FINAL REPORT

POCSITRON STUDIES OF DEFECTED METALS, METALLIC SURFACES

DOE Contract DE-FG02-85ER45223 (7/1/85 - 12/1/91)

Prepared by: A. Bansil, p.I.

Physics Department

Northeastern University

Boston MA 02115

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I. Abstract

The final report for the DOE project DE-FG02-85ER45223 is presented. Specific problems proposed under this project included the treatment of electronic structure and momentum density in various disordered and defected systems. Since 1987, when the new high-temperature superconductors were discovered, the project focused extensively on questions concerning the electronic structure and Fermiology of high- T_c superconductors, in particular, (i) momentum density and positron experiments, (ii) angle-resolved photoemission intensities, (iii) effects of disorder and substitutions in the high- T_c 's. The specific progress made in each of these problems is summarized.

II. Project Overview

This is the final report for the DOE project DE-FG02-85ER45223, "Positron Studies of Defected Metals, Metallic Surfaces", for the period 7/1/85 through 12/1/91, spanning about 6 years. The principal Investigator for this project was Arun Bansil, Professor of Physics, Northeastern University.

The broad scope of the project encompassed the development of first principles realistic methods for investigating the electronic structure and spectroscopy of ordered as well as disordered materials. A focused effort on the Fermiology of the high- T_c superconductors, as an example of complex unit cell materials, was planned. The specific spectroscopies that were intended to be investigated were, the positron annihilation (two-dimensional correlation, 2D-ACAR), and the angle-resolved photoemission (ARPES) experiments, in addition to the development of the first-principles KKR-CPA approach to treat effects of substitutions and oxygen-vacancy disorder in materials of the complexity of the high- T_c 's. The broad as well as the specific goals of the program were realized exceptionally well. While the supporting technical details are given in Sections III and V below, here we outline some of the non-technical and general aspects.

A vigorous two-way interaction between the theory and experiment was built deliberately into our program and has proven most effective. This may be seen by the example of the success of our studies of positron annihilation 2D-ACAR spectra of binary alloys and $YBa_2Cu_3O_x$, and the angle-resolved photoemission spectra of Y123-(001) surface. In each case fundamental new insights into the nature of the spectra and the Fermiology of the materials has been obtained. It will be seen that many of our publications involve joint theory-experiment papers.

Our research program attracted many graduate and post-graduate students during the length of the project (e.g. S. N. Khanna, A. K. Ibrahim, R. S. Rao, R. Prasad, W. Dlugosz, R. Pankaluoto, A. S. Serageldin, E. Arola, S. Kaprzyk, M. Lindroos, among others). Effective collaborations at a national and international level were forged, including very extensive interactions with the Argonne National Laboratory (Campuzano, Veal, Smedskjaer, Liu, and students), Tampere University of Technology (Finland), The Netherlands Energy Research Foundation (Holland), Indian Institute of Technology, Kanpur, and Poland, among others. Many of the younger researchers have found a longer range bond with the present problems and would likely continue to contribute to these areas for many years to come.

Our results have been published extensively in the open literature, and reported in numerous national and international conferences and meetings, resulting in 33 publications, some 16 major invited talks at meetings, and many contributed papers at some 12 national and international meetings, and 3 Ph. D. thesis under the direct supervision of the p.I.

It may be noted that the p.I. was accorded several honors during the period of this grant. These are, Honorary Professor in Solid State Theory at Tampere University of Technology, Tampere, Finland (1989-). Scientific Consultant, Netherlands Energy Research Foundation, Petten, The Netherlands (1987-). Member, Commission on Charge, Spin, and Momentum Densities of I. U. Cryst.

(1992-). Resident Associate, Argonne National Laboratory (1991-).

The p.I has been involved in the organizational activities at a national and international level. Current and recent activities include: Conference Chairman, First Workshop on Fermiology of High- T_c Superconductors, Argonne National Lab., March 1991; Conference Chairman (US side), US/Japan Seminar on Electronic Structure and Fermiology of High- T_c Superconductors, Sendai, Japan, July, 1992; Co-Chair, Spectroscopies of Novel Materials, Santa Fe, March 1993; Member, International Committee, Workshop on Electronic Structure of Materials, Madras, India, Feb. 1992. Member, Program Committee, 10th International Positron Annihilation Conference, Beijing, 1994.

