NASA-CR-201114

FINAL REPORT
JUNE, 1996

RESEARCH ON HIGH Tc SUPERCONDUCTING COMPOUNDS

FREDERICK W. OLIVER, P.I.
Department of Physics
Morgan State University
Baltimore, Maryland 21239
410-319-3033

NASA GRANT NAG 5-2375

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 $Bi_2Ca_{0.5}Eu_{0.5}Sr_2Cu_2O_x$ and $EuBa_2Cu_3O_{7-x}$.

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 .69 ± 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 .73 mm/s ±0.02 for all samples made. One of these was irradiated with 3.5 x 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 EuF_3. Results from these investigations were reported previously to NASA in the various annual reports(4,5,6).

TABLE 1.

Pellet	Tc(K)	Transition Width (K)
CCD	92.1	0.2
BBC	96.1	0.5
BBB	95.0	1.4
ABB	102.7	1.0
BBA	94.4	1.4

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.

Sample	L.W. (mm/s) (± .05)	L.W. Ratio	I.S. (mm/s) (± .02)
EuF_3	2.90	1.00	0.00
BBC	2.67	0.92	0.74
BBA	2.83	0.98	0.77
BBB	2.92	0.99	0.69
BAB	2.58	0.89	0.78
CCD	2.66	0.92	0.70
ABB	2.61	0.90	0.69

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 3.5×10^{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 3.

Sample	Linewidth Ratio	Isomer shift(mm/s)
EuF_3	1	0
$EuBa_2Cu_3O_{7-x}$	.90 ± .05	.82 ± .01
$EuBa_2Cu_3O_{7-x}$ (Irradiated)	.85 ± .05	.94 ± .01

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 theorys 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

1. Oliver, F.W., Hoffman, E., Tarleton, D., May, L.,Violet,C.E., and Seehra,M.S.," ^{151}Eu Mossbauer Investigation on a Bismuth High-Tc Superconductor", Bull. of the A.P.S. ,Vol.40, No. 2(1995)p998.

2. Oliver, F.W., May, L., and Violet, C.E., " Mossbauer Studies on High Temperature Superconductors", Proceedings of the HBCU Workshop on the Physics of Materials and Materials Science, October 13-15, 1994.

3. Oliver, F.W., Hoffman, E., Seifu,D., Hammond, E., Pierre, F., Kureishy, Z., Howard, J., and Wynter, C.,"A Mossbauer Study of the Effects of Neutron Irradiation on a High Temperature Superconductor", Bull of the A.P.S., Vol. 41, No.1 (1996)p340.

4. Oliver, F.W., NASA Annual Report, October 1, 1993 - September 30, 1994.

5. Oliver, F.W., NASA Status Report, October 1, 1994-February 28, 1995, Grant NAG 5-2375.

6. Oliver, F.W., NASA Status Report, March 1, 1995-November 30, 1995, Grant NAG 5-2375.

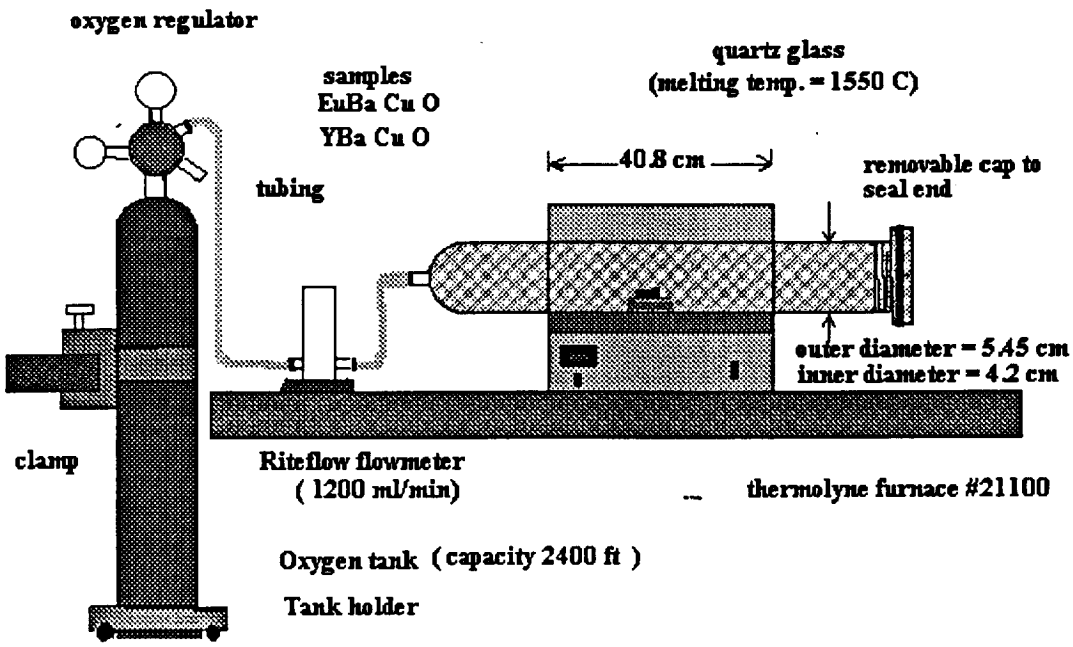
7. Edwards, M.A., Howard, J.W., private communication.

8. Edwards, M.A., Howard, J.W., Radcliffe, D., Wynter, C.I., Oliver, F.W., et al., (To be submitted to Physica C).

9. Blackstead, H.A., and Dow, J.D., JETP Lett., Vol. 59, 283(1994).

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

11. Cost, J. R., Willis, J. O., Thompson, J.D., and Peterson, D.E., Phys. rev. B, Vol. 37, No. 4, 1563(1988).



Setup for the sintering and annealing process for producing superconductors

Figure 1.

BLOCK DIAGRAM OF MOSSBAUER SPECTROMETER

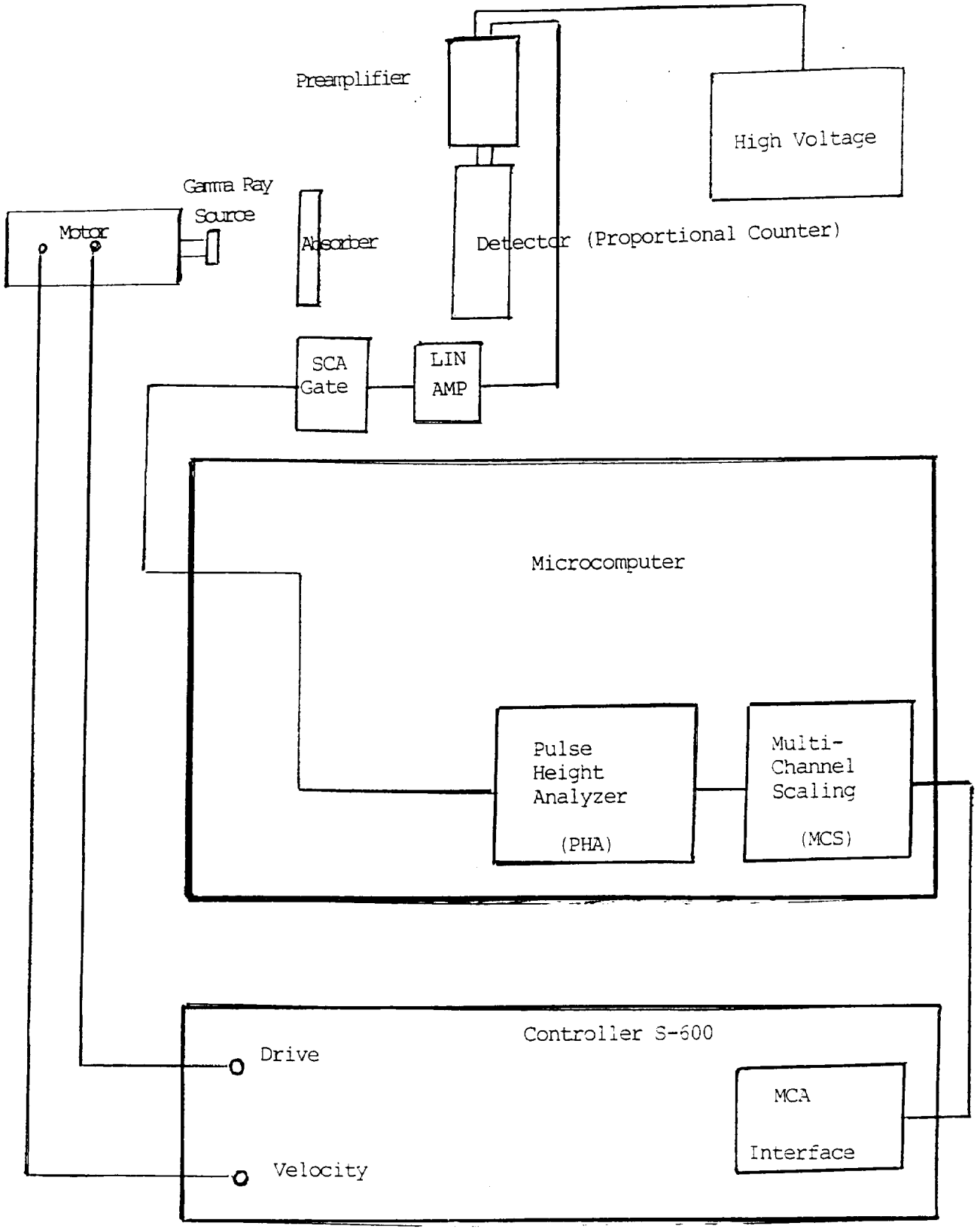


Figure 2.

