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**DATA ACQUISITION AND ANALYSIS SYSTEM FOR THE
ION MICROPROBE MASS ANALYZER**

D. M. Darby
S. S. Cristy

February 1979

**UNION
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**OAK RIDGE Y-12 PLANT
OAK RIDGE, TENNESSEE**

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DATA ACQUISITION AND ANALYSIS SYSTEM FOR THE ION MICROPROBE MASS ANALYZER

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Oak Ridge Y-12 Plant

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ABSTRACT

A computer was interfaced to an ion microprobe mass analyzer for more rapid data acquisition and analysis. The interface is designed to allow data acquisition, independent of the computer. A large data analysis package was developed and implemented. Performance of the computerized system was evaluated and compared to manual operation.

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SUMMARY

The ion microprobe mass analyzer (IMMA) is used for in situ mass analysis of microvolumes near the surface of a solid. In order to more fully utilize the capabilities of the instrument and speed analysis of the large volumes of data generated, the IMMA was interfaced to the multiuser computer system in the Instrumentation and Characterization Department at the Oak Ridge Y-12 Plant.^(a) The interface design allows the IMMA to operate independently of the computer. The interface acquires information from pulse-counting scalers, a timer/scaler control system, a field monitor, a primary ion beam sweep control, and a mass scanning control. The interface uses a cassette tape system for local data storage and is able to control the pen lift and paper advance on an X-Y recorder.

A large data analysis package, including the CARISMA^(b) analysis program, was implemented for the computer. The computer manipulates the data and outputs in digital form on a teleprinter or in graphical form on an X-Y recorder. Performance of the computerized system was evaluated and compared to manual operation.

(a) Operated by the Union Carbide Corporation's Nuclear Division for the Department of Energy.

(b) Trademark of the Applied Research Laboratories, Sunland, California.

INTRODUCTION

The IMMA (Figure 1) is one of a relatively new class of instruments for in situ mass analysis of a microvolume near the surface of a solid.^{1 - 5} Analyses are performed by bombarding

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Figure 1. ION MICROPROBE MASS ANALYZER AND COMPUTER INTERFACE.

the sample with a beam of 1 - 22.5-keV ions which causes atoms and molecules to be sputtered from the surface. A fraction of the sputtered atoms and molecules are ionized and accelerated into a mass spectrometer for separation according to their mass-to-charge ratio (m/e). Mass analysis provides sensitivity for all elements and allows the determination of isotope ratios. Full mass spectra may be taken, or one or two secondary-ion masses may be monitored as successive surface layers are sputtered for in-depth composition profiles. With its high sensitivity for most elements and good spatial resolution ($2\ \mu\text{m}$ on the surface in the X-Y direction and 10 nm in depth), the ion microprobe is often the instrument of choice when a combination of thin layers or low concentrations and spatial resolutions on a micrometer scale is involved.^{6 - 8} The ion microprobe is unique in its capability to provide isotopic composition, high sensitivity for low-Z elements, and micrometer spatial resolution.

The ion microprobe is capable of generating large quantities of data in short periods of time. For example, 100 to 300 secondary-ion mass peaks may be generated in a mass scan of two minutes duration. This scan is likely to be followed by several more mass scans as an analysis with depth is often desired. Since all these results may be from a microvolume of sample ($0.5 \mu\text{m}^3$ in size), usually a number of additional microvolumes need to be analyzed. For analysis purposes, the m/e ratio and intensities of each or many of the peaks will have to be determined. Similarly, one or two ions may be monitored at time intervals as short as 0.1 second for concentration-in-depth profiles. Plots as a function of time and, in the case of two-ion monitoring (ratio switching), ratios, plots, and ratio plots of the data are generally desired.

