FINAL REPORT
JUNE, 1996

RESEARCH ON HIGH T_c
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$_{0.5}$Eu$_{0.5}$Sr$_2$Cu$_2$O$_x$ and EuBa$_2$Cu$_3$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 $0.73 \pm 0.02$ mm/s for all samples made. One of these was irradiated with $3.5 \times 10^{16}$ 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 a 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 linewidths 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>

TABLE 1.
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>
<thead>
<tr>
<th>Sample</th>
<th>L.W. (mm/s) (± 0.05)</th>
<th>L.W. Ratio</th>
<th>I.S. (mm/s) (± 0.02)</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$</em>{7-x}$</td>
<td>.90 ± .05</td>
<td>.82 ± .01</td>
</tr>
<tr>
<td>EuBa$_2$Cu$<em>3$O$</em>{7-x}$ (Irradiated)</td>
<td>.85 ± .05</td>
<td>.94 ± .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. A
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.

9.
Superconductor CCD

Velocity in mm/sec relative to europium fluoride

Figure 4.
Superconductor BBA

Channel Number

Percent Absorption

Velocity in mm/sec relative to europium fluoride

Figure 5
Superconductor BBC

Velocity in mm/sec relative to europium fluoride

Figure 6
Superconductor ABB

Velocity in mm/sec relative to europium fluoride

Figure 7.
Superconductor ABB (irradiated)

Velocity in mm/sec relative to europium fluoride

Figure 8.
APPENDIX A - PAPERS PRESENTED
Determination of Gap Distortion and Longitudinal Resonance Frequency in Superfluid $^3$He-B. M.R. RAND, D.T. SPRAGUE, T.M. HAARD, J.B. KYCIA, P.J. HAMOT, Y. LEE, D.M. MARKS, W.P. HALPERIN, Northeastern University. We have performed pulsed transverse nuclear magnetic resonance in superfluid $^3$He-B. We derived and then numerically solved the Leggett equations for the high field limit. From our experiments and our analysis of the Leggett equations we have determined the temperature dependence of the longitudinal resonance frequency and the distortion of the energy 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 $\phi = 120^\circ$, 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.

Theory of Pulsed NMR Studies in Solid D$_2$. T. DINESE, B. C. SANCTUARY, M. GILL, and H. MEYER, Duke U. Density matrix theory is used to calculate the response signal of D$_2$ (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 o-H$_2$ and p-D$_2$ (both with J=1 and I=1), but had 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 another representation 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 t between the pulses and their respective phases $\Phi$, is compared with that observed for several D$_2$ crystals of various J=1 concentrations. We also discuss the satellite echoes, predicted for the I=2 spin system, which have been observed in D$_2$ adsorbed on MgO but not in solid D$_2$.

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SESSION III: DAMOP: ATOMIC AND MOLECULAR STRUCTURE AND SPECTROSCOPY
Thursday morning, 20 April 1995
Room 3 at 8:00
R. Pratt, presiding

8:00
III 1 Rovibronic Spectroscopy of the Ethoxy Radical in a Supersonic Jet Environment. PRABHAKAR MISRA, Howard University. The ethoxy (C$_2$H$_5$O) radical is generated as a chemical intermediate in combustion and atmospheric processes. It belongs to the C$_3$ point group and has 18 fundamental vibrational frequencies. C$_2$H$_5$O was produced in situ by photolyzing freshly synthesized C$_2$H$_5$NO in a pulsed supersonic expansion with KrF ($\lambda$ 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 C$_2$H$_5$O have been recorded in the 310-350 nm region with 0.15 cm$^{-1}$ resolution. Wavelength-resolved emission spectra have also been obtained with an Optical Multichannel Analyzer system, which employed CCD detection in conjunction with a 0.275 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 C$_2$H$_5$O radical.

8:12
III 2 151Eu Mössbauer Investigation on a Bismuth High-T$_c$ Superconductor. F.W. OLIVER, E. HOFFMAN, D. TARLETSON, Morgan State U., L. MAY, The Catholic University of America, C.E. VIOLET, LLNL, and M.S. SEEHR, West Virginia University. We report on Mossbauer studies on Bismuth high-temperature superconductors with a particular emphasis on our findings on the superconductor Bi$_2$Ca$_2$CuO$_{5.5}$ using $^{151}$Eu. Magnetic susceptibility measurements show a transition temperature of 87 K. Mossbauer measurements were performed between liquid nitrogen and room temperature. Isomer shift measurements show the Eu to be trivalent and is similar to those found for Eu based 1,2,3 high-T$_c$ superconductors. Evidence of phonon softening is observed about the Eu atom during transition to the superconducting state. A discussion on the isomer shift and f factor as a function of temperature will be reported and compared with previous results found in Eu based high-T$_c$ superconductors.

Supported by NASA - NAG 5-2375.

8:24
III 3 Microwave Dielectric Behavior of Transition Metal Oxides. J.R. DAHLIA, Southeast Missouri State University. A microwave resonant cavity in the $T_{2u}$ mode is used to study the dielectric properties of a sample of cobalt oxide and nickel oxide. The microwave data of these crystals is taken as a function of frequency and temperature. A fixed length of the sample is inserted into the resonant cavity and the perturbation of the signal are recorded in terms of the frequency shifts and width changes. Slater's perturbation equations are used to calculate the real and imaginary parts of the complex dielectric constant. A very sensitive heating and cooling technique is used to study the dielectric behavior of these crystals at various temperatures. Debye's theory is used to calculate the relaxation times of these crystals.

Supported by a grant from Grants and Research Funding Committee at Southeast Missouri State University.