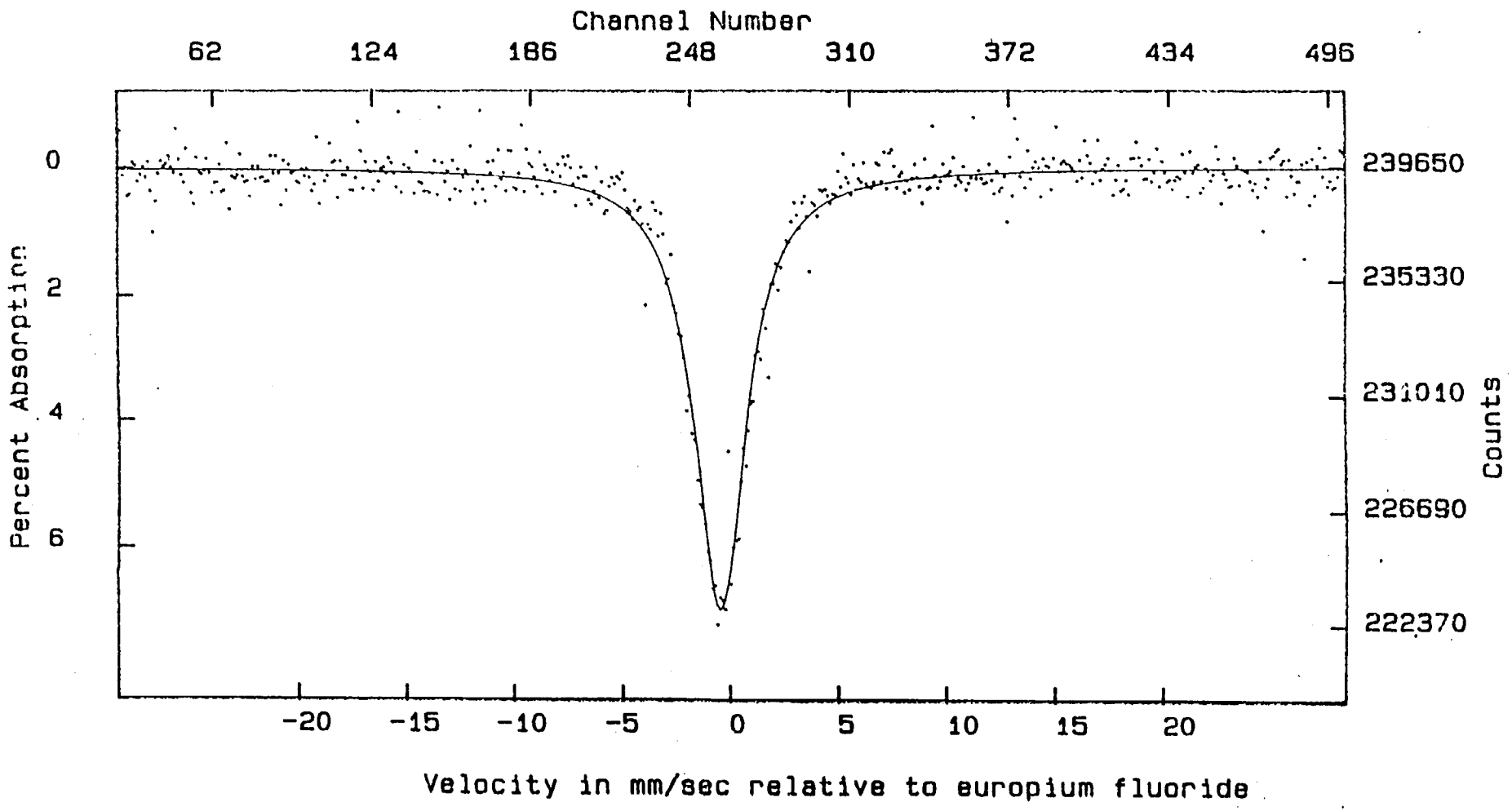

M.S.U. PHYSICS 08-16-1995 Time: 10:31:40
Superconductor BBB
Channel Number
62
124
186
248
310
372
434
496
Percent Absorption
0
2
4
6
239650
235330
231010
226690
222370
Counts
-20
-15
-10
-5
0
5
10
15
20
Velocity in mm/sec relative to europium fluoride

Figure 3.

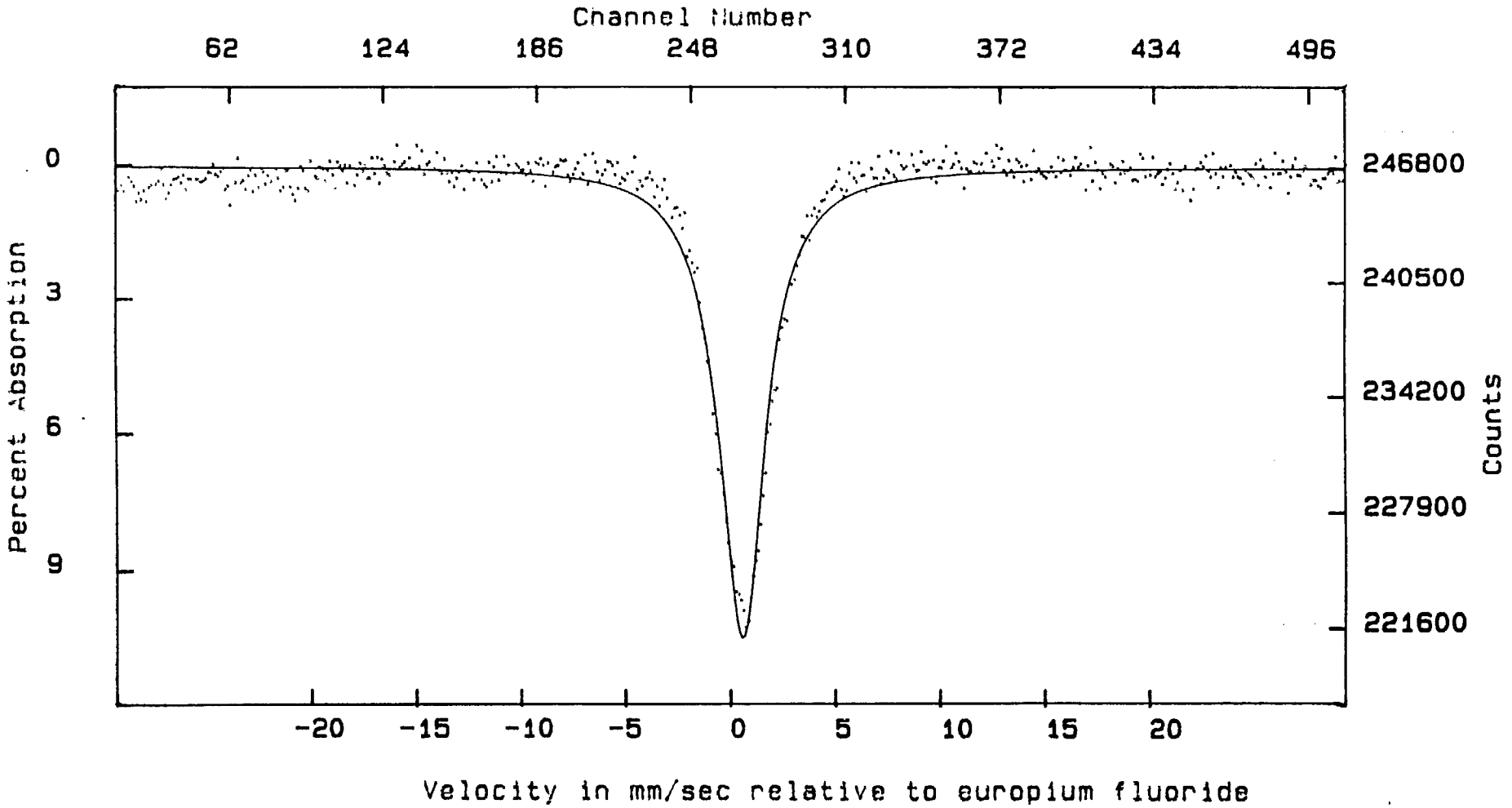

M.S.U. PHYSICS 08-18-1995 Time: 14: 46: 42
Superconductor CCD
Channel Number
62
124
186
248
310
372
434
496
0
3
6
9
Percent Absorption
246800
240500
234200
227900
221600
Counts
-20
-15
-10
-5
0
5
10
15
20
Velocity in mm/sec relative to europium fluoride

Figure 4.

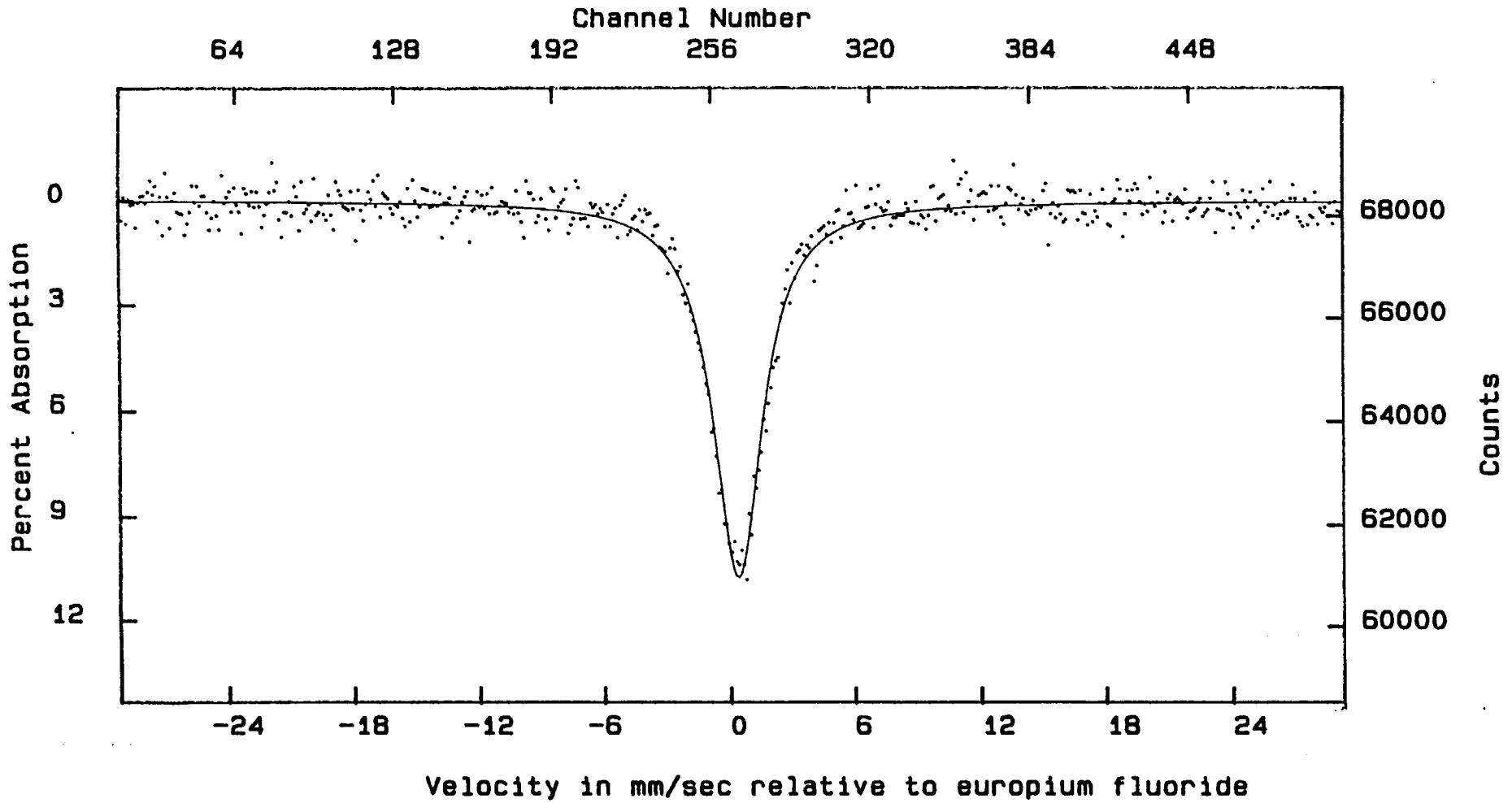

M.S.U. PHYSICS 08-15-1995 Time: 16: 45: 12
Superconductor BBA
Channel Number
64
128
192
256
320
384
448
0
3
6
9
12
Percent Absorption
68000
66000
64000
62000
60000
Counts
-24
-18
-12
-6
0
6
12
18
24
Velocity in mm/sec relative to europium fluoride

