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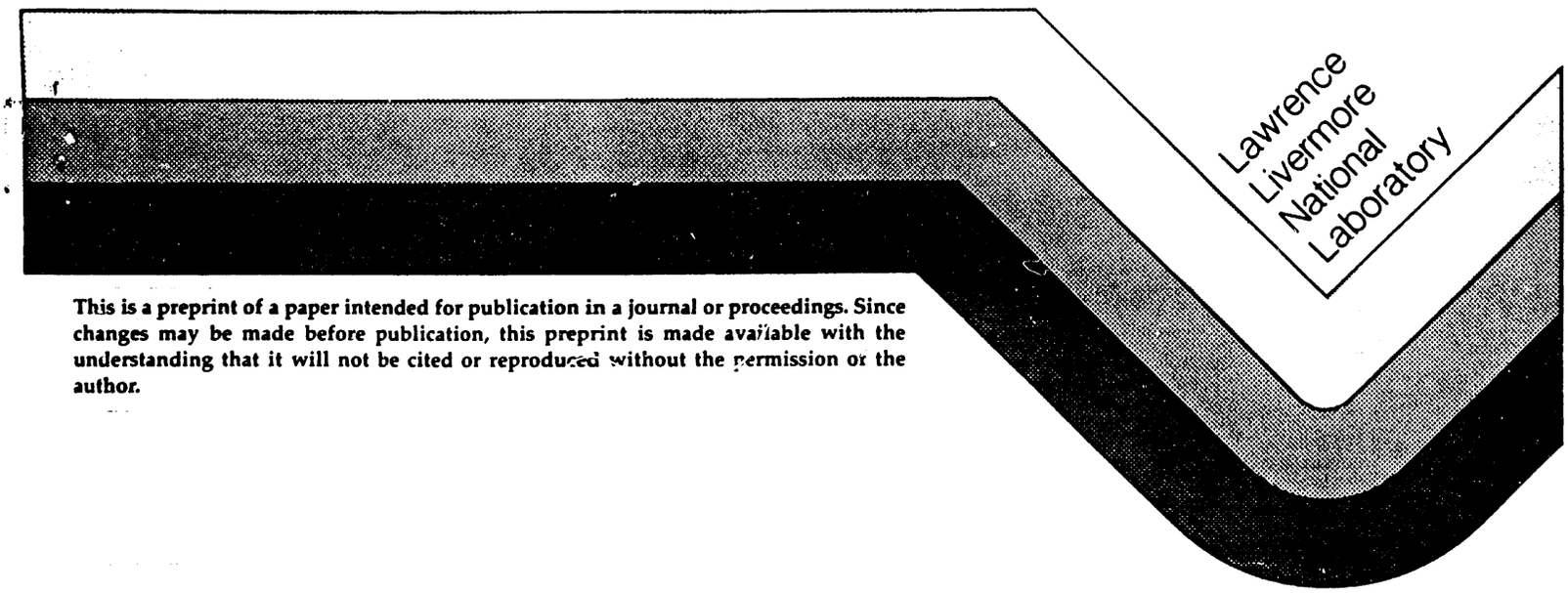

DISCLAIMER

DIRECT, EXPERIMENTAL EVIDENCE OF THE FERMI SURFACE IN $YBa_2Cu_3O_{7-x}$

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INTRODUCTION

We report new measurements of the electron-positron momentum spectra of $YBa_2Cu_3O_{7-x}$ performed with ultra-high statistical precision. These data differ from previous results in two significant respects: They show the D_2 symmetry appropriate for untwinned crystals and, more importantly, they show unmistakable, statistically significant, discontinuities that are evidence of a major Fermi surface section.

These results provide a partial answer to a question of special significance to the study of high temperature superconductors i.e. the distribution of the electrons in the material, the electronic structure. Special consideration has been given both experimentally and theoretically to the existence and shape of a Fermi surface in the materials and to the superconducting gap. There are only three experimental techniques that can provide details of the electronic structure at useful resolutions. They are angular correlation of positron annihilation radiation, ACAR, angle resolved photo emission, PE, and de Haas van Alphen measurements.

