FINAL REPORT
JUNE, 1996

RESEARCH ON HIGH Tc
SUPERCONDUCTING COMPOUNDS

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NASA GRANT NAG 5-2375
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SUMMARY OF RESULTS

This document represents a final report of our research on the grant NAG 5-2375 from NASA during the period October 1, 1993 through March 31, 1996. We successfully performed Mossbauer research using the 21.54 kev resonance radiation of $^{151}$Eu on the high temperature superconductors Bi$_2$Ca$_y$Eu$_{0.5}$Sr$_2$Cu$_2$O$_{x}$ and EuBa$_2$Cu$_2$O$_{x}$. For the Bismuth compound the Mossbauer measurements gave a weak signal at room temperature but improved at lower temperatures. Experimental data indicated that europium is located at only one crystallographic site. Isomer shift measurements were $0.69 \pm 0.02$ mm/s with respect to EuF$_3$. The linewidth at room temperature was found to be $2.54$ mm/s. This value falls within the values observed by other researchers on Eu based 1,2,3 high-Tc compounds. Our results also show the Eu to be trivalent with no trace of divalent europium present. 

Superconducting europium based 1,2,3 compounds were prepared and measurements completed. Our results show the Eu to be trivalent with no trace of divalent europium present. These compounds had an average isomer shift of $0.73$ mm/s $\pm 0.02$ for all samples made. One of these was irradiated with $3.5 \times 10^{18}$ neutrons and a comparison made of the Mossbauer parameters for the irradiated and non-irradiated samples. Experimental results showed no difference between linewidths but a measurable effect was seen for the isomer shift.
INTRODUCTION

There have been extensive studies on high temperature superconductors, however the exact mechanism for superconductivity in these compounds is not understood. We undertook this scientific investigation in order to gain a better understanding of some of the characteristics of this very important class of compounds. We are pleased to report the successful results of our Mossbauer study on high temperature superconductors. Results from the research have been presented at the 1995 Spring Washington Meeting of The American Physical Society (1), the HBCU Workshop on the Physics of Materials and Materials Science in Washington, DC in October of 1994 (2), and the 1996 March Meeting of The American Physical Society in St. Louis (3). A full length paper is being prepared for submission to Physica C for publishing which includes some of the results from these investigations(4). We are also planning to submit a paper to the journal, Computer Physics Communications detailing the usefulness of the MATLAB software package in analyzing Mossbauer data.

In addition to the above, we greatly improved our research capability with the addition of new equipment and the development of improved software which was written under the auspices of this grant.

RESEARCH RESULTS

We were highly successful in our attempt to use the Mossbauer Effect to study high temperature superconductors by substituting the Mossbauer active rare-earth element europium. Figure (1) shows the apparatus used to make compounds. Figure (2) shows a block diagram of the experimental set-up of the Mossbauer spectrometer. Work studied by our laboratory during the grant period included a particle size investigation, an irradiation study, and a phonon study. Several 1,2,3 superconductors were made with transition temperatures between 90.8°K and 102.7°K. Table 1 shows the transition temperatures and widths for the samples made. Mossbauer measurements showed all samples to be trivalent, nonmagnetic, and to have an excellent linewidth when compared to the standard EuF₃. Results from these investigations were reported previously to NASA in the various annual reports(4,5,6).

<table>
<thead>
<tr>
<th>Pellet</th>
<th>Tc(K)</th>
<th>Transition Width (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CCD</td>
<td>92.1</td>
<td>0.2</td>
</tr>
<tr>
<td>BBC</td>
<td>96.1</td>
<td>0.5</td>
</tr>
<tr>
<td>BBB</td>
<td>95.0</td>
<td>1.4</td>
</tr>
<tr>
<td>ABB</td>
<td>102.7</td>
<td>1.0</td>
</tr>
<tr>
<td>BBA</td>
<td>94.4</td>
<td>1.4</td>
</tr>
</tbody>
</table>
**Particle Size Study**

We were part of a group effort looking at the relationship of starting particle size for the various compounds used to make a superconductor with the final superconductor. Our laboratory did the Mossbauer studies. We looked at the Mossbauer parameters of linewidth and isomer shift. Linewidth renders information about the site locations, and isomer shifts gives information about the electronic structure and s-electron interaction at the Mossbauer active atom. Mossbauer spectra were taken in transmission geometry at room temperature in the constant acceleration mode and fitted by a least squares analysis. Table 2. shows the Mossbauer results for the various superconductors. Europium fluoride was used as a standard for isomer shift calculations and an iron foil was used to calibrate the system. Figures 3 through 7 show the Mossbauer experimental data for the various particle sizes. The experimental results did not show any systematic relationship between the Mossbauer parameters and starting particle size. This is understandable since the Mossbauer effect investigates particles on the atomic level. This also agrees with the results found by Howard et al on their study on relationship between particle size and transition temperature for high Tc compounds(8). A paper is being written which includes our Mossbauer results(9).

**TABLE 2.**

<table>
<thead>
<tr>
<th>Sample</th>
<th>L.W. (mm/s) (± .05)</th>
<th>L.W. Ratio</th>
<th>I.S. (mm/s) (± .02)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EuF₃</td>
<td>2.90</td>
<td>1.00</td>
<td>0.00</td>
</tr>
<tr>
<td>BBC</td>
<td>2.67</td>
<td>0.92</td>
<td>0.74</td>
</tr>
<tr>
<td>BBA</td>
<td>2.83</td>
<td>0.98</td>
<td>0.77</td>
</tr>
<tr>
<td>BBB</td>
<td>2.92</td>
<td>0.99</td>
<td>0.69</td>
</tr>
<tr>
<td>BAB</td>
<td>2.58</td>
<td>0.89</td>
<td>0.78</td>
</tr>
<tr>
<td>CCD</td>
<td>2.66</td>
<td>0.92</td>
<td>0.70</td>
</tr>
<tr>
<td>ABB</td>
<td>2.61</td>
<td>0.90</td>
<td>0.69</td>
</tr>
</tbody>
</table>

L.W. = line width
I.S. = isomer shift
Irradiation Studies

There has been several investigations to observe irradiation effects in other types of materials using the Mossbauer isotope $^{57}$Fe, but this is the first reported attempt using $^{151}$Eu. Previous researchers discovered that neutron irradiation increased the important critical current density in high Tc superconductors (11). This improvement was attributed to the creation of defects in the material. We undertook this study to see what observables one could identify due to neutron irradiation using $^{151}$Eu Mossbauer spectroscopy. Superconductors were irradiated with $3.5 \times 10^{16}$ neutrons and a comparison made of the Mossbauer parameters for the irradiated and non-irradiated samples. Our experimental results showed no substantial difference between linewidths, but a measurable effect was brought out by the computer fitting for the isomer shift. Figure (8) shows the spectrum for the irradiated superconductor and table 3. summarizes the results of the investigation. No increase in linewidth means that all the europium atoms are found in similar atomic sites. The change in isomer shift due to irradiation implies that there is an increase in the s electron density at the nucleus of the europium atom. This suggests to get a higher current density in superconducting materials, one needs to modify the superconductor to increase its s electron density. Another competing mechanism may be due to the europium absorbing the neutrons and causing a difference in the isomer shift. Europium is sometimes used in control rods in nuclear reactors because of its ability to absorb neutrons. The isomer shift is known to be dependent on the nuclear radius and the absorption of neutrons may cause a detectable change in the nuclear radius which may be what we are observing. If this is true then this effect would have application in nuclear physics. Additional studies need to be done, perhaps with higher dosages to see if the trends cited above are consistent and more pronounced.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Linewidth Ratio</th>
<th>Isomer shift (mm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EuF$_3$</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>EuBa$_2$Cu$<em>2$O$</em>{y-x}$</td>
<td>$.90 \pm .05$</td>
<td>$.82 \pm .01$</td>
</tr>
<tr>
<td>EuBa$_2$Cu$<em>2$O$</em>{y-x}$ (Irradiated)</td>
<td>$.85 \pm .05$</td>
<td>$.94 \pm .01$</td>
</tr>
</tbody>
</table>
Phonon Studies

We reported on our previously observed phonon anomaly (1) in a Bi high Tc compound at the March 1995 American Physical Society meeting in Washington D.C. This work indicated that other sites besides the commonly accepted copper planes are effected by the superconductivity mechanism. At the time of the presentation this was a unique concept. Since then however there have been other theories that predict the possibility of the superconducting mechanism occurring at other locations besides the copper planes (9). Our results also indicate that the s electron density as shown by isomer shift measurements are similar for the different types (2112 vs 1,2,3) of superconductors.

