Two-photon momentum density in La$_{2-x}$Sr$_x$CuO$_4$ and Nd$_{2-x}$Ce$_x$CuO$_4$

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We present calculations of the electron-positron momentum density for the high-$T_c$ superconductors La$_{2-x}$Sr$_x$CuO$_4$ and Nd$_{2-x}$Ce$_x$CuO$_4$, together with experimental two-dimensional angular correlation of annihilation radiation (2D-ACAR) for Nd$_{2-x}$Ce$_x$CuO$_4$. The calculations are based on first-principles electronic structure obtained using the full-potential linearized augmented-plane-wave and the linear muffin-tin orbital methods. Our results indicate a non-negligible overlap of the positron wave function with the CuO$_2$ plane electrons responsible for the Fermi surfaces in these compounds. Therefore, these compounds may be well suited for investigating Fermi-surface-related effects. After the folding of umklapp terms according to Lock, Crisp and West, the predicted Fermi-surface breaks are mixed with strong effects induced by the positron wave function in La$_{2-x}$Sr$_x$CuO$_4$, while their resolution is better in Nd$_{2-x}$Ce$_x$CuO$_4$. A comparison of our calculations with the most recent experimental results for La$_{2-x}$Sr$_x$CuO$_4$ shows good agreement. For Nd$_{2-x}$Ce$_x$CuO$_4$ good agreement is observed between theoretical and experimental 2D-ACAR profiles.

I. INTRODUCTION

Despite a great amount of experimental and theoretical work, there are still open questions concerning the electronic structure of the high-$T_c$ oxide superconductors. In particular, it still remains to be determined how well the picture provided by highly precise local-density-band-structure calculations works in describing the electronic states of these materials in their normal state. The existence of a Fermi surface (FS) is one of the issues where many efforts have been devoted. Angle-resolved photoemission$^1$ and positron-annihilation experiments$^2-^4$ have now pointed out the existence of a FS for some of these systems, in good agreement with band-structure calculations.$^5,^6$

Positron-annihilation spectroscopy$^7$ has been largely used to investigate the FS in high-$T_c$ superconductors. Two-dimensional angular correlation of annihilation radiation (2D-ACAR) experiments have been applied to YBa$_2$Cu$_3$O$_{7-\delta}$, La$_{2-x}$Sr$_x$CuO$_4$, and Bi$_2$Sr$_2$CaCu$_2$O$_8$ (Refs. 2-4 and 8-14) by several groups. However, due to many experimental problems, only very recent experiments$^2,^3,^15$ on unwinned YBa$_2$Cu$_3$O$_{7-\delta}$ crystals could show FS features related to the Cu-O chains, in reasonable agreement with band-structure calculations.$^5$

Having excellent unwinned samples has been recognized as a crucial element in order to detect a FS in YBa$_2$Cu$_3$O$_{7-\delta}$. In the Bi-Sr-Ca-Cu-O systems, recent experiments$^16$ also seem to indicate the existence of a FS in agreement with band-structure calculations,$^6$ although due to the presence of superlattice modulations in the Bi-O layers, the interpretation of experiments is not straightforward.$^17$

From the theoretical point of view, 2D-ACAR predictions based on local-density-approximation (LDA) band-structure calculations were reported.$^8,^10,^16,^18-^20$ Generally, good agreement has been found among these different calculations.

Although the work already done is of crucial importance, still in both Bi-Sr-Ca-Cu-O and Y-Ba-Cu-O superconductors the positron density has been shown to be quite low near the Cu-O planes, sampling mainly the Bi-O layers and the Cu-O chains in the two systems, respectively. It is therefore important to perform experiments, and to provide the corresponding theoretical predictions, on materials where there is a larger overlap between the positron and the interesting Cu-O planes. Good candidates would be the Tl-Ba-Ca-Cu-O,$^10$ the Nd- Ce-Cu-O and, to a smaller extent, the La-Sr-Cu-O superconductors.