Quantitative elemental analysis with the ion microprobe is not simple and straight forward because analytical sensitivity varies over two or three orders of magnitude and is dependent upon the surface chemistry of the sample. In general, two approaches are used—either a standards comparison method or a theoretical model and a computer program such as CARISMA⁹ which makes corrections based upon a local thermal equilibrium (LTE) model.¹⁰

In view of the preceding comments, computerization of the ion microprobe was considered to be necessary to reduce analysis time or allow more thorough analyses to be made. The first part of a proposed two-part implementation is reported here.

COMPUTERIZATION OF THE ION MICROPROBE MASS ANALYZER

INSTRUMENT DESCRIPTION

The Oak Ridge Y-12 Plant ion microprobe mass analyzer (IMMA) is based on a design by Liebl.¹¹ A schematic of this instrument^(c) is presented in Figure 2. A duoplasmatron

Figure 2. PRINCIPAL COMPONENTS AND OPERATION OF THE ION MICROPROBE MASS ANALYZER.

provides a high brightness ion source for either positive or negative ions. Ions accelerated from the duoplasmatron are mass analyzed by using a 90-degree-sector magnet to provide a pure, monoisotopic ion beam (primary) for sputtering the sample. A two-lens system provides for focusing the beam to a minimum diameter of about $2\ \mu\text{m}$, with current densities of $5\ \text{mA}/\text{cm}^2$ readily attained. Beam-sweep plates provide for moving the beam in a line or raster pattern over the sample. An optical microscope is provided for viewing the sample and the area being analyzed.

(c) The schematic is furnished by the manufacturer, Applied Research Laboratories.

The sample is biased at ± 1.5 kV for accelerating either the positive or negative ions that are formed in the sputtering process into the secondary mass spectrometer. This spectrometer consists of a pickup electrode at ground potential, deflection plates to adjust the secondary-ion beam on axis, a focusing Einzel lens, a 45-degree spherical condenser electric sector, and a 90-degree magnetic sector. The wedge-shaped magnetic sector and spherical electric sector are designed to produce a spectrometer that is double focusing and stigmatic imaging with high transmission efficiency.¹¹

After mass analysis, the secondary ions are detected with a detector of the Daly¹² type which allows efficient collection of either positive or negative ions and single-ion counting. Ions passing through the secondary (exit) slit of the mass spectrometer are accelerated through 15 kV to an aluminum target. A photomultiplier tube then produces a current pulse when these electrons are accelerated into a scintillator connected to the photomultiplier by means of a light pipe. Analog conversion of the photomultiplier pulses provides for graphic display on the X-Y recorder or oscilloscope screen. High-speed pulse-counting hardware transmits counts to the timer/scaler at rates which may exceed 10^7 cts/sec.

Two pairs of deflection plates just ahead of the secondary slit provide for rapidly switching two secondary ions alternately into the detector when their m/e values are within $\pm 7.5\%$ of the mean mass.

TIMER/SCALER AND COUNTING HARDWARE

The last dynode of the photomultiplier tube is capacitively coupled to the input of a high-speed pulse amplifier. The output of this amplifier passes through a second pulse amplifier, identical to the first, to a discriminator which performs pulse-shaping and noise-rejection duties. The timer/scaler provides a timer gate for the discriminator output. Parallel outputs from the discriminator are routed to a dual coincidence unit which functions during ratio switching to route output pulses to the appropriate scaler, in phase with voltage to the secondary-ion beam switching plates. In the normal counting mode, only one scaler (Scaler A) receives pulses. The timer/scaler provides the controlling gate signals. Each output from the dual coincidence unit feeds a 200-MHz decade scaler. In the system, these scalers are designated as Prescalers A and B. Every tenth count sends a carry pulse of 20-nsec width to the tens counter (second digit) on the timer/scaler. A separate binary coded decimal (BCD) signal transfers the digit displayed on the prescaler to the units position of the timer/scaler. In this manner, the inherent 20-MHz capability of the timer/scaler is multiplied by a factor of 10 for displaying 200-MHz counting results.