8:36
III 4 Quantized Magnetic Flux in Atomic Systems. R.L. COLLINS, retired, HCO1 Box 106C, Rockport, TX 78382. Magnetic flux within a superconducting ring is quantized in units of $\Phi_0=\frac{h}{2e}$. 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 $<p>$ operator, $-i\hbar \nabla \psi$ becoming $-i\hbar \nabla + q \Phi$. (Where $\Phi$ is the vector potential). Following Feynman (3), a wave function written as $\psi(r) = \int^{|\Phi(r)|} \exp[i\Phi(r)]$ leads to a current density $J=(\hbar/2m)(\partial/\partial r \psi^* \psi - \psi \partial/\partial r \psi^*)$ or $m = (\hbar/2e)\Phi$. On integrating these last equations 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 electrically 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 logarithmic 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 $O_2 \rightarrow O_3$ transformations.

H31 115

Growth Induced Alignment and Assignment of the Vibrational Modes of C in AIGaAs.* J.-F. ZENG, MICHAEL STAVOLA, Lehigh University. C.R. ABERNATHY and S.J. PEARTON, University of Florida. Seven infrared absorption bands observed in C doped AIGaAs near 600 cm$^{-1}$ have been assigned to the vibrations of $C_{60}$. The complexity of this spectrum has prevented the assignment of the vibrational bands to specific C$_6$ modes that are associated with different numbers of Al neighbors, although considerable progress has been made$^2$ toward understanding C$_6$ by studying the C-H complexes in hydrogenated AIGaAs. We have recently discovered that the vibrational absorption due to C$_6$ in AIGaAs grown by metalorganic MBE is polarized along specific (110) directions in the (001) growth plane. A similar growth-induced alignment was discovered previously$^3$ for a (C$_{60}$)$_2$-H complex in epitaxial GaAs. We assign the polarized absorption bands in AIGaAs to C$_6$ atoms with Al neighbors that have been aligned along specific directions during growth and use the additional information that the alignment provides to assign the C$_6$ 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 Born-von Karman conditions. In the first case, and for solids where the value of the surface charge is not imposed by 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 $O(1/L)$ divergence in the small-wavevector limit, confirming previous theoretical discussions.

H31 117

Dynamics of rough Ge(001) surfaces at low temperatures E. 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 10-360 minutes and imaged at room temperature. The activation energy for surface smoothing is $1.9\pm0.25$ eV. The dependence of the relaxation rate on the in-plane length scale is inconsistent with the continuum model of Mullins: the time constant $\tau$ is proportional to $L^2$, $n=2.2\pm0.4$. 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$_2$Te$_2$O$_5$. L.A. KAPPERS and R.H. BARTRAM, Univ. of Conn. Storrs, CT. I. FÖLDVÁRI and A. PÉTER, Research Lab. for Crystal Physics, Budapest, Hungary. — Bismuth tellurite is a new nonlinear optical material with interesting photoresponsive 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 photoresponsive and photochromic properties of the material. Chromium shows a non-typical absorption spectrum in Bi$_2$Te$_2$O$_5$ 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, P. Fenten, Z. Kureishi, Morgan State Univ., Baltimore, MD. J. Howard, Hofstra University, Hempstead, N.Y., C. Wynter, Nassau Community College, Nassau, N.Y. It has been found that neutron irradiation of high temperature superconductors change properties of the material [1]. 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 x 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 - NASA 5-2375
HISTORICALLY BLACK COLLEGES AND UNIVERSITIES 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. Malozovskiy, 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-Tc Superconductivity in Cuprates—T. Tsang, Howard University
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)
hhold = 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

23.
\[ q(k,i) = l + hh(k) \cdot x(k,i)^2; \]
\[ qqsq(k,i) = q(k,i)^2; \]

\%tt = zeros(3+3*L, nd);
for il=i0:nd;
for kl=0:L-1;
    tt(1+3*kl,il) = l./qq(l+kl,il);
    tt(2+3*kl,il) = xp(l+kl,il)./qqsq(l+kl,il);
    tt(3+3*kl,il) = xpsq(l+kl,il)./qqsq(l+kl,il);
end
end
for il=i0:nd;
    tt(4+3*(L-1),il) = 1;
    tt(5+3*(L-1),il) = x(il);
    tt(6+3*(L-1),il) = x(il)^2;
end

mm = zeros(3*L+3,3*L+3);
for nl=1:3*L+3;
    for n2=1:3*L+3;
        mm(nl,n2) = sum(tt(n2,:).*tt(nl,:));
    end
end

\%nn = zeros(3*L+3,1);
for n3=1:3*L+3;
    nn(n3,1) = sum(y.*tt(n3,:));
end

\det(mm)
zz = inv(mm)\cdot nn;
for k2=1:L;
    aa(k2) = zz(1+3.\cdot (k2-1));
    gama(k2) = zz(2+3.\cdot (k2-1))/(2.\cdot aa(k2).\cdot hh(k2));
    delta(k2) = -zz(3+3.\cdot (k2-1))/aa(k2);
end
ee = zz(4+3*(L-1));
ff = zz(5+3*(L-1));
gg = zz(6+3*(L-1));

for k3=1:L;
    hh(k3) = hh(k3) + delta(k3);
    pp(k3) = pp(k3) + gama(k3);
end
for i=i0:nd;
    xsq(i) = x(i)^2;
    for k4=1:L;
        xmppsq(k4,i) = (x(i) - pp(k4))^2;
    end
end

24.
yt=\left(\frac{aa(1,1)}{1. + hh(1,1) \cdot \text{xmpsq}(1,:))} + \frac{aa(1,2)}{1. + hh(1,2) \cdot \text{xmpsq}(2,:))} + \frac{aa(1,3)}{1. + hh(1,3) \cdot \text{xmpsq}(3,:))} + \frac{aa(1,4)}{1. + hh(1,4) \cdot \text{xmpsq}(4,:))} + \frac{aa(1,5)}{1. + hh(1,5) \cdot \text{xmpsq}(5,:))} + \frac{aa(1,6)}{1. + hh(1,6) \cdot \text{xmpsq}(6,:))} \right) + ee + ff \cdot x + gg \cdot x^2;