This paper reports calculations of the theoretical two-photon momentum distribution (TPMD) of La$_{2-x}$Sr$_x$CuO$_4$ and Nd$_{2-x}$Ce$_x$CuO$_4$ as well as experimental positron results in Nd$_{2-x}$Ce$_x$CuO$_{4+\delta}$. The cal-
culations are based on the results of band-structure calculations performed within LDA using the full-potential linearized augmented-plane-wave (FLAPW) and linear muffin-tin orbital (LMTO) methods. A rigid band model is used to treat the Sr and Ce doping. After Lock, Crisp, and West (LCW) folding, our results for $La_{2-x}Sr_xCuO_4$ show good agreement with the most recent experiments performed by Howell et al. on this system. As for $Nd_{2-x}Ce_xCuO_4$, the experiments performed in Geneva do not reveal the calculated FS. This discrepancy may be due to the insufficient quality of our single crystals.

II. METHODS

A. Measurements

The $Nd_{2-x}Ce_xCuO_4$ single crystals used for 2D-ACAR measurements were grown by a flux technique described in detail in Ref. 24. These compounds, like the structurally similar $La_{2-x}Sr_xCuO_4$, have a semiconductor to metal transition for a finite value of $x$ and are superconducting in a narrow range of Ce concentration ($x = 0.13-0.17$) once reduced by an appropriate annealing ($\delta \sim 0.04$). Two series of $Nd_{2-x}Ce_xCuO_4$ crystals were used for our measurements. The first was insulating with a composition of Ce $x = 0.11$ determined by energy dispersive x-ray analysis (EDAX). The second was metallic with $x = 0.14$ and had a superconducting transition temperature of 18–20 K. All measured crystals were reduced at 900°C for 15 h in argon atmosphere. We suppose that the samples were not completely homogeneous because the resistivity of the metallic one was not strictly zero in the superconducting state.

For each material composition we have attached three samples of $1.5 \times 4 \times 0.05$ mm$^2$ with Formvar to gold-plated tungsten wires of 50 $\mu$m diameter. Alignments were achieved within 2 degrees in an orientation suited for measuring 2D-ACAR spectra in the $c$ plane, where the Brillouin zone (BZ) has the largest projection. We thus have [100] and [010] lying along $p_x$ and $p_y$, respectively. 2D-ACAR measurements were performed with the spectrometer described in Ref. 8 using positrons from a $^{22}$Na source of about 20 mCi and a focusing magnetic field of 1.8 T. Data were taken at 10 K in a vacuum of $10^{-6}$ Torr. An acquisition rate of 60 cps was obtained with sample-detector distances of 7.72 m. Total statistics of $2 \times 10^8$ coincidences were obtained for each data set, sufficient to provide a fine resolving power of breaks generated by FS sheets. The 2D-ACAR were accumulated with a bin width of $0.15 \times 0.15$ mrad$^2$, a value smaller than the angular resolution of $0.4 \times 0.5$ mrad$^2$ FWHM (1 mrad = 0.137 a.u.). Data treatment is as usual: correction with the measured angular efficiency function of the spectrometer, smoothing by direct convolution with a square function ($0.75 \times 0.75$ mrad$^2$ in the present case), symmetrization after centering of the 2D-ACAR, extraction of its anisotropic part by subtracting in each point the average value of all data with the same $p$ radius, LCW remapping of the smoothed, and centered 2D-ACAR.

B. Calculations

Through 2D-ACAR, one measures a two-dimensional projection of the two-photon momentum density $\rho^{2\gamma}(p)$, which is discontinuous in correspondence of bands crossing the Fermi level, $E_F$. The latter quantity can be calculated (in the independent particle model, IPM) as

$$\rho^{2\gamma}(p) = \sum_{n,k} \delta(p-k-G) \times \left| \int_{\text{cell}} e^{-i p \cdot r} \psi_n(k)(r) \psi_+(r) \, dr \right|^2,$$

where $\psi_n$ and $\psi_+$ are the (occupied) electron and positron wave functions and where $n$ and $k$ label the band and $k$ point, respectively.