Figure 3 is a block diagram of the high-speed counting system and the gates and signals between the counting system and the timer/scaler. In a normal one-ion counting mode (NORM/MASS), the timer gate enables the discriminator when a "start" signal is generated manually, or automatically when the display time elapses or in the "hold" position, after a reset has occurred at the end of a print cycle. The timer gate disables the discriminator when a manual, preset time, or preset count "stop" is generated. In this mode, the Scaler A gate is always enabled, and the Scaler B gate is always disabled. Not shown in the diagram is the

Figure 3. HIGH-SPEED COUNTING SYSTEM FOR THE ION MICROPROBE MASS ANALYZER.

voltage-to-frequency converter and associated circuitry which convert the Hall-effect field monitor voltage from the secondary magnet to a mass number which is displayed on Scaler B in the NORM/MASS mode. In the peak-switching (RATIO) mode, Scaler Gates A and B are enabled alternately for one millisecond with the timer gate, providing a 0.1-millisecond blanking during switching.

The timer also provides gating signals to the ratio-switching circuitry (voltage switch on the secondary-ion deflection plates) for synchronization with the scaler gates. Scalers A and B have an eight-digit display of accumulated counts. In NORM/MASS mode, Scaler B displays a five-digit representation of the secondary mass number in tenths of mass units. The timer displays six digits in milliseconds to 999.999 seconds. A coupler provides for automatic or manual teleprinter printing of the data in Scalers A and B and the timer at the end of a preset time or counting interval.

SECONDARY-MAGNET FIELD CONTROLLER AND MONITOR

A block diagram of the magnet field control system is included as Figure 4. A sweep-voltage generator supplies a reference voltage at Point V_{IN} . An imbalance between V_{IN} and the amplified Hall-effect field voltage at A1 drives the differential power amplifier until the field

Figure 4. SECONDARY-MAGNET-FIELD CONTROL SYSTEM.

strength changes to balance the inputs at A1. The Hall probe is thus seen to have a dual purpose: (1) It is a vital link in the field-control system providing a voltage proportional to the field strength for feedback control, and (2) it provides m/e identification for the X-Y recorder, the analog mass meter on the IMMA console, the timer/scaler, and the IMMA computer interface. Mass/charge (m/e) indication is a result of the Hall-probe voltage being proportional to the field strength, H , and the relationship:

$$m/e = \frac{H^2 r^2}{2Vc^2}, \quad (1)$$

where:

- m represents the mass,
- e the charge on the ion,
- r the radius of deflection,
- V the accelerating potential, and
- c the velocity of light in a vacuum.

For a given instrument of given radius, r , and fixed accelerating potential, V , the equation simplifies to:

$$m/e = KH^2, \quad (2)$$

where the constant $K = r^2/2V_c^2$.

Thus, the expression:

$$m/e = K' V_h^2, \quad (3)$$

where V_h represents the Hall-probe voltage, and K' is a proportionality constant (which includes K).

ANALYSIS MODES

The instrument just described is used, primarily, in six analysis modes, namely: single-peak profiling, peak switching or ratio profiling, X-line profiling, mass scan, ion imaging, and multichannel scaling. The computer interface data-acquisition system involves the first four of these, which are briefly described in the subsections to follow, with a word about quantitation under **Mass Scan**.

Single-Peak Profiling

Single-peak profiling consists of sputtering a sample at a constant rate while monitoring the secondary-ion current of a selected m/e . The result is a profile of the secondary-ion intensity with depth into the sample. This mode is used to determine the thickness of thin layers, establish diffusion profiles, and determine the location of elements for studies of oxidation, plating, diffusion, corrosion, cleaning, and other characteristics of a similar nature.

The sputtering-ion beam may be focused into a spot, swept in a line, or rastered. To obtain a sputtering pattern with a minimum edge/area ratio and a flat-bottomed crater for maximum depth resolution, a large (50 - 500- μ m-diameter) defocused spot is sometimes used; however, a raster pattern with a smaller spot is the more common method. With the raster mode, an electronic aperture system can be used which accepts the secondary-ion signal only when the primary beam is located in a preselected center portion of the raster. In the raster mode, ion imaging may also be done as a function of sputter time or depth.