Positron ACAR measurements occupy a spot between angle resolved photo emission measurements and de Haas van Alphen measurements. The first, PE, can in one spectrum supply the energy spectrum for some selected momentum in the Brillion zone. This momentum selection is achieved by limiting the angular acceptance in the electron detector. In order to map the entire electron momentum distribution to see the full shape of the Fermi surface the measurement must be performed for each momentum bin. This is rarely done. Best photo emission angular acceptances are of the order of 2 degrees and the full momentum of the Brillion zone depends on photon energy but is typically 18 degrees[1,2]. This results in a momentum resolution of about 11 % of the reciprocal lattice vector and is the limit on which the momentum position of bands crossing the Fermi surface can be determined in photo emission. Photo emission is also performed on cleaved crystals at low temperatures and thus may not be determining normal state properties and is vulnerable to effects of surface contamination.

De Haas van Alphen measurements on the other hand measure the area enclosed by the Fermi surface in a plane defined by an external magnetic field. These are measurements of bulk magnetic properties in the normal state. However at present only orientated polycrystalline samples have been measured by this technique[3].

Positron ACAR measurements determine only the momentum of the electron in each annihilation event. Therefore there is no distinction of between electrons in bound and unbound states at the same momentum. Fortunately the Fermi surface is defined by limit in the momentum for occupied states set and can be easily seen as a sharp break or discontinuity in the measured distributions. More importantly the ACAR measurement maps out the entire momentum space even into higher order zones in a single experiment. Thus the continuous shape of a Fermi surface is determined in the same measurement and broadening of the Fermi surface can be detected by the sharpness of the discontinuity. These measurements have been very successful in studying Fermi surface driven order-disorder transitions in binary alloys where the shape and broadening of the Fermi surface are central issues in the physics of the transitions. Since the positron is a bulk probe there is no vulnerability to surface effects in the ACAR measurement. Also the sample temperature of the positron measurement can be set at any temperature so that the measurements can clearly be those of a normal state property.

Predictions of the existence of a continuously connected Fermi surface are not specific to all proposed theories for describing superconducting oxides. Consequently the analysis of the positron data for the existence of a Fermi surface must first be done independently of the predictions of any particular theory. This restriction presents a special challenge to the positron technique and requires levels of precision in the measurement beyond those of any previous experiments on elemental metals or alloys.

There have been several attempts to clearly demonstrate a Fermi surface using positrons[4-6]. Unfortunately the interpretation of earlier data on YBCO was complicated by low statistical precision in the earliest measurements and the use of highly twinned crystals throughout. Those significant features in earlier data sets that were statistically reproducible were in reasonable agreement with features expected from the effects of distortion of the positron and electron wave functions by the non-uniform charge densities in the oxide lattice[7].

EXPERIMENT

We have completed ACAR measurements on twin-free crystals of YBCO to ultra-high levels of statistical precision. The measurements were performed at the University of Texas at Arlington and the data were collected on their spectrometer. Untwinned YBCO samples were prepared by the LLNL program at the University of California at Davis.

The YBCO measurement was performed on a matrix of crystals that were made twin-free by annealing under compression along the a direction. This resulted in crystals that were twin-free over 90% of their surface. Measurements of the DC magnetic susceptibility showed that all of the crystals had an onset of superconductivity above 92 K. Two of the crystals had transitions significantly broader than the rest with mid points at 85 K. These data indicate that the level of oxygenation was high in all but isolated parts of two samples.

The samples were mounted in a matrix of six crystals, attached by epoxy to a web of 25 micron wires. The crystals were brought to a common alignment within 0.5 degrees by a process of repeated attachment, guided by Laue X-ray photography. This matrix was then mounted so that the c axis of the samples was along the line connecting the detector centers and the a and b sample axes were along the x and y data axes respectively. Data were collected in a 256 X 256 matrix with .143 mrad wide bins. The data were stored every 2 x 10^7 counts and after individual analysis to assure stability of the detection system were later summed into full distributions. Two distributions of 2.5 10^8 counts were obtained with the sample-detector alignment rotated by 90°between the two.