Figure 5

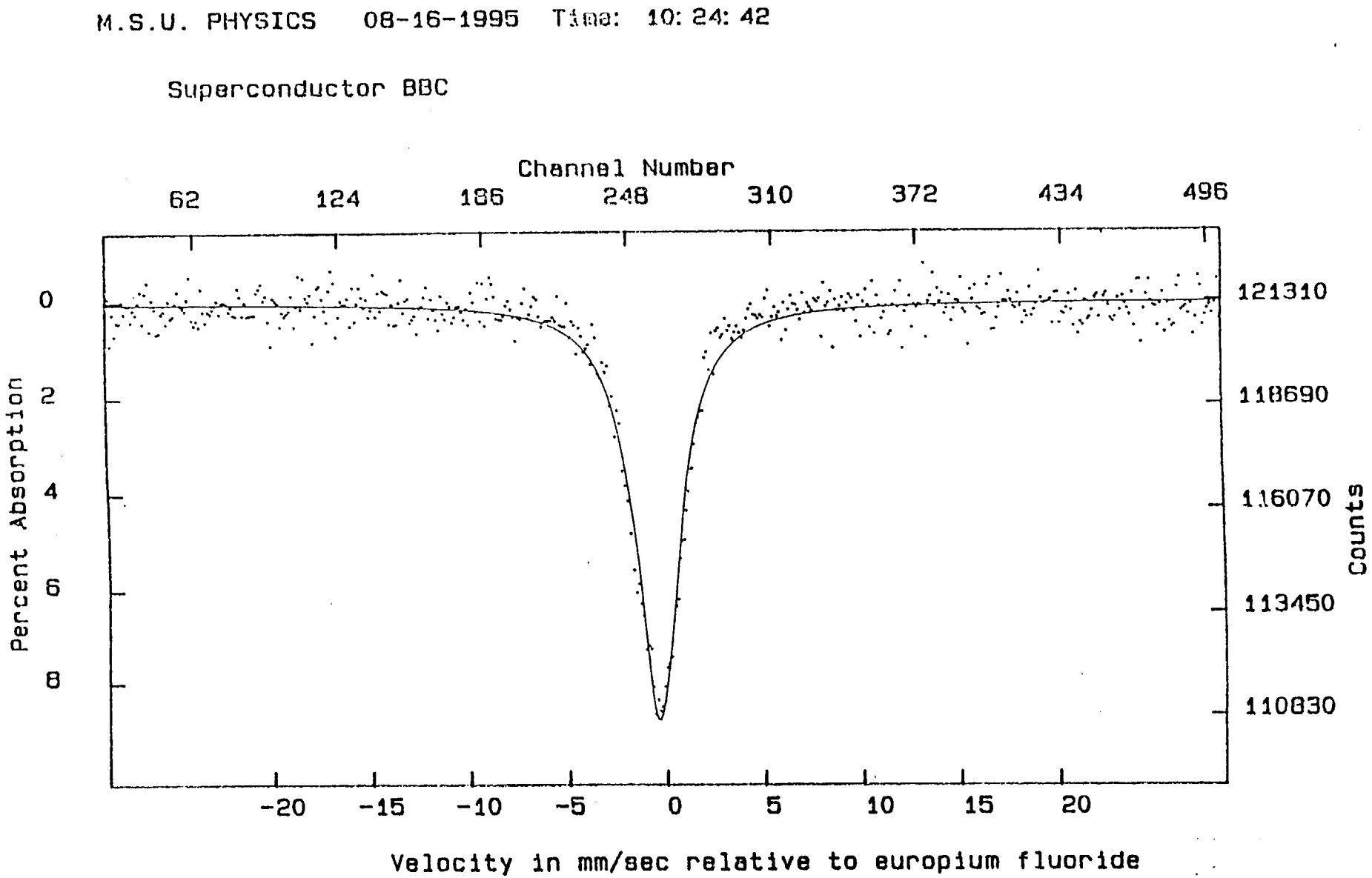

M.S.U. PHYSICS 08-16-1995 Time: 10:24:42
Superconductor BBC
Channel Number
62
124
186
248
310
372
434
496
0
2
4
6
8
Percent Absorption
121310
118690
116070
113450
110830
Counts
-20
-15
-10
-5
0
5
10
15
20
Velocity in mm/sec relative to europium fluoride

Figure 6

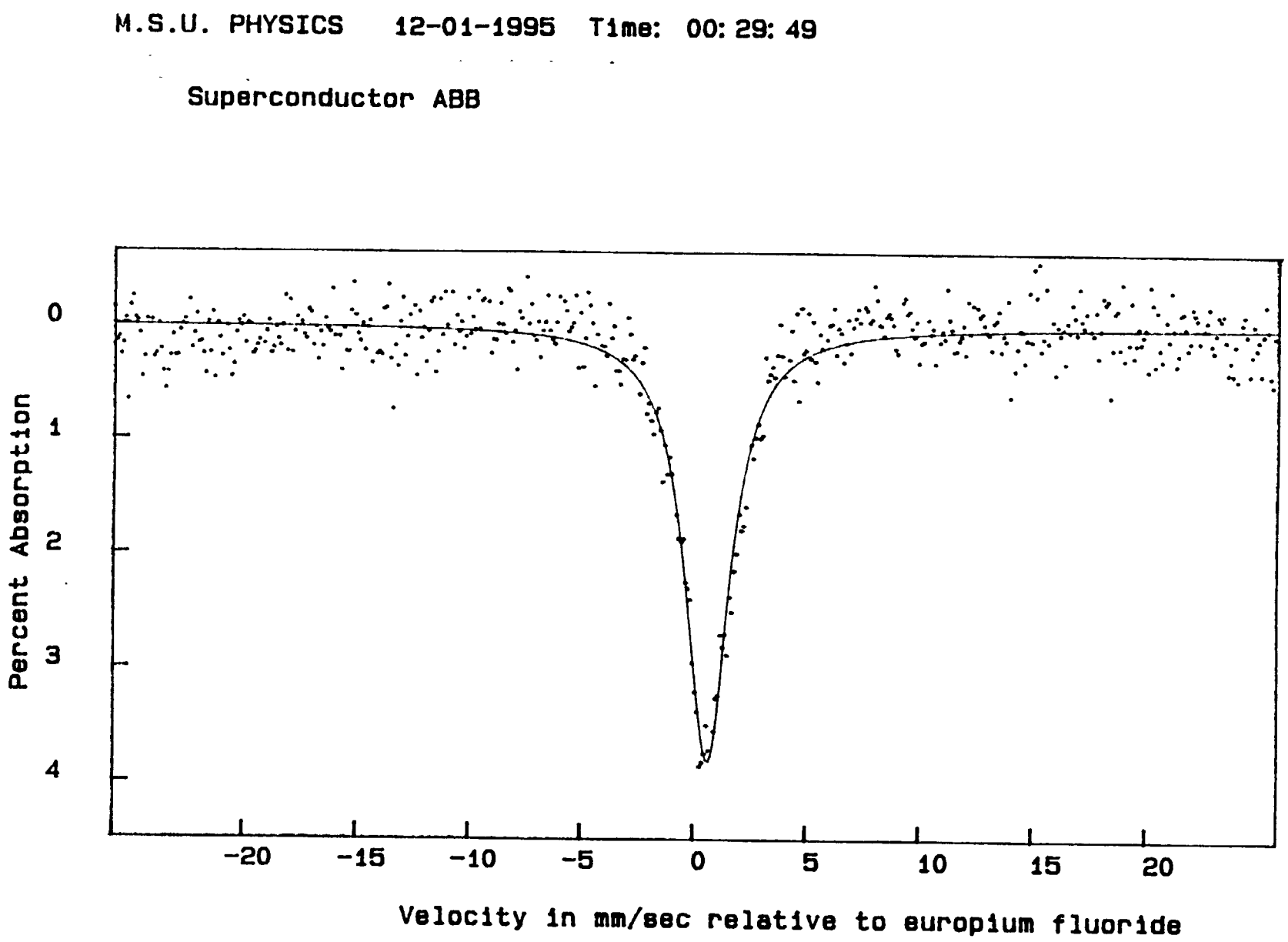

M.S.U. PHYSICS 12-01-1995 Time: 00: 29: 49
Superconductor ABB
Percent Absorption
0
1
2
3
4
-20
-15
-10
-5
0
5
10
15
20
Velocity in mm/sec relative to europium fluoride

Figure 7.