\text{chisq} = \text{sum}(\sqrt{\frac{ly - yt}{2}}) \cdot \frac{1}{\text{nd}}

yp=ee + ff \cdot x + gg \cdot x^2;

xpmin = - \frac{ff}{2 \cdot gg};

xpmnsq = xpmin^2;

ypmin = ee + ff \cdot xpmin + gg \cdot xpmnsq;

\text{if (count) } \leq 2
\begin{align*}
y &= y - yp + ypmin; \\
yt &= yt - yp + ypmin;
\end{align*}
\text{end}
\text{end}
\text{delta}
\text{gama}
\text{pp}
\text{hh}
bb = 1./\sqrt{hh}
baseline = ee + ff \cdot xpmin + gg \cdot xpmnsq

for i=1:16;
\text{y}(i)=baseline;
\text{end};

width = bb \cdot (\text{nd} - 1.);
peak = pp \cdot (\text{nd} - 1.) + 1.
\text{cal}499 = 2.245 ./(\{(\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 (\text{nd} - 1.) \cdot \text{cal}499
x = (x - c499./nd) \cdot \text{cal}499 \cdot (\text{nd} - 1.);
\text{y} = (y + \text{yminbs}./(\text{ymaxbs} - \text{yminbs})) \cdot (\text{baseline} + \text{yminbs}./(\text{ymaxbs} - \text{yminbs}));
\text{yt} = (yt + \text{yminbs}./(\text{ymaxbs} - \text{yminbs})) \cdot (\text{baseline} + \text{yminbs}./(\text{ymaxbs} - \text{yminbs}));
\text{ppc} = (pp - c499./nd) \cdot \text{cal}499 \cdot (\text{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)
\text{plot}(X,y,'o',x, yt);
\text{legend}('data','fit')
\text{title}('Fe (B600-09)')
\text{xlabel}('Velocity [mm/s]')
\text{ylabel}('Relative Transmission')
\text{print}('plot.ps')

25.
MOSSPLOT.BAS

10 REM
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"
66 GOSUB 10050: REM Delay
68 FS$ = "FS": REM so that NEWFQ$ = FS$
70 CLS
72 ON KEY(10) GOSUB 10100: KEY(10) ON: REM Setting F10 for
returning to the menu at any time
73 PR = 0
74 ON KEY(5) GOSUB 10160: KEY(5) ON: REM Setting F5 for
use of the line printer
75 LOCATE 10, 12: PRINT "IF YOU WISH THE LINE PRINTER TO
RECORD THE OPERATION,"
76 PRINT: PRINT: PRINT " PRESS
FUNCTION KEY F5"
77 BEEP: GOSUB 10050: GOSUB 10050: CLS
78 LOCATE 25, 8
79 PRINT "TO RETURN TO THE MENU AT ANY TIME PRESS FUNCTION
KEY F10 (Enter)"
80 NUTEMS = ";": NEWFQ$ = "": DAT$ = "": BOX$ = ""
82 LOCATE 1, 35
84 PRINT "MENU": PRINT
85 PRINT " 1) Plot a theoretical curve from parameters
given by the"
86 PRINT " MOSS curve-fitting program (on the
VAX)"
90 PRINT " 2) Print out the data from 512-channel
*.spm files created"
91 PRINT " by the ASA-modified The Nucleus PCA"
PRINT
95 PRINT " 3) Create a .inp file for input into the
MOSS program: PRINT
100 PRINT " 4) For a *.spm file, calculate velocity
from interferometer data;"
101 PRINT " plot counts versus velocity"
102 PRINT " 4') For a *.spm file run without the
interferometer,"
103 PRINT " plot counts versus channel number;"
PRINT
105 PRINT " 5) Overplot a fitted curve from parameters
given by the MOSS program: PRINT
107 PRINT " 6) Plot data points and overplot the
fitted curve from a .DAT"
108 PRINT " file downloaded from the VAX: PRINT
110 PRINT " 7) Exit MossPlot"
120 PRINT: INPUT " Enter your choice from the
menu by number: ", NUTEMS
124 ITEMS = NUTEMS
125 ON ERROR GOTO 10300
126 IF ITEMS <> "7" AND PR=1 THEN LPRINT : LPRINT " 
"; DATES: "; TIMES: " MOSSPLOT Menu Choice: ";
ITEMS: LPRINT
127 ON ERROR GOTO 0
129 PNTXS = 512: REM Item 6 may alter this
130 IF ITEMS = "6" THEN CLS : GOTO 6000
131 IF ITEMS = "6" THEN CLS : GOTO 6000
132 IF ITEMS = "6" THEN CLS : GOTO 3000
133 IF ITEMS = "6" THEN CLS : GOTO 3000
134 IF ITEMS = "6" THEN CLS : GOTO 6000
135 IF ITEMS = "6" THEN VELSTDS = " by interferometry"
136 IF ITEMS = "6" OR ITEMS = "6" 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 = "7" THEN CLS : GOTO 600
200 GOTO 130