The completion of the present project has opened up many new directions of research. These include studies of the spectral intensities in positron annihilation, and angle-resolved photoemission spectroscopies in high- T_c superconductors and other more complex materials, such as the organic superconductors and fullerenes. Many questions concerning the changes in the Fermiology of materials around the metal/insulator transition need to be explored. Among other topics, we may note the development of the high-resolution Compton scattering technique as a probe of the Fermiology of materials, as well as wider application of the alloy theory approach to investigate the electronic structure and properties of substituted phases of the high- T_c 's. Some of these areas are being explored currently by the p.I. and others.

III. Technical Summary of Results, Motivation

While a great deal of work was devoted to the electronic structure and spectroscopy of the high- T_c 's, as seen from Sections IIIA through IIIC below, we also made very substantial progress on many other problems as summarized in Sections IIID - IIJ below.

IIIA. Momentum Densities in High- T_c Superconductors

The main purpose of this project was to compute the momentum density of the electron-positron pair, $\rho_{2\gamma}(\mathbf{p})$; in a two-dimensional positron experiment where one measure the angular correlation of the 2γ annihilation radiation, the observed intensity for momentum $\mathbf{p}$ is related to a suitable two-dimensional projection of $\rho_{2\gamma}(\mathbf{p})$. For studying the Fermiology of layered compounds much of the early attention was focused on the c-projection, although the a-axis and b-axis projected momentum density is of intrinsic interest also. One main advantage of the positron spectroscopy is that this technique does not require long mean free paths of the electrons, compared to the methods like the de Haas van Alphen. On the other hand, the positron annihilates with all the electrons in the solid, and therefore the Fermi surface signal is typically only a few percent of the total signal. The positron spectroscopy has proven itself as a valuable probe of the Fermi surface and the momentum density of the electron gas in materials more generally, including more recently the high- T_c 's. The crucial importance of parallel theoretical model computations for interpreting the experiments is also well-recognized.

The aims of the project were eminently realized. A first principles methodology, based on the Korringa-Kohn-Rostoker (KKR) band structure approach, for calculating momentum density and its 2-dimensional integrals was formulated and implemented for the first time in complex ordered crystals. The approach was applied to analyze the positron annihilation two-dimensional angular correlation (2D-ACAR) experiments in the 90K high- T_c superconductor $YBa_2Cu_3O_7$. By folding the local density band theory (LDA) based electron-positron momentum density in the first Brillouin zone (the LCW-folding), we find for the first time that clear signatures from all the Fermi surface sheets can be obtained in $YBa_2Cu_3O_7$, including in particular the Cu-O plane sheets. Our computations also show for the first time that insofar as the analysis of the Fermi surfaces via folded spectra is concerned, the intrinsic positronic effects in the 123-compound are quite small. These results are of fundamental importance in establishing the usefulness of the conventional LDA band theory for describing the ground state

of the 123-compound.

These results have had a very large impact on the field. Specifically, new positron annihilation (2D-ACAR) data from nearly untwinned single crystals of the 123 was compared after a proper background subtraction with our band theory computations and excellent accord has been obtained for various sections through the 2D-ACAR distribution, and also for the anisotropies in the form of difference sections between various pairs of high-symmetry directions. We emphasize that the comparisons were on an *absolute* scale and showed for the first time agreement in not only the shape but also the absolute size of the undulations in the anisotropic spectra. The crucial role of the theory in interpreting the spectra is clear. In particular, the characteristic signatures of the electron ridge Fermi surface sheets have been established in the measurements clearly. The presence of the pillbox Fermi surface is also indicated. These results are important, since the ridge states have not been observed directly by any other spectroscopy to date.