Software Development

During the period of the grant, we developed many new computer subroutines to reduce the tedious task of analyzing data. Several codes developed were cited in earlier reports to NASA (4,5). Significant codes developed included MOSSPL13.BAS which enabled us to modify the software provided by the company who designed our Mossbauer system into software that could feed experimental data directly into another program we developed for curve fitting using the software package MATLAB. The advantage of MATLAB is that one can use a pc instead of a mainframe computer to analyze Mossbauer experimental data. We found this program to give us the same results as that found using the mainframe. This capability frees any Mossbauer research laboratory from the restrictions imposed by using a mainframe computing system. We plan to submit this program for publication in a computer physics journal (7). A copy of this code MOXXX.m is found in Appendix B. An example of the results of this fitting routine is shown for the iron standard used in our experiments in figure (7).

Laboratory Development

We greatly increased our research capability with the addition of new equipment and the development of improved software. The Mossbauer Laboratory now has two research grade Mossbauer spectrometers. Currently there are only three locations in Maryland where Mossbauer spectroscopy can be done. Those three being Morgan State, Johns Hopkins University, and UMBC. As a result of this grant we strengthened our collaborative ties with both Hopkins and UMBC and this cooperation will enhance the state of Mossbauer research in the state of Maryland and the nation and will be of great benefit in this era of decreasing funds for scientific research. Many individuals strengthened their research capability because of working on this grant. Seven students working on the project subsequentially graduated ( 4 graduates, 3 undergraduates). Seven additional undergraduates are still in college in physics or engineering and two high school students have indicated that they will major in physics or engineering when they enter college.
list of participants and their duties is located in appendix c.

REFERENCES


10. Seifu, D., Oliver, F.W., and Hoffman, E., "Curve Fitting of Mossbauer Data using MATLAB" (to be submitted to Computer Physics Communication)

Setup for the sintering and annealing process for producing superconductors

Figure 1.
Figure 2.
Superconductor BBB

Velocity in mm/sec relative to europium fluoride

Figure 3.
Superconductor BBA

Channel Number

Percent Absorption

Counts

Velocity in mm/sec relative to europium fluoride

Figure 5
Superconductor BBC

Velocity in mm/sec relative to europium fluoride

Figure 6
Superconductor ABB

Figure 7.
Superconductor ABB  (irradiated)

Velocity in mm/sec relative to europium fluoride

Figure 8.
FeFoil

Figure 9.
APPENDIX A - PAPERS PRESENTED
**Theory of Pulsed NMR**

The precession frequency agrees with the gap. Numerical solutions show that the tipping angle dependent precession frequency generally differs substantially from the prediction of stationary solutions and depends on the magnitude of the transverse tipping field. However, for tipping angles of \( \phi < 60^\circ \) and also for \( \phi = 125^\circ \), the precession frequency agrees with the stationary solution, being insensitive to the magnitude of the tipping field. This work is supported by the National Science Foundation through grants DMR-9214025 and DMR-9211918.

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**Theory of Pulsed NMR**

The theory of pulsed NMR studies in solid \( ^2\text{He-B} \) T. Dinesen, B. C. Sanctuary, M. Gill, and H. Meyer, Duke U. Density matrix theory is used to calculate the response signal of \( ^2\text{He-B} \) (with rotational angular momentum \( J = 0 \) and nuclear spin \( I = 2 \)) in two- and three-pulse NMR experiments. A closed-form method has been successfully applied to the solid echo properties of \( ^2\text{He} \) and \( ^2\text{B} \) (with \( J = 1 \) and \( I = 1 \)), but not previously been developed for the \( I = 2 \) spin system. We find, as expected, similar functional dependence upon the experimental parameters of both ortho and para systems and arrive at a detailed account of the intermolecular dipolar field. While this closed-form method considers individual contributions to the echo amplitude, greater physical insight is gained by considering the rotational invariance properties of the line shape. Results from a spherical tensor and product operator basis are then compared with one another as representations of the quadrupolar solid echo response problem. Finally, the predicted solid echo amplitude ratio of the \( I = 1 \) and \( I = 2 \) components, expressed as a function of the time \( \tau \) between the pulses and their respective phases \( \Phi \), is compared with that observed for several \( ^2\text{He} \) crystals of various \( J = 1 \) concentrations. We also discuss the satellite echoes, predicted for the \( I = 2 \) system, which have been observed in \( ^2\text{O} \) absorbed on MgO but not in solid \( ^2\text{D} \).

1. I. Yu et al., J. Low Temp. Physics 51, 369 (1983) for \( ^2\text{He} \).

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**SESSION II1: DAMOP: ATOMIC AND MOLECULAR STRUCTURE AND SPECTROSCOPY**

Thursday morning, 20 April 1995

Room 3 at 8:00

R. Pratt, presiding

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**III1 1**

Rovibronic Spectroscopy of the Ethoxy Radical in a Supersonic Jet Environment. Prabhakar Misra, Howard University — The ethoxy \( (\text{C}_2\text{H}_5\text{O}) \) radical is generated as a chemical intermediate in combustion and atmospheric processes. It belongs to the \( C_2 \) point group and has 18 fundamental vibrational frequencies. \( \text{C}_2\text{H}_5\text{O} \) was produced in a jet of \( \text{KrF} \) gas (248 nm) excimer laser pulses. A frequency-doubled Nd:YAG-pumped dye laser with a nominal linewidth of 0.07 cm\(^{-1}\) served as the probe beam for excitation of the radical. Extensive laser excitation spectra of jet-cooled \( \text{C}_2\text{H}_5\text{O} \) have been recorded in the 310–350 nm region with 0.16 cm\(^{-1}\) resolution. Wavelength-resolved emission spectra have also been obtained with an Optical Multi-channel Analyzer system, which employed CCD detection in conjunction with a 0.257 m monochromator equipped with a 1200 grooves/mm grating that provided a resolution of 0.5 nm. Several new vibrational frequencies have been identified for the \( \text{C}_2\text{H}_5\text{O} \) radical.

**III1 4**

Quanized Magnetic Flux in Atomic Systems. R.L. Collins, retired, HC01 Box 106C, Rockport, TX 78382 — Magnetic flux within a superconducting ring is quantized in units of \( \Phi = h/2e \). This same flux quantum also plays a role within atomic systems. An oscillating charge \( q \) creates, about itself, an encircling and transient magnetic field. The Schrodinger equation requires correction of the \( \langle \psi | \vec{p} \cdot \vec{r} \rangle \) becoming \( \langle \psi | \vec{p} \cdot \vec{r} \rangle = \frac{\hbar}{2} \langle \psi | \vec{r} \rangle \). Following Feynman, a wave function written as \( \psi(r) = (\vec{p} \cdot \vec{r})^N \exp(i\vec{p} \cdot \vec{r}) \) leads to a current density \( J = (\hbar/2m)(V^0 - (2\vec{q} \cdot \vec{p})/\hbar) \) or \( n = (h/2\pi)(V^0 - qA) \). On integrating this last equation along the displacement between turning points of the motion, the magnetic flux \( \Phi \) is readily obtained. The first term is
were calculated based upon the nucleation rate theory assuming that the molecular volume and the surface free-energy of the electronically active oxygen clusters are not affected by the presence of hydrogen in the silicon matrix. From the present analysis, it was found that the activation energies of interstitial oxygen diffusion in silicon containing hydrogen are between 0.13 and 0.28 eV lower than the normal value of 2.53 eV. Based upon the result showing a logarthmic dependence of the activation energy on hydrogen supersaturation in the silicon matrix, it is proposed that enhanced oxygen diffusion is governed mainly by hydrogen supersaturation and not the presence of hydrogen in the matrix alone.