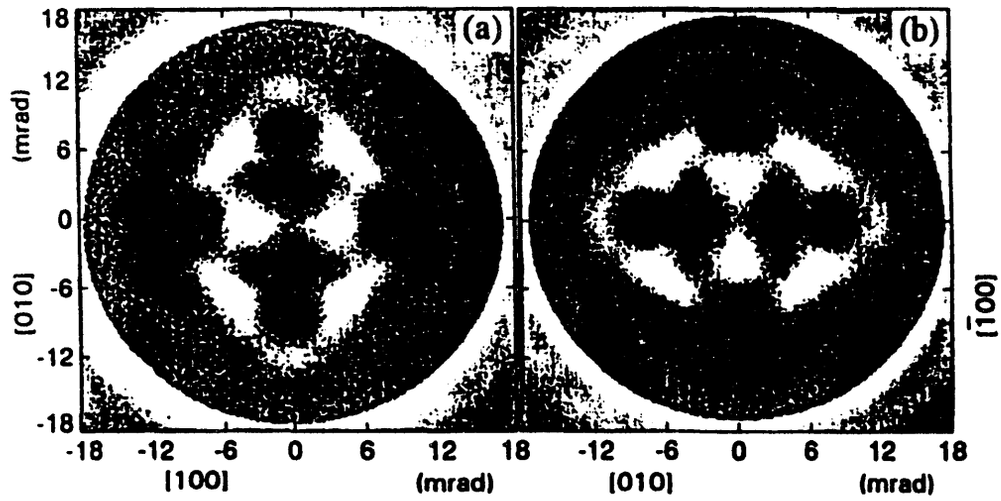

Figure 1. Residual anisotropy distributions for the two subsets of the data. The sample-spectrometer orientation has been rotated by 90° for data set b.

These data were then corrected for the efficiency function of the detector and the isotropic portion of the spectrum was subtracted producing anisotropic residuals as seen in figure 1 a and b. The data in figure 1 show a clear D2 symmetry in alignment with the crystalline axis as would be expected from contributions related to the Cu-O chains in untwinned samples and are identical within the statistics of the measurement. The data distributions were then rotated to the same orientation and summed to produce a single distribution containing 5 10^8 counts. Also since the underlying symmetry of the data are apparent it is permissible to bring the four equivalent quadrants into one. The anisotropic residual of this combined distribution is seen in figure 2 a and b in contour and isotropic views.

DISCUSSION

The data as displayed have several remarkable features. There are four-fold symmetric areas of positive or negative excursions that are consistent with the features observed in twinned samples and can be attributed to wave function effects. These effects are due in part to the non-uniform spatial distribution of the positron. Positron densities have been calculated to be highest in the region surrounding the CuO chains, high in the region of the CuO planes and low everywhere else. This has been verified in measurements on twinned crystals where the wavefunction effects were the statistically significant feature.