IIIB. Angle-Resolved Photoemission Spectra in High- T_c 's

In an angle-resolved photoemission experiment, one shines light of a given frequency (and preferably polarization) on the surface of an oriented single crystal, and measures the intensity of the photoemitted electrons of a given energy and momentum. In principle, angle-resolved photoemission is a powerful spectroscopy capable of giving spectral peaks corresponding to *individual* Bloch states of a given crystal momentum $\mathbf{k}$, as shown by numerous studies of simple metals. The technique is however surface sensitive because the photoelectrons possess a mean free path of typically a few interatomic layers for the ultraviolet photon energies typically employed in the experiment. The first photoemission experiments on Y-123 were not successful due to oxygen loss from the surface, but these experimental difficulties have now been overcome by cleaving Y-123 samples *in situ*, and high quality data is available. The value of parallel theoretical model

computations for interpreting the complex photoemission spectra has been well recognized even in simpler materials.

These considerations provide a strong motivation for obtaining band theory predictions of the spectral intensities in the high- T_c 's. Such theoretical computations are expected to provide unique information concerning the signatures and observability of the specific electronic states in the photoemission spectra. The theory-experiment comparisons of this type at the spectral level constitute a more discriminating meeting point between theory and experiment than a comparison of the positions of bands alone. Such comparisons help settle controversies concerning the interpretation of various features, and thus help establish the extent to which the conventional band theory picture can be used to describe the normal state of the high- T_c 's.

Under this project we have completed the development of the methodology and computer codes for first principles computation of the angle-resolved spectra in complex crystal structures, together with extensive computations on the (001)-surface of Y-123. We note that the previous photoemission codes were able to treat only a maximum of 2 atoms per layer unit cell, while in the 123-compound, we require 3 atoms in the layer unit cell for the (001)-surface and 9 basis atoms for the (100)-surface. Furthermore, the layers in the high- T_c compounds are 'buckled', i.e., they show small deviations from perfect flatness, which significantly complicates the computations. Additionally, since heavy atoms are involved in most high- T_c materials, the treatment must at least be semi-relativistic.

We have used the 'one step' approach for calculating the angle-resolved photoemission spectra. In this approach, the photoemission process is treated as a single quantum mechanical event, and the artificial distinctions between the processes of excitation, transport, and transmission of the electron through the surface barrier invoked in the earlier 'three-step' type models are removed. Specifically we have developed and extensively tested a semi-relativistic 'one-step' photoemission code, TUTNU, capable of treating essentially an arbitrary number of

atoms in the layer unit cell, including the buckling of the layers.

One important result of the project was the demonstration for the first time that the shape and polarization dependence of the spectral feature associated with the CuO_2 planes predicted by the conventional band theory framework is in remarkable agreement with the angle-resolved photoemission measurements from the (001)-Y123 surface. This result constitutes a discriminating test of the underlying band theory based wavefunctions implicit in the computations. A surprising finding of the study was that the ARPES spectra from Y123 are well described by a unique surface termination, i.e., the BaO layer in the top is followed by the CuO_2 plane layers. The effects of different surface terminations on the ARPES spectra from the Y123-(001) surface were extensively delineated.

IIIC. First Principles Treatment of Disorder Effects in High- T_c 's

The binary substitutionally disordered alloys, in which a lattice is occupied randomly by two different chemical species, the CuZn solid solutions being an ancient example, are well-known materials. The high- T_c 's display wide variations in properties, including the superconducting transition temperatures, with various substitutions, and with oxygen concentration which can be varied more or less continuously over wide ranges. The theory of ordered phases is not suited for discussing the electronic structure of the disordered phases. In connection with the binary disorderd phases, during the 70's and the 80's a first-principles theory, the so-called KKR-CPA was developed, and has proven its value as the modern 'band theory' of disorderd alloys; here KKR refers to the Korringa-Kohn-Rostoker band structure scheme, and CPA to the coherent-potential-approximation, which is a scheme for treating the disorder effects, and amounts to replacing the disordered system by an ordered one of effective 'CPA-atoms'. Oxygen non-stoichiometry may be modeled by considering the oxygen sublattice to be a 'disordered alloy' of oxygen and vacancy 'atoms'; such a description has been used successfully for the transition metal hydrides. Extensive experience with binary alloys shows clearly

the need for a first principles framework if one is to obtain a realistic description of the electronic structure. The need for developing a similar KKR-CPA type parameter free description in the high- T_c 's is thus clear; with many atoms per unit cell, it will be very difficult to make any serious theoretical predictions concerning the electronic structure without a first-principles basis.