Typically, the secondary-ion current is monitored with a plot of the analog secondary-ion current on the X-Y recorder and by printing counts accumulated in Scaler A for selected time intervals, using a teleprinter. The time interval may be set from 0.1 to 1000 seconds on the timer/scaler, but a 3-second delay for printing between counting intervals must be considered when the interface system described later is not used.

Peak Switching or Ratio Profiling

The ratio-switching deflection plates and circuitry described earlier make it possible to monitor two peaks (within a 15% mass range) simultaneously as the sample is sputtered. This capability is often useful for isotope measurements; monitoring a metal and its oxide or fluoride; monitoring surface-layer interactions or reactions using isotopically altered

substrates, layers, or reagents, and performing diffusion or migration studies involving elements not widely different in mass. Sputtering modes are the same as for single-peak profiling. Monitoring is limited to printing counts accumulated in Scalers A and B, using the teleprinter. An analog plot, if done in real time, is an average of the two signals. Often it is desirable to plot the individual secondary-ion intensity profiles and the ratio of the two ions monitored. These plots are very time consuming if done by hand.

X-Line Profile

In the X-line profile mode, the primary ion beam is swept in a line across the surface of the sample. The X axis of the recorder is swept synchronously with the ion beam and the Y axis records photomultiplier or sample current. This mode is very useful for observing changes in concentrations when crossing certain features such as grain boundaries, cracks, inclusions, and other visible features. Often X-line profiles are desired as a function of sputtering depth into the sample. X-line profiles allow mapping of surfaces with more quantitative information than is obtainable with secondary-ion videographs (ion imaging).

Mass Scan

The mass-scan mode is used for qualitative and quantitative determinations of sample composition. Typically, the secondary-magnet field is swept while photomultiplier current versus m/e (Hall-probe voltage squared) is recorded on the X-Y recorder. Any primary-ion-beam mode can be used according to the requirements of the analysis. A rapid mass scan gives qualitative information concerning the elements and isotopes present. For quantitative purposes, the peak heights of the relevant secondary ions may be measured. For more accurate measurements, the mass spectrum is manually scanned, and each secondary ion of interest is individually counted by using the timer/scaler, as in the single-peak mode.

Counting individual peaks is the most accurate and also the most time consuming when large numbers of peaks are to be counted. When the sample composition is changing rapidly, a trade off of accuracy for speed or limitation of the number of peaks counted must be accepted. As discussed later, the computer-interface data-acquisition system provides an alternative which is nearly as accurate and operates at the automatic scan speed.

Semiquantitative comparisons between two spots on a sample, or two similar samples, often involve normalizing the data to a matrix element such that quick comparisons of intensities of other elements can be made. Quantitative work generally requires development of relative sensitivity factors for the elements of interest, using standards of similar matrix to that of the unknown. Several theoretical models of the sputtering process have led to development of computer programs for the analysis of ion-microprobe, secondary-ion mass-spectrometry data. The most accurate at this time is probably the CARISMA program, based on a local thermal equilibrium model.¹ This program has had good success in a number of natural silicate matrices,² but has been found to be poor in certain matrices such as uranium.³ Once CARISMA is found to be suitable for a given type of matrix with empirical corrections for a few elements, it is a useful tool for relatively rapid quantitative analysis.

COMPUTER INTERFACE HARDWARE

The computer interface for IMMA (Figures 5 and 6) collects data from the timer/scaler, the Hall probe, and the prescaler. These data are then stored by a

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Figure 5. DISPLAY PANEL FOR THE ION MICROPROBE MASS ANALYZER COMPUTER INTERFACE.

magnetic-tape cassette unit and may optionally be transmitted to the remotely located multiuser computer where they are stored, manipulated, and returned for display. The type of test determines the particular format and analysis of the data. Identification (sample number, run number, and test type) is stored with every test (Appendix A). Capability is provided for either automatic or manual data acquisition (Appendix B) and cassette control. File identification is displayed to the operator to provide assistance during manual search and is transferred to the computer from the IMMA interface for an automatic search. For the operator's benefit, indicators display the type of test, the status of the test, a datum-acquisition strobe, the buffer storage status, and the computer status. Finally, the interface controls and X-Y recorder pen lift and paper advance for graphic display. A teleprinter is used for operator/computer interaction and data display.

