distances could be compared directly with the superconducting electronic structure inside the same unit cell did not exist.

To investigate how the geometry of a CuO₅ pyramid affects superconductivity locally, an ideal experiment would be to continuously perturb the dimensions of a single unit cell (Fig. 1B) and measure the resulting changes in superconducting

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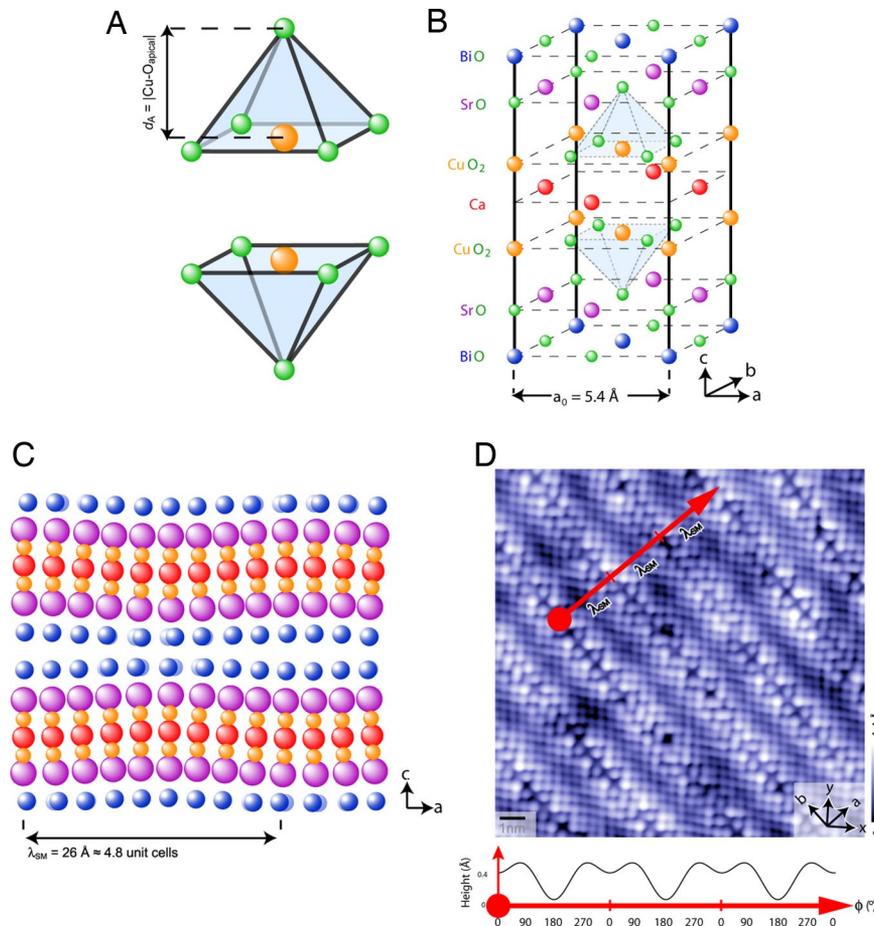


Fig. 1. Crystal structure and periodic unit cell distortion due to bulk incommensurate supermodulation. (A) The CuO_5 pyramidal coordination of oxygen atoms surrounding each copper atom in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$. (B) Top half of the $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ unit cell (the lower half is identical except for a translation by $a_0/2$ along the a axis). Crystal axes a , b , and c are indicated. (C) Schematic view along the b axis of the crystal, showing representative displacements of all non-O atoms (adapted from ref. 14). Supermodulation displacements can be seen in both the a and c directions. (D) A 14.6-nm-square topographic image of the exposed BiO layer of a cleaved crystal of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$. The x and y axes (aligned along the Cu–O bonds), and the crystalline a and b axes, are indicated in the figure. The c axis supermodulation effect is visible as corrugations of the surface. A simulated cross-section is shown, illustrating the periodic profile of the modulations. [Profile calculated by phase-averaging the topographic height and fitting the first two harmonics of the resulting function $z(\phi)$.]

