

Effect of Symmetry Distortions on Photoelectron Selection Rules and Spectra of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$

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We derive photoelectron selection rules along the glide plane in orthorhombic $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (Bi2212). These selection rules explain the reversed intensity behavior of the shadow and the main band of the material as a natural consequence of the varying representation of the final state as a function of k_{\parallel} . Our one-step simulations strongly support the structural origin of the shadow band but we also introduce a scenario for detecting antiferromagnetic signatures in low doping.

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Angle resolved ultraviolet photoelectron spectroscopy (ARUPS) is probably the most important tool to study the electronic structure of complex materials such as the high T_c superconductors. It has been shown that matrix element effects must be taken into account in interpreting experimental data [1,2]. Using the one-step model of ARUPS and optical matrix elements, light has been shed on the strong variation of intensities due to the matrix element effects [3–5]. However, there are more strict rules dictating intensities in ARUPS, selection rules due to crystal symmetry. High resolution angular resolved photoemission measurements along high symmetry lines have been carried out recently to investigate the origin of the shadow bands in Bi2212 [6,7]. Based on one-step computations, it was proposed that the shadow Fermi surface (FS) in Bi2212 has its origin in the orthorhombic (orth.) structure of the material [6]. In this study, a need for selection rules emerged. In the orth. structure, a mirror plane is broken into a glide plane. In this Letter, we give a group theoretical analysis for the selection rules along the glide plane and demonstrate the derived rules with one-step ARUPS simulations. We focus on Bi2212, but the derived selection rules may be applied to any cuprate superconductor with a similar structure.

The space group of the commonly used body-centered tetragonal (tetr.) structure for Bi2212 is number 139 in the International Tables for Crystallography. In x-ray diffraction experiments, an orth. structure has been found [8]. In this structure, atoms are moved from their tetr. positions and the symmetry group is changed. The nonsymmorphic space group of the orth. structure is group number 66. The geometric structure of the superconducting cuprates may be described by a pile of planes of atoms. In the orth. structure, the movements of the atoms from tetr. positions in the Cu-O planes are small. Displacements are more clear in the Bi-O plane, which is sketched in Fig. 1. Figure 1(a) represents the tetr. Bi-O plane and Fig. 1(b) the orth. Bi-O plane, where empty circles representing Bi atoms and solid circles representing O atoms are displaced. In the tetr. structure, there are mirror planes corresponding to the dashed lines in Fig. 1(a), but in the orth. structure only

the mirror plane parallel to the x axis remains. The mirror plane parallel to the y axis is changed into a glide plane, which is plotted with a dashed-dotted line in Fig. 1(b). This glide plane corresponds to the glide operation $\{\sigma_x|\mathbf{b}/2\}$, a reflection (σ_x in the $x = 0$ plane) followed by a translation by half the primitive lattice vector in the y axis.

The model FS of Bi2212 (only one sheet is shown for clarity) is sketched in Fig. 1(c). The figure shows the main band (FS of the tetr. structure) as thick circles and the shadow band as thin circles. In the figure, the first tetr. Brillouin zone is approximately plotted with a dashed line and the first orth. Brillouin zone with a solid line. Two-dimensional k_{\parallel} points of high symmetry $\bar{\Gamma}$, \bar{X} , and \bar{Y} are also marked. The direction from $\bar{\Gamma}$ to \bar{X} that is parallel to the mirror plane in real space is denoted by $\bar{\Sigma}$ and the direction from $\bar{\Gamma}$ to \bar{Y} that is parallel to the glide plane by $\bar{\Lambda}$ [9]. These directions are commonly known as the nodal directions.

The formula, based on Fermi's golden rule, for the photocurrent by Feibelman and Eastman [10] can be manipulated into the form

$$I(E, k_{\parallel}) \propto \text{Im} \left(\sum_{ij} \langle \psi_{f, k_{\parallel}}^{(\text{final})} | \mathbf{A} \cdot \mathbf{p} | \psi_{i, k_{\parallel}}^{(\text{initial})} \rangle \times G_{ij} \langle \psi_{j, k_{\parallel}}^{(\text{initial})} | \mathbf{A} \cdot \mathbf{p} | \psi_{f, k_{\parallel}}^{(\text{final})} \rangle \right), \quad (1)$$

where \mathbf{A} is the vector potential of the incident photon and G_{ij} is a hole Green function. Photoemission selection rules