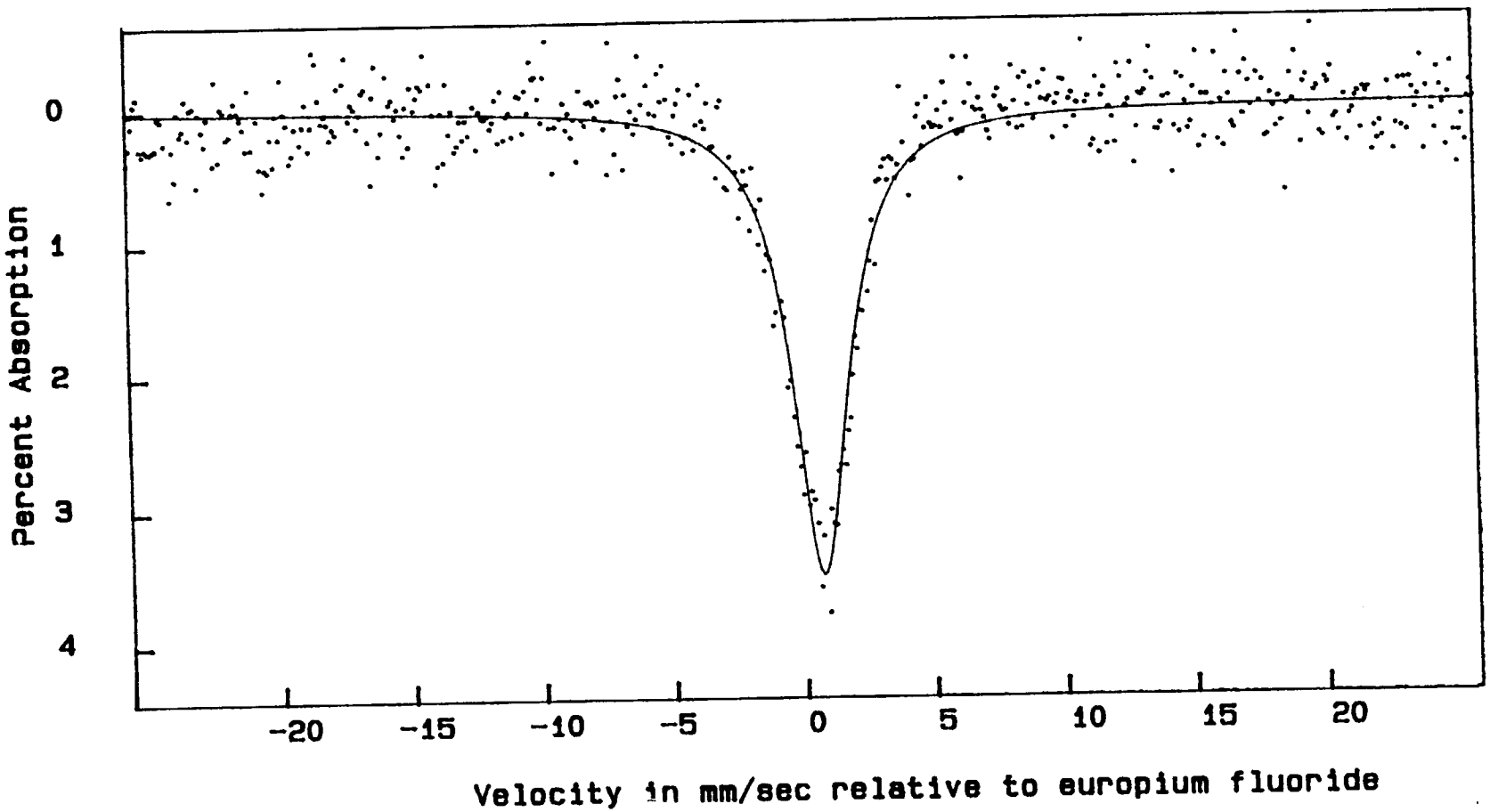

M.S.U. PHYSICS 12-01-1995 Time: 00: 48: 03
Superconductor ABB (irradiated)
Percent Absorption
0
1
2
3
4
-20
-15
-10
-5
0
5
10
15
20
Velocity in mm/sec relative to europium fluoride

Figure 8.

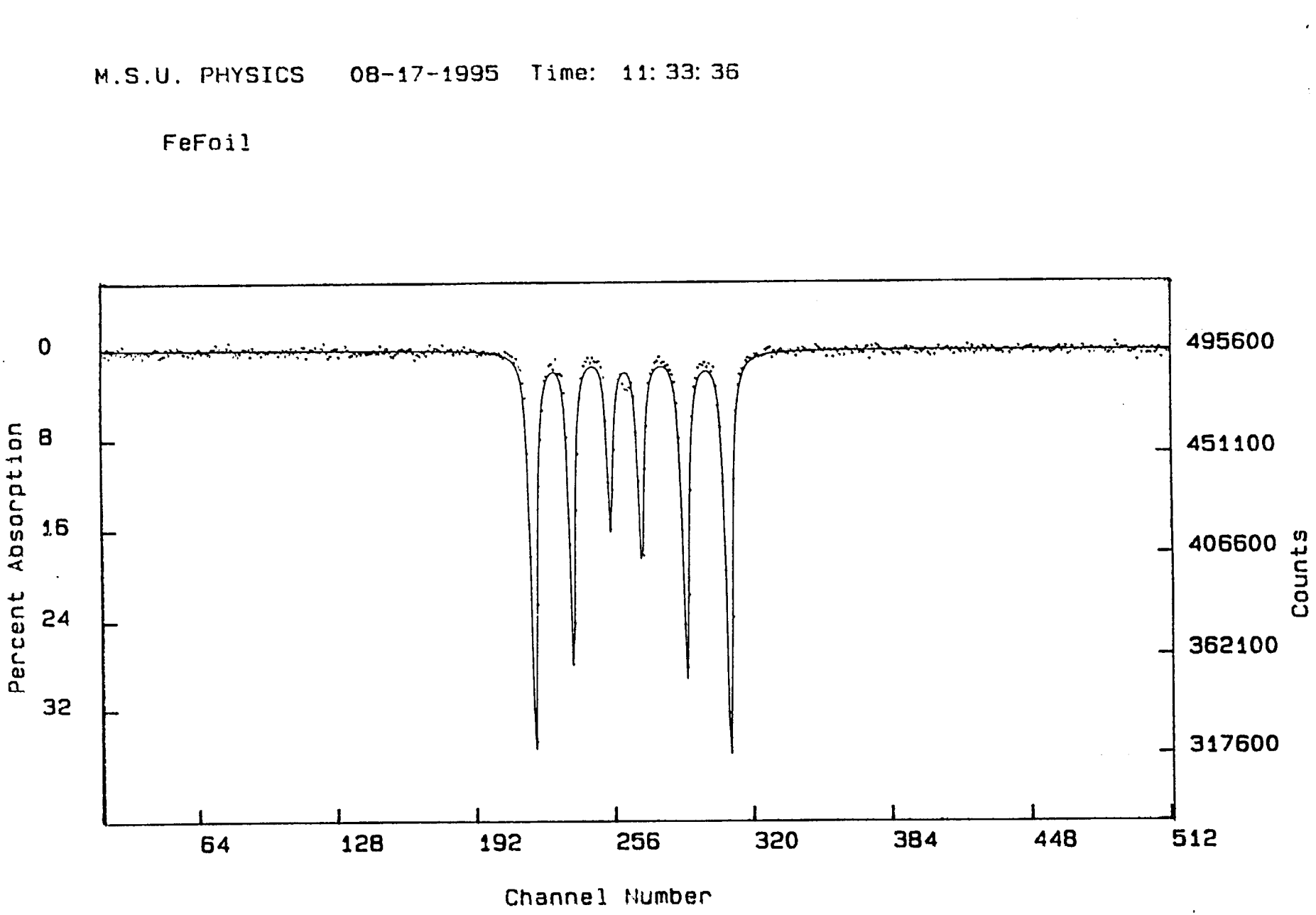

M.S.U. PHYSICS 08-17-1995 Time: 11:33:36
FeFoil
Percent Absorption
0
8
16
24
32
Counts
495600
451100
406600
362100
317600
64
128
192
256
320
384
448
512
Channel Number

Figure 9.

APPENDIX A - PAPERS PRESENTED

10:00
I10 11

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, *Northwestern 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 $\phi < 60°$ and also for $\phi \approx 125°$, 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-9314025 and DMR-9311918.

10:12
I10 12 Theory of Pulsed NMR Studies in Solid D_2 T. DINESEN, B. C. SANCTUARY, Mc. Gill U. and H. MEYER, Duke U. Density matrix theory is used to calculate the response signal of o-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[1] 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 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 τ between the pulses and their respective phases Φ, is compared with that observed[1] for several D_2 crystals of various J=1 concentrations. We also discuss the satellite echoes, predicted for the I=2 system, which have been observed[2] in D_2 adsorbed on MgO but not[1] in solid D_2.

1) I.Yu et al., J. Low Temp. Physics **51**, 369 (1983) for H_2.
D. Clarkson, X. Qin and H. Meyer, J. Low Temp. Physics **91**, 119 (1993) for D_2.
2) M.P. Volz et al. Phys. Rev. Lett. **63**, 2582 (1989)

SESSION I11: DAMOP: ATOMIC AND MOLECULAR STRUCTURE AND SPECTROSCOPY

Thursday morning, 20 April 1995
Room 3 at 8:00
R. Pratt, presiding

8:00
I11 1 **Rovibronic Spectroscopy of the Ethoxy Radical in a Supersonic Jet Environment** PRABHAKAR MISRA, *Howard University* — The ethoxy (C_2H_5O) radical is generated as a chemical intermediate in combustion and atmospheric processes. It belongs to the C_s point group and has 18 fundamental vibrational frequencies. C_2H_5O was produced in situ by photolyzing freshly synthesized C_2H_5ONO in a pulsed supersonic expansion with KrF (@ 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_2H_5O 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_2H_5O radical.

*Supported by EPA grant R81-9720-010, NASA grant NAG3-1677 and CSTEA (NAGW-2950).

8:12
I11 2 ^{151}Eu Mössbauer Investigation on a Bismuth High-T_c Superconductor. F. W. Oliver, E. Hoffman, D. Tarleton, Morgan State Univ., L. May, The Catholic Uni. of America, C.E. Violet, LLNL, and M. S. Seehra, West Virginia Univ. We report on Mössbauer studies on Bismuth high -temperature superconductors with a particular emphasis on our findings on the superconductor $Bi_2Ca_{0.5}Eu_{0.5}Sr_2Cu_2O_x$ using ^{151}Eu. Magnetic susceptibility measurements show a transition temperature of 87 K. Mössbauer 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
I11 3

Microwave Dielectric Behavior of Transition Metal Oxides. J. N. DAHIYA, Southeast Missouri State University.--A microwave resonant cavity in the TE_{011} 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
I11 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 $\Phi=h/2e$. (1,2) 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, $-i(h/2\pi)\nabla$ becoming $-i(h/2\pi)\nabla-qA$ (where A is the vector potential). Following Feynman (3), a wave function written as $\Psi(r)=[\rho(r)]^{1/2}\exp[i\theta(r)]$ leads to a current density $J=(h/2\pi m)(\nabla\theta-(2\pi q/h)A)\rho$ or $mv=(h/2\pi)\nabla\theta-qA$. On integrating this last equation along the displacement between turning points of the motion, the magnetic flux Φ 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 $O_h^7 \rightarrow O^{6,7}$ transformations.