600 CLS
605 LOCATE 25, 2
610 INPUT "Exit MOSSPLOT (yes, no)"; FS$20 IF FS$ = "y" OR FS$ = "y" THEN GOTO 720
700 REM Loading a *.spm file
702 IF FS$ = "m" THEN GOTO 720
708 PRINT " Do you want to process "; FS$: " again
(y, n)?"
709 INPUT "", REFILES
710 IF REFILES = "y" OR REFILES = "y" THEN GOTO 750
720 DIM X(4000): PRINT : PRINT: PRINT
723 INPUT "Menu of .spm file (you may type it without the
.spm extension): ", NEWFQ$
732 PRINT : PRINT
740 DGT = 1: REM Initializing at the first digit
745 WHILE CH$ <> CHR$(46) AND DGT < (LEN(NEWFQ$) + 2):
REM Up to the dot if there is one
750 CH$ = MID$(NEWFQ$, DGT, 1): REM Filename
character
755 DGT = DGT + 1
760 WEND
762 NEWFQ$ = LEFT$(NEWFQ$, DGT-2): REM Filename without
dot or extension
764 IF NEWFQ$ = FS$: THEN RETURN
765 FS$ = NEWFQ$
765 FY$ = FS$ + ".spm"
767 ON ERROR GOTO 10175
768 rem error 53
770 OPEN FS$ FOR RANDOM AS #1 LEN = 64
772 ON ERROR GOTO 0
775 FIELD #1, 64 AS A$
780 GET #1, 1
785 FOR I = 1 TO 40
790 GET #1, I
800 FOR J = 1 TO 64
810 X(I) = 64 * (I - 1) + J
820 B$ = MID$(A$, J, 1)
830 (X(I)) = ASC(B$)
840 NEXT J
845 NEXT I
850 FOR I = 1 TO PNTXS
860 N = 504 + 4 * I
870 Y(I) = X(N + 1) + 256 * (X(N + 2) + 256 * (X(N + 3)))
880 NEXT I
883 CLOSE #1
885 FOR I = 1 TO 512
886 IF Y(I) <> 0 GOTO 890
887 NEXT I
888 ERROR 53
889 ERROR GOTO 0
890 IF PR=1 THEN LPRINT : LPRINT "Data File Loaded: "; FS$: LPRINT
900 RETURN
1000 REM Raw data printout routine
1020 GOSUB 700
1040 FOR I = 1 TO 512 STEP 8
1049 ON ERROR GOTO 10300
1050 LPRINT USING "###; ";
1051 ON ERROR GOTO 0
1060 FOR J = 0 TO 7
1065 DIM A(512)
1070 A(J) = Y(I + J)
1080 LPRINT USING "##### "; A(J)
1090 IF J = 7 THEN LPRINT ""
1500 NEXT J
1510 NEXT I
1520 GOTO 70
2000 REM Processing a *.DAT file
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 "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 ";
2230 PRINT "The hyperfine splitting = 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 = the average of the spacings"
2245 IF PR=1 THEN LPRINT: LPRINT "between peaks 1-2, 2-3, 4-5, and 5-6 = "; HFS; " channels"
2255 HFSSTD = 2.245: REM Standard HFS in mm/s
2260 B = HFSSTD / HFS: REM Slope of the velocity vs. channel no. curve
2261 PRINT "The calibration constant = "; HFSSTD; "/HFS; " = "; B; " (mm/s)/channel"
2262 IF PR=1 THEN LPRINT: LPRINT "The calibration constant = "; HFSSTD; "/HFS; " = "; B; " (mm/s)/channel"
2263 PRINT " : IF PR=1 THEN LPRINT: LPRINT "The calibration constant = "; HFSSTD; "/HFS; " = "; B; " (mm/s)/channel"
2264 IF EFS = "E" THEN D = (B - EFS) / HFS: REM Use this shift in all subsequent calculations
2265 IF D = 0 THEN D = 0: REM This is to avoid division by zero
2266 IF D = 0 THEN D = 0: REM This is to avoid division by zero
2270 A = -B * ISSTD: C = 0: REM V = A + BX + CX^2; linearity assumed here
2275 REM To get the isomer shift for the sample
2282 READPK$ = DATS
2285 IF EFS = "E" OR EFS = "e" THEN GO SUB 12600
2287 IF EFS = "E" OR EFS = "e" THEN GO SUB 2600
2290 IS = B*(PEAK - ISSSTD)
2295 PRINT: PRINT "Isomer shift"; VELSTD$; " for "
2296 PRINT " "; HFS$; " "; HFS$; " "; HFS$; " "; HFS$; " "; HFS$;
2297 PRINT:PRINT: PRINT " "; B; "X(1);PEAK; " - " ; ISSSTD; ");"
2300 IF PR=1 THEN LPRINT: LPRINT "Isomer shift"; VELSTD$; "; for "; HFS$; "; "
2301 IF PR=1 THEN LPRINT " "; B; "X(1);PEAK; " - " ; ISSSTD; " "; IS; " "; mm/s
2310 PRINT: PRINT " Do you want an extra x and y scale?"
2320 PRINT " "; REPEATSTD$ = "Y" OR REPEATSTD$ = "y";
2330 PRINT " "; (answer "; CHRS(34); "; n"; ";"
2340 PRINT " "; CHRS(34); "; for a plot being"
2345 PRINT " prepared for publication"
2350 PRINT " "; (y, n)
2360 IF SS$ = "n" OR SCALES$ = "N" THEN ITMS$ = "PUBS"
2365 IF YS = 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 PRINT " "; automatically-maximized scale (y, ";"
2405 REPEATSC$ = "Y" OR REPEATSC$ = "y"
2410 PRINT " "; GOSUB 6029
2500 OPEN DAT$ FOR INPUT AS #2
2505 ENDFK$ = "CAL FIT": REM For theoretical points
2510 GO SUB 2800
2520 CLOSE #2
2590 ITMS$ = "Y": GOTO 4618
2600 REM Reading peak positions and calculating average
2603 ON ERROR GOTO 10225
2605 OPEN READPK$ FOR INPUT AS #3
2606 ON ERROR GOTO 0
2610 JUNK$ = ""
2615 WHILE RIGHTS(JUNK$, 6) <> "TO 0.5"
2620 READLINE INPUT #3, JUNK$
2621 WEND
2625 INPUT #3, JUNK$
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))