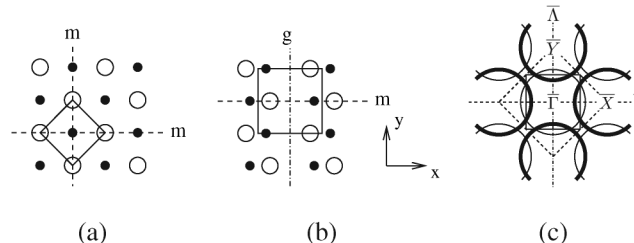


FIG. 1. Sketch of the positions of atoms in Bi2212. (a) Tetr. Bi-O layer, (b) orth. Bi-O layer, (c) sketch of the Fermi surface.

arise from the symmetries of the initial (ψ_i) and final (ψ_f) states and the dipole operator $\mathbf{A} \cdot \mathbf{p}$ in the matrix elements of Eq. (1). These selection rules are especially relevant along the mirror and glide planes, the directions $\bar{\Sigma}$ and $\bar{\Lambda}$ in Fig. 1(c). In the following analysis, the dipole approximation is used, but the derivations are exact beyond the approximation if the wave vector of the radiation lies in the symmetry plane that is under discussion.

In the mirror plane, since there is a well defined parity about the reflection in the plane, the selection rules can be derived by considering the parities of the components of the matrix element [11]. The transition is allowed if the entire dipole matrix element $\langle \psi_f | \mathbf{A} \cdot \mathbf{p} | \psi_i \rangle$ is even. With respect to reflection, the final state with its momentum lying in the mirror plane is even. The operator $\mathbf{A} \cdot \mathbf{p}$ is even (odd) if the polarization is parallel (perpendicular) to the plane, which can be explained by considering parities of the initial state ψ_i and its derivative $\mathbf{A} \cdot \mathbf{p} \psi_i$, where $\mathbf{p} = -i\hbar \nabla$. The initial state at the Fermi level is similar to a Bloch sum of copper $d_{x^2-y^2}$ orbitals [12]. With respect to reflection, this orbital and the Bloch sum with its momentum lying in the plane are odd. Thus, for photointensity to be nonzero, the operator $\mathbf{A} \cdot \mathbf{p}$ must be odd, and, respectively, polarization must be perpendicular to the mirror plane. This result is presented in combined form in Table II. The even (identity) representation is denoted by Σ and the odd representation by Σ' .

Along the glide plane in the orth. structure, the full machinery of the group theory has to be used. Photoemission selection rules due to a glide plane have been considered previously by Pescia *et al.* [13] A good account of a more general procedure has been given by Bassani and Parravicini [14]. The dipole matrix element $\langle \psi_f^{(\mu)} | (\mathbf{A} \cdot \mathbf{p})^{(\alpha)} | \psi_i^{(\nu)} \rangle$ will vanish if the irreducible representation (irrep) of the final state does not appear in the product of irreps of the initial state and the operator. The number of times it appears is given by [14]

$$c(\mathbf{k}, \mu; \alpha; \mathbf{k}, \nu) = \frac{1}{h_{\mathbf{k}}} \sum_{\{R_{\mathbf{k}}|\mathbf{f}\}} \chi^{(\mu)}(\{R_{\mathbf{k}}|\mathbf{f}\})^* \chi^{(\alpha)}(R_{\mathbf{k}}) \chi^{(\nu)}(\{R_{\mathbf{k}}|\mathbf{f}\}), \quad (2)$$

where $h_{\mathbf{k}}$ is the order (number of elements $\{R_{\mathbf{k}}|\mathbf{f}\}$) of the relevant little group for a particular \mathbf{k} point in the first Brillouin zone. $\chi^{(\nu)}(\{R_{\mathbf{k}}|\mathbf{f}\})$ is the character of the little group irrep $D^{(\nu)}(\{R_{\mathbf{k}}|\mathbf{f}\})$ for the initial state, $\chi^{(\mu)}(\{R_{\mathbf{k}}|\mathbf{f}\})$ the character of the irrep of the final state, and $\chi^{(\alpha)}(R)$ is the character of the small point group representation $D^{(\nu)}(R_{\mathbf{k}})$ of the dipole operator. The little group of a particular \mathbf{k} point contains operations $\{R|\mathbf{f}\}$ of the full space group that satisfy

$$R\mathbf{k} = \mathbf{k} + \mathbf{G}, \quad (3)$$

i.e., leaving \mathbf{k} unchanged. The small point group of \mathbf{k} contains the rotational parts of the little group operations.

In the glide plane determined by direction $\bar{\Lambda}$ in Fig. 1(c), the little group (operations that keep $k_{\parallel} = k_y \hat{\mathbf{k}}_y$ and k_z unchanged) of the \mathbf{k} vector in the plane contains two operations, identity operation $\{E|0\}$ and glide operation $\{\sigma_x|\mathbf{b}/2\}$. Both of the two operations form a class of their own, and the eigenstates in the plane can be classified by two irreps. A character table for the little group is in Table I.