The capabilities of the interface are portrayed in Figure 7. Each component will be described in the following subsections.

Figure 6. ION MICROPROBE MASS ANALYZER SYSTEM.

External Environment

Figure 7. INTERRELATIONSHIP OF THE INTERFACE BETWEEN THE INTERNAL AND EXTERNAL ENVIRONMENTS.

Timer/Scaler Control

The timer/scaler (Figure 8) which accumulates and displays ion counts, count-collection time, and mass number is read when the interface is in the semiautomatic mode. The time or

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Figure 8. DISPLAY PANEL FOR THE TIMER/SCALER.

count preset of the timer/scaler determines the interface acquisition of the BCD data and is used for both single and ratio peak modes because the timer/scaler displays data after a selected time interval or count total. Operated in this manner, the interface appears as a passive high-speed teleprinter.

In automatic mode, the interface can stop, start, read, and reset both the timer/scaler and the prescaler. Pulses from the prescaler are converted to transistor-transistor logic (TTL) signals and are used to detect peak start and end conditions, and are counted during a clock period to determine the peak amplitude. This mode is used for a mass scan and allows accumulation of the area while moving across a single mass peak. This action results in an accurate determination of the relative intensity of each secondary-ion peak detected by the peak detector.

In the manual mode, the interface is completely isolated from the timer/scaler; thus, no interaction is allowed. This mode is used to return to the normal operation and capabilities of the ion microprobe.

Data Buffer and Cassette Storage

Data acquired during a test is double buffered into either of the two 512 x 8-bit shift register buffers with automatic buffer swap. When a buffer is full, it can be read by the computer (on-line condition), and it is always written onto the cassette tape. A memory-full indicator is lit whenever a buffer is unavailable for filling (ie, being emptied by the cassette or computer).

A nine-track digital magnetic cassette tape unit is used for all local data storage (Figure 9). Multiple tests may be stored on a single cassette. Eight tracks of the cassette are used for data; the other track is used to mark the end of the file. This marker is written at both the start and end of every test, and the File Marker indicator is lit when a file is being written or read. The Sample # and Run # dialed on the thumbwheel switches are stored in the first buffer at the start of a test and always follow the marker on the tape; thus, when the end-of-file marker is detected, the following number can be displayed as the file identification on the LED display panel. When the only other possible combination occurs

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Figure 9. ION MICROPROBE MASS ANALYZER DATA STORAGE SYSTEM.

(marker, marker), the first marker is ignored. The front panel of the IMMA data storage system, besides displaying file markers and file identification, provides for a manual reset, fast or incremental searches in a forward or reverse direction, and a load forward. If the cassette is being read by the computer, a READING TAPE indicator on the IMMA interface is lit.

Hall-Probe Monitor

The Hall probe, which converts the secondary-ion deflecting magnetic field strength to a corresponding voltage, is used in a closed-loop magnetic field controller in the mass-analyzer portion of the IMMA. This output is also isolated, amplified, offset, and digitized (12 bits) by the interface. In this manner, the instantaneous mass number (between 0 and 300) is accurately determined. Expansion capabilities were included for a possible 0 - 600 mass-number range. This capability is used in a mass-scan test where the values are buffered temporarily in a 12-bit register.

Additionally, the current mass number is compared with the digital numbers representing Masses 75 and 125, and this information is used in the peak detector and clock circuitry because, before Mass 75, no peaks can overlap; and, by Mass 125, the peak width increases enough to require that the data synchronizer be slowed.

During a mass scan, some background noise and peak tailing must be ignored. Therefore, a peak start-and-end detector is used to define "acceptable" peaks (Figure 10).