2663 INPUT #3, PK(1): INPUT #3, JUNK$: INPUT #3, JUNK$
2665 NEXT I
2666 CLOSE #3
2670 PEAK = 0
2675 FOR I = (4 - (N/2)) TO (3 + (N/2))
2680 INPUT #3, JUNK$
2685 NEXT I
2690 NEXT I
2691 PEAK = PEAK / N: REM Isomer shift = avg. of N positions
2699 RETURN
REM Reading the converged baseline value
3030 FR$ = FQ$ + INP.
REM
2925 "INP": REM
2920 'if (y(i)=O) and (y(i-1)=O) goto 2920
2910 next i:
2898 'if (y(i)=O) and (y(i-1)=O) goto 2920
2890 INPUT #2, Y(1)
2870 I = 1: Y(O) = 1
2860
2830 JUNKS =
2750 INPUT #2, JUNK_
2710 JUNKS =
2700 REM Reading the converged baseline value
3175 NEXT I
3170 FOR I = 1 TO PNTS% + 1
3165 PRINT #I, USING "######. "; Y(I + J);
5)/16)); I;
3120 LSET EORF$ =
3100 FOR K = 1 TO N
3080 'print: print "; Y(I-1) = ";
3070 PRINT : PRINT "Velocity formula calculation:"
3050 PRINT : PRINT "A file is being saved suitable for input into the MOSS program." The new filename will be named : FR$
3052 IF PS <> "" THEN GOTO 3700
3060 PRINT "Type any description you wish to add to the filename (< 64 characters):"
3070 PRINT "How many lines in the spectrum? n
3090 PRINT "Enter estimated parameters (ENTER for zero spacers):" GOSUB 5100
3100 OPEN FR$ FOR OUTPUT AS #1
3120 LSET EORFS = CHR$(13) + CHR$(10): REM Carriage retn.
3121 Y(J) = STR$(Y(I05)): REM Counts in channel 105 used as a sample
3130 REM The next line strips the space added by STR$ from the left
3122 REM The next line strips the space added by STR$ from the left
3123 Y(J) = RIGHT$(Y(J), LEN(Y(J)) - 1)
3124 IF LEN(Y(J)) = 7 THEN GOSUB 3500: REM For stripping off the first 1
3140 PRINT #1, "(10F7.0)"
3145 PRINT #1, CHR$(35): FR$: = " "; DESCFS
3150 PRINT #1, USING "####.": PNTS%; (15 + INT(PNTS% -
3155 PRINT #1, " ";
3160 PRINT #1, USING "####.": ; B3;
3165 FOR I = 1 TO N
3167 AREA(I) = ABS(AREA(I))
3170 PRINT #1, USING "####.": ; AREA(I);
3175 IF (I+1) = 7 THEN PRINT #1, EORFS
3180 FOR J = 1 TO N
3184 PRINT #1, USING "####.": LWEJ;
3186 IF (I+N+J) = 7 OR (1+N+J) = 14 OR (1+N+J) = 21
3188 NEXT J
3192 FOR K = 1 TO N
3194 PRINT #1, USING "####.": NRG(K);
3196 IF (I+(2*N)+K) = 7 OR (1+(2*N)+K) = 14 OR
3198 NEXT K
3200 FOR I = 1 TO PNTS% STEP 10
3205 FOR J = 0 TO 9
3210 IF (I + J) > PNTS% GOTO 3300
3215 'print: print "; I; " Y(I) = ";
3216 Y(I) = (Y(I-1) - Y(I-1)); Y(I-1) = "; Y(I-1) = ";
3219 'print: print " PNTS% = "; PNTS% = "; PNTS%
3230 PRINT #1, USING "####.": Y(I + J);
3240 IF J = 9 THEN PRINT #1, EORFS
3250 NEXT J
3260 NEXT I
3300 REM The following are NBAD(I), the channel numbers to be omitted by MOSS
3310 PRINT #1, EORFS
3320 FOR I = 1 TO 14: REM Discarding the 1st 14 points(non-data)
3340 PRINT #1, USING "####.": I;
3350 NEXT I
3360 PRINT #1, EORFS
3365 K = 0: REM Counter for 14-digit lines
3370 FOR I = 16 TO PNTS% STEP 16
3380 PRINT #1, USING "####.": I;
3385 K = K + 1
3390 IF INT(K/14) = (K/14) THEN PRINT #1, EORFS
3400 NEXT I
3470 CLOSE #1
3480 FR$ = " ";
3490 GOSUB 10000
3495 GOTO 70
3500 REM Routine for handling 7-digit counts
3510 YADDX = 1
3540 FOR I = 1 TO 512
3550 Y$ = STR$(Y(I))
3560 REM The next line strips the space added by STR$ AND the 1 from the left
3570 Y$ = RIGHTS(Y$, LEN(Y$) - 2)
3580 Y(I) = VAL (Y$)
3590 NEXT I
3600 RETURN
3700 PRINT: PRINT "Would you like "; CHR$(34); P$; CHR$(34)
3710 INPUT " to be printed as a description in the file"; PAGAINS
3720 IF PAGAINS = "Y" OR PAGAINS = "Y" THEN DESCFS = P$:
3730 GOTO 3080
3730 GOTO 3060
4000 REM Velocity formula calculation
4005 'print "PROGRAM ASSUMES 512 CHANNELS, FLYBACK MODE"
4100 'print "LASER MULTIPLEXES INTO EVERY 16TH CHANNEL"
4140 'print "TIMING INFO. ASSUMED:"";
4145 'print "CH 9, ZERO VEL. IN CH 264"
4150 'print "IF NOT, CHANGE DATA IN LINE 4160."
4159 'print "PRINT: PRINT "Velocity formula calculation:"
4160 A7 = 9: A9 = 264
4170 N = 0: A0 = 0: A1 = 0: A2 = 0: A3 = 0: A4 = 0: A5 = 0: A6 = 0
4180 REM STARTING AND ENDING CH. NOS. ARE 11% AND 72%
4190 TRUE = 95: T2K = 432: REM, 8/95, Setup B reliable only in this range
4200 M1 = Y(9)
4240 B1 = 7.91024B
4250 FOR X = 11% TO 12% STEP 16
4260 M = Y(X)
4300 M = M * B1 / M1
5300 FOR X = 11% TO T2%: REM Initializing Y(X)
5301 Y(X) = 0
5302 NEXT X
5303 FOR X = 11% TO T2%
5304 Y(X) = Y(X) + YY(I) / (1 + (X - YY(N + I)) + X - YY(N + I)) / (YY(2 * N + I) * YY(2 * N + I))
5305 NEXT I
5306 Y(X) = B3 - Y(X)
5307 NEXT X
5308 RETURN