To proceed, it has to be found out how to assign symmetry labels to particular final (and initial) states. The matching of the wave function at the surface of the sample rules out some of the possible final states. The final state in ARUPS is a time-reversed LEED state [10]. The irrep of this state may be obtained from the plane wave state $\psi_{\mathbf{k}_f} = e^{i(\mathbf{k}_f \cdot \mathbf{r})}$ that arrives to the detector [11]. The state is transformed under the glide operation according to

$$\begin{aligned} O_{\{\sigma_x|\mathbf{b}/2\}} \psi_{\mathbf{k}_f}(\mathbf{r}) &= \psi_{\mathbf{k}_f}(-x, y - b/2, z) = e^{i(k_{fy}(y-b/2) + k_{fz}z)} \\ &= e^{-ik_{fy}b/2} \psi_{\mathbf{k}_f}(\mathbf{r}) = e^{-i(k_y + G_y)b/2} \psi_{\mathbf{k}_f}(\mathbf{r}) \\ &= \delta e^{-in\pi} \psi_{\mathbf{k}_f}(\mathbf{r}), \end{aligned} \quad (4)$$

where k_y lies in the first Brillouin zone and \mathbf{G} is a reciprocal lattice vector. The glide operation is represented by $\delta e^{-in\pi}$, where n is an integer. The irrep of the final state is a function of the magnitude of the parallel component of its wave vector. It belongs to the irrep Λ in the 1., 3., 5., ... repeated Brillouin zone and to the representation Λ' in the 2., 4., 6., ... zone. This fundamental result for ARUPS and glide plane was first shown by Pescia *et al.* [13] and has been exploited for Ni(100) - p(2 × 2)C [15] and TiO₂ [16].

The operator $\mathbf{A} \cdot \mathbf{p}$ belongs to representation Λ of the small point group if the polarization vector lies in the glide plane and to representation Λ' if it is perpendicular to the plane (parallel to the x axis). Photoemission selection rules follow from Eq. (2). They are presented in Table II. In summary, the initial state must belong to the same irrep as the final state if the polarization is parallel to the symmetry plane and to the other irrep if the polarization is perpendicular to the plane.

To finish, the symmetry labels of the initial states forming the FS have to be determined. As was discussed, the movements of the atoms from the tetr. sites are very small in the copper-oxide layers, and it can be assumed that the shape of the initial state is very close to the tetr. case, which can also be shown in the band structure calculations. Thus, the initial state at the FS belongs to the same irrep as a Bloch state of copper $d_{x^2-y^2}$ orbitals. A Bloch sum of

TABLE I. Character table of the little group in plane $\bar{\Lambda}$. δ is $e^{-i\mathbf{k} \cdot \mathbf{b}/2}$.

	E	$\{\sigma_x \mathbf{b}/2\}$
Λ	1	δ
Λ'	1	$-\delta$

TABLE II. Dipole selection rules in the planes of high symmetry.

k_f in the mirror plane $\bar{\Sigma}$							
Repeated zone of $k_{f\parallel}$...	1.	2.	3.	4.	5.	...
Allowed final state irrep	...	Σ	Σ	Σ	Σ	Σ	...
Allowed initial state if $\mathbf{A} \perp \bar{\Sigma}$...	Σ'	Σ'	Σ'	Σ'	Σ'	...
Allowed initial state if $\mathbf{A} \parallel \bar{\Sigma}$...	Σ	Σ	Σ	Σ	Σ	...
k_f in the glide plane $\bar{\Lambda}$							
Repeated zone of $k_{f\parallel}$...	1.	2.	3.	4.	5.	...
Allowed final state irrep	...	Λ	Λ'	Λ	Λ'	Λ	...
Allowed initial state if $\mathbf{A} \perp \bar{\Lambda}$...	Λ'	Λ	Λ'	Λ	Λ'	...
Allowed initial state if $\mathbf{k} \parallel \bar{\Lambda}$...	Λ	Λ'	Λ	Λ'	Λ	...

copper $d_{x^2-y^2}$ orbitals at a position $\mathbf{d}_1 = 0.251\mathbf{a} + 0.5\mathbf{b} - 0.303\mathbf{c}$ is defined as

$$\phi_{d_{x^2-y^2}, \text{Cu}_1}(\mathbf{r}) = \sum_{\tau_\nu} e^{i\mathbf{k} \cdot \tau_\nu} \phi_{d_{x^2-y^2}}(\mathbf{r} - \mathbf{d}_1 - \tau_\nu). \quad (5)$$