H31 115 Growth Induced Alignment and Assignment of the Vibrational Modes of C in AlGaAs.* 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 AlGaAs near 600 cm^{-1} have been assigned to the vibrations of C_{As}.[1,2] The complexity of this spectrum has prevented the assignment of the vibrational bands to specific C_{As} modes that are associated with different numbers of Al neighbors, although considerable progress has been made[2] toward understanding C_{As} by studying the C-H complexes in hydrogenated AlGaAs. We have recently discovered that the vibrational absorption due to C_{As} in AlGaAs 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 $(C_{As})_2$-H complex in epitaxial GaAs. We assign the polarized absorption bands in AlGaAs to C_{As} 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_{As} modes.

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

1. H. Ono and N. Furuhata, Appl. Phys. Lett. 59, 1881 (1991).
2. R.E. Pritchard *et al.*, Phys. Rev. B 50, 10628 (1994).
3. Y. Cheng *et al.*, Phys. Rev. B 49, 2469 (1994).

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 $O(\frac{1}{q^2})$ divergence in the small-wavevector limit, confirming previous theoretical discussions [1].

[1]X. Gonze, Ph. Ghosez and R. W. Godby, Phys. Rev. Lett. 74, 4035 (1995)

H31 117 Dynamics of rough Ge(001) surfaces at low temperatures S. JAY CHEY, 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±0.25 eV. The dependence of the relaxation rate on the in-plane length scale is inconsistent with the continuum model of Mullins: the time constant τ of the smoothing process increases with increasing lateral length scale L as $\tau \propto L^n$, 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_2TeO_5. L.A. KAPPERS and R.H. BARTRAM, Univ. of Conn. Storrs, CT. I. FÖLDVÁRI and Á. PÉTER, Research Lab. for Crystal Physics, Budapest, Hungary. — Bismuth tellurite is a new non-linear 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 5 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_2TeO_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).

1. I. Földvári, H. Liu, R.C. Powell and A. Péter, J. Appl. Phys. 71, 5465 (1992); and Opt. Mater. 2.175 (1993).
2. D. Mercurio, M. El Farissi, B. Frit and P. Goursat. Mat. Chem. Phys. 9, 467 (1983).

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. Kureishy, Morgan State Univ., Balto., 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[1,2]. We report on a Mössbauer investigation of neutron irradiated $EuBa_2Cu_3O_x$ using the 21.53 kev transition of ^{151}Eu. A sample was irradiated with approximately 3.5×10^{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.

1. B. Roas, B. Hensel, G. Saemann-Ischenko, and L. Schultz, Appl. Phys. Lett., 54(11), (March 1989) p.1051.
2. J.-W. Lee, H.S. Lessure, D.E. Laughlin, M.E. McHenry, and S. G. Sankar, J. O. Willis, J.R. Cost, and .M. Maley, Appl. Phys. Lett. 57(20) (November, 1990) p.2150.

Supported by NASA - NAG 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

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

E4 *The Effect of Intrinsic and Trapped Magnetic Flux Lines on the Resistive Properties of YBCO Superconductor*—G. Miller, **W. Small**, J. T. Wang, S. Tsai, W. Williams, and S. SubbaRao, Lincoln University

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)
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;
```

```
qq(k,i)=1+hh(k).*xp(k,i).^2;
qqsq(k,i)=qq(k,i).^2;
end
end

%tt = zeros(3+3*L,nd);
for i1=i0:nd;
for k1=0:L-1;
tt(1+3*k1,i1) =1./qq(1+k1,i1);
tt(2+3*k1,i1)=xp(1+k1,i1)./qqsq(1+k1,i1);
tt(3+3*k1,i1)=xpsq(1+k1,i1)./qqsq(1+k1,i1);
end
end
for i1=i0:nd;
tt(4+3*(L-1),i1)= 1;
tt(5+3*(L-1),i1)= x(i1);
tt(6+3*(L-1),i1)= x(i1).^2;
end

mm = zeros(3*L+3,3*L+3);
for n1=1:3*L+3;
  for n2=1:3*L+3;

mm(n1,n2) = sum(tt(n2,:).*tt(n1,:));

   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)*nn;

for k2=1:L;
aa(k2)     = zz(1+3.*(k2-1));
gama(k2)   = zz(2+3.*(k2-1))/(2.*aa(k2).*hh(k2));
delta(k2) =-zz(3+3.*(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
```

```
yt=(aa(1,1)./(1. + hh(1,1).*xmppsq(1,:))) + (aa(1,2)./(1. + hh(1,2).*xmppsq(2
,:))) + (aa(1,3)./(1. + hh(1,3).*xmppsq(3,:))) +(aa(1,4)./(1. + hh(1,4).*xmpp
sq(4,:))) +(aa(1,5)./(1. + hh(1,5).*xmppsq(5,:))) +(aa(1,6)./(1. + hh(1,6).*x
mppsq(6,:))) + ee + ff.*x + gg.*xsq;


chisq = sum((y - yt).^2)./(nd-L)

yp=ee + ff.*x + gg.*xsq;
xpmin = - ff./(2.*gg);
xpminsq = xpmin.^2;
ypmin = ee + ff.*xpmin + gg.*xpminsq;

if (count) <= 2
y = y - yp + ypmin;
yt = yt - yp + ypmin;
end

end

delta
gama
pp
hh
bb=1./sqrt(hh)
baseline = ee + ff.*xpmin + gg.*xpminsq

for i=1:16;
y(i)=baseline;
end;

width = bb.*(nd-1.)
peak = pp.*(nd-1.) + 1.

cal499 = 2.245 ./(((peak(2)-peak(1))+(peak(3)-peak(2))+(peak(5)-peak(4))+(pea
k(6)-peak(5))))./4.)

c499 = (peak(3) + peak(4))./2.
LW499 = bb.*(nd-1.).*cal499

x = (x - c499./nd).*cal499.*(nd-1.);
y = (y + yminbs./(ymaxbs - yminbs))./(baseline  + yminbs./(ymaxbs - yminbs));
yt= (yt+ yminbs./(ymaxbs - yminbs))./(baseline  + yminbs./(ymaxbs - yminbs));

ppc = (pp - c499./nd).*cal499.*(nd-1.);

Hypfld = ((ppc(2)-ppc(1))+(ppc(3)-ppc(2))+(ppc(5)-ppc(4))+(ppc(6)-ppc(5))).*3
6.81

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')
```

```
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
60 PRINT "                                        Welcome to":
PRINT
65 PRINT "                                      M O S S P L O
T": PRINT
66 GOSUB 10050: REM Delay
67 DIM Y(515): DIM G(515): DIM M(515): DIM V(1515)
68 FQ$ = "FQ": REM so that NEWFQ$ <>FQ$

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 NUTEM$ = "": NEWFILE$ = "": 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)": PRINT
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: ", NUTEM$
124 ITEM$ = NUTEM$
125 ON ERROR GOTO 10300
126 IF ITEM$ <> "7" AND PR=1 THEN LPRINT : LPRINT "
"; DATE$; "    "; TIME$; "   MOSSPLOT Menu Choice: ";
ITEM$: LPRINT
127 ON ERROR GOTO 0

129 PNTS% = 512: REM Item 6 may alter this
130 IF ITEM$ = "1" THEN CLS : GOTO 6000
140 IF ITEM$ = "2" THEN CLS : GOTO 1000
150 IF ITEM$ = "3" THEN CLS : GOTO 3000
155 IF ITEM$ = "4" THEN VELSTD$ = " by interferometry"
160 IF ITEM$ = "4" OR ITEM$ = "4'" THEN CLS : GOTO 6000
170 IF ITEM$ = "5" THEN CLS : BOX$ = "DRAWN": GOTO 6180
180 IF ITEM$ = "6" THEN CLS : GOTO 2000
190 IF ITEM$ = "7" THEN CLS : GOTO 600
200 GOTO 130


600 CLS
605 LOCATE 25, 2
610 INPUT "Exit MOSSPLOT (yes, no)"; EX$
620 IF EX$ = "Y" OR EX$ = "y" THEN COLOR 7,0: CLS: END
630 GOTO 70

700 REM Loading a *.spm file
702 IF FS$ = "" THEN GOTO 720
708 PRINT "       Do you want to process "; FS$; " again
(y, n)?"
709 INPUT "                                ", REFILE$
710 IF REFILE$ = "Y" OR REFILE$ = "y" THEN RETURN
720 DIM X(4000): PRINT : 'PRINT: PRINT
730 INPUT "Name of .spm file (you may type it without the
.spm extension):  ", NEWFILE$
732 PRINT : PRINT
740 DGT = 1: REM Initializing at the first digit
745 WHILE CH$ <> CHR$(46) AND DGT < (LEN(NEWFILE$) + 2):
REM Up to the dot if there is one
750       CH$ = MID$(NEWFILE$, DGT, 1): REM Filename
character
755    DGT = DGT + 1
760 WEND
762 NEWFQ$ = LEFT$(NEWFILE$, DGT-2): REM Filename without
dot or extension
764 IF NEWFQ$ = FQ$ THEN RETURN
766 FQ$ = NEWFQ$
765 FS$ = FQ$ + ".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 = 9 TO 40
790     GET #1, I
800     FOR J = 1 TO 64
810             K = 64 * (I - 1) + J
820             B$ = MID$(A$, J, 1)
830             X(K) = ASC(B$)
840     NEXT J
845 NEXT I
850 FOR I = 1 TO PNTS%
860     N = 504 + 4 * I
870     Y(I) = X(N + 1) + 256 * (X(N + 2) + 256 * X(N +
3))
880 NEXT I
883 CLOSE #1
885 FOR I = 1 TO 512
886     IF Y(I) <> 0 GOTO 890
887 NEXT I
888 ERROR 53
889 ON ERROR GOTO 0
890 IF PR=1 THEN LPRINT : LPRINT "Data File Loaded:
  "; FS$:  LPRINT
900 RETURN

1000 REM Raw data printout routine
1010 GOSUB 700
1440 FOR I = 1 TO 512 STEP 8
1449 ON ERROR GOTO 10300
1450    LPRINT USING "###"; I;
1451 ON ERROR GOTO 0
1460    FOR J = 0 TO 7
1465             DIM A(512)
1470             A(J) = Y(I + J)
1480             LPRINT USING "######## "; A(J);
1490             IF J = 7 THEN LPRINT ""
1500    NEXT J
1510 NEXT I
1520 GOTO 70