The 2D-ACAR experiments measure the projection $N(p_x, p_y) = \int \rho^{2\gamma}(p) \, dp_x$ of the momentum density over a given plane (which in the present case is chosen to be perpendicular to the $c$ axis of these materials) convoluted by the experimental resolution. The standard Lock, Crisp, and West procedure enhances FS breaks, by coherently superposing the umklapp terms according to

$$\tilde{\rho}^{2\gamma}(k) = \sum_G \rho^{2\gamma}(k + G),$$

where $G$ represents a reciprocal lattice vector and $k$ is now restricted to the first BZ. This procedure is justified when the positron wave function has little influence and when electron-positron correlation effects are small.

When the enhancement factor $\gamma(r_x(r))$ is included in a local density approach, the TPMD is given by$^{26}$

$$\rho^{2\gamma}(p) = \sum_{n,k} \delta(p-k-G) \int_{\text{cell}} dr \exp(-i p \cdot r) \psi_+(r) \psi_n(k)(r) \sqrt{\gamma(r_x(r))},$$

and the zone reduced momentum density can be reduced to$^{22,27}$

$${\tilde{\rho}}^{2\gamma}(k) = \text{const} \sum_G \rho(k + G),$$

$$= \text{const} \int dr \gamma(r) |\psi_+(r)|^2 n(k, r),$$

where $\gamma^{2\gamma}(k)$ and $n(k, r)$ are, respectively, the positron-annihilation rate and the electron density arising from occupied electronic states at $k$. If $\psi_+ = \text{const}$ and $\gamma = 1$, one obtains the electron momentum density (EMD) in the reduced space as in the LCW theorem. The effects of the positron wave function and of the enhancement factor is to modulate the FS structures given by the EMD.
Formula (4) results in significant computational simplification, but to compare theory with extended zone experimental data, formula (3) must be used.

Our calculations have been carried out using both the FLAPW and the LMTO methods within the local density approximation. The FLAPW band-structure calculations for La$_2$-xSr$_x$CuO$_4$ have been performed by Yu et al. in the body-centered tetragonal structure; the details of the calculation are described in Ref. 21. The positron wave function is calculated with a potential equal to the inverted crystal Coulomb potential plus a potential due to electron-positron correlation effects within a LDA scheme as suggested by Boronski and Nieminen. The electron-positron annihilation enhancement was also included; the effects of these corrections will be discussed below. About 650 G vectors were used to fold $\rho^{2p}(p)$. We then integrated along the c-axis direction to obtain $\hat{N}(k_x, k_y) = \int \rho^{2p}(k) \, dk_z$. The contribution of core levels, expected to be rather small, was not included but the outermost La and Nd semicore p electrons were included in the valence bands.

In the LMTO calculations, we performed the self-consistent calculation using 270 k points in the irreducible BZ. Then, the positron wave-function calculation is carried out near the Fermi surface, by using an LMTO basis limited to s and p orbitals only, in order to avoid numerical instabilities. Isotropic core contributions are calculated and included in the ACAR and in the LCW background. Singh and Jarlborg showed how to use the LMTO method to calculate formula (3) and derived an efficient method to correct the overlapping spheres. The small effect of the electron-positron correlation potential was neglected in the LMTO calculations.

The total annihilation rate (i.e., the inverse of the positron lifetime) is obtained by summing over all momenta and is given by

$$ R = \frac{1}{\tau} = 0.05047 \left( \frac{a.u.}{p^8} \right) \int dr|\psi_+(r)|^2 n(r). \quad (5) $$

$R$ is very sensitive to the description of the enhancement factor and for that reason it is a crucial test for the theory. The lifetime calculations have been performed using the LMTO method as in Ref. 31.