This can be decomposed into components belonging to different irreducible representations of the little group of \mathbf{k} by [14]

$$\begin{aligned} \phi_{d_{x^2-y^2}}^{(\Lambda)}(\mathbf{r}) &= \frac{1}{2} [\phi_{d_{x^2-y^2}, \text{Cu}_1}(\mathbf{r}) - e^{-i\mathbf{k} \cdot \mathbf{b}/2} \phi_{d_{x^2-y^2}, \text{Cu}_2}(\mathbf{r})], \\ \phi_{d_{x^2-y^2}}^{(\Lambda')}(\mathbf{r}) &= \frac{1}{2} [\phi_{d_{x^2-y^2}, \text{Cu}_1}(\mathbf{r}) + e^{-i\mathbf{k} \cdot \mathbf{b}/2} \phi_{d_{x^2-y^2}, \text{Cu}_2}(\mathbf{r})], \end{aligned} \quad (6)$$

where $\phi_{d_{x^2-y^2}, \text{Cu}_2}(\mathbf{r})$ is a Bloch sum of an identical $d_{x^2-y^2}$ orbital at $\mathbf{d}_2 = -0.251\mathbf{a} + 0\mathbf{b} - 0.303\mathbf{c}$. These states can be pictured at Γ as bonding-antibonding states which have the opposite dispersion as a function of \mathbf{k}_y . $\phi_{d_{x^2-y^2}}^{(\Lambda')}$ is the bonding state with lower energy and $\phi_{d_{x^2-y^2}}^{(\Lambda)}$ the antibonding state. In the repeated zone scheme, the state $\phi_{d_{x^2-y^2}}^{(\Lambda')}$ represents the main band, i.e., the band of the tetr. structure, and the state $\phi_{d_{x^2-y^2}}^{(\Lambda)}$ the shadow band.

We have performed first-principles simulations of ARUPS spectra in Bi2212 using the one-step model of photoemission [17,18]. Figure 2 shows the calculated FS of the orth. Bi2212 in the normal incidence setup. Double-headed arrows indicate polarization of the incident light. Photon energy was 54 eV. First, we remark that there seems to be no general correspondence between the intensities of the main band and the shadow band. The effect of selection rules is seen in high symmetry directions $\bar{\Sigma}$ and $\bar{\Lambda}$. The FS map is probed at the Fermi level, and the initial state belongs to representation Λ' in the glide plane and to the representation Σ' in the mirror plane. In Fig. 2(a), polarization is parallel to the mirror plane and neither the shadow or the main band is visible in the $\bar{\Sigma}$ direction, whereas only the main band is visible in the $\bar{\Lambda}$ direction. In Fig. 2(b), polarization is parallel to the glide plane and both of the bands are visible in the $\bar{\Sigma}$ direction, whereas only the shadow band is visible in the $\bar{\Lambda}$ direction. This phenomenon has also been shown experimentally [6,7].

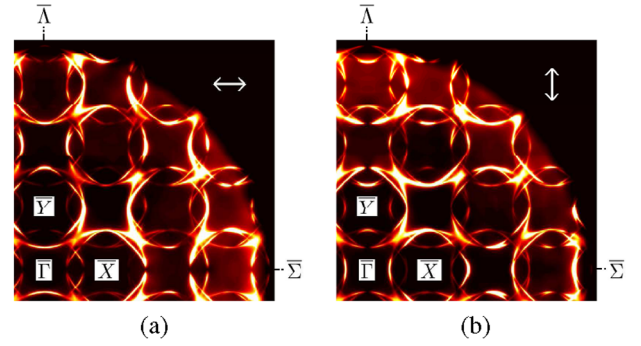


FIG. 2 (color online). Bi2212 FS map. Normal incidence. (a) Polarization parallel to the x axis. (b) Polarization parallel to the y axis.

The strange behavior of the shadow band follows from the varying irrep of the final state in the consequent Brillouin zones.

Figure 3 shows photointensity as a function of binding energy and k_{\parallel} . Calculations were performed within the normal incidence setup; photon energy was 40 eV. The Fermi function was ignored. Figures 3(a) and 3(b) show results along the glide plane with polarization perpendicular to the plane [Fig. 3(a), main band visible] and parallel to the plane [Fig. 3(b), shadow band visible]. Figures 3(c) and 3(d) show the corresponding results along the mirror plane. Along the glide plane, the main and the shadow bands seem to give continuous intensity as a function of \mathbf{k}_{\parallel} even when crossing the zone barrier. This can again be explained with Table II. When an initial state band crosses the zone barrier, it can be mapped to the other band in the first Brillouin zone and its irrep, as the irrep of the final state, will change.