6000 REM PLOT ROUTINE FOR HP 7440A COLORPRO PLOTTER
6010 PRINT "PRINT: PRINT: PRINT: PRINT"
6021 IF ITEMS = "I" THEN CLS: PRINT " Enter a title to be printed at the top: ", FSS$: GOTO 6031
6022 IF ITEMS = "M" THEN INPUT " upper left above the plot: ", FSS$: GOTO 6031
6025 GOSUB 700
6185 GOSUB 9000: REM for plotter setup codes
6186 IF ITEMS = "S" THEN GOTO 7000
6188 PRINT#1, "SP1"
6200 REM y axis scales
6205 T1K = 17
6210 IF ITEMS = "T1" AND ITEMS = "6" AND ITEMS = "CAL6" AND ITEMS = "PUBL" THEN GOSUB 11000
6220 IF ITEMS = "T1" OR ITEMS = "6" OR ITEMS = "CAL6" OR ITEMS = "PUBL" THEN MAXCNT = B3: GOSUB 11065
6290 REM for x axes
6295 IF ITEMS = "T1" OR ITEMS = "4" OR ITEMS = "6" THEN GOTO 6340
6300 P6 = -P6
6301 PRINT "At line 6301, P4 = "; P4; "; and P6 = "; P6
6302 'while inkey$ = ""
6303 'wend
6321 F3 = V(PNTS%): V(T1K): REM for scaling x axis
6322 REM F3 = B*(PNTS%*T1K) + C*(PNTS%*2020): REM Collins had F3 from 25 to PNTS%
6323 WHILE P6 <= P4: REM New x-axis velocity labelling routine
6324 GOSUB 8600
6325 P6 = P6 + P5
6326 WEND: IF ITEMS = "PUBL" GOTO 6360
6327 'FOR X = T1K TO T2K: REM Collins' routine
6330 'IF (VX) - P6 >= 0 THEN GOSUB 8900: REM x axis labelling with velocity
6335 NEXT X
6340 PNTS2% = PNTS% - (PNTS MOD 8)
6345 FOR X = PNTS2% / 8 TO PNTS% STEP PNTS2% / 8
6351 IF ITEMS = "T1" OR ITEMS = "4" OR ITEMS = "6" THEN GOSUB 8800: REM x axis labelling in Ch. No.
6352 IF ITEMS = "T1" OR ITEMS = "CAL6" THEN GOSUB B700: REM Upper x axis labelling in Ch. No.
6355 NEXT X
6360 PRINT #1, "PA": 1000; 7500; "D11,0": "LB": "M.S.U. PHYSICS": " "; "DATES": " "; "Time": "TIME1"
6362 PRINT #1, "PA": 1000; 7200; "D11,0": "LB": "FSS": " "; "M.S.U. PHYSICS": " "; "DATES": " "; "Time": "TIME1"
6365 PRINT #1, "PA": 1500; 7000; "D11,0": "LB": "PS": " "; "M.S.U. PHYSICS": " "; "DATES": " "; "Time": "TIME1"
6367 IF ITEMS = "CAL6" THEN PRINT #1, "PA": 2000; 6800; "D11,0": "LB": "Peak isomer shift = "; IS; " mm/s "; " "; "M.S.U. PHYSICS": " "; "DATES": " "; "Time": "TIME1"
6370 GOSUB 10000
6371 GOSUB 10000
6380 IF ITEMS = "PUBL" THEN PRINT #1, "PA 10000 3500 0010,1 LBCounts": " "; " 
6382 GOSUB 10000
6384 GOSUB 10000
6390 PRINT #1, "PA 400 3000 D11,0 LBPercent Absorption": " "; " 
6392 GOSUB 10000
6394 GOSUB 10000
6395 IF ITEMS = "T1" OR ITEMS = "4" OR ITEMS = "6" THEN GOTO 6440
6400 PRINT #1, "PA 3000 1400 D11,0 LBVelocity in mm/sec": "VELSTD$
6405 GOSUB 10000
6410 GOSUB 10000
6415 GOSUB 10000
6420 IF ITEMS = "PUBL" AND ITEMS = "4" THEN PRINT #1, "PA 4000 6400 D11,0 LBChannel Number"
6425 GOSUB 10000
6430 GOSUB 10000
6435 GOSUB 10000: GOTO 7000
6440 PRINT #1, "PA 4000 1400 D11,0 LBChannel Number"
6450 GOSUB 10000
6460 GOSUB 10000
6470 GOSUB 10000
7000 REM Point or curve plotting routine, from 61B6, 6435, or 6470
7010 FOR X = T1K TO PNTS%
7020 IF ITEMS = "T1" THEN GOTO 7030
7022 REM G(X), no interf. calibr.
7023 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
7055 IF P6 - ABS(VX(X)) >= 0 THEN G(X) = 5000 + INT(8000 * VX(X) / F3)
7561 'print "At line 7561, X = "; X; "; VX(X) = "; VX(X); "; and G(X) = "; G(X)
7562 'while inkey$ = ""
7563 'wend
7570 GOTO 7570
7570 GOTO 7570
7580 YF = (Y(X) * CF83 / B3: REM CF83 = OldB3/Y$: see line 11410
7585 M(X) = IDN + (((IUP - IDN) / (CFUP - CFDN)) * (YF - CFDN))
7587 NEXT X
7590 IF ITEMS = "T1" OR ITEMS = "S" THEN PRINT #1, "SP4": GOSUB 10000: REM Pen 4 for curve
7591 FOR X = T1K TO PNTS%: REM Plotting
7592 IF M(X) > 6000 OR M(X) < 2000 GOTO 7580
7595 IF G(X) < 1000 OR G(X) > 9000 THEN 7580
7596 IF ITEMS = "4" OR ITEMS = "4" OR ITEMS = "6" OR ITEMS = "CAL6" OR ITEMS = "PUBL6" THEN PRINT #1, "PA;"
7599 PRINT #1, "PA; G(X); M(X); "PD": REM for points
7600 PRINT #1, "PA; G(X); M(X); "PD": REM for curve
7605 NEXT X
7607 PRINT #1, "SPD;"
7608 CLOSE #1: CLOSE #2
7610 IF ITEMS = "6" OR ITEMS = "CAL6" OR ITEMS = "PUBL6" THEN RETURN: REM to 2500
7630 ERASE YY, BB, ZZ, GG, AA, AREA1, LW1, NRG1: GOTO 70
8600 REM Subroutine from 6324 for lower x axis labelling in mm/s
8610 I = 5000 + (8000 * (P6 - P2) / F3)
8620 IF I < 1000 OR I > 9000 THEN RETURN
8630 PRINT #1, "PA; I; 2000; "PD": I; 2100; "PD"
8640 PRINT #1, "PA; I - 100; 1800; "D11,0"; "LB": P6; " 
8650 GOSUB 10000
8660 GOSUB 10000
8670 RETURN
8700 REM Subroutine from 6352 for upper x axis labelling in Ch. No.
8710 I = 5000 + (8000 * (VX(X) - P2) / F3): REM Same as 8905, but no "INT"
8720 IF I < 1000 OR I > 9000 THEN RETURN
8730 PRINT #1, "PA; I; 6000; "PD": I; 5900; "PD"
8740 PRINT #1, "PA; I - 250; 6200; "D11,0"; "LB": X; " 
8750 GOSUB 10000
8760 GOSUB 10000
8770 RETURN
8800 REM Subroutine from 6351 for lower x axis labelling in Ch. No.
8810 I = 1000 + (8000 * (X - T1) / (PNTS% - T1))
8820 IF I < 1000 OR I > 9000 THEN RETURN
8830 PRINT #1, "PA": I; 2000; "PD": I; 2100; "PD"
REM Collins' subroutine (unused) from line 6330
REM from line 6220