properties within that same unit cell. At first glance, this might seem merely a *gedanken* experiment. Fortunately, however, significant variations in cell dimensions and geometry occur naturally at the nanoscale in the $\text{Bi}_2\text{Sr}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_{4+2n}$ ($n = 1, 2, 3$) family. These variations take the form of a bulk incommensurate periodic modulation (12–17) perturbing the atoms from their mean positions (18), as shown schematically in Fig. 1C and D. This so-called crystal “supermodulation” is believed to originate from a misfit between the preferred bond lengths of the perovskite and rock-salt layers of the crystal. In each of the 14 layers of the $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (Bi-2212) unit cell, atoms are displaced from their mean locations (i.e., where they would be located in an idealized average unit cell) by up to 0.4 \AA , following a functional form repeating, on average, every 26 \AA (≈ 4.8 unit cells) along the a axis. These distortions are represented schematically in Fig. 1C. Here we exploit the associated modulations of interatomic distances (whose largest fractional change is to the Cu–O_{apical} distance) to directly explore associated changes to the superconducting state.

Results

Topographic and Spectroscopic Imaging of Bi-2212. We use floating-zone-grown single crystals of Bi-2212, cleaved in cryogenic ultrahigh vacuum to reveal the BiO layer (Fig. 1B). These

crystals are inserted into the scanning tunneling microscope (STM) head at 4.2 K. The CuO_2 plane is $\approx 5 \text{ \AA}$ beneath the BiO surface and separated from the STM tip by insulating BiO and SrO layers. Fig. 1D shows a 14.6-nm-square topographic image of the BiO surface, revealing the distorted, grid-like arrangement of Bi atoms; the Cu atoms lie $\approx 5 \text{ \AA}$ below each Bi atom. The blotchy appearance of the topograph is due to the heterogeneous high-energy spectral weight shifts near each dopant atom (19). Most importantly, the effects of the crystal supermodulation at the BiO layer can be seen in Fig. 1D as a surface corrugation. A simulated cross-section of this surface corrugation along the red line in the figure is displayed below the topograph and shows the primary BiO modulation with its weaker second harmonic. We choose to label the phase of the supermodulation as $\phi = 0^\circ$ (180°) where the first-order maximum (minimum) c axis Bi atom positions occur [see [supporting information \(SI\) Text](#) for details].

Homogeneous Low-Energy Excitations with $E = \Delta$ Nanoscale Electronic Disorder. To explore the CuO_2 electronic local density of states (LDOS) (\mathbf{r}, E) at each point within the supermodulation, we use STM-based imaging of the differential conductance $g(\mathbf{r}, V) \equiv dI/dV(\mathbf{r})$. If spatial variations of the tunneling matrix elements do not predominate, this technique results in a spatial