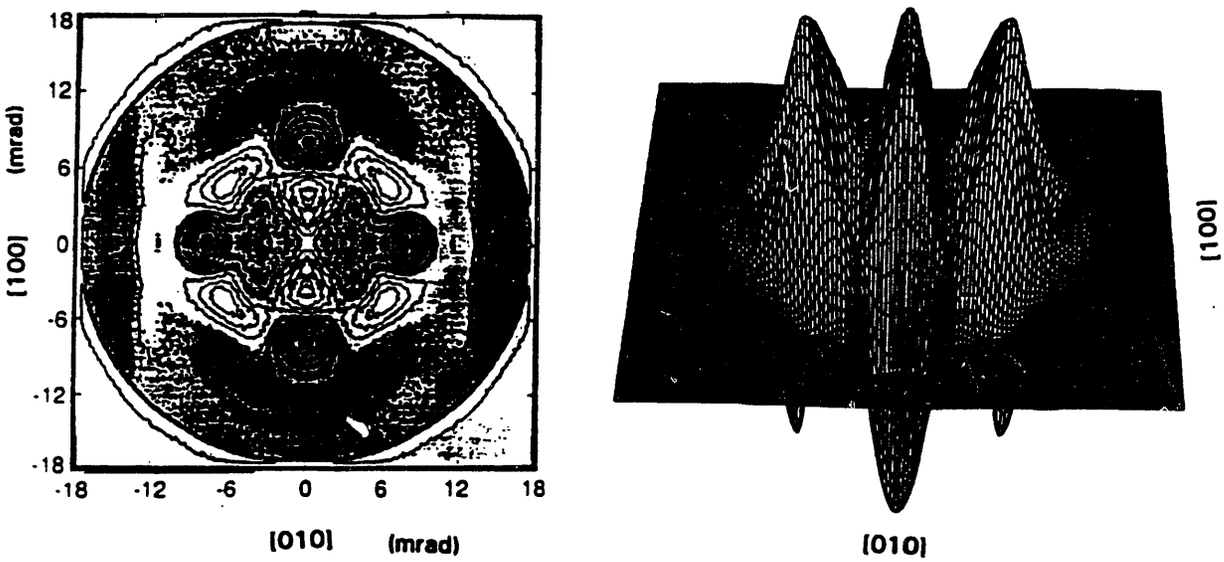

Figure 2. Residual anisotropy of the full data set shown in contour and isometric displays. The sharp changes in the data having two fold symmetry are continuous along the chains, vertical direction, for both low and high momentum values.

New features in the present data are the line discontinutites running parallel to the gamma-x direction seen both in the central, p=0, zone and at positions symmetrically placed at about +/- 4 pi/b, roughly 13 mrad from the distribution center. There is also evidence of a ridge at +/- 2 pi/b but it is obscured in both data displays by the peaks resulting from the wavefunction effects. The breaks at high momentum are significant at 10 standard deviations in the data in figure 2. They stand as convincing evidence of a Fermi surface at that momentum.

The ACAR distributions are measured in real momentum space and consequently are an extended pattern of the electronic distribution in the Brillion zone. Because of this any demonstration of the Fermi surface must be evident at momenta greater than the reciprocal lattice momentum. Observation of the breaks seen at high momenta in figure 2 is sufficient to justify further data manipulation. It is permissible in cases where there is a Fermi surface to sum all of the data back into a single zone using the LCW theorem.

Since we clearly see breaks in the data at high momentum we have applied the LCW operation to our data and the results are seen in figure 3. The Fermi surface sheets with D2 symmetry seen at momenta inside the central zone are now reinforced by the data from other zones and are clearly seen as breaks centered on gamma and running in the gamma-x direction.