H31 114

Phase diagrams for structural phase transformation in spinels -

V. F. Shifrin and B. N. N. Achar, The University Of Memphis. We have investigated the structural phase transformation in spinels on the basis of a six component order-parameter Landau theory. Phase diagrams plotted in the plane of two thermodynamic variables can account for the experimentally observed $O_2 \rightarrow O^+_2$ transformations.

H31 115

Growth Induced Alignment and Assignment of the Vibrational Modes of $C$ in $\text{AIGaAs}^*$. - J.-F. Zheng, Michael Stavola, Lehigh University, C. R. Abernathy and S. J. Pearton, University Of Florida. Seven infrared absorption bands observed in $C$ doped $\text{AlGaAs}$ near 600 cm$^{-1}$ have been assigned to the vibrations of $C_{6h}$. The complexity of this spectrum has prevented the assignment of the vibrational bands to specific $\text{C}_{6h}$ modes that are associated with different numbers of $\text{Al}$ neighbors, although considerable progress has been made toward understanding $\text{C}_{6h}$ by studying the $C-H$ complexes in hydrogenated $\text{AlGaAs}$. We have recently discovered that the vibrational absorption due to $C_{6h}$ in $\text{AlGaAs}$ grown by metalorganic MBE is polarized along specific $C_{6h}$ directions in the $(001)$ growth plane. A similar growth-induced alignment was discovered previously for a $(C_{4v})^2$-H complex in epitaxial $\text{GaAs}$. We assign the polarized absorption bands in $\text{AlGaAs}$ to $C_{6h}$ atoms with $\text{Al}$ neighbors that have been aligned along specific directions during growth and use the additional information that the alignment provides to assign the $C_{6h}$ modes.

$^*ONR$ Grant No. N00014-94-1-0117 and N00014-93-1-0857.

H31 116

Density Functional Theory of Insulators : Exchange-Correlation Electric fields -

Xavier Gonze, Philippe Ghosez, Unité PCPM, Université Catholique de Louvain, Belgium, REX Godby, Department of Physics, University of York, United Kingdom. We examine the density functional theory of periodic, infinite, insulators, obtained either from the limit of a finite piece of matter for increasing volumes, or with the symmetry of the bulk solid. A homogeneous exchange-correlation electric field will appear, in order to induce the correct value of the surface charge. In contrast, in the second case, the topology of the problem precludes a homogeneous exchange-correlation electric field, and the Berry's phase computation of the polarization from the Kohn-Sham orbitals will not give the same value as that derived from the many-body wavefunctions. This effect is exhibited for a model 1-D semiconductor. The exchange-correlation kernel of the latter is also obtained, and exhibits a $O(\frac{1}{\hbar})$ divergence in the small-wavenumber limit, confirming previous theoretical discussions.


H31 117

Dynamics of rough Ge(001) surfaces at low temperatures. S. JAY CREY, JOSEPH VAN NOSTRAND, DAVID G. CAHILL, Department of Materials Science, University of Illinois, Urbana, IL. The relaxation of nonequilibrium surface morphologies is studied on nanometer length scales and at temperatures far below roughening using in-situ scanning tunneling microscopy. Controlled multilayer surface roughness is produced by low-energy ion etching of Ge(001) at 270°C, the characteristic in-plane length scale of the roughness is varied from 37-118 nm. These surfaces are subsequently annealed at temperature in the range 220-325°C for 10-300 minutes and imaged at room temperature. The activation energy for surface smoothing is 1.9±0.2 eV. The dependence of the relaxation rate on the in-plane length scale is inconsistent with the continuum model of Mullins; the time constant $t$ depends on the smoothing rate increases with increasing lateral length scale $L$ as $t \approx L^2$, $n=2.2±0.4$. The results are consistent with a simple model based on step mobility, step-step interactions, and uncorrelated motion of adjacent steps.

H31 118

Optical Absorption of Chromium in Bismuth Tellurite -

Bi$_2$TeO$_5$. L. A. KAPPERS and R. H. BARTRAM, Univ. of Conn.

S. Nest, CT. I. FOLDVARI and A. PETER, Research Lab. for Crystal Physics, Budapest, Hungary. Bismuth tellurite is a nonlinear optical material with interesting photorefractive properties including a long lived signal component [1]. It crystallizes in a perturbed CaF$_2$ structure which contains large numbers of open oxygen positions [2]. This results in unusual coordination numbers of 7 and 8 around Bi and around $Te$ ions. Ambivalent impurities, like Cr, are important because of their role in the photorefractive and photochromic properties of the material. Chromium shows a non-typical absorption spectrum in Bi$_2$TeO$_5$ that covers the visible and near infrared range. White light exposure and thermal annealing modify the spectrum in opposite directions. The original spectrum and its changes could only be explained by assuming the presence of Cr$^{6+}$ and Cr$^{5+}$ valence states. The coordination symmetry of the lattice points and the possibility of filling the open anion positions with excess O$_2^-$ ions support this model.

Supported by NSF Grant INT-9222297, Univ. of Conn. Res. Found., and Hungarian Res. Found. (OTKA-T-014884).


H31 119

A Mössbauer Study of the Effects of Neutron Irradiation on a High Temperature Superconductor, F. W. Oliver, E. Hoffman, D. Seifu, E. Hammond, F. Pierre, Z. Kureishi, Morgan State Univ. Baltimore, MD. J. Howard, Hofstra University, Hempstead, N.Y.; C. Wynder, Nassau Community College, Nassau, N.Y. It has been found that neutron irradiation of high temperature superconductors change properties of the material. We report on a Mössbauer investigation of neutron irradiated EuBa$_2$Cu$_3$O$_y$ using the 21.53 keV transition of $^{151}$Eu. A sample was irradiated with approximately $3.5 \times 10^{16}$ neutrons and a comparison made of the Mössbauer parameters for the irradiated and non-irradiated samples. Experimental results showed no difference between line-widths for this level of radiation but a measurable effect was seen for the isomer shift. A discussion of the isomer shift will be reported and compared with previous results found on irradiated low temperature superconductors.


Supported by NASA - NAG 5-2735


HISTORICALLY BLACK COLLEGES AND UNIVERISITIES WORKSHOP ON THE PHYSICS OF MATERIALS AND MATERIALS SCIENCE (HBCU PMMS'94)

Crystal Gateway Marriott Hotel
Washington, D. C.
October 13–15, 1994

Tentative Schedule

Wednesday, October 12, 1994

7:00–9:00 p.m. Registration and Reception, Salon I, Crystal Gateway Marriott Hotel

Thursday, October 13, 1994

7:00–8:30 a.m. Breakfast (Salons H and J) and Conference Registration

8:30–9:00 Opening Ceremony (Salons B and C)

Dr. William T. Oosterhuis, Branch Chief
Division of Materials Sciences, Office of Basic Energy Sciences
United States Department of Energy

Dr. Earl Richardson, President
Morgan State University

Dr. Bill R. Appleton, Associate Director for the Advanced Neutron Source, Oak Ridge National Laboratory

ELECTRONIC AND OPTOELECTRONIC PROPERTIES OF MATERIALS

Session Chairman—Michael D. Williams
AT&T Bell Laboratories

9:00–9:40 Ab Initio Study of the Structural and Electronic Properties of Solid Cubane—Steven L. Richardson, Howard University, and José Luís Martins, INESC, Lisboa, Portugal