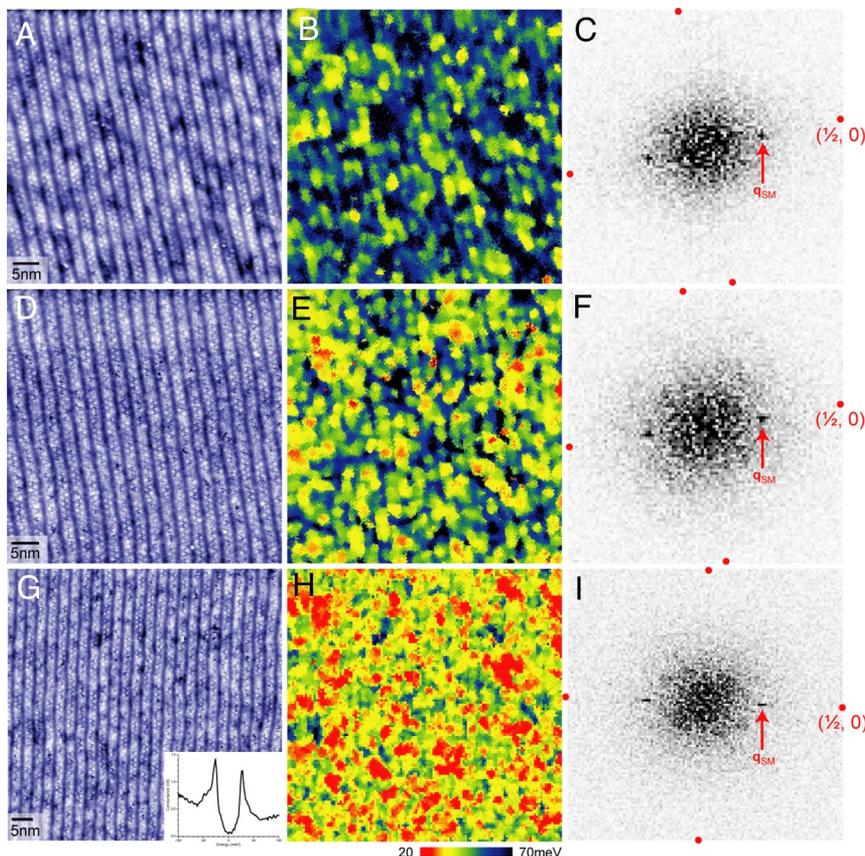


Fig. 2. Appearance of gap modulations at the same wavevector \mathbf{q}_{SM} as the crystal supermodulation. Topographic images of underdoped (mean gap, 5 meV) (A), optimally doped (mean gap, 47 meV) (D), and overdoped (mean gap, 37 meV) (G) samples of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8-\delta}$. Gap maps B, E, and H correspond to adjacent topographs A, D, and G, respectively, alongside their respective Fourier transforms C, F, and I. Clear peaks are visible in the Fourier-transformed gap maps at \mathbf{q}_{SM} (indicated). Points corresponding to $(\pm\frac{1}{2}, 0)$ and $(0, \pm\frac{1}{2})$ are indicated, in units of $2\pi/a_0$.

image of LDOS ($\mathbf{r}, E = eV$) $\propto g(\mathbf{r}, V)$. To generate an atomic resolution “gap map,” we then determine, at each point, half the energy difference between the two peaks in each $g(\mathbf{r}, V)$ spectrum (Fig. 2G Inset) and ascribe this difference to the maximum value of the d -wave superconducting energy gap $\Delta(\mathbf{r})$. For this work, we studied gap maps from 11 distinct samples of Bi-2212 at a sequence of different hole-dopings, $0.08 < p < 0.23$. Fig. 2 B, E, and H shows gap maps produced from three representative samples at $p \approx 0.13, 0.15,$ and 0.17 . An identical color scale represents Δ in these panels. The panels exhibit intense disorder in the gap maxima, with values ranging from 20 to >70 meV within adjacent ≈ 3 -nm-diameter domains; the disorder in gap maxima occurs in association with the nonstoichiometric dopant oxygen atom locations (19), with gap values strongly increased in their vicinity. However, this disorder in gap maxima always coexists with a $dI/dV(\mathbf{r}, E)$ that is spatially homogeneous below some lower energy (20–22) [because the $\Delta(\mathbf{k})$ for any range of energies where quasiparticle interference (23, 24) is detected must be spatially homogeneous throughout that region]. The detailed agreement between results from $g(\mathbf{r}, V)$ imaging (21) and angle-resolved photoemission (25) provides confidence that tunneling matrix element effects do not prevent the STM from accessing an undistorted \mathbf{k} -space electronic structure.