III. RESULTS AND DISCUSSION

A. Positron densities

In Fig. 1 we show the positron charge distribution calculated for La$_2$CuO$_4$ [Fig. 1(a)] and Nd$_2$CuO$_4$ [Fig. 1(b)] with inclusion of the electron-positron correlation potential in a (100) plane cutting the Cu-O bonds and in a (110) plane passing through the La(Nd) atoms. The overlap of the ground-state positron wave function with the Cu-O planes is substantial in Nd$_2$CuO$_4$ and non-negligible in La$_2$CuO$_4$, leading to sizable contributions to the momentum density from the corresponding bands. The effect of including correlation is small in both compounds, bringing more positron charge close to the Cu-O planes, and depleting the interstitial regions defined by the La (Nd) ions.

![FIG. 1. Positron density for La$_2$CuO$_4$ (a), and Nd$_2$-xCe$_x$CuO$_4$ (b) in the vertical (100) plane (left frame) and diagonal (110) plane (right frame) as calculated with inclusion of the electron-positron correlation potential (see text). The CuO$_2$ plane is perpendicular to both (100) and (110) planes. Contours are spaced by 0.0005 e$^+$/a.u.$^3$ and grow away from atomic positions.](image)

B. La$_2$-xSr$_x$CuO$_4$

We show in Fig. 2 lines from the calculated 2D-ACAR spectrum of La$_2$-$x$Sr$_x$CuO$_4$ for $x \approx 0.17$ (within a rigid-band model) along the $\Gamma-Z$ (100) and $\Gamma-X$ (110) directions, as well as their difference. These results are obtained with the inclusion of both $e^+ - e^-$ correlation and enhancement. Test calculations have shown a relatively weak dependence of the 2D-ACAR spectra (normalized to equal volumes) upon inclusion of these corrections to IPM (larger changes are instead observed in the LCW folded distribution, as discussed later). The signature of the FS is apparent along the $\Gamma-Z$ direction, but not along $\Gamma-X$. This is a consequence of the symmetry of the Cu-O $dp$ band for $k$ along $\Gamma-X$; in fact, nonvanishing contributions to the LCW only arise from the umklapp terms with $G_x \neq G_y$, which do not contribute to the $N(p_x, p_y)$ lines in Fig. 2. We note that the signature of

![FIG. 2. 2D-ACAR along the $\Gamma-Z$ (solid line) and $\Gamma-X$ (dashed line) directions, as calculated by the FLAPW method for La$_2$-$x$Sr$_x$CuO$_4$ ($x \approx 0.17$). The difference between the $\Gamma-Z$ and the $\Gamma-X$ lines is also shown multiplied by two for clarity reasons. Correlation and enhancement effects have been included.](image)
the FS is only evident in the first BZ. In Fig. 2 we also show the difference between the Γ-Z and Γ-X 2D-ACAR lines. We see a positive region followed, between ≈3 and ≈10 mrad, by a deep negative region. While some of the structures around 3 mrad have a FS related structure, the main origin of this anisotropy can be explained by positron wave-function modulation effects. The results shown in Fig. 2 are in good agreement with the corresponding experimental line difference by Howell et al.23

In order to emphasize the structures related to the FS, we show in Fig. 3 the 2D-ACAR derivatives along the Γ-Z and Γ-X directions. We see clear structures along Γ-Z related to the FS around ≈2.5–4 mrad, but almost no images of these discontinuities in the higher zones.