10100 REM F10 key event handler from line 72
10110 LOCATE 25, 1;
10120 INPUT "Return to menu (yes, no)"; akey$  
10130 IF akey$ = "Y" OR akey$ = "y" THEN ERASE YY, BB, ZZ,  
10140 FOR J = 1 TO 10000  
10150 IF J = 1 TO 30000  
10160 NEXT J  
10170 RETURN

101100 REM F5 key event handler from line 74
101165 PR = 1: RETURN

10175 REM error handler for FS$ (line 770)
10180 BEEP: PRINT "FILE NOT FOUND"
10185 PRINT "(F10 to return to menu)"
10190 PRINT: RESUME 730

10200 REM error handler for DAT$ (line 2020)
10205 BEEP: PRINT "FILE NOT FOUND"
10210 PRINT "(F10 to return to menu)"
10215 PRINT: RESUME 2005

10225 REM error handler for READPK$ = STDFES$ (line 2605)
10230 BEEP: PRINT "FILE NOT FOUND"
10235 PRINT "(F10 to return to menu)"
10240 PRINT: IF EFS = "E" OR EFS = "e" THEN RESUME 12070

10245 PRINT: IF EFS = "F" OR EFS = "f" THEN RESUME 2105

10250 REM error handler for STDEUS$ (line 12605)
10255 BEEP: 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 and RETURN when ready"