20.
Poster Session D: WIDE BAND GAP MATERIALS
4:00–5:30 p.m., Salon C

D1 An FT Raman and FTIR Investigation of PAN-Based Carbon Fibers—Chai-Pei Chang, Georgia Institute of Technology; Subhash C. Bhatia, Spelman College; and Satish Kumar, Georgia Institute of Technology

D2 Optical Emission Analysis of Pulsed-Laser Deposition of Diamondlike Carbon Films—Alessandro Rengan, Central State University

D3 Carrier Velocity in Wide Band-Gap Materials—Craig J. Scott, Ronald Green, and Carl White, Morgan State University, and André D. Cropper, Virginia Polytechnic Institute and State University

D4 Synthesis and Characterization of Homoepitaxial Diamond Films—L. F. Sutcu, Clark Atlanta University; C. J. Chu, R. H. Hauge, and J. L. Margrave, Rice University; and M. P. D’Evelyn, Rensselaer Polytechnic Institute

D5 Fabrication of Beta Silicon Carbide Diodes Using Proton Isolation—J. Coleman and G. L. Harris, Howard University

Poster Session E: HIGH-TEMPERATURE SUPERCONDUCTORS
4:00–5:30 p.m., Salon C

E1 A Possible Mechanism of High-Temperature Superconductivity—J. D. Fan and Y. M. Malozovsky, Southern University and A&M College

E2 Impurity Studies on Some High-Temperature Superconductors—A. B. Kebede, C. Buford, and S. Mtingwa, North Carolina A&T University

E3 Mössbauer Studies on High-Temperature Superconductors—F. W. Oliver, Morgan State University; L. May, The Catholic University of America; and C. E. Violet, Lawrence Livermore National Laboratory


E5 Theory of High-\( T_c \) Superconductivity in Cuprates—T. Tsang, Howard University
APPENDIX B - SOFTWARE DEVELOPMENT
i0=1;
x=i0:1:nd;
y = reshape(M',1,nd);
for i=1:31;
   ii = i.*16;
   y(ii) = (y(ii-1) + y(ii+1))./2.:
end;
y(512) = y(511);
for i=1:16;
y(i)=y(17);
end;
plot(x,y,'o')
end
chisq=1;

ymin = y(i0);
ymax = y(i0);
for i=i0:nd;
   if y(i)<ymin
      ymin=y(i);
      imin=i;
   end
   if y(i)>ymax
      ymax=y(i);
   end
end

yminbs = ymin;
ymaxbs = ymax;

y = (y - ymin)./(ymax - ymin);
x = (x - 1)./(nd-1.);

pp = (pp - 1.)/(nd-1.)
bb = bb/(nd-1.)

hh = 1./(bb.^2)
hold = hh;