Over higher masses, where peaks start to overlap, a digital peak-and-valley detector¹¹ is enabled. Figure 11 indicates the simplest overlapping peak and the data taken at each point, while Figure 12 shows the effect of peak digitization.

X-Line Sweep Monitor

In the X-line test, the primary ion beam is swept in a line across the sample while focusing a single secondary-ion on the detector. The X axis of the recorder is swept synchronously with the beam sweep, while the Y axis can be set to accept photomultiplier current, log of photomultiplier current, or sample current. Many consecutive X-line scans result in a depth profile across the sample. In an X-line test, the interface detects the sweep reset and drops the recorder pen at the appropriate moment following the reset. The number of sweeps are counted, and the pen is dropped on the first sweep after the test starts and then only every first, second, third, . . . Delta Records, as preset by the operator. The paper is automatically advanced after each recorded sweep. When the number of Delta Records recorded equals the Number of Records, the test is ended. Delta Records and Number of Records are dialed and then entered by means of the adjacent EXECUTE button (Figure 13).

X-Y-Plotter Control

The X-Y plotter (11 x 17.5 inches), with automatic paper feed and pen lift, can be driven by the computer. Two 12-bit digital-to-analog converters (DACs) are used for the X and Y values, giving 4096 increments. The computer generates a paper feed or pen lift and allows enough time for the operation to complete. Since the response of the plotter is very slow, the plot routines rapidly drive the plotter in one continuous motion to a new position if the pen is up; if the pen is down, many small steps at a 40-Hz rate (approximately) must be taken to avoid both hysteresis problems and amplifier jitter. Computer plotting is selected for both axes by means of two 6-position switches located immediately below the plotter (Figure 14). Computer pen lift and paper advance are also switch selectable.

Figure 10. ION MICROPROBE MASS ANALYZER SINGLE PEAK. [Recorded: Mass Number (M_1), Total Peak Area (A_1) (timer/scaler readings)]

Figure 11. ION MICROPROBE MASS ANALYZER MULTIPLE PEAK. [Code Explanations: P_1 and P_2 - Counts per Clock, Remains a Maximum for 3 Consecutive Clock Times, Recorded for Each "P" are the Mass Number (M_1 and M_3), Counts per Clock (P_1 and P_2), and Peak Code; V_1 - Counts per Time Remain a Minimum (but not zero) for 3 Consecutive Clock Times, Recorded as M_2 and V_1 , Valley Code; M_1 - M_3 - Mass Number is Read at an Inflection Point; Restraints: (1) All Peaks are Separated by Valleys (or end of peak), (2) Mass Number must be Greater than 75 before Multiple Peaks are Detected]

Figure 12. COMPARISON OF RUN DATA AND THE RESULTANT DIGITIZED PEAKS.

Manual Control and Indicators

The manual controls on the IMMA interface hardware (Figure 15) allow the operator to stop and start a test, clear the system (computer reset), disable the computer control (off line), select a test (test mode and execute), select X-line test parameters (Delta Record and Number of Records), and select test identification (Sample ID, Run Number). The cassette tape unit controls have previously been explained.

Figure 13. X-LINE THUMBWHEEL, LOCATED ON THE ION MICROPROBE MASS ANALYZER INTERFACE PANEL.

Computer Control and Transmission Cable

Most of the manual controls are paralleled by computer controls. The computer can select, start, and stop a test, read the cassette, and

Figure 14. X-Y RECORDER INPUT SELECTOR.

Figure 15. FRONT PANEL OF THE INTERFACE.

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load the test parameters and sample identifications. This capability allows real-time data acquisition, and the data may be returned for the operator's information during the test.

All data and signals transferred to and from the computer on the transmission cable are buffered and line driven to eliminate noise and ground problems. All of the line receivers are capable of being disabled. At the computer, enabling/disabling is done via a program request. At the interface, the line receivers are disabled by either the manual Computer Reset control located on the front panel or by the interface when it detects that the lines are "floating" due to loss of power to the drivers.