We emphasize that a brute force attempt to treat systems of present complexity using the KKR-CPA methodology commonly used for the binary alloys will rapidly become unfeasible due to computational demands. In order to make a serious headway in this connection, we have developed and implemented a linear tetrahedron type $\vec{k}$ -space integration method for disordered muffin-tin systems. Our approach yields orders of magnitude gains in efficiency and also allows us to treat for the first time the limiting cases of an ordered compound and a single impurity within the KKR-CPA framework in a unified manner.

We have studied extensively the electronic structure of the simple cubic perovskites, $Ba_xK_{1-x}BiO_3$ (BKB) and $BaPb_{1-x}Bi_xO_3$ (BPB). Our computations involve no free parameters and are fully charge as well as spin (if needed) self-consistent and include semi-relativistic corrections. We note that selfconsistent first principles treatment of electronic structure and properties of disorder effects in materials with complexity of crystal structures exhibited by the high- T_c 's has so far not been obtained by any other group.

A brief summary of the results for BKB and BPB is as follows. Electronic structures of $Ba_xK_{1-x}BiO_3$ and $BaPb_{1-x}Bi_xO_3$ were computed selfconsistently using the semi-relativistic KKR-CPA for $x=0.1, 0.2, \dots, 0.9$, as well as the single impurity cases $x=0$ and $x=1.0$, a total of 11 compositions in each compound. These results permit us for the first time an ab-initio discussion of the rigid band and non-rigid band effects in the electronic spectra of BKB and BPB. McMillan-Hopfield parameters over the entire range of compositions were also computed and discussed. The density of states at E_F is found to reasonably well described by the $BaBiO_3$ based rigid band model. The shape of the underlying density

of states around E_F is virtually unchanged however only in the case of BKB; in BPB, the shape is changed substantially and the aforementioned agreement should be considered fortuitous. In considering density of states away from E_F , some conclusions of the present study are similar to earlier simpler virtual crystal and tight-binding model studies and some are not. Our computed McMillan-Hopfield parameters give insight into mechanism of superconductivity in these classic compounds.

Some work has also been completed in exploring the effects of substitutions on the La-site in the La214 superconductor in the bct phase. We emphasize that we have in mind here the doped 214 in the *metallic* range, the band theory is of course not expected to be satisfactory for the undoped 214. Our first-principles computations show that the van Hove singularity is indeed not seriously affected by La/Sr, La/Ca, and La/Ba replacement of the La-site. The Fermi energy is lowered as expected by the replacement of the trivalent La by divalent atoms. Significant changes away from the Fermi energy in the density of states are however induced by these substitutions. We emphasize that in order to reliably delineate the rather small changes in the Fermi energy (of the order of 10 mRy) the computations must be highly accurate.

IIID. Momentum Density in Binary Alloys

After several years of developmental work on the theoretical as well as the experimental side, the first extensive momentum density (3-D and 2-D) computations were completed on $Cu_{95}Pd_5$, $Cu_{85}Pd_{15}$, and $Cu_{90}Ge_{10}$ disordered alloys, just as the first 2D-ACAR measurements on CuPd and CuGe single crystals from Argonne and The Netherlands became available. Comparisons showed a tantalizing accord between theory and experiment in a variety of striking features of the data.

A brief summary of the most noteworthy results in this connection is as follows. Surprisingly large effects of alloying are seen on the momentum density

for the first time. Particularly exciting is the fact that the characteristic alloying effects on the momentum density near $p=0$ leave signatures in the theoretical 2D-ACAR curves and that these signatures are also seen in the corresponding 2D-ACAR measurements. We emphasize that the momentum density near $p=0$ arises mainly from states near the valence band edge. This is the first time that these states, which are not accessible directly in any other experiment (for example in photoemission), have been found to give observable effects in the 2D-ACAR experiments. Our results provide the first direct evidence for the existence of an s-p like impurity band far below the Fermi energy in CuGe. In CuPd we were able to confirm experimentally for the first time the theoretically predicted flattening of the FS of Cu along (110) upon adding Pd. We were also able to deduce for the first time the disordered induced smearings of the (100) and (110) radii in CuGe.