It is customary to calculate the anisotropy of the 2D-ACAR distribution in the p_x-p_y plane, obtained by subtraction of the cylindrical average of the distribution itself (different definitions of the anisotropy have also been used in the literature). The resulting structures can be a consequence of both FS effects and wave-function modulation effects. In order to distinguish them, we calculated the anisotropy of La_{2-x}Sr_xCuO_4 for two different positions of the Fermi level, corresponding in a rigid-band model to z ≈ 0.17 (shown in Fig. 4), and to a hypothetical system in which the full Cu-O d_{p_z} band has been filled up. In both cases the main structures of the anisotropy are (i) four small maxima along the p_x and p_y directions in the low momentum region (entirely contained in the first BZ) and (ii) four larger maxima along the diagonal directions (including X and equivalent points) centered outside the first BZ. These main structures do not derive from FS effects, which only produce a few modifications, such as the displacement of the crosslike structure in the first BZ and the occurrence of the small plateau along the diagonal directions, just before the large maxima, for a realistic band filling. We notice that since we interpolated N(p_x,p_y) on a relatively spaced mesh, the FS discontinuities, such as those in Fig. 2, are smoothed out. The main structures found in our calculations are in overall agreement with the recent experimental results of Howell et al.23

We applied the LCW folding procedure22 to our calculated momentum density. Figure 5 shows the LCW distribution without (left) and with (right) the experimental (≈ 0.5 mrad) smoothing, for a Fermi-level position corresponding, in a rigid-band scheme, to z = 0.17. In order to show the effect of the electron-positron interaction, we show in Fig. 5 the results obtained with the FLAPW method in the independent particle model [Figs. 5(a) and 5(b)] (IPM) and with the inclusion of correlation and enhancement (CE)26,28 [Figs. 5(c) and 5(d)], together with the LMTO results including the enhancement effects. Although the general shape of the calculated LCW is similar in the two cases, the inclusion of the above corrections produces significant differences. At the Γ point we always have a relative minimum, but the depth of this minimum is significantly larger when correlation and enhancement (CE) effects are taken into account. The FS shows up clearly in the LCW plots, producing a low density region around X. The value of the discontinuity in ρ_{2D}(k) at the FS is larger along Γ-Z than Γ-X, 2 and 1.3 %, respectively, relative to the value at the Γ point. This is probably due to the symmetry arguments discussed in connection with N(p_x,p_y). The k_z dispersion of the FS smears the discontinuity out (see Xu et al.22), especially close to the Γ-Z line.

The relative discontinuities are almost the same in the IPM calculation and after the inclusion of CE. However, the strong variations observed in the LCW distribution away from Fermi-surface breaks (and ascribed to positron wave-function effects), are larger when we include the CE effects. As a consequence, the FS shows up more clearly in the IPM calculation. The importance of the FS break is large enough to be visible in a 2D-ACAR experiment, even when considering the experimental resolution.

The agreement between the FLAPW and LMTO results shown in Figs. 5(e) and 5(f) appears to be reasonable, and the amplitude of Fermi breaks, relative to the Γ value, is similar in the two calculations. The value of having results from two completely different methods is to control the sensitivity of different approximations. It allows us to conclude that the effect of using spherical

FIG. 3. Calculated derivatives (solid line) of the 2D-ACAR spectra of Fig. 2 for La_{2-x}Sr_xCuO_4 (z ≈ 0.17) along the Γ-Z (solid line) and Γ-X (dashed line) directions.
MT potentials in the LMTO calculations does not affect very much the TPMD results.

It is known that La$_{2-z}$Sr$_z$CuO$_4$ has a little orthorhombic distortion in the low temperature phase, where measurements were performed. Also, the samples measured by Howell et al.\textsuperscript{23} were twinned. The tetragonal-to-orthorhombic distortion can be viewed at the simplest level as an approximate \( \sqrt{2} \times \sqrt{2} \) superlattice formation, in which \( a' \approx b' \approx \sqrt{2}a \) and \( c' \approx c \). Howell et al.\textsuperscript{23} have reduced the data into a twinned orthorhombic BZ and found a break near the zone boundary suggestive of a single FS. Since the electronic-structure calculations were performed in the tetragonal structure, we folded point \( X \) on point \( \Gamma \) in order to simulate the orthorhombic BZ. The corresponding results, shown in Fig. 6, are quite consistent with the experiments,\textsuperscript{23} showing a minimum of intensity at \( \Gamma/X \) and a shallow, almost linear groove due to the Fermi surface.