The design criteria for the IMMA were to acquire data with or without the computer and to allow real-time or posttest analysis/display of data. The hardware just described has successfully performed its part of this task over the past two years. The IMMA interface, though, is only half the story. The supporting software described in the following section is equally important for computer-assisted data collection and analysis.

COMPUTER INTERFACE SOFTWARE

The IMMA software executes as one of several tasks which operates under the supervision of a real-time monitor system (RSX) on a medium-sized PDP-15/35 computer (Figure 16). The 18-bit word computer has an input/output (I/O) processor separate from the central

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Figure 16. OVERALL VIEW OF THE PDP-15/35 COMPUTER.

processing unit, thus allowing concurrent task execution and I/O processing. This capability, together with a large instruction set and powerful peripheral devices, makes the PDP-15/35 an ideal multiuser computer.

The configuration of the RSX-15 system used for this project allows four tasks to operate simultaneously (interleaved). These tasks are priority driven and currently may belong to any one of eight different users performing control, data acquisition, or analysis. Each task operates in a specified region of core, called a "partition", with an optional common area external to this partition. Each task may consist of an extensive overlay of routines. In addition to disks, magnetic tapes, lineprinter, reader/punch, and teleprinter, the system supports a scratch-pad memory system designed and built in Y-12. This provision allows large arrays of data to be accessed quickly and inexpensively.

The computer software package consists of 78 routines overlayed into five tasks. IMMA represents one task and CARISMA four tasks, both of which utilize: (1) 8K words of core memory (2 - 4K partitions), (2) a 0.5K external common memory, (3) a 10K scratch-pad memory, (4) a 50K disk (40K for program storage, 10K for data), (5) a teleprinter, and (6) a lineprinter. IMMA and CARISMA operate in a foreground/background mode with great

advantage since CARISMA is a long (occasionally several hours) series of calculations requiring no operator intervention, while IMMA is totally interactive (ie, the operator directs the flow of execution by selecting an appropriate option).

Each task operates as a "mini system", and many privileges are granted a task that would normally be reserved for the executive system. Along with the privileges go the responsibilities of monitoring system integrity. Therefore, throughout the tasks, the following conventions have been established:

$\text{LOG}(A)$ for $A \leq 0$, = 1,

$1/A$ for $A = 0$, = 1, and

$\sqrt{A}$ for $A < 0$, = 0.

Additionally, disk transfers are monitored where necessary to prevent an overflow of the allowable region. Scratch-pad transfers are likewise monitored, and the actual transfer instructions operate uninterruptably. The interrupt capability of the teleprinter is disabled when the task is not executing, and the interrupt capability of the IMMA interface is enabled for data acquisition only.

Software System

To get computer assistance, the operator requests initiation of his task from computer personnel. Initiation is done at the computer console. An LED display panel is maintained at the computer site to show the status of this and other tasks. After initiation, the task types on the local teleprinter the main program identifier.

From this main program, several data-acquisition routines can be selected, a mass scan can be read from cassette tape, and data from a single peak or ratio test can either be read from tape or taken in real time (see Figure 17). The format and interpretation of the data are different for each test, as are the analysis algorithms. The single-peak routines allow display of counts/second versus elapsed time on a graph or hard-copy device. The ratio-test routine allows display of counts/second for both masses and the ratios of Mass A/Mass B and Mass B/Mass A. The mass-scan test allows the operator to calibrate the Hall probe by fitting a voltage-versus-mass number curve; additionally, he may separate overlapping peaks and display data on a graph or hard-copy device, normalize data, and apply a correction factor to the data (mass number^{-1/2}). CARISMA may be invoked from the main program as well as its output routine; and, finally, a routine allowing calibration of the X-Y plotter may be called from the main program. The main IMMA program identifies itself by typing:

```
ION MICROPROBE MAIN . . . HR:MIN:SEC DAY/MON/YR
OPTION?
```

Figure 17. ION MICROPROBE MASS ANALYZER MAIN OPTIONS.