IIIE. Mono-vacancy in Cu and Alloys

We completed an extensive study of the two-photon annihilation momentum density $\rho_{2\gamma}(\vec{p})$ for a vacancy trapped positron in metals and alloys within the KKR-CPA type framework. Application of the theory to the case of a mono-vacancy in Cu has been carried out; these are the first realistic $\rho_{2\gamma}(\vec{p})$ computations on a d-band metal. Our decomposition of $\rho_{2\gamma}(\vec{p})$ into contributions from various sites offers new insights into the nature of $\rho_{2\gamma}(\vec{p})$ for a vacancy trapped positron in metals. Contrary to common expectation, we find that the contribution from the nearest-neighbor-(110)-shell and not from the central vacant site determines the characteristic bell-shape of the $\rho_{2\gamma}(\vec{p})$ curve. In fact, in the low $\vec{p}$ -region (p less than about 5 mrad), $\rho_{2\gamma}(\vec{p})$ is dominated by the nn-shell contributions; the central site contribution is found to be rather broad and featureless.

IIIF. Compton Profiles in Metals and Alloys

For the first time Compton profile, $J(\vec{q})$, for a disordered alloy using the modern alloy KKR-CPA theory was obtained. Theoretical results for the $Cu_{1-x}Ni_x$

alloys over the entire solid solution composition range were compared with high-resolution Compton measurements on corresponding polycrystalline alloy samples. This constitutes the first comprehensive study of this kind. The theory reproduces the main features of the observed Compton profiles. The relationship of $J(\vec{q})$ and its derivatives with the Fermi surface dimensions was discussed. Our results suggest that more information about the Fermi surface may be possible to extract from Compton measurements than has usually been assumed, especially if single alloy crystals are used.

IIIG. Surface States in Metals and Alloys

Using the Greens's function matching approach, we have developed the theory of surface states on the alloy surfaces. In the first application of the theory, we have focussed on the Shockley type surface states (SSS); the Tamm type surface states are known to arise from the perturbation of the atomic potential in the surface layer and require a somewhat more elaborate treatment. Since the Shockley state on the (100) surface of Cu and Cu-based alloys has not been observed, we focused our attention on the (110) and (111) surfaces of Cu and Cu-based solid solutions, where we have previously reported Shockley states in several cases via angle-resolved-photoemission experiments. Extensive calculations on CuAl, CuGe, CuNi, CuPd, and CuAu surfaces have been carried out. The binding energies of the SSS's is found to decrease roughly linearly with decreasing e/a ratio, but significant deviations from such a rigid band behavior are noted for various impurities.

IIIH. Metallic Glasses

The first realistic computations on the electronic structure of Ni-P glasses have been completed. This study was carried out by modelling the glass as an appropriate substitutional alloy. Our results show strong deviations from the commonly assumed rigid band picture for the electronic structure of this classic metal-metalloid system and consistently explain a variety of experiments. The

Ni-d-holes are found to persist over the entire glass-forming range. Most interestingly, we find that upon adding P or B the host s-p-free-electron band is lowered as a whole and the associated pseudo-gap begins to fall below the Fermi energy. The recent Hall effect measurements on Ni-P glasses at Northeastern University were also analyzed in terms of our model. We suggest a new explanation for the observed reversal of the classical Hall coefficient in $Ni_{1-x}P_x$ around 23 at% P, namely that this reversal may be attributed to a decrease in the s-p density of states at the Fermi energy so that the Ni d-holes begin to dominate the conductivity.

IIIJ. Relativistic KKR-CPA Study of Binary Alloys

We have modified our KKR-CPA codes in order to make these codes fully relativistic. A number of calculations on the $Cu_{75}Au_{25}$, $Cu_{90}Au_{10}$, $Au_{70}Pd_{30}$, and $Cu_{75}Pt_{25}$ have been completed. The results have been compared with the angle resolved photoemission experiments on the one hand and the non-relativistic calculations on these alloys on the other. The characteristic relativistic effects on the electronic spectrum of these important alloys have been delineated in a series of articles.