count = 1
while (count) < 24
   count = count + 1
   for i=i0:nd;
      for k=1:L;
         xp(k,i)=x(i)-pp(k);
         xpsq(k,i)=xp(k,i).^2;
      end
   end
end
\[ q(k,i) = 1 + hh(k) \cdot xp(k,i)^2; \]
\[ qqsq(k,i) = q(k,i)^2; \]
\[ tt = \text{zeros}(3+3*L, nd); \]
\[ \text{for } il=0 : nd; \]
\[ \text{for } kl=0 : L-1; \]
\[ tt(1+3*kl,il) = 1./q(k+kl,il); \]
\[ tt(2+3*kl,il) = xp(1+k1,il)/qqsq(1+k1,il); \]
\[ tt(3+3*kl,il) = xpsq(1+k1,il)/qqsq(1+k1,il); \]
\[ \text{end} \]
\[ \text{end} \]
\[ m = \text{zeros}(3*L+3,3*L+3); \]
\[ \text{for } n1=1:3*L+3; \]
\[ \text{for } n2=1:3*L+3; \]
\[ m(n1,n2) = \text{sum}(tt(n2,:).*tt(n1,:)); \]
\[ \text{end} \]
\[ \text{end} \]
\[ \text{nn} = \text{zeros}(3*L+3, 1); \]
\[ \text{for } n3=1:3*L+3; \]
\[ \text{nn(n3,1)} = \text{sum}(y.*tt(n3,:)); \]
\[ \text{end} \]
\[ \text{det}(m) \]
\[ z = \text{inv}(m) * n; \]
\[ \text{for } k2=1:L; \]
\[ a(k2) = z(1+3*(k2-1)); \]
\[ gama(k2) = z(2+3*(k2-1))/(2.*a(k2).*hh(k2)); \]
\[ \text{delta}(k2) = -z(3+3*(k2-1))/a(k2); \]
\[ \text{end} \]
\[ \text{ee} = z(4+3*(L-1)); \]
\[ ff = z(5+3*(L-1)); \]
\[ gg = z(6+3*(L-1)); \]
\[ \text{for } k3=1:L; \]
\[ hh(k3) = hh(k3) + \text{delta}(k3); \]
\[ pp(k3) = pp(k3) + \text{gama}(k3); \]
\[ \text{end} \]
\[ \text{for } i=0 : nd; \]
\[ xsq(i) = x(i)^2; \]
\[ \text{for } k4=1:L; \]
\[ xmpsq(k4,i) = (x(i) - pp(k4))^2; \]
\[ \text{end} \]
\[ \text{end} \]
\[
\begin{align*}
\text{MOXXX.M} \\
yt &= \left( \frac{aa(1,1)}{1 + hh(1,1) \cdot xmppsq(1,:) \cdot xmppsq(2,:) \cdot xmppsq(3,:) \cdot xmppsq(4,:) \cdot xmppsq(5,:) \cdot xmppsq(6,:) \cdot xmppsq(7,:)} \right) + \left( \frac{aa(1,2)}{1 + hh(1,2) \cdot xmppsq(2,:) \cdot xmppsq(3,:) \cdot xmppsq(4,:) \cdot xmppsq(5,:) \cdot xmppsq(6,:) \cdot xmppsq(7,:)} \right) + \left( \frac{aa(1,3)}{1 + hh(1,3) \cdot xmppsq(3,:) \cdot xmppsq(4,:) \cdot xmppsq(5,:) \cdot xmppsq(6,:) \cdot xmppsq(7,:)} \right) + \left( \frac{aa(1,4)}{1 + hh(1,4) \cdot xmppsq(4,:) \cdot xmppsq(5,:) \cdot xmppsq(6,:) \cdot xmppsq(7,:)} \right) + \left( \frac{aa(1,5)}{1 + hh(1,5) \cdot xmppsq(5,:) \cdot xmppsq(6,:) \cdot xmppsq(7,:)} \right) + \left( \frac{aa(1,6)}{1 + hh(1,6) \cdot xmppsq(6,:) \cdot xmppsq(7,:)} \right) + ee + ff \cdot x + gg \cdot x^2; \\
\text{chisq} &= \text{sum}(y - y_t)^2 / (nd - 1) \\
yp &= ee + ff \cdot x + gg \cdot x^2; \\
xpmin &= - ff / (2 \cdot gg); \\
xpminsq &= xpmin^2; \\
ypmin &= ee + ff \cdot xpmin + gg \cdot xpminsq; \\
\text{if (count) <= 2} \\
y &= y - yp + ypmin; \\
yt &= yt - yp + ypmin; \\
\text{end} \\
\text{end} \\
\delta \text{}\ \text{gama} \\
p \text{p} \\
\text{bb} = 1 / \text{sqrt}(hh) \\
\text{baseline} = ee + ff \cdot xpmin + gg \cdot xpminsq \\
\text{for } i = 1:16; \\
\text{y}(i) = \text{baseline}; \\
\text{end;} \\
\text{width} = bb \cdot (nd - 1) \\
\text{peak} = pp \cdot (nd - 1) + 1. \\
\text{cal}499 = 2.245 \cdot ((\text{peak}(2) - \text{peak}(1)) + (\text{peak}(3) - \text{peak}(2)) + (\text{peak}(5) - \text{peak}(4)) + (\text{peak}(6) - \text{peak}(5)) \cdot 4. \\
\text{c}499 = (\text{peak}(3) + \text{peak}(4)) / 2. \\
\text{LW}499 = bb \cdot (nd - 1) \cdot (\text{cal}499 \\
x = (x - c499 / nd) \cdot (\text{cal}499 \cdot (nd - 1)); \\
y = (y + yminbs / (ymaxbs - yminbs)) / (\text{baseline} + yminbs / (ymaxbs - yminbs)); \\
yt = (yt + yminbs / (ymaxbs - yminbs)) / (\text{baseline} + yminbs / (ymaxbs - yminbs)); \\
\text{ppc} = p - c499 / nd \cdot (\text{cal}499 \cdot (nd - 1)); \\
\text{Hypfld} = (\text{ppc}(2) - \text{ppc}(1)) + (\text{ppc}(3) - \text{ppc}(2)) + (\text{ppc}(5) - \text{ppc}(4)) + (\text{ppc}(6) - \text{ppc}(5)) \cdot 3. \\
\text{6.81} \\
\text{- subplot(2,1,1) \\
plot(x, y, 'o', x, yt); \\
legend('data', 'fit') \\
title('Fe (B600-09)') \\
xlabel('Velocity [mm/s]') \\
ylabel('Relative Transmission') \\
print('plot.ps')
\end{align*}
\]
10 REM MOSSPLOT.BAS
15 COLOR 1, 11
20 CLS : KEY OFF
22 LOCATE 2, 1
25 PRINT "Adapted from a program by R.L. Collins, Austin Science Associates, Inc."
30 PRINT "Austin TX 78745"
40 PRINT "Fall, 1995, version by E.J. Hoffman, Morgan State University Physics Dept."
50 PRINT : PRINT : PRINT : PRINT : PRINT
60 PRINT "Welcome to":
PRINT
65 PRINT "MOSSPLOT"
70 GOSUB 10050: REM Delay
72 DIM Y(515): DIM G(515): DIM M(515): DIM V(1515)
78 FGS = "FGS": REM so that NEWFOS$ = FGS
79 CLS
80 PRINT "If you wish the line printer to receive data at any time"
81 PRINT "press function key F5"
82 PRINT: PRINT: PRINT "FUNCTION KEY F5"
83 BEEP: GOSUB 10050: GOSUB 10050: CLS
84 PRINT "To return to the menu at any time press function key F10 (Enter)"
85 PRINT "NOITEMS = "": NEWFILES = "": DATES = "": BOX = "":
86 INPUT "LOCATE 1, 35"
87 PRINT "1) Plot the theoretical curve from parameters given by the"
88 PRINT "MOSS curve-fitting program (on the VAX)"
90 PRINT "2) Print out the data from 512-channel *.sm file created"
91 PRINT "by the ASA-modified The Nucleus PCA"
92 PRINT "3) Create an INP file for input into the"
93 PRINT "MOSS program: PRINT"
94 PRINT "4) For a *.sm file, calculate velocity from interferometer data"
95 PRINT "plot counts versus velocity"
96 PRINT "5) Overplot a fitted curve from parameters"
97 PRINT "given by the MOSS program: PRINT"
98 PRINT "6) Plot data points and overplot the fitted curve from a .DAT"
99 PRINT "file downloaded from the VAX";
100 PRINT "7) Exit MOSSPlot"
120 PRINT : INPUT "Enter your choice from the menu by number: "; NOITEMS
124 ITEMS = NOITEMS
125 GOSUB ERGOTO 10300
126 IF ITEMS = "6" THEN CLS : GOTO 2000
129 PRINT "Menu by number:
130 IF ITEMS = "7" THEN CLS : GOTO 600
131 IF ITEMS = "2" THEN CLS : GOTO 1000
132 IF ITEMS = "3" THEN CLS : GOTO 3000
133 IF ITEMS = "4" THEN VELSTDS = "by interferometry"
134 IF ITEMS = "5" OR ITEMS = "9" THEN CLS : GOTO 6000
137 IF ITEMS = "5" THEN CLS : BOX = "DRAWN": GOTO 6180
180 IF ITEMS = "6" THEN CLS : GOTO 2000
190 IF ITEMS = "76" THEN CLS : GOTO 600
200 GOTO 130
260 CLS
265 LOCATE 25, 2
269 INPUT "Exit MOSSPLOT (yes, no)"; YES
270 IF YES = "y" OR YES = "y" THEN CLS : END
273 PRINT "Do you want to process "; FS$ = "": REM Again (y, n)?"
271 INPUT "", REFILITIES
272 IF REFILITIES = "y" OR REFILITIES = "y" THEN RETURN
273 OPEN FS$ FOR RANDOM AS #I LEN = 64
274 GOSUB OPENFILE: FS$ = NEWFS$ + ".sm": PRINT "": PRINT PRINT
275 PRINT "Filename character":
276 OPEN FS$ FOR RANDOM AS #I LEN = 64
277 1) MOSSPL13.BAS
278 GET #I, 1
279 IF Y(I) + J)"
280 BS = MID$(AS, J, 1)
281 X(K) = ASC(BS)
282 NEXT J
283 NEXT I
284 NEXT I
285 FOR I = 1 TO PNTS
286 N = 504 + 4 * I
287 Y(I) = (X(N + 1) + 256 * (X(N + 2) + 256 * (X(N + 3))
288 NEXT I
289 CLOSE #1
291 FOR I = 1 TO 64
292 IF Y(I) <> 0 GOTO 890
293 IF PR = 1 THEN LPRINT: LPRINT "Data File Loaded: "; FS$: LPRINT
294 RETURN
299 REM Raw data printout routine
300 GOSUB 700
301 PRINT USING "##**: #;"; TIMES; " MOSSPLOT Menu Choice: ";
302 PRINT: PRINT: PRINT: PRINT: PRINT
2209 REM hyperfine splitting calculation follows
2210 IF N = 6 THEN HFS = ((PK(6) - PK(4)) + (PK(3) - PK(1)))/4
2215 IF N = 4 THEN HFS = ((PK(5) - PK(4)) + (PK(3) - PK(2)))/2
2220 PRINT "Print "Peak of the Fe standard run = the average of "; N; " positions = Channel "; CALIBRE
2225 IF PR=1 THEN LPRINT: LPRINT "Peak of the Fe standard run = the average of "; N; " positions = Channel "; CALIBRE
2230 PRINT "The hyperfine splitting is the average of the spacings"
2235 PRINT "; between peaks 1-2, 2-3, 4-5, and 5-6 = "; HFS; " channels"
2240 IF PR=1 THEN LPRINT: LPRINT "The hyperfine splitting is the average of the spacings"
2245 IF PR=1 THEN LPRINT = "between peaks 1-2, 2-3, 4-5, and 5-6 = "; HFS; " channels"
2255 HFSTD = 2.245: REM Standard HFS in mm/s
2260 B = HFSTD / HFS: REM Slope of the velocity vs. channel no. curve
2261 PRINT "Print "HFSSTD / HFS = "; B; " (mm/s)/channel"
2265 IF PR=1 THEN LPRINT: LPRINT "The calibration constant = "; HFSSTD / HFS; " = B; " (mm/s)/channel"
2270 A = -8 * ISSTD: C = 0: REM V = A + BX + CX^2; linearity assumed here
2275 REM To get the isomer shift for the sample
2285 IF EFS = "H" OR EFS = "e" THEN GOSUB 12600
2287 IF EFS = "F" OR EFS = "f" THEN GOSUB 2600
2290 IS = B*(PEAK - ISSTD)
2295 PRINT: PRINT "Isomer shift = "; IS; " (mm/s)
2300 IF PR=1 THEN LPRINT: LPRINT "Isomer shift = "; IS; " (mm/s)
2301 IF PR=1 THEN LPRINT "B; "X("; PEAK; " - ISSTD; ") = "; IS; " (mm/s)
2310 PRINT: PRINT "Do you want an extra x and y scale?"
2320 PRINT "for channel number and for counts,"
2330 PRINT "Name "; CHRS(34); " for a plot being"
2340 PRINT "prepared for publication"
2350 INPUT "(y, n)"; SCALES$ = "; REPEATS$ = "n"
2355 IF SCALES$ = "n" OR SCALES$ = "N" THEN ITEMS = "n"
2365 IF Y = 0 OR SCALES$ = "y" OR SCALES$ = "Y" THEN GOTO 2410
2370 PRINT: PRINT "Would you like to re-use the same"
2380 PRINT "Absorption axis scaling as in the"
2390 PRINT "last plot, rather than an auto-"
2400 INPUT "Automatically-maximized scale (y, n)"; REPEATS$ = "n"
2405 PRINT: PRINT "4010 GOSUB 6029"
2500 OPEN DAT$ FOR INPUT AS #2
2505 ENDFJUNKS = "CAL FIT": REM For theoretical points
2510 GOSUB 2600
2520 CLOSE #2
2590 ITEMS = "n": GOTO 6183
2600 REM Reading peak positions and calculating average
2603 ON ERROR GOTO 10229
2605 OPEN READPK$ FOR INPUT AS #3
2606 ON ERROR GOTO 0
2610 JUNK$ = "n"
2615 WHILE RIGHT$(JUNK$, 6) <> "TO 0.5"
2620 LPRINT "; INPUT #3, JUNK$"
2625 WEND
2626 INPUT #3, JUNK
2627 INPUT #3, JUNK
2628 INPUT #3, JUNK
2629 INPUT #3, JUNK
2630 INPUT #3, NRPARAMS
2635 N = (NRPARAMS - 1)/3
2636 IF N <= 6 AND N <= 4 THEN GOTO 10325
2640 JUNK = 0
2645 WHILE JUNK <= (1 + 2*N + 1)
2650 INPUT #3, JUNK
2655 WEND
2660 FOR I = (4 - (N/2)) TO (3 + (N/2))
2669 NEXT I
2668 CLOSE #3
2670 PEAK = 0
2680 FOR I = (4 - (N/2)) TO (3 + (N/2))
2689 PEAK = PEAK + PK(I)
2690 NEXT I
2691 PEAK = PEAK / N: REM Isomer shift = avg. of N positions
2699 RETURN
3000 REM To save the data as a .INP file suitable for input into the MOSS program
3010 YADDX = 0: REM Assume 6-digit counts until line 3124
3020 GOSUB 700
3030 FRS$ = FRS$ + "INP": REM New filename is the same with ",INP" instead of ",spm"
3040 PRINT : PRINT ": A file is being saved suitable for input into the MOSS program."
3050 PRINT : PRINT ": The new filename will be "; FRS$
3052 IF P$ = "" THEN GOTO 3700
3060 PRINT "Type any description you wish to add to the filename (< 64 characters);"
3070 INPUT ": ; DESCRS$"
3080 PRINT ; INPUT : INPUT ": How many lines in the spectrum? N"
3090 PRINT : PRINT ": Enter estimated parameters (ENTER for zero spacers);"; GOSUB 5100
3100 OPEN FRS$ FOR OUTPUT AS #1
3110 LET EORFS = CHR$(13) + CHR$(10): REM Carriage retn. + linefeed
3120 YIJS = STR$(Y(105)); REM Counts in channel 105 used as a sample
3122 REM The next line strips the space added by STR$ from the left
3123 YIJS = RIGHTS(YIJS, LEN(YIJS) - 1)
3124 IF LEN(YIJS) = 7 THEN GOSUB 3500: REM For stripping off the first 1
3140 PRINT #1, ",1 (10F7.0)"
3145 PRINT #1, CHR$(35); FOS$ = " "; DESCRS$
3150 PRINT #1, USING "#####": PNTS%; (15 + INT(CPNTS% - 51/16)); ; N; (3*N + 1); 0; 0; 1; 1; 1; 0; 0; YADDX;
3155 PRINT #1, ", "
3160 PRINT #1, USING "#####. "; B3;
3165 FOR I = 1 TO N
3167 AREA(I) = ABS(AREA(I))
3170 PRINT #1, USING "#####. "; AREA(I);
3175 IF (I+1) = 7 THEN PRINT #1, EORFS
3180 NEXT I