The total annihilation rate (the inverse of the positron lifetime) is very sensitive to the enhancement factor and is a crucial test for the theory.\textsuperscript{31} In the IPM, \( \tau = 541 \) ps while including the enhancement \( \tau = 167 \) ps, which compares rather well with the experimental value of about 180 ps.\textsuperscript{33}

C. Nd$_{2-z}$Ce$_z$CuO$_4$

In Fig. 7 we show the experimental and calculated 2D-ACAR of Nd$_{2-z}$Ce$_z$CuO$_4$ (\( x = 0.16 \) in a rigid-band scheme) along the \( \Gamma-X \) and \( \Gamma-Z \) directions. The agreement between measured and calculated results is rather good; more in detail, the FLAPW calculations give a profile slightly broader than the experimental one, while the opposite tendency is observed in the LMTO calculations. This difference might be due to the inclusion of the core (with use of enhancement corrections) in the latter results.

The anisotropic part is shown in Fig. 8. With respect to the La compound case, one can notice more structures which are more extended in \( p \) space. However, the amplitude of the anisotropy is much stronger in the La compound for low momentum values. Some of the important structures appear to be turned 45 degrees compared to
the La compound. This is probably one effect of the different structural positions of the two interplane oxygens. The measured anisotropies in the (doped) Nd compound are compatible with the calculations, but their amplitudes are smaller (see Fig. 7). This gives the impression that the expected signal is present, but it is drowned by some other, stronger signal, which has no particular anisotropy.

When the LCW folding is applied, one finds good agreement between FLAPW and LMTO in predicting important Fermi breaks (Fig. 8). This is due to the fact that the calculations find a large overlap in the Cu-O planes. The amplitude of the discontinuities is \( \approx 5 \) and \( \approx 4\% \) in the FLAPW and in the LMTO calculations, respectively. The positron wave-function effects are much less important than in \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \), which also contributes to make FS signals much more clear in the present case. Despite these promising theoretical findings, no Fermi surface can be identified in the experimental LCW spectrum. An explanation for this would be that a possible impurity phase masks the FS signal. The lifetime calculations also indicate the presence of defects or vacancies with positron trapping properties. A conclusion from all these results is that the measured Nd compound still suffers from impurity phases. Another reason for the lack of FS signal in the experimental LCW could be the localization of positrons in shallow traps. But this hypothesis is ruled out by the lack of temperature dependence of the measured lifetimes, which is of course an important quantity to look at.

Lifetime measurements performed in \( \text{Nd}_2\text{CuO}_4 \) single crystals show one component increasing from 204 to 207...
ps with temperature between 100 and 300 K. Under 100 K, it decreases down to 200 ps at low temperature, and a second component of 320 ps appears that reaches 5% intensity. In the superconducting \( \text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4-\delta \) compound, the first lifetime component is identical to the insulating case. However, the second component is larger (440 ps) and appears below 140 K with an intensity between 2.1 and 2.8%. The main component is in good agreement with the value of 200 ps measured in the superconductor by Howell et al. The calculated lifetime using enhancement amounts to 145 ps (the IPM calculation gives 420 ps), and does not agree with the previous experimental values. This might indicate that in Nd compounds the problem of defects (positron traps) is still important.

IV. CONCLUSION

We have calculated positron characteristics of the two high-\( T_c \) superconducting compounds \( \text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4-\delta \) and \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \). The positron distributions in real space, evaluated using the FLAPW method, show that positrons are more homogeneously distributed in \( \text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4-\delta \) than in other oxide compounds like \( \text{YBa}_2\text{Cu}_3\text{O}_{7-\delta} \) and \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8 \). This makes \( \text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4-\delta \) an attractive material for the study of Fermi surface by 2D-ACAR. One expects that the CuO\(_2\) Fermi surface may be observed experimentally, while in \( \text{YBa}_2\text{Cu}_3\text{O}_{7-\delta} \) the repulsion of positrons from CuO\(_2\) planes makes it difficult to see the related Fermi surface sheets.