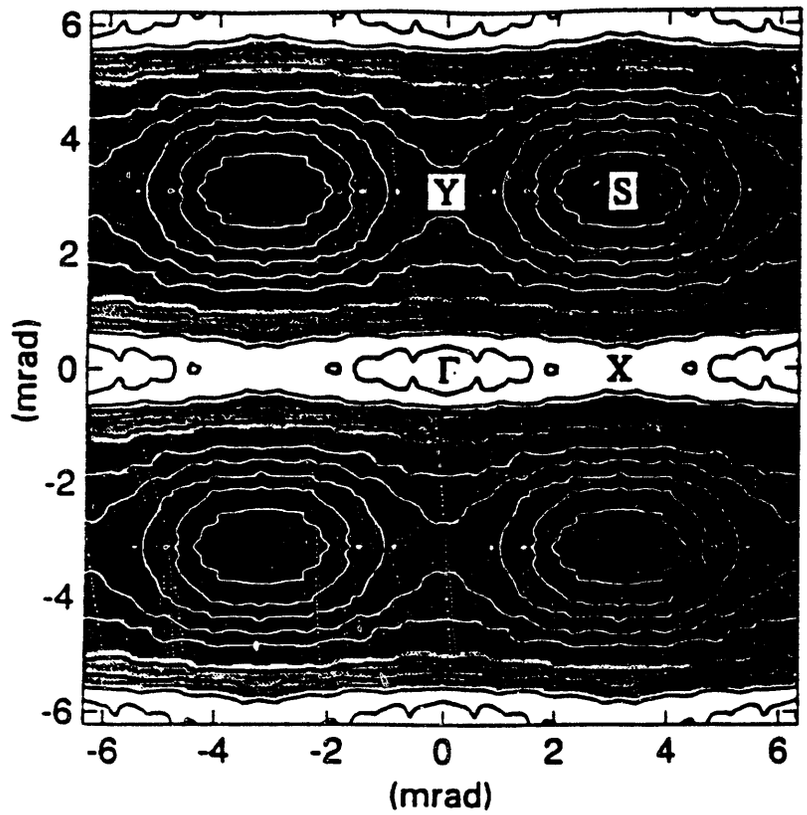

Figure 3. The full ACAR distribution reduced into a single zone using the LCW theorem.

The position of the experimentally observed Fermi surface is in good agreement with that expected from band theory[8-11]. Both real momentum calculations[10] , single zone calculations[11] and our own LMTO results, shown in figure 4 predict the Fermi surface sheet that we see from the crossing of a band associated with the Cu-O chains. Fermi surface crossings in both the gamma and z plane are shown. There is even agreement between the data and the shape of the calculated Fermi surface through the zone. Theory predicts that there are other Fermi surface features in the form of closed loops centered on the S point and associated with either CuO plane bands or hybrid states. We have no independent confirmation of these features in our data. Although there is a general depression at the S point, there are no sharp discontinutiies and it is known that a depression at S can be the result of wave function effects. Also these same wave function effects tend to diminish the size of any Fermi surface breaks associated with the CuO planes due to the propensity of the positron to overlap on the chains.

To obtain an unambiguous answer to the question of a Fermi surface on the CuO planes requires either much higher statistics or a different system. We are performing a similar experiment on single crystals of $La_{1.874}Sr_{.126}CuO_4$ with a sharp superconducting transition at 30 K using the LLNL spectrometer At the time of this report the data lack the statistical precision of the YBCO experiment just described.

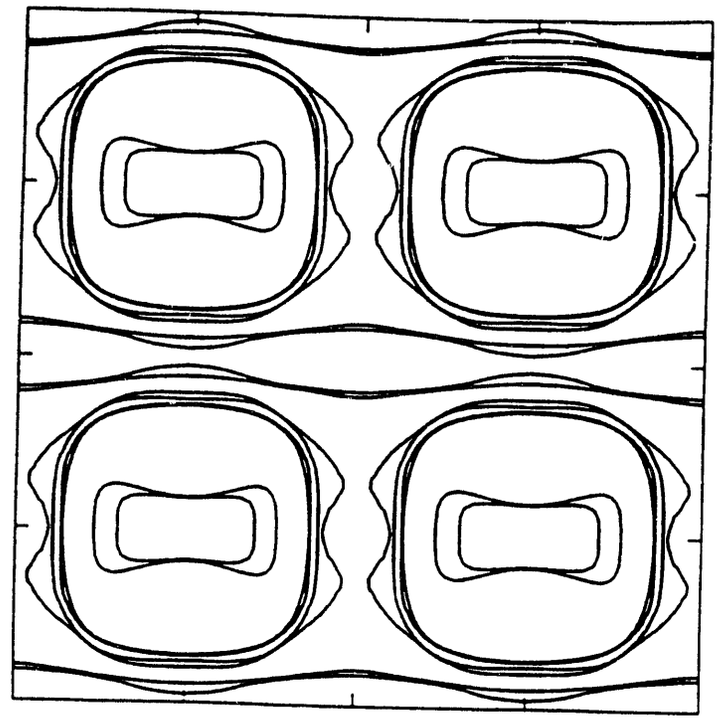

Figure 4. LMTO calculations of the Fermi surface crossings in both the gamma and z planes. The repeated zones are shown in the same format as the data of figure 3.

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