In all $\Delta(\mathbf{r})$, we find a variation of the gap magnitude that has the same wavevector \mathbf{q}_{SM} as the crystal supermodulation. The three gap maps of Fig. 2 B, E, and H are presented alongside their simultaneously acquired topographs (Fig. 2 A, D, and G). In the three topographs, each ≈ 45 nm square, the minima ($\phi = 180^\circ$) of the supermodulation distortion can be seen as a series of dark parallel lines ≈ 2.6 nm apart. The mean gap energy falls from the

underdoped sample (Fig. 2B; 55 meV), through the near-optimally doped sample (Fig. 2E; 47 meV), to the moderately overdoped sample (Fig. 2H; 37 meV). Careful comparison of the gap maps with the topographs reveals that each gap map exhibits periodic features with the same wavevector \mathbf{q}_{SM} as its simultaneous topograph. This becomes more obvious in the Fourier transforms of the gap maps (Fig. 2 C, F, and I), which exhibit clear peaks, labeled \mathbf{q}_{SM} , at positions corresponding to the average wavevector of the crystalline supermodulation. The obvious difficulty is how to quantify the local relationship between the supermodulation and Δ variations at \mathbf{q}_{SM} in the presence of both the irregularity in the supermodulation and the dopant-induced gap disorder.

Supermodulation Phase Map. The supermodulation itself is an incommensurate, approximately periodic, displacive modulation of the atomic sites of the crystal. The periodicity and direction of the modulation can be given (14) by wavevector $\mathbf{q}_{\text{SM}} = q_1\mathbf{a}^* + q_2\mathbf{b}^* + q_3\mathbf{c}^*$, where \mathbf{a}^* , \mathbf{b}^* , and \mathbf{c}^* are the reciprocal basis vectors of the lattice, $q_1 = 0$, $q_2 \approx 0.212$, and $q_3 = 1$. The effect of the supermodulation is to displace each atom, μ , whose unperturbed position within the unit cell we denote \mathbf{x}^μ , by a displacement vector $\mathbf{u}^\mu(\phi)$. We call ϕ the “supermodulation phase,” and set $\mathbf{u}^\mu(\phi) = \mathbf{u}^\mu(\phi + 2\pi)$ for all ϕ . The supermodulation phase at an atomic site μ is given by $\phi = 2\pi\mathbf{q} \cdot (\mathbf{n} + \mathbf{x}^\mu)$, where \mathbf{n} is the position of the unit cell in which the atom resides. Thus, because of the periodicity of the displacements $\mathbf{u}^\mu(\phi)$, the dimensions of any unit cell at \mathbf{r} in the crystal can be labeled by $\phi(\mathbf{r})$, and all unit cells with the same value of ϕ will, in general, have the same interatomic dimensions. If the supermodulation were sufficiently regular, knowing \mathbf{q}_{SM} and the