2000 REM Processing a *.DAT file
```

```
2005 INPUT "Name of source (downloaded *.DAT) file:  ",
DAT$
2010 PRINT
2015 FS$ = DAT$
2018 ON ERROR GOTO 10200
2020 OPEN DAT$ FOR INPUT AS #2
2021 ON ERROR GOTO 0
2025 ENDJUNK$ = "AL DATA": REM For experimental points
2030 GOSUB 2800
2035 GOSUB 2700: REM For baseline
2055 PRINT: PRINT "Is this a europium run or an iron run?
(Answer "; CHR$(34); "E"; CHR$(34); " or "; CHR$(34); "F";
CHR$(34); ")"
2057 INPUT "                                        ", EF$
2060 IF EF$ <> "E" AND EF$ <> "e" AND EF$ <> "F" AND EF$
<> "f" THEN GOTO 12900
2070 IF EF$ = "F" OR EF$ = "f" THEN VELSTD$ = " relative
to iron": STDEU$ = "": GOTO 2100
2071 VELSTD$ = " relative to europium fluoride"
2075 GOTO 12000

2100 IF STDFE$ <> "" THEN INPUT "Want to use the same Fe
standard run for calibration"; REPEATSTD$
2103 IF REPEATSTD$ = "Y" OR REPEATSTD$ = "y" THEN GOTO
2111
2105  PRINT  :  PRINT  "Name  of  Fe  standard  run  for
calibration"
2110 PRINT "     ("; CHR$(34); "Enter"; CHR$(34); : INPUT
"if no calibration desired):", STDFE$
2111 PRINT : PRINT
2130 IF STDFE$ = "" THEN GOTO 2410
2135 ITEM$ = "CAL6"
2136 IF REPEATSTD$ = "Y" OR REPEATSTD$ = "y" THEN PRINT :
GOTO 2287
2137 dim pk(10)
2140 READPK$ = STDFE$: GOSUB 2600
2150 CALIBRFE = PEAK
2155 IF VELSTD$ = " relative to iron" AND STDFE$ <> ""
THEN FS$ = FS$ + ", calibrated using " + STDFE$
2160 IF STDEU$ <> "" THEN FS$ = FS$ + ", calibrated using
" + STDEU$ + " and " + STDFE$
2170 IF PR=1 THEN LPRINT: LPRINT "Data File:      "; FS$:
LPRINT
2180 IF STDEU$ <> "" AND PR=1 THEN LPRINT "Peak of the Eu
standard run is at channel "; CALIBREU

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 "; CALIBRFE
2225 IF PR=1 THEN LPRINT : LPRINT "Peak of the Fe standard
run = the average of "; N; " positions = Channel ";
CALIBRFE
2230 PRINT : 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 "         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 : 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 : PRINT : IF PR=1 THEN LPRINT : LPRINT
2265 IF EF$ = "E" OR EF$ = "e" THEN ISSTD = CALIBREU
2267 IF EF$ = "F" OR EF$ = "f" THEN ISSTD = CALIBRFE
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$ = DAT$
2285 IF EF$ = "E" OR EF$ = "e" THEN GOSUB 12600
2287 IF EF$ = "F" OR EF$ = "f" THEN GOSUB 2600
2290 IS = B*(PEAK - ISSTD)
2295 PRINT: PRINT "Isomer shift"; VELSTD$; " for "
2296 PRINT "  "; FS$; ":"
2297 PRINT:PRINT "     "; B; "X(";PEAK ; " - "; ISSTD; ")
= "; IS; " mm/s"
2300 IF PR=1 THEN LPRINT: LPRINT "Isomer shift"; VELSTD$;
" for "; FS$; ": "
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 "                    (answer "; CHR$(34); "n";
CHR$(34); " for a plot being"
2340 PRINT "                                prepared for
publication)"
2350 INPUT "                              (y, n)"; SCALES$
2360 IF SCALES$ = "n" OR SCALES$ = "N" THEN ITEM$ = "PUB6"
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 INPUT "                 ically-maximized scale (y,
n)"; REPEATSC$
2405 PRINT : PRINT
2410 GOSUB 6029

2500 OPEN DAT$ FOR INPUT AS #2
2505 ENDJUNK$ = "CAL FIT": REM For theoretical points
2510 GOSUB 2800
2520 CLOSE #2
2590 ITEM$ = "5": GOTO 6183

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 RIGHT$(JUNK$, 6) <> "TO 0.5"
2620    LINE INPUT #3, JUNK$
2621 WEND
2623 INPUT #3, JUNK
2624 INPUT #3, JUNK
2625 INPUT #3, JUNK
2626 INPUT #3, JUNK
2627 INPUT #3, JUNK
2628 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
2680 FOR I = (4 - (N/2)) TO (3 + (N/2))
2683    INPUT #3, PK(I): INPUT #3, JUNK: INPUT #3, JUNK
2685 NEXT I
2686 CLOSE #3
2687 PEAK = 0
2688 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
```

```
2700 REM Reading the converged baseline value
2710 JUNK$ = ""
2720 WHILE RIGHT$(JUNK$, 9) <> "DEVIATION"
2730    LINE INPUT #2, JUNK$
2740 WEND
2750 INPUT #2, JUNK%
2770 INPUT #2, B3
2790 RETURN

2800 REM Read-in loops
2810 JUNK$ = ""
2820 WHILE RIGHT$(JUNK$, 7) <> ENDJUNK$
2830    LINE INPUT #2, JUNK$
2840 WEND
2850 LINE INPUT #2, JUNK$ : 'print " JUNK$ = "; JUNK$
2860 LINE INPUT #2, JUNK$ : 'print " JUNK$ = "; JUNK$
2870 I = 1: Y(0) = 1
2880 'WHILE (Y(I) <> 0) OR (Y(I-1) <> 0)
2885 FOR I = 1 TO PNTS%
2890    INPUT #2, Y(I)
2895    'print: print "       I = ";I; "       Y(I) = ";
Y(I):rem ; "    Y(I-1) = "; Y(I-1)
2896    'gosub 10050: 'gosub 10050: GOSUB 10050:  GOSUB
10050
2898    'if (y(i)=0) and (y(i-1)=0) goto 2920
2900    'I = I + 1
2910 next i: 'WEND
2911 'gosub 10050
2915    'print: print "       I = ";I; "       Y(I) = ";
Y(I); "    Y(I-1) = "; Y(I-1)
2920 'PNTS% = I - 3
2925    'print: print "      PNTS% = ";PNTS%
2930 RETURN


3000 REM To save the data as a .INP file suitable for
input into the MOSS program
3010 YADD% = 0: REM Assume 6-digit counts until line 3124
3020 GOSUB 700
3030 FR$ = FQ$ + ".INP": REM New filename is the same with
".INP" instead of ".spm"
3040 PRINT : PRINT : PRINT "           A file is being
saved suitable for input into the MOSS program."
3050 PRINT : PRINT "                                  The new
filename will be "; FR$
3052 IF P$ <> "" THEN GOTO 3700
3060 PRINT "Type any description you wish to add to the
filename (< 64 characters):"
3070 PRINT: INPUT  "  ", DESCR$
3080 PRINT : PRINT : INPUT "        How many lines in the
spectrum"; N
3090 PRINT: PRINT "     Enter estimated parameters (ENTER
for zero spacers)": GOSUB 5100
3100 OPEN FR$ FOR OUTPUT AS #1
3120 LSET EORF$ = CHR$(13) + CHR$(10): REM Carriage retn.
+ linefeed
3121 YIJ$ = 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 YIJ$ = RIGHT$(YIJ$, LEN(YIJ$) - 1)
3124 IF LEN(YIJ$) = 7 THEN GOSUB 3500: REM For stripping
off the first 1

3140 PRINT #1, "1     (10F7.0)"
3145 PRINT #1, CHR$(35); FQ$; "  "; DESCR$
3150 PRINT #1, USING "#####"; PNTS%; (15 + INT((PNTS% -
5)/16)); 1; N; (3*N + 1); 0; 0; 0; 1; 1; 1; 0; 0; YADD%;
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);
3173    IF (1+I) = 7 THEN PRINT #1, EORF$
3175 NEXT I
3182 FOR J = 1 TO N
3184    PRINT #1, USING "##.#      "; LW!(J);
3186    IF (1+N+J) = 7 OR (1+N+J) = 14  OR (1+N+J) = 21
THEN PRINT #1, EORF$
3188 NEXT J
3192 FOR K = 1 TO N
3194    PRINT #1, USING "###.      "; NRG!(K);
3196      IF (1+(2*N)+K) = 7 OR (1+(2*N)+K) = 14 OR
(1+(2*N)+K) = 21 OR K = N THEN PRINT #1, EORF$
3198 NEXT K

3200 FOR I = 1 TO PNTS% STEP 10
3205    FOR J = 0 TO 9
3210          IF (I + J) > PNTS% GOTO 3300
3230          PRINT #1, USING "######."; Y(I + J);
3240          IF J = 9 THEN PRINT #1, EORF$
3250    NEXT J
3260 NEXT I

3300 REM The following are NBAD(I), the channel numbers to
be omitted by MOSS
3310 PRINT #1, EORF$
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, EORF$
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, EORF$
3400 NEXT I

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

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

3700  PRINT: PRINT "Would you like "; CHR$(34); P$;
CHR$(34)
3710 INPUT "      to be printed as a description in the
file"; PAGAIN$
3720 IF PAGAIN$ = "y" OR PAGAIN$ = "Y" THEN DESCR$ = P$:
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 T1% AND T2%
4190 T1% = 96: T2% = 432: REM, 8/95, Setup B reliable only
in this range
4200 M1 = Y(9)
4240 B1 = 7.910248
4250 FOR X = T1% TO T2% STEP 16
4260 M = Y(X)
4300 M = M * B1 / M1
```