IV. Statement of Impact on Energy Problems

In connection with the rationale for the present investigations, it may be noted that electrons play a central role in determining the electrical, optical, magnetic, thermal, and probably also the mechanical properties of materials in general and metals in particular. The application of the quantum theory to the ordered solids (i.e. those possessing a perfect lattice symmetry with each lattice site occupied by atoms of the same chemical species in the given magnetic state), which was begun in the 1930's has greatly enhanced our understanding of materials. The question of the nature of electron states in 'imperfect' materials, i.e. those possessing some form of deviation from perfect crystalline order have

drawn an increasing attention in the recent years. It is clear that if we are to fully utilize various materials in the present and future technologies we must develop a firm understanding of their electronic structures. In the context of this project, we especially note the high- T_c superconductors which are particularly relevant materials for the energy sciences.

V. Project Output

VA. List of Publications

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 30. E. Arola, C. J. Barnes, R. S. Rao, A. Bansil, and M. Pessa: “Electronic Structure of a $Cu_{75}Pt_{25}$ Disordered Alloy”,
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 31. A. Bansil: “Positron Annihilation 2D-ACAR Spectra in $YBa_2Cu_3O_7$: LDA Predictions”, **J. Phys. Chem. Solids** **52**, 1493(1991).
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 33. L. C. Smedskjaer, A. Bansil, U. Welp, Y. Fang, and K. G. Bailey: “Positron Studies of Metallic $YBa_2Cu_3O_{7-x}$ ”,
J. Phys. Chem. Solids **52**, 1541(1991).

VB. Invited Talks at Meetings and Conferences, 1986-

1. Workshop on Electronic Structure of Defects in Metals and Alloys, Argonne National Lab., June 1986.

2. International School on Electronic Structure Methods and Applications, Kanpur, India, October 1986.
3. NATO Institute on Alloy Phase Stability, Crete, Greece, June 1987.
4. U.S./Japan Workshop on Defects in Metals and Alloys, Hawaii, May 1987.
5. 8th International Positron Annihilation Conference, Gent, Belgium, 1988.
19. DOE/DMS Seminar on Properties of Materials, Gatlinberg, Tennessee, 1989.
6. High- T_c Meeting (STC), University of Chicago, 1989.
7. Fermiology of High- T_c Superconductors, Argonne National Lab., 1991.
8. 9th International Positron Annihilation Conference, Hungary, 1991.
9. Material Research Society (MRS) Meeting, Boston, Dec. 1991.
10. Int. Electronic Structure of Materials Workshop, Madras, India, 1992.
11. US/Japan Seminar on High- T_c Superconductors, Sendai, Japan, 1992.
12. Sagamore X, Charge, Spin, Momentum Density, Konstanz (Germany), Sept. 1991
13. International Summer School on Mag. and Materials, Poland (1992).
14. Enrico Fermi School on Positron Annihilation, Milan (1993).
15. Spectroscopy of Novel Materials, Santa Fe (1993).

VC. Contributed Papers at National and International Meetings, 1986-

A. Bansil authored/co-authored contributed papers at these meetings.

1. Workshop on Electronic Structure of Defects in Metals and Alloys, Argonne National Lab, June 1986.
2. International School on Band Structure Methods and Applications, Kanpur, India, October 1986.
3. APS Meeting in New York, March 1987.
4. APS Meeting in New Orleans, March 1988.
5. APS Meeting in St. Louis, March 1989.
6. APS Meeting in Anaheim, March 1990.
7. APS Meeting in Cincinnati, March 1991.
8. MRS Meeting in Boston, Dec. 1991.
9. APS Meeting in Indianapolis, March 1992.
10. Joint Nordic Spring Meeting, Nyborg, Denmark, May 1992.
11. MRS Meeting, Anaheim (April, 1992).
12. MRS Meeting, Boston (December 1992).

VD. Ph. D. Thesis

1. E. Arola; "The Relativistic KKR-CPA Method: A Study of Electronic Structure of CuAu, AuPd, and CuPt Disordered Alloys", 1991, Tampere University of Technology, under A. Bansil.
2. R. Pankaluoto; " Topics on the Application of the LMTO Method with Emphasis on the High- T_c Superconductor $YBa_2Cu_3O_x$ ", 1992, Tampere University of Technology, under A. Bansil.
3. A. S. Serageldin; "A Study of Shockley States on Ideal Semi-Infinite Surfaces of Compositionally Disorderd Alloys", 1990, Northeastern University, under A. Bansil.

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