3300 REM The following are NBAD(I), the channel numbers to be omitted by MOSS
3310 PRINT #1, EORFS
3320 FOR I = 1 TO 14: REM Discarding the 1st 14 points(non-data)
3340 PRINT #1, USING "#####"; I;
3350 NEXT I
3360 PRINT #1, EORFS
3365 K = 0: REM Counter for 14-digit lines
3370 FOR I = 16 TO PNTS% STEP 16
3380 PRINT #1, USING "#####"; I;
3385 K = K + 1
3390 IF INT(K/14) = (K/14) THEN PRINT #1, EORFS
3400 NEXT I

3470 CLOSE #1
3480 FSS$ = ""
3490 GOSUB 10000
3495 GOTO 70

3500 REM Routine for handling 7-digit counts
3510 YADDX = 1
3540 FOR I = 1 TO 512
3550 YIS$ = STR$(Y(I))
3560 REM The next line strips the space added by STR$ and the 1 from the left
3570 YIS$ = RIGHTS(YIS$, LEN(YIS$) - 2)
3580 Y(I) = VAL(YIS$)
3590 NEXT I
3600 RETURN

3700 PRINT: PRINT "Would you like "; CHRS$(34); P$: CHRS$(34)
3710 PRINT " to be printed as a description in the file"; PAGAINS$ = "Y" OR PAGAINS$ = "Y" THEN DESCRS$ = P$: GOTO 3080
3730 GOTO 3060

4000 REM Velocity formula calculation
4005 REM "PROGRAM ASSUMES 512 CHANNELS, FLYBACK MODE"
4100 REM "LASER MULTIPLEXES INTO EVERY 16TH CHANNEL"
4140 REM "TIMING INFO. ASSUMED:"
4145 REM "PRINT " CH 9, ZERO VEL. IN CH 264"
4150 REM "PRINT " IF NOT, CHANGE DATA IN LINE 4160."
4159 REM PRINT: PRINT "Velocity formula calculation:"
4160 A7 = 9: A9 = 264
4170 N = 0: AO = 0: A1 = 0: A2 = 0: A3 = 0: A4 = 0: A5 = 0: A6 = 0
4180 REM STARTING AND ENDING CH. NOS. ARE 11% AND 12%
4190 TIX = 95: TIX = 432: REM, 8/95, Setup B reliable only in this range
4200 M1 = Y(9)
4240 B1 = 7.910248
4250 FOR X = 11% TO 12% STEP 16
4260 M = Y(X)
4300 M = M * B1 / M1

28.
5100 REM Routine for calculating Y(X), the fitted curve
5001 CLS
5005 T1% = 5: T2% = 511
5010 PRINT: PRINT: INPUT "How many lines in the spectrum": N
5020 P1% = 4 * ATN(1): REM Pi = 4 X arctan(1)
5030 PRINT: PRINT "Enter values from the converged curvefit:
5050 DIM NRG(I): DIM AREA(I): DIM LW(I)
5100 PRINT: PRINT "Enter the baseline", B3
5101 IF P1%=1 THEN LPRINT: "Values entered:"
5105 IF P1%=1 THEN LPRINT: "Baseline (counts): "; B3
5110 PRINT: PRINT "Enter the parameters for each line:"
5111 FOR I = 1 TO N
5112 IF N = 1 THEN PRINT: GOTO 5120
5115 PRINT: PRINT "For Line ": I; ": ":
5120 PRINT: PRINT "Absolute value of area under curve (channels X counts): ", AREA(I)
5130 PRINT: PRINT "Line width (channels): ", LW(I)
5140 PRINT: INPUT "Position: Channel No. ", NRG(I)
5160 IF N = 1 THEN GOTO 5180
5170 IF P1%=1 THEN LPRINT: "For Line No. ", I
5180 IF P1%=1 THEN LPRINT: "Absolute value of area under curve" X counts): ", AREA(I)
5190 IF P1%=1 THEN LPRINT: "Line width (channels): ", LW(I)
5200 IF P1%=1 THEN LPRINT: "Position: Channel No. ", NRG(I)