```
4310 IF X < A9 THEN 4330
4320 GOTO 4340
4330 M = -M
4340 N = N + 1
4350 A0 = A0 + X
4360 A1 = A1 + X * X
4370 A2 = A2 + M
4380 A3 = A3 + X * X * X
4390 A4 = A4 + X * M
4400 A5 = A5 + X * X * X * X
4410 A6 = A6 + X * X * M
4420 NEXT X
4430 REM NOW TO FIND PARAMETERS IN VEL(X)=A+BX+CXX
4440 D = N * (A1 * A5 - A3 * A3) - A0 * (A0 * A5 - A1 * A3) + A1 * (A0 * A3 - A1 * A1)
4450 N1 = A2 * (A1 * A5 - A3 * A3) - A0 * (A4 * A5 - A3 * A6) + A1 * (A4 * A3 - A1 * A6)
4460 N2 = N * (A4 * A5 - A3 * A6) - A2 * (A0 * A5 - A1 * A3) + A1 * (A0 * A6 - A1 * A4)
4465 N3 = N * (A1 * A6 - A3 * A4) - A0 * (A0 * A6 - A1 * A4) + A2 * (A0 * A3 - A1 * A1)
4470 A = N1 / D: B = N2 / D: C = N3 / D
4480 IF PR=1 THEN LPRINT "VEL(X)="; A; "+ "; B; "*X+ "; C; "*X^2"
4481 IF PR=1 THEN LPRINT "            where X is channel number"
4483 IF PR=1 THEN LPRINT : LPRINT
4484 PRINT "VEL(X)= "; A; "+ "; B; "*X+ "; C; "*X^2"
4485 PRINT "where X is channel number"
4487 PRINT : PRINT "            NOTE THAT THE QUADRATIC COEFFICIENT IS ": PRINT
4488 PRINT "                    "; C: PRINT
4492 PRINT "       For the best linearity the quadratic coefficient should vanish."
4494 PRINT "      Use the UltraLin program for easy adjustment of the ultralinear control."
4500 RETURN: REM To line 6078


5000 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 PI! = 4 * ATN(1): REM Pi = 4 X arctan(1)
5030 PRINT: PRINT "     Enter values from the converged curvefit: "
5040 DIM YY(3 * N): DIM BB(3 * N): DIM ZZ(3 * N): DIM GG(3 * N): DIM AA(3 * N, 6 * N)
5050 'DIM NRG!(N):  DIM AREA!(N): DIM LW!(N)
5100 PRINT : PRINT : INPUT "Enter the baseline ", B3
5101 IF PR=1 THEN LPRINT : LPRINT "            Values entered:"
5105 IF PR=1 THEN LPRINT : LPRINT "Baseline (counts): "; B3
5110 PRINT : 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 No. "; I; ":"
5120    PRINT : INPUT "     Absolute value of area under curve (channels X counts): ", AREA!(I)
5130     PRINT : INPUT "      Line width (channels): ", LW!(I)
5140     PRINT : INPUT "      Position:  Channel No. ", NRG!(I)
5160    IF N = 1 THEN GOTO 5180
5170    IF PR=1 THEN LPRINT : LPRINT "      For Line No. "; I
5180    IF PR=1 THEN LPRINT : LPRINT "     Absolute value of area under curve"
5185    IF PR=1 THEN LPRINT "                    (channels X counts): ", AREA!(I)
5190    IF PR=1 THEN LPRINT "      Line width (channels): ", LW!(I)
5200    IF PR=1 THEN LPRINT "      Position:  Channel No. ", NRG!(I)
5205    IF ITEM$="3" THEN GOTO 5250
5210    YY(N + I) = NRG!(I)
5230     YY(I) = AREA!(I) / (PI! * LW!(I)): REM Assumes AREA! =  PI x LW! x DEPTH OF DIP
5240   YY(2 * N + I) = (LW!(I)) / 2: REM Austin's program uses half-width
5250 NEXT I
5255    IF ITEM$="3" THEN RETURN

5260 FOR X = T1% TO T2%: REM Initializing Y(X)
5280    Y(X) = 0
5290 NEXT X

5300 FOR X = T1% TO T2%
5330    FOR I = 1 TO N
5340      Y(X) = Y(X) + YY(I) / (1 + (X - YY(N + I)) * (X - YY(N + I)) / (YY(2 * N + I) * YY(2 * N + I)))
5350    NEXT I
5360    Y(X) = B3 - Y(X)
5370 NEXT X

5380 RETURN


6000 REM PLOT ROUTINE FOR HP 7440A COLORPRO PLOTTER
6010 PRINT : PRINT : PRINT : PRINT
6021 IF ITEM$ = "1" THEN CLS : PRINT "     Enter a title to be printed at the"
6022 IF ITEM$ = "1" THEN INPUT "     upper left above the plot: ", FS$: GOTO 6031
6025 GOSUB 700
6029 PRINT: PRINT "  "; CHR$(34); FS$; CHR$(34);
6030 PRINT : PRINT "        will be printed at the upper left above the plot."
6031 PRINT : PRINT "             Enter anything else you wish to appear as "
6032 PRINT "                    a subtitle ("; CHR$(34); "Enter"; CHR$(34); " for nothing else): "
6033 PRINT : INPUT "              ", P$
6034 IF ITEM$ = "1" THEN PRINT "                    "; FS$: GOSUB 5000
6035 IF ITEM$ = "CAL6" OR ITEM$ = "PUB6" THEN GOTO 6080
6037 IF ITEM$ = "1" OR ITEM$ = "6" OR ITEM$ = "4'" THEN GOTO 6090
6046 SOURCE$ = "Co-57": MATRIX$ = "Rh": P2 = .14
6047 PRINT : PRINT "     NOTE: This program assumes a "; SOURCE$; "source in a "; MATRIX$; " matrix:"
6048 PRINT "                    velocity offset = "; P2; " mm/s"
6075 GOSUB 4000: REM For velocity formula
6080 FOR X = 1 TO 1200
6082    V(X) = A + B * X + C * X * X
6084 NEXT X
6085 P4 = INT(V(INT(.9 * (PNTS%))))
6086 IF P4 > 4 AND INT(P4 / 2) <> (P4 / 2) THEN P4 = P4 - 1
6087 IF P4 > 4 AND INT(P4 / 4) <> (P4 / 4) THEN P4 = P4 + 2
6088 IF P4 = 3 THEN P5 = 1 ELSE P5 = (P4) / 4: REM Max. vel. and tic spacing
6090 PRINT : PRINT
6091 PRINT "          LOAD BLANK SHEET OF PAPER, AND SET SWITCH BOX TO "; CHR$(34); "A"; CHR$(34)
6095 GOSUB 10000: PRINT : 'PRINT : 'PRINT : PRINT
6160 PRINT : INPUT "IS PLOTTER READY (yes, no) "; AA$: REM Plot routine for curve or points
6174 IF AA$ = "N" OR AA$ = "n" THEN CLS : GOTO 6090
6175 CLS : LOCATE 9, 30
6176 PRINT "PLOTTING "; FS$
6180 IF ITEM$ = "5" THEN GOSUB 5000
6182 ON ERROR GOTO 10275
6183 OPEN "COM2:9600,S,7,1,RS,CS65535,DS,CD" FOR RANDOM AS #1
6184 ON ERROR GOTO 0
```

```
6185 GOSUB 9000: REM For plotter setup codes
6186 IF ITEM$ = "5" THEN GOTO 7000
6188 PRINT#1, "SP1";
6200 REM y axis scales
6205 T1% = 17
6210 IF ITEM$ <> "1" AND ITEM$ <> "6" AND ITEM$ <> "CAL6"
AND ITEM$ <> "PUB6" THEN GOSUB 11000
6220 IF ITEM$ = "1" OR ITEM$ = "6" OR ITEM$ = "CAL6" OR
ITEM$ = "PUB6" THEN MAXCNT = B3: GOSUB 11065

6290 REM For x axes
6295 IF ITEM$ = "1" OR ITEM$ = "4'" OR ITEM$ = "6" THEN
GOTO 6340
6300 P6 = -P4
6301    'print "At line 6301, P4 = "; P4; ", and P6 = ";
P6
6302    'while inkey$ = ""
6303    'wend
6321 F3 = V(PNTS%) - V(T1%): REM For scaling x axis
6322  REM  F3  =  B*(PNTS%-T1%)  +  C*(PNTS%^2-20^2):  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 ITEM$ = "PUB6" GOTO 6360
6327 'FOR X = T1% TO T2%: REM Collins' routine
6330    'IF (V(X) - 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 ITEM$ = "1" OR ITEM$ = "4'" OR ITEM$ = "6" THEN
GOSUB 8800: REM x axis labelling in Ch. No.
6352    IF ITEM$ = "4" OR ITEM$ = "CAL6" THEN GOSUB 8700:
REM Upper x axis labelling in Ch. No.
6355 NEXT X

6360 PRINT #1, "PA"; 1000; 7500; "DI1,0"; "LB"; "M.S.U.
PHYSICS"; "   "; DATE$; "  "; "Time: "; TIME$
6362 PRINT #1, "PA"; 1000; 7200; "DI1,0"; "LB"; FS$; "  "
6365 PRINT #1, "PA"; 1500; 7000; "DI1,0"; "LB"; P$; "  "
6367 IF ITEM$ = "CAL6" THEN PRINT #1, "PA"; 2000; 6800;
"DI1,0"; "LB"; "Peak isomer shift = "; IS; " mm/s "; " "
6370 GOSUB 10000
6371 GOSUB 10000
6380 IF ITEM$ <> "PUB6" THEN PRINT #1, "PA 10000 3500
DI0,1 LBCounts"; "  "
6382 GOSUB 10000
6384 GOSUB 10000
6390 PRINT #1, "PA 400 3000 DI0,1 LBPercent Absorption";
"  "
6392 GOSUB 10000
6394 GOSUB 10000
6395 IF ITEM$ = "1" OR ITEM$ = "4'" OR ITEM$ = "6" THEN
GOTO 6440
6400 PRINT #1, "PA 3000 1400 DI1,0 LBVelocity in mm/sec";
VELSTD$
6405 GOSUB 10000
6410 GOSUB 10000
6415 GOSUB 10000
6420 IF ITEM$ <> "PUB6" AND ITEM$ <> "4'" THEN PRINT #1,
"PA 4000 6400 DI1,0 LBChannel Number"
6425 GOSUB 10000
6430 GOSUB 10000
6435 GOSUB 10000: GOTO 7000
6440 PRINT #1, "PA 4000 1400 DI1,0 LBChannel Number"
6450 GOSUB 10000
6460 GOSUB 10000
6470 GOSUB 10000

7000 REM Point or curve plotting routine, from 6186, 6435,
or 6470
7010 FOR X = T1% TO PNTS%
7020    IF ITEM$ = "4" 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
7060    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
7070    GOTO 7520


7520    YF = Y(X) * CFB3 / B3: REM CFB3 = OldB3/YS (see
line 11410)
7530    M(X) = IDN + (((IUP - IDN) / (CFUP - CFDN)) * (YF
- CFDN))
7532 NEXT X