Furthermore, there is one surprising consequence of the selection rule due to the glide plane. As this rule states, the final states for the shadow and the main bands must belong to a different irrep along the $\bar{\Lambda}$ line. Consequently, when picturing the band structure, the final state for the shadow band cannot be an umklapp of the final state for the main band, but, on the contrary, it must lie in some other available band with a fixed final state energy. This means that the intensities of the bands vary, e.g., as a function of photon energy in an uncorrelated way, which can also be seen as a function of binding energy in Figs. 3(a) and 3(c).

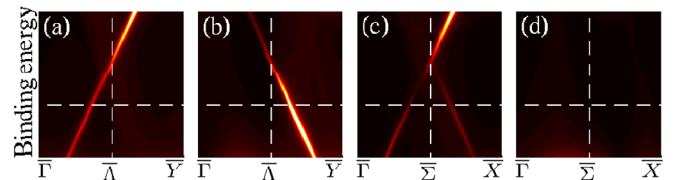


FIG. 3 (color online). Photoelectron spectra along high symmetry lines as a function of energy. (a) Along the glide plane, perpendicular polarization. (b) Along the glide plane, parallel polarization. (c) Along the mirror plane, parallel polarization. (d) Along the mirror plane, perpendicular polarization.

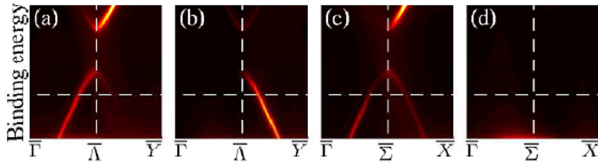


FIG. 4 (color online). Photoelectron spectra along the high symmetry lines as a function of energy, including the AFM effect, $u = 0.9$ eV. (a) Along the glide plane, perpendicular polarization. (b) Along the glide plane, parallel polarization. (c) Along the mirror plane, perpendicular polarization. (d) Along the mirror plane, parallel polarization.

Actually, because of the fact that the width (due to Σ_f'' and k_{\perp} dispersion [19]) of the final state is relatively large, both the main and the shadow bands can be observed with the same single photon energy.

Available experimental data are consistent with our predicted intensities due to structural distortions, but we also point out that the intensity variation along the glide plane strongly masks any weak sign of antiferromagnetism (AFM) induced spectral features. We have modeled the molecular field of the AFM interaction with planar ordering, which is known to exist in $\text{La}_2\text{CuO}_{4-y}$ [20], by an *ad hoc* parameter u on copper sites. Our computations reveal that, to produce shadow bands in ARUPS by AFM, a relatively large u has to be used.

But there is one interesting possibility. If both the structural and the AFM interactions were present, as must be with low doping, the selection rules would change again. The correct magnetic group should be determined, but, because the specification of the magnetic moments in Bi2212 is not available and because of limitations of our program code, we can only discuss the AFM selection rules qualitatively. While maintaining the reflection symmetry, the *ad hoc* planar ordering breaks the glide symmetry, and, consequently, the derived selection rules along the glide plane would no longer be valid. In practice, this would mean that, in those high symmetry directions where the structural distortions forbid intensity, there could exist signatures of the FS due to the AFM interaction. In Fig. 4, we have calculated the effect of the AFM on ARUPS spectra. The magnitude of u was 0.9 eV, which induces an energy gap of the same magnitude. In contrast to Fig. 3, along the glide plane [Figs. 4(a) and 4(b)], there are no longer strict selection rules for the polarization, and the main and the shadow bands are, though weakly, visible with both polarizations. Along the mirror plane [Figs. 4(c) and 4(d)], the selection rules remain strict. We thus urge experimentalists to focus some measurements with high flux and precise polarizations to look for possible signatures of AFM features. A development of the AFM gap with lowered doping and maybe other signatures of the AFM may be seen in this way.

We have shown that structural modifications in Bi2212 from a body-centered tetragonal lattice to a base-centered orthorhombic lattice change selection rules in ARUPS along the high symmetry lines. Because of the glide plane in orthorhombic structure, it turns out that the irreducible representation of the final state changes alternatively in the repeated zone scheme of k_{\parallel} space. With fixed polarization, this yields opposite intensity behavior for the main and the shadow FS in the adjacent Brillouin zones. The calculated FS is consistent with available experimental data, which is strong evidence against the antiferromagnetic scenario, but a possibility of detecting AFM features in low doping is proposed.

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