6000 REM PLOT ROUTINE FOR HP 7440A COLORPRO PLOTTER
7022    G(X) = 1000 + 8000 * (X - T1%) / (PNTS% - T1%)
7025    G(X) = INT(G(X))
7027    GOTO 7520
7030    REM G(X) for interferometer-calibrated points
7031    'print "At line 7031 P6 = "; P6
7040    REM The next line skips the laser data
7050    IF ((X - 16) / 16) = INT((X - 16) / 16) THEN X = X + 1
7050    IF P6 - ABS(V(X)) >= 0 THEN G(X) = 5000 + INT(8000 * V(X) / F3)
7561    'print "At line 7561, X = "; X; "", V(X) = "; V(X); ";", and (G(X) = "; G(X)
7562    'while inkey$ = "" 
7563    'wend 
7564    GOTO 7570
7570    REM For tower x axis
7570
7575    IF ITEMS = "1" OR ITEMS = "4" OR ITEMS = "6" THEN GOTO 7560
7570
7570    FOR X = 1 TO 20; REM: Items = "1" OR ITEMS = "4" OR ITEMS = "6"
7576    REM: Subroutine from 6324 for lower x axis labelling in Ch. No.
7578    REM: Integer division in Ch. No.
7578
7578    FOR X = 1 TO 20; REM: Items = "1" OR ITEMS = "4" OR ITEMS = "6"
7578    REM: Subroutine from 6324 for lower x axis labelling in Ch. No.
7578
7578    FOR X = 1 TO 20; REM: Items = "1" OR ITEMS = "4" OR ITEMS = "6"
7578    REM: Subroutine from 6324 for lower x axis labelling in Ch. No.
7578
7578    FOR X = 1 TO 20; REM: Items = "1" OR ITEMS = "4" OR ITEMS = "6"
7578    REM: Subroutine from 6324 for lower x axis labelling in Ch. No.
7578
7578    FOR X = 1 TO 20; REM: Items = "1" OR ITEMS = "4" OR ITEMS = "6"
7578    REM: Subroutine from 6324 for lower x axis labelling in Ch. No.
7578
7578    FOR X = 1 TO 20; REM: Items = "1" OR ITEMS = "4" OR ITEMS = "6"
7578    REM: Subroutine from 6324 for lower x axis labelling in Ch. No.
7578
7578    FOR X = 1 TO 20; REM: Items = "1" OR ITEMS = "4" OR ITEMS = "6"
7578    REM: Subroutine from 6324 for lower x axis labelling in Ch. No.
7578
7578    FOR X = 1 TO 20; REM: Items = "1" OR ITEMS = "4" OR ITEMS = "6"
7578    REM: Subroutine from 6324 for lower x axis labelling in Ch. No.
10245 PRINT: IF EFS = "F" OR EFS = "f" THEN RESUME 2105
10250 REM error handler for STDEUS (line 12605)
10255 BEEP: PRINT: PRINT " "; STDEUS;
10260 PRINT " "FILE NOT FOUND"
10260 PRINT " "(F10 to return to menu)"
10265 PRINT: RESUME 12050
10275 REM error handler for OPENing plotter (line 6183)
10280 CLS: LOCATE 9, 20
10285 BEEP: PRINT "Plotter not responding: check switch box and connectors";
10290 RESUME 6095
10300 REM error handler for printer (line 126 and 1450)
10305 CLS: LOCATE 9, 20
10310 BEEP: PRINT "Printer not responding: check paper, power switch, connectors, etc.";
10315 PRINT: PRINT " Press the p key
10317 PRINT: PRINT " and RETURN when ready"
10320 IF PRINTS = "Y" OR PRINTS = "y" THEN RESUME
10321 IF PRINTS = "N" OR PRINTS = "n" THEN PR = 0: RESUME
10325 CLOSE #3: REM Error handling from line 2636
10340 PRINT: PRINT " "STANDARD RUN"
10345 PRINT: PRINT " "STDFS$; " shows "; N; " lines and a
total of "; NRPARAMS; " parameters.";
10350 PRINT " "Choose an Fe standard run with
4 or 6 lines."
10355 PRINT: PRINT " "Press F10 if you wish to
10360 PRINT: PRINT: PRINT: CLOSE #3: GOTO 2410
11000 REM The y axis scales: REM from line 6210
11005 REM Setting the baseline to maximum counts
11030 MAXCNT = 0
11039 'print: print "At 11039 T1%, PNTXS%, MINCNT,
11040 FOR I = T1% TO PNTXS
11045 PRINT " "M INE " T 1 0 4 5 "
11050 IF Y(I) > MAXCNT THEN MAXCNT = Y(I)
11051 'print: print " For I = "; i; " "Y(I) = " "
11056 y(i); " MAXCNT = "; mAXcnt
11052 'gosub 10050: gosub 10050: gosub 10050
11060 NEXT I
11065 IF REPEATS$ = "Y" OR REPEATS$ = "y" THEN GOTO
11050; REM from line 6220
11067 IF ITEMS = "H" OR ITEMS = "h" THEN B3 = MAXCNT
11068 'print "MAXCNT = "; mAXcnt
11069 MINCNT = MAXCNT
11070 'print: print "MINCNT = "; mincnt
11071 'gosub 10050: gosub 10050
11078 FOR I = T1% TO PNTXS STEP 16
11080 FOR J = I TO (I + 14)
11085 IF J > PNTXS THEN GOTO 11120
11090 IF Y(J) < MINCNT THEN MINCNT = Y(J)
11091 'print: print " For j = "; j; " and j = "; j; ",
11096 Y(J) = "; y(j); " MINCNT = "; mincnt
11092 'gosub 10050: gosub 10050: gosub 10050
11100 NEXT J
11101 'print: print " For i = "; i; " and j = "; j; ",
11106 Y(J) = "; y(j); " MINCNT = "; mincnt
11102 'gosub 10050: gosub 10050: gosub 10050
11110 NEXT I
11120 MAXCNT = STR$(MAXCNT): MINCNT = STR$(MINCNT)
11124 REM The next line strips the space added by STRS
from the left
11125 MAXCNT = RIGHT$(MAXCNT, LEN(MAXCNT) - 1): MINCNT
+ RIGHT$(MINCNT, LEN(MINCNT) - 1)
11130 MAXPNT% = INSTR(MAXCNT, ":"); MINPNT% =
11140 IF MAXPNT% = 0 THEN MAXEXP% = LEN(MAXCNT$) - 1 ELSE MAXEXP% = MAXPNT% - 2
11150 IF MINPNT% = 0 THEN MINEXP% = LEN(MINCNT$) - 1 ELSE MINEXP% = MINPNT% - 2