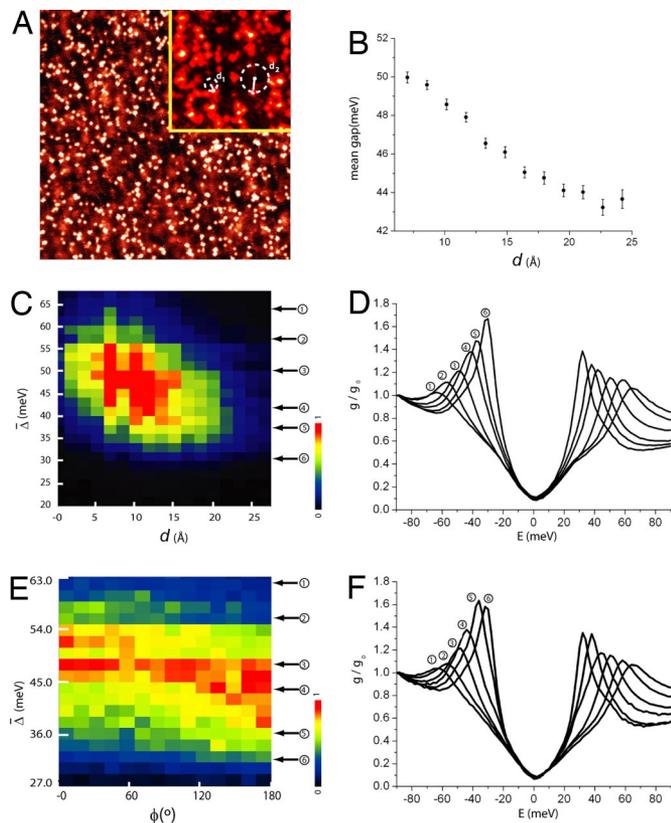


Fig. 4. Response of gap to interstitial dopant ions and supermodulation. (A) A $dI/dV(r, V)$ map at $V = -0.96$ V, showing locations of dopant ions. *Inset*, two examples of the definition of d , the distance from any point to the nearest dopant atom. (B) Mean gap value as a function of d . (C) Histogram of gap values vs. d . (D) Average spectra associated with different nearest-dopant-atom distances, as labeled in C. (E) Gap magnitudes sorted by the phase of the supermodulation. (F) Average spectra associated with different values of supermodulation phase, as labeled in E. We emphasize that the spectra in D and F are not sorted by gap values. The arrows in C and E are merely guides to indicate the resulting average gap values after the spectra are sorted by d and ϕ , respectively.

conductivity to these apparently different perturbations. Fig. 4A shows a $g(r, V)$ map at $V = -0.9$ V that is believed to reveal the locations (19) of interstitial dopant ions in Bi-2212. Fig. 4A *Inset* provides two examples of the definition of d , the distance of any point to the nearest dopant atom: all points on the surface \mathbf{r} can be labeled with a particular value of $d(\mathbf{r})$. The $g(r, V)$ spectra are then sorted according to $d(\mathbf{r})$, with the results shown in Fig. 4B, C, and D. Fig. 4B shows the mean gap value as a function of d , falling >7 meV within a d range of 2 nm. Fig. 4C shows the histogram of gap values vs. d , whereas Fig. 4D shows the average spectra associated with various d (as labeled in Fig. 4C). For the range of gap variations due to dopant disorder, the key spectra are labeled 2, 3 and 4. For comparison, Fig. 4E shows the gap magnitudes sorted by the phase of the supermodulation $\phi(\mathbf{r})$ (in the same sample), and Fig. 4F shows the average spectra associated with different values of $\phi(\mathbf{r})$ (as labeled in Fig. 4E). Here, the key spectra are labeled 2, 3, 4, and 5. Comparing Fig. 4D and F, we see that the anticorrelation between coherence peak height and Δ seen in the random gap disorder (19, 20, 22) (Fig. 4D) appears indistinguishable, although the primary perturbation is not random dopant atoms but the crystalline supermodulation. Empirically, then, we detect no difference between the evolution of $g(V)$ spectra as a function of dopant distance d and supermodulation phase ϕ .

Discussion and Conclusions

In these studies, we show a direct link between the dimensions of individual unit cells and the local gap maximum in a high-temperature superconductor. The gap maxima Δ are modulated cosinusoidally by the changes in unit cell dimensions of Bi-2212, with the gap maxima occurring in association with the minima of $O_{\text{apical}}\text{-Cu}$ distance (when only the first harmonic of the crystal refinement is considered). The range of the gap modulation is found to be $\approx 9\%$ of the mean gap maximum independent of doping. We note that the modulating superconducting gap, albeit induced by a crystal modulation, now makes it possible to study a “pair-density wave” (26–29) in cuprates. Overall, our data confirm directly at atomic scale the theoretical concept of a strong influence of unit cell geometry on cuprate electronic structure and superconductivity (2, 9, 11).