7535 IF ITEM$="1" OR ITEM$="5" THEN PRINT #1,"SP4;":GOSUB
10000: REM Pen 4 for curve

7538 FOR X = T1% TO PNTS%: REM Plotting
7542    IF M(X) > 6000 OR M(X) < 2000 GOTO 7580
7550    IF G(X) < 1000 OR G(X) > 9000 THEN 7580
7560    IF ITEM$ = "4" OR ITEM$ = "4'" OR ITEM$ = "6" OR
ITEM$ = "CAL6" OR ITEM$ = "PUB6" THEN PRINT #1, "PA";
G(X); M(X); "PD PU;": GOTO 7580: REM For points
7570    PRINT #1, "PA"; G(X); M(X); "PD"; : REM For curve
7580 NEXT X
7590 PRINT #1, "PU";

7592 REM Box drawing
7693 IF BOX$ = "DRAWN" THEN GOTO 7607
7597 PRINT #1, "PA 1000 2000 PR PD 0 4000 8000 0 0 -4000
-8000 0 PU PA;": REM Box drawing
7605 BOX$ = "DRAWN"
7607 PRINT #1, "SP0;"
7608 CLOSE #1: CLOSE #2
7610 IF ITEM$ = "6" OR ITEM$ = "CAL6" OR ITEM$ = "PUB6"
THEN RETURN: REM to 2500
7630 ERASE YY, BB, ZZ, GG, AA, AREA!, LW!, NRG!: 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; "PU"
8640    PRINT #1, "PA"; I - 100; 1800; "DI1,0"; "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 * (V(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; "PU"
8740    PRINT #1, "PA"; I - 250; 6200; "DI1,0"; "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; "PU"
```

```
8840    PRINT #1, "PA"; I - 100; 1800; "DI1,0"; "LB"; X;
" "
8850    GOSUB 10000
8860    GOSUB 10000
8870    RETURN

8900    REM Collins' subroutine (unused) from line 6330
for lower x axis labelling in mm/s
8905    I = 5000 + INT(8000 * (V(X) - P2) / F3)
8910    IF I < 1000 THEN 8950
8920    IF I > 9000 THEN 8950
8930    PRINT #1, "PA"; I; 2000; "PD"; I; 2100; "PU";
8940    PRINT #1, "PA"; I - 100; 1800; "DI1,0"; "LB"; P6;
"   "
8945    GOSUB 10000
8946    GOSUB 10000
8950    P6 = P6 + P5
8970    RETURN

9000 RESTORE: REM READing plotter codes
9005 FOR X = 1 TO 6
9010    READ K$
9020    PRINT #1, K$
9030 NEXT X
9040 RETURN
9050 DATA CHR$(27).CHR$(64);0:
9060 DATA CHR$(27).I64;;17:
9070 DATA CHR$(27).N;19:
9080 DATA CHR$(27).J
9090 DATA IN;
9110 DATA DT

10000 FOR J = 1 TO 10000
10005 NEXT J
10010 RETURN

10050 FOR J = 1 TO 30000!
10060 NEXT J
10070 RETURN

10075 FOR J = 1 TO 1000
10080 NEXT J
10085 RETURN


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,
GG, AA, AREA!, LW!, NRG!: GOTO 70
10140 LOCATE 25, 1: PRINT SPACE$(78): REM Deletes prompt
10150 RETURN

10160 REM F5 key event handler from line 74
10165 PR = 1: RETURN

10175 REM error handler for FS$ (line 770)
10180 BEEP: PRINT: PRINT "                    "; FS$; "
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: PRINT "                    "; DAT$; "
FILE NOT FOUND"
10210 PRINT "                          (F10 to return to
menu)"
10215 PRINT: RESUME 2005

10225 REM error handler for READPK$ = STDFE$ (line 2605)
10230 BEEP: PRINT: PRINT "                    "; READPK$;
" FILE NOT FOUND"
10235 PRINT "                          (F10 to return to
menu)"
10240 PRINT: IF EF$ = "E" OR EF$ = "e" THEN RESUME 12070
10245 PRINT: IF EF$ = "F" OR EF$ = "f" THEN RESUME 2105

10250 REM error handler for STDEU$ (line 12605)
10255 BEEP: PRINT: PRINT "                    "; STDEU$;
" 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 "
10317 PRINT:INPUT  "    (RETURN only if you don't want
the printer to record your operation)", PRINT$
10320 IF PRINT$ = "P" OR PRINT$ = "p" THEN RESUME
10321 IF PRINT$ = "" OR PRINT$ = "" THEN PR = 0: RESUME


10325 CLOSE #3: REM Error handling from line 2636
10340 PRINT: PRINT "                          FAULTY Fe
STANDARD RUN!"
10345 PRINT: PRINT "  "; STDFE$; " 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 #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%, PNTS%, MINCNT,
MAXCNT    =     "; T1%; PNTS%; MINCNT; MAXCNT
11040 FOR I = T1% TO PNTS%
11045 'print "L i n e     1 1 0 4 5"
11050   IF Y(I) > MAXCNT THEN MAXCNT = Y(I)
11051   'print: print " For I = "; i;  ", Y(I)    =    ";
y(I); "  MAXCNT   =   "; mAXcnt
11052   'gosub 10050: gosub 10050:  GOSUB 10050
11060 NEXT I

11065 IF REPEATSC$ = "Y" OR REPEATSC$ = "y" THEN GOTO
11500: REM from line 6220
11067 IF ITEM$ = "4" OR ITEM$ = "4'" 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 PNTS% STEP 16
11080   FOR J = I TO (I + 14)
11085   IF J > PNTS% THEN GOTO 11120
11090   IF Y(J) < MINCNT THEN MINCNT = Y(J)
11091   'print: print " For I = "; i; "  and J = "; j; ",
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; ",
Y(J)    =    "; y(j); "  MINCNT   =   "; mincnt
11102  'gosub 10050: gosub 10050:  GOSUB 10050
11110 NEXT I
11120 MAXCNT$ = STR$(MAXCNT): MINCNT$ = STR$(MINCNT)
11124 REM The next line strips the space added by STR$
from the left
11125 MAXCNT$ = RIGHT$(MAXCNT$, LEN(MAXCNT$) - 1): MINCNT$
= RIGHT$(MINCNT$, LEN(MINCNT$) - 1)
11130   MAXPNT%   =   INSTR(MAXCNT$,   "."):   MINPNT%   =
```

```
INSTR(MINCNT$, ".")
11140 IF MAXPNT% = 0 THEN MAXEXP% = LEN(MAXCNT$) - 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 WHILE MINDIG% = MAXDIG%
11190   J = J + 1
11200    MAXDIG% = VAL(MID$(MAXCNT$, J, 1)): MINDIG% =
VAL(MID$(MINCNT$, J, 1))
11210 WEND
11213 IF (MAXDIG% - MINDIG%) <= 1 THEN Q% = 4: GOTO 11225
11215 IF (MAXDIG% - MINDIG%) <= 2 THEN Q% = 3: GOTO 11225
11220 IF (MAXDIG% - MINDIG%) <= 4 THEN Q% = 2 ELSE Q% = 1
11225 YS = 10 ^ (MAXEXP% + 2 - J - Q%)
11230  CFUP$ = LEFT$(MAXCNT$, J + Q% - 1): CFUP =
VAL(CFUP$): CFUP = CFUP + 1
11240  CFDN$ = LEFT$(MINCNT$, J + Q% - 1): CFDN =
VAL(CFDN$): GOTO 11290
11250 REM Routine for wide count spread
11260 DIFF% = MAXEXP% - MINEXP%
11270 CFUP$ = LEFT$(MAXCNT$, DIFF% + 1): CFUP = VAL(CFUP$)
+ 1
11280 CFDN$ = LEFT$(MINCNT$, 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 ITEM$ = "PUB6" 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)
11325   I = IDN + (((IUP - IDN) / (CFUP - CFDN)) * (CF -
CFDN))
11330    PRINT #1, "PA"; 8900; I; "PD"; 9000; I; "PU";
11340    PRINT #1, "PA"; 9020; (I - 10); "DI1,0"; "LB";
(CF * YS); "    "
11350    GOSUB 10000
11360 NEXT CF
11370 GOSUB 10000

11400 REM Left y axis (percent absorption)
11410 ABSNUP2 = 1 - (YS * CFDN / B3)
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 ABSNSP = (ABSNUP3) / 4
11480 CFB3 = B3 / YS
11485 CFUP3 = (CFB3) * (1 - ABSNUP3)
11490 IUP3 = IDN + (((IUP - IDN) / (CFUP - CFDN)) * (CFUP3
- CFDN))
11495 IF ABSNUP3 > .02 AND IUP3 > 2400 THEN ABSNUP3 =
ABSNUP3 + ABSNSP
11500 ABSN = 0
11510 WHILE ABSN <= ABSNUP3
11520   CF = (CFB3) * (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; "DI1,0"; "LB"; (100 *
ABSN); "    "
11560   GOSUB 10000
11570   ABSN = ABSN + ABSNSP
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 STDEU$ <> "" THEN INPUT "Want to use the same Eu
and Fe standard runs for calibration"; REPEUSTD$
12030 IF REPEUSTD$ = "Y" OR REPEUSTD$ = "y" THEN GOTO
12090
12050 PRINT : PRINT "Name of Eu standard run for
calibrating v = 0"
12060 PRINT "    ("; CHR$(34); "Enter"; CHR$(34); : INPUT
"if no calibration desired):  ", STDEU$
12065 IF STDEU$ = "" THEN GOTO 2410
12066 READPK$ = STDEU$: GOSUB 12600
12068 CALIBREU = PEAK
12070 PRINT : PRINT "Name of Fe standard run for
calibrating the v scale"
12080 INPUT "             (do not omit this):  ", STDFE$
12090 PRINT : PRINT
12200 GOTO 2135

12600 REM Reading Eu peak position (from line 12066 or
2285)
12603 ON ERROR GOTO 10250
12605 OPEN READPK$ FOR INPUT AS #4
12606 ON ERROR GOTO 0
12610 JUNK$ = ""
12615 WHILE RIGHT$(JUNK$, 9) <> "DEVIATION"
12620    LINE INPUT #4, JUNK$
12621 WEND
12640 JUNK = 0
12645 WHILE JUNK <> 4
12650    INPUT #4, JUNK
12655 WEND
12683 INPUT #4, PEAK
12686 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
```

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.