11170 IF MAXEXP% <> MINEXP% THEN GOTO 11250
11180 MAXDIG% = 1: MINDIG% = 1: J = 0
11185 IF HAXDIG% = 1: MINDIG% = VAL(MIDS(MINCNT$, J, 1)): MINPNT% = HAXOIG% = VAL(MID$(MAXCNT$, J, 1)): MINDIG% = J = J + 1
11190 HAYOIG% = 1: MINDIG% = 1: J = 0
11200 IF HAXEXP% + 1
11210 REM Routine for wide count spread
11213 IF (MAXDIG% - MINDIG%) <= 1 THEN Q% = 5 ELSE Q% = 1
11215 WEND
11220 IF HAXDIG% - MINDIG% <= 1 THEN Q% = 2 ELSE Q% = 1
11225 YS = 10
11230 IF (HAXDIG% - MINDIG%) <= 1 THEN Q% = 2 ELSE Q% = 1
11235 WEND
11240 CFUP$ = LEFT$(MAXCNT$, J + Q%)
11250 CFUP = CFUP + 1
11260 CFUP$ = LEFT$(MAXCNT$, J + Q% - 1): CFUP = 11270 CFUP = VAL(CFDN$): GOTO 11290
11280 CFUP$ = LEFT$(MINCNT$, J + Q% - 1): CFUP = VAL(CFDN$): GOTO 11290
11290 CFUP = 5500: REM Highest tic on the right y axis (counts)
11300 IDN = 2500
11305 REM IUP - IDN = 3000
11310 REM (IUP - IDN)/(CFUP = CFDN) = 3000/10 = 300
11315 IF ITEMS = "PUB" THEN GOTO 11400
11320 CFSTEP = (CFUP - CFDN)/4
11325 FOR CF = CFDN TO CFUP STEP CFSTEP: REM Right y axis (counts)
11330 PRINT #1, "PA": 8900; I; "PD": 9000; I; "PU":
11340 PRINT #1, "PA": 9020; (I - 10); "DI,0": "LB":
11350 GOSUB 10000
11360 NEXT CF
11370 GOSUB 10000
11380 CFUP = CFUP + Q%
11390 REM Left y axis (percent absorption)
11400 REM Left y axis (percent absorption)
11410 ABSNUP2 = 1 - (YS * CFDN / 83)
11413 IF ABSNUP2 <= 0.02 THEN ABSNUP2 = 0.02: GOTO 11470
11417 IF ABSNUP2 < 0.02 THEN ABSNUP3 = ABSNUP2: GOTO 11470
11420 ABSNUP3 = 0: K = 1
11430 WHILE ABSNUP3 = 0
11440 ABSNUP3 = (INT(ABSNUP2 * (10 * K))/ (10 * K)
11450 K = K + 1
11460 WEND
11470 ABSN = (ABSNUP3) / 4
11480 CF3 = 83 / YS
11485 CFUP3 = (CF3) * (1 - ABSNUP3)
11490 IUP3 = IDN + (((IUP - IDN) / (CFUP - CFDN)) * (CFUP - CFDN))
11495 IF ABSNUP3 > 0.02 AND IUP3 > 2400 THEN ABSNUP3 =
11500 ABSN + ABSN
11510 WHILE ABSN <= ABSNUP3
11520 CF = (CF3) * (1 - ABSN)
11530 I = IDN + (((IUP - IDN) / (CFUP - CFDN)) * (CF - CFDN))
11535 IF I > 5800 OR I < 2200 THEN 11570
11540 PRINT #1, "PA": 1000; I; "PD": 1100; I; "PU":
11550 PRINT #1, "PA": 440; I; "DI,0": "LB": (100 *
11550 GOSUB 10000
11570 ABSN = ABSN + ABSN
11575 IF ABSNUP3 > 0.02 THEN ABSN = (CINT(100*ABSN))/100: REM ABSN sometimes is ragged
11580 WEND

11590 GOSUB 10000
11600 RETURN REM to line 6290
12000 REM Eu standard
12010 IF STDEUSE = "Y" THEN INPUT "Want to use the same Eu and Fe standard runs for calibration": REPREUSTD$ = "Y" THEN GOTO 12090
12050 PRINT : PRINT "Name of Eu standard run for calibrating v = O" 12060 PRINT "("; CHR$(34); "Enter": CHR$(34); : INPUT "if no calibration desired): ", STDEUSE$ 12065 IF STDEUSE$ = "Y" THEN GOTO 12610
12066 READPKS$ = STDEUSE$: GOSUB 12600
12068 CALIBREU = PEAK 12070 PRINT : PRINT "Name of Fe standard run for calibrating the v scale" 12080 INPUT "(do not omit this): ", STDFES$ 12090 PRINT : PRINT 12200 GOTO 2055
12600 REM Reading Eu peak position (from line 12066 or 2285)
12603 ON ERROR GOTO 10250
12605 OPEN READPKS$ FOR INPUT AS #4
12606 ON ERROR GOTO 10250
12610 JUNK$ = "" 12615 WHILE RIGHTS(JUNK$, 9) < "DEVIATION" 12620 LINE INPUT #4, JUNK$ 12621 WEND 12640 JUNK$ = 4 12645 WHILE JUNK$ <= 4 12650 INPUT #4, JUNK$ 12655 WEND 12683 INPUT #4, PEAK 12666 CLOSE #4 12687 RETURN
12900 PRINT: PRINT "This program can only process Eu and Fe runs (press F10 to return to menu)" 12910 GOTO 2055

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32.
APPENDIX C - PERSONNEL SUPPORTED
PERSONNEL INVOLVED

Frederick W. Oliver
Professor - Physics Department
Principal Investigator.

Eugene Hoffman
Assistant Professor - Physics Department
Research Scientist
Professor Hoffman was responsible for developing computer codes for plotting on a pc the data fit by the mainframe computer. He also assisted with many of the administrative duties of the grant.

Clive Wynter
Professor - Chemistry Department - Nassau Community College
Research Scientist
Professor Wynter made the superconducting compounds and coordinated writing of scientific papers.

Richard Lockhart
Professor - Prince Georges Community College
Research Scientist
Professor Lockhart worked on the project during the summer of 1995. He was responsible for ordering equipment and setting up the laboratory for making superconducting compounds.

Jeyasingh Nithianadam
Lecturer - Electrical Engineering
Research Associate
Professor Nithianadam worked on the project during the summer of 1994. He developed software and assisted with instrumentation.

Christopher Brown
Graduate student - UMCP
Mr. Brown was responsible for assisting in the laboratory to make superconducting samples.

Dereje Seifu, Lecturer - Physics Department
Research Associate
Dr. Seifu, a theoretical physicist, worked on developing software for analyzing experimental data on the mainframe computer.

Zarfar Kureishy
Research Associate
Mr. Kureishy assisted with the many technical and administrative tasks associated with carrying out the objectives of the research.

Freydoun Borhani - Research Technician
Received M.S. in science in May of 1994.
Mr. Borhani analyzed experimental data.
The students below assisted with analyzing data, writing software, and preparing samples for experimental measurements.

Laura Gardner - M.S. Science (Currently in graduate school - Environmental Engineering, Johns Hopkins University).

Aaron Bowman - Undergraduate physics student (senior)

James Chavis - B.S. Engineering Physics, May 1996 (Currently in graduate School, Science Morgan State University)

Grace Gregory - Undergraduate physics student (junior)

Mia Nicholson - Undergraduate physics student (junior)

Takisha Miller - Undergraduate physics student (senior)

Lester Richardson - B.S. Engineering physics (currently in graduate school - Physics, Hampton University)

Xavier Preston - B.S. Physics, May 1995 (Currently employed at U.S. Patent Office)

Evan Tolson - Undergraduate physics student (junior)

Daryle Strickland - Undergraduate electrical engineering student (senior)

Carolyn Cox - M.S. Science, 1995 (Currently employed as a high school science teacher in Baltimore)

William Evans - M.S. Science, 1995 (Currently employed at Veterans Hospital as a Biomedical engineer)

Ernest Jackson - Graduate student (Currently employed as a high school science teacher in Baltimore)

Mohammad Ranjbar - M.S. Science, 1994

Dacia Tarleton - Undergraduate electrical engineering student (senior).

Farrah Pulce - High School student, NASA Sharpe Program.

Fritz Pierre - High school student, NASA Sharpe Program.