Two-photon momentum distributions, 2D-ACAR distributions, and their anisotropies have been calculated by both the FLAPW and LMTO methods. In general, the agreement between the two calculations is good. Some discrepancies are noticed which may be related to differences in the assumed electronic configurations. From the total annihilation rate we have evaluated the positron lifetime by the LMTO method. It is very important to use an adequate description of the enhancement and correlations to obtain a precise value of lifetime.

The LCW folding procedure has been applied to calculated 2D-ACAR in order to look for the manifestation of the Fermi surface and to study the deformations induced by nonconstant positron wave functions and correlation effects. We find a clear and intense Fermi surface signal in \( \text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4-\delta \). It should be clearly observed experimentally. In \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) we have simulated the twinning induced in samples by the tetragonal to orthorhombic distortion. We show that the Fermi surface gives a weak break near the edge of the new Brillouin zone. Such breaks were recently experimentally observed by Howell et al.

We also report 2D-ACAR measurements on both superconducting and insulating \( \text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4-\delta \) single crystals. Comparison with FLAPW and LMTO calculations is presented. While the general shapes of calculated and experimental 2D-ACAR agree, it is not possible to detect any signal related to the Fermi surface in the measured LCW distributions. This may be due to a large trapping by either structural defects or shallow traps (the measurements have been performed at low temperature) or impurity phase. In fact, the experimental lifetimes are larger than the calculated ones, suggesting a significant trapping in our samples. Another explanation may be that there is no Fermi surface in high-\( T_c \) superconducting compounds as it is suggested by some theoretical approaches. We are not in favor of this explanation for two reasons: Fermi surfaces have been observed in other high-\( T_c \) compounds and we know that we are very dependent on the quality of the samples for our measurements.

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4For a general overview see, for instance, the Proceedings of the Workshop on the Ferromagnetism of High-T$_c$ Superconductors, Argonne National Laboratory [J. Phys. Chem. Solids 52 (1991)].


FIG. 4. 2D-ACAR anisotropy of \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) (calculated by the FLAPW method) obtained by subtracting from the 2D-ACAR its spherical average. Correlation (Ref. 28) and enhancement (Ref. 26) effects have been included. a.u. are used in (b); the range considered goes from \(-15\) to \(15\) mrad. Shaded regions are negative.
FIG. 5. Calculated LCW distribution of La$_{2-x}$Sr$_x$CuO$_4$ ($x \approx 0.17$) in the tetragonal Brillouin zone before [(a), (c), and (e)] and after [(b), (d), and (f)] convolution with the experimental resolution ($\approx 0.5$ mrad); (a) and (b) are obtained in the IPM model with the FLAPW method, while (c), (d), (e), and (f) include correlation and enhancement effects and are calculated with the FLAPW [(c) and (d)] and LMTO methods [(e) and (f)]. The LMTO results are within IPM and with enhancement effects, respectively.
FIG. 6. LCW distribution of La$_{2-x}$Sr$_x$CuO$_4$ ($x \approx 0.17$) after folding in the orthorhombic Brillouin zone and twinning, as explained in the text. Both the corners and the midpoint of the figure are a superposition of the $\Gamma$ and $X$ points of the tetragonal BZ. Calculations by the FLAPW (a) and LMTO (b) methods.
FIG. 8. 2D-ACAR anisotropy of Nd$_{2-x}$Ce$_x$CuO$_4$ (calculated by the LMTO method) obtained by subtracting from the 2D-ACAR its spherical average. Enhancement effects have been included. a.u. are used in (b); the range considered goes from $-15$ to $15$ mrad.
FIG. 9. LCW distribution for Nd$_{2-x}$Ce$_x$CuO$_4$ as calculated by the FLAPW (a) and LMTO (b) methods.