10325 CLOSE #5: REM Error handling from line 2636
10340 PRINT: PRINT "STANDARD RUN!"
10350 PRINT: PRINT "STDFES$; " 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 return to the menu"
10360 PRINT: PRINT: PRINT: CLOSE #5: 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%, PNTSX%, MINCNT, MAXCNT = "; T1%; PNTSX%; MINCNT; MAXCNT  
11040 FOR I = T1% TO PNTSX%  
11045 "print "I i e 1 1 0 4 5"  
11050 IF Y(I) > MAXCNT THEN MAXCNT = Y(I)  
11051 "print: print "For I = "; I; " "; Y(I) = ";  
11052 "MAXCNT = "; MAXCNT  
11055 "goSUB 10050: gOSUB 10050: gOSUB 10050  
11060 NEXT I  
11065 IF repeaTSCS = "Y" OR repeaTSCS = "y" THEN GOTO  
11070 REM from line 6220
11067 IF ITEM$ = "N" OR ITEM$ = "n" THEN B3 = MAXCNT  
11068 "print "MAXCNT = "; MAXCNT  
11069 "MINCNT = MAXCNT  
11070 "print: print "MINCNT = "; mincnt  
11071 "goSUB 10050: gosub 10050  
11072 FOR I = T1% TO PNTSX% STEP 16  
11080 FOR J = I TO (I + 14)  
11085 IF J > PNTSX% THEN GOTO 11120  
11090 IF Y(J) < MINCNT THEN MINCNT = Y(J)  
11095 "print: print "For J = "; J; " and J = "; j; "  
11097 Y(J) = "; y(J); " MINCNT = "; mincnt  
11098 "goSUB 10050: gosub 10050: gosub 10050  
11100 NEXT J  
11101 "print: print "For J = "; J; " and J = "; j; "  
11103 Y(J) = "; y(J); " MINCNT = "; mincnt  
11104 "goSUB 10050: gosub 10050: gosub 10050  
11110 NEXT I  
11120 MAXCNTS = STR$(MAXCNT); MINCNTS = STR$(MINCNT)
11124 REM The next line strips the space added by STR$  
11125 MAXCNTS = RIGHTS(MAXCNTS, LEN(MAXCNTS) - 1); MINCNTS = RIGHTS(MINCNTS, LEN(MINCNTS) - 1)  
11130 MAXPNT% = INSTR(MAXCNTS, "%."); MINPNT% =
INSTR(MINCNTS, ",")
11140 IF MAXPNT% = 0 THEN MAXEXP% = LEN(MAXCNTS) - 1 ELSE
MAXEXP% = MAXPNT% - 2
11150 IF MINPNT% = 0 THEN MINEXP% = LEN(MINCNTS) - 1 ELSE
MINEXP% = MINPNT% - 2
11170 IF MAXEXP% < MINEXP% THEN GOTO 11250
11180 MAXDIG% = 1: MINDIG% = 1: J = 0
11185 WHILE MAXDIG% = MAXDIG%
11190 J = J - 1
11200 MAXDIG% = VAL(MIDS(MAXCNTS, J + 1)) \ MINDIG% = VAL(MIDS(MINCNTS, J + 1))
11210 WEND
11215 IF (MAXDIG% - MINDIG%) <= 1 THEN Q% = 0 ELSE
11220 IF (MAXDIG% - MINDIG%) <= 4 THEN Q% = GOTO 11225
11225 YS = 10^((MAXEXP% - 2 - J - 0.5))
11230 CFUP$ = LEFTS(MAXCNTS, J + 0.5 - 1): CFUP = VAL(CFUP$)
+ 1
11240 CFDN$ = LEFTS(MINCNTS, J + 0.5 - 1): CFDN = VAL(CFDN$)
11250 REM Routine for wide count spread
11260 DIFF% = MAXEXP% - MINEXP%
11270 CFUP$ = LEFTS(MAXCNTS, DIFF% + 1): CFUP = VAL(CFUP$)
+ 1
11280 CFDN$ = LEFTS(MINCNTS, 1): CFDN = VAL(CFDN$)
11290 IUP = 5500: REM Highest tic on the right y axis
(counts)
11300 IDN = 2500
11305 REM IUP - IDN = 3000
11310 REM (IUP - IDN)/(CFUP - CFDN) = 3000/10 = 300
11315 IF ITEMS(1) = "PUB4" THEN GOTO 11400
11317 CFSTEP = (CFUP - CFDN)/4
11318 CFSTEP = INT(CFSTEP)
11320 FOR CF = CFDN TO CFUP STEP CFSTEP: REM Right y axis
(counts)
11322 I = IDN + (((IUP - IDN) \ (CFUP - CFDN)) \ (CF - CFDN))
11330 PRINT #1, "PA": 9000; I; "PD": 9000; I; "PU":
11340 PRINT #1, "PA": 9020; (I - 10): "D11.0": "LB";
(CF \ 10) \ "Y": "
11350 GOSUB 10000
11360 NEXT CF
11370 GOSUB 10000
11400 REM Left y axis (percent absorption)
11410 ABSNUP2 = 1 - (YS \ CFDN / 83)
11413 IF ABSNUP2 <= .02 THEN ABSNUP3 = .02: GOTO 11470
11417 IF ABSNUP2 < .05 THEN ABSNUP3 = ABSNUP2: GOTO 11470
11420 ABSNUP3 = 0: K = 1
11430 WHILE ABSNUP3 = 0
11440 ABSNUP3 = (INT(ABSNUP2 * (10 \ K))) / (10 \ K)
11450 K = K + 1
11460 WEND
11470 ABSNP = (ABSNUP3) / 4
11480 CF3$ = 83 / YS
11485 CFUP3 = (CF3$) \ (ABSNU3)
11490 IUP3 = IDN + (((IUP - IDN) \ (CFUP - CFDN)) \ (CFUP3
- CFDN))
11495 IF ABSNUP3 > .02 AND IUP3 > 2400 THEN ABSNUP3 =
ABSNU3 + ABSNP
11500 ABSN = 0
11510 WHILE ABSN <= ABSNUP3
11520 CF = (CF3$) \ (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; "D11.0": "LB"; (100 *
ABSN): "
11560 GOSUB 10000
11570 ABSN = ABSN + ABSNP
11575 IF ABSNUP3 > .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 STDEUS = "" THEN INPUT "Want to use the same Eu
and Fe standard runs for calibration"; REPEUSTD$
12030 IF REPEUSTD$ = "" OR REPEUSTD$ = "y" THEN GOTO 12090
12050 PRINT : PRINT "Name of Eu standard run for
calibrating y = 0"
12060 PRINT "("; CHR$(34); "Enter"; CHR$(34); : INPUT
"if no calibration desired): ", STDEUS$
12065 IF STDEUS = "" THEN GOTO 2410
12066 READPKS* = STDEUS: GOSUB 12600
12068 CALIBREU = PEAK
12070 PRINT : PRINT "Name of Fe standard run for
calibrating the v scale"
12080 INPUT "(do not omit this): ", STDFE$
12090 PRINT : PRINT
12100 GOTO 2135
12120 REM Reading Eu peak position (from line 12066 or 2285)
12130 ON ERROR GOTO 12250
12150 OPEN READPKS* FOR INPUT AS #4
12160 ON ERROR GOTO 0
12180 JUNK$ = ""
12190 WHILE RIGHTS$(JUNK$, 9) <> "DEVIA"
12200 LINE INPUT #4, JUNK$
12210 WEND
12240 JUNK = 0
12245 WHILE JUNK <> 4
12260 INPUT #4, JUNK$
12255 WEND
12263 INPUT #4, PEAK
12266 CLOSE #4
12287 RETURN
12290 PRINT: PRINT "This program can only process Eu and
Fe runs (press F10 to return to menu)"
122910 GOTO 2055
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.