However, a key question emerging from these studies is whether the random gap disorder associated with the dopant atoms (19) and the periodic gap modulations herein could be caused by the same atomic-scale mechanism. In neither case are the observations consistent with variations of in-plane hole density because the high Δ regions occur when the negatively charged oxygen atom (dopant or apical) is most attractive to holes and should, therefore, tend to diminish Δ , but the opposite is detected in both cases. For this reason, both types of Δ variations appear to be more consistent with some other strong out-of-plane effect unrelated to hole density variations. This issue is important because, if there is a single out-of-plane influence that can alter gap magnitudes by large factors, it is obviously key to understanding the superconductivity and achieving maximum T_c . An important observation is that the modulation in Δ reported here also preserves the anticorrelation between coherence peak height and Δ seen in the random gap disorder (19, 20, 22) (Fig. 4F): the spectra evolve in both cases from having small gaps and sharp coherence peaks to wide gaps and low coherence peaks, as if both gap energy and quasiparticle lifetimes are affected in opposite directions by a single parameter. Thus, there is no empirical reason to conjecture two different microscopic mechanisms for the dopant disorder-induced effects and the new supermodulation-induced effects reported here. Conversely, the supermodulation effects on Δ would be empirically consistent with those of the random dopant disorder on Δ if (i) the supermodulation’s first-harmonic of atomic displacements predominates, and (ii) the proposal that the interstitial dopant atoms displace the apical oxygen atom (30) and tilt the CuO_5 pyramid is correct. In that case, dopant- and supermodulation-induced gap variations would have a closely related out-of-plane trigger effect, probably involving either the alteration of d_A or the tipping to the CuO_5 cage, which is central to the electron-pairing process.

Studies of local variations in superconducting electronic structure are becoming a key area for atomic-scale tests of proposed mechanisms for cuprate superconductivity (31–35). But because such analysis has, in the past, relied on correlations between random dopant locations (19) and electronic disorder, definite conclusions have been difficult to achieve. With the finding of a nonrandom modulation in superconducting electronic structure due to unit cell dimension modulations, we point to a far more controlled avenue for testing models of the pairing mechanism at atomic scale. Theoretical approaches (36–38) to this challenge have emerged rapidly. Yin and Ku (36) derive an effective one-band Hamiltonian but emphasizing the effects of out-of-plane apical oxygen atoms by using a Wannier function and LDA+U approach. The parameters emphasize an intersite “superrepulsion” term V_{ij} , which is controlled by the energy of the apical oxygen p_z orbital; V_{ij} weakens local pairing strength. These authors propose that the dopant atoms and the crystal supermodulation both perturb the energy levels of the apical

oxygen p_z orbital (2), which in turn modulates V_{ij} and thus Δ . Andersen *et al.* (37) use a d -wave Bardeen–Cooper–Schrieffer Hamiltonian whose pairing strength is modulating along with the supermodulation reproducing the effects reported here. This type of model has been quite successful in reproducing the random effects due to dopant disorder (11). Although dopant-disorder and supermodulation effects on Δ can, therefore, be consistent within the model, the microscopic cause of the pairing modulation and dopant effect has not yet been identified. Yang *et al.* (38) use a t - t' - J model within a renormalized mean field theory to account for the strong correlations. This model appears to be related to that used by Zhu (34) to describe dopant-disorder effects. Here, by modulating t , t' , and J along with the crystalline supermodulation, a Δ modulation can be simulated in agreement with experiment, but with the t' modulation leading to a significant carrier concentration modulation. Yang *et al.* ascribe the random gap disorder (19–22, 31–35) to a different microscopic effect, possibly emerging from local hole-density variation through Sr/Bi intersubstitution.

Identification of a predominant out-of-plane influence controlling the superconductivity could transform both the material science approach to raising T_c and efforts to understand the microscopic electron-pairing mechanism in cuprate high- T_c su-

perconductivity (1). The powerful and nonrandom effects on superconductivity of varying the interatomic distances within individual crystal unit cells, as reported here, provide opportunities to address both this issue and the physics of pair density waves directly at the atomic scale. The small spatial scale on which these effects occur also means that sophisticated quantitative, but numerically intensive, theoretical models can now be brought to bear on the observations. An immediate challenge for this research focus will be to relate a controlled change in T_c to electronic structure changes resulting from interatomic distance alterations, as determined directly by spectroscopic imaging scanning tunneling microscopy.

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