Like all requests for options, a carriage return (CR) in the first column results in a list of available options; ie:

ION MICROPROBE MAIN ... 10:15:15 15/ 7/75

OPTION?

OPTIONS ARE:

PKS RECORD COUNTS FOR SPECIFIED PEAKS.

CAR RUN CARISMA.

CAP OUTPUT CARISMA.

SCN MASS SCAN.

EXT EXIT PROGRAM.

XLE X LINE SCAN.

PSU SETUP PLOTTER.

ION MICROPROBE MAIN ... 10:15:52 15/ 7/75

EXIT (EXT) terminates the IMMA task. Options CAR and CAP are described in Appendix C. Plotter setup (PSU) allows the operator to adjust the plotter's X,Y offset and scale. (All computer inputs are followed with a CR.) The computer responds:

PLOTTER SETUP,

and adjusts the two DACs to a zero-volt output. The first CR adjusts the DACs to a full-scale, 10-volt output; a second CR restores them to zero and returns to the IMMA main.

Mass Scan

The mass-scan option (Figure 18) reads mass-scan information from the cassette tape and allows calibration, peak separation, manipulation, and graphic display of the data. The computer asks for a file name, and the operator responds with the two-digit sample number and two-digit run number that was dialed in at the beginning of the mass-scan test. The interface is turned on line, and the tape is searched for this file name. (Whenever the interface is on line, pushing the "computer reset" button forces a return to IMMA MAIN.) All of the file names which are read are reported. When the proper file has been located, the data are read and stored on the disk. A maximum of 500 masses may be stored. If the calibration curve already exists, all peaks closer than 0.3 atomic mass unit (amu) which are not on the boundary of overlapping peaks are combined. Information concerning overlapping peaks is outputted (Figure 18). After all data are inputted, the computer asks the operator if this data set is to be used for calibration. A "yes" answer is used when the operator wishes to update coefficients for the cubic, voltage-versus-mass equation stored in the computer. This updating is done by utilizing a least-squares fit of known peak location and the corresponding voltage reading. The peak location is determined by the operator from the optional plot of counts versus volts.² Overlapping peaks will have the unique characteristics of unit height for all except the last whose height is that of the total envelope.

The next calibration step is to input a position-versus-mass number table (Figure 18) with the integer information right justified under the appropriate columns. Whether

```

CION MICROPROBE MAIN... 10:27:12  20/ 1/78
OPTION?
SCN
FILE IDENTIFICATION?
0759

FILE NAMES:
      8
      759
PEAK MASS 135.28 COUNTS      258.
PEAK MASS 136.46 COUNTS      694.
PEAK MASS 137.40 COUNTS      861.
PEAK MASS 138.47 COUNTS     1232.
PEAK MASS 139.31 COUNTS     7928.
PEAK MASS 141.47 COUNTS      94. AREA  322641.

PEAK MASS 151.53 COUNTS      19.
PEAK MASS 152.78 COUNTS      63.
PEAK MASS 153.79 COUNTS      71.
PEAK MASS 154.80 COUNTS     107.
PEAK MASS 155.81 COUNTS     624.
PEAK MASS 157.08 COUNTS       8.
PEAK MASS 157.85 COUNTS     65. AREA  29856.

CALIBRATE USING THIS DATA SET?
Y
PLOT CALIBRATION DATA?
N
PEAK NUMBER AND ASSOCIATED MASS NUMBER?
TERMINATE WITH PEAK NUMBER=999.
PPP MMM
001 001
002 010
006 023
010 030
012 040
018 050
020 064
026 090
029 094
030 106
034 130
040 138
041 140
045 152
054 181
057 198
058 206
059 207
060 208
999
PROCESSING OPTION?

```

Figure 18. MASS-SCAN CALIBRATION.

the operator chooses to calibrate or not, overlapping peak areas are determined by proportioning amplitudes to the total area (Figure 19).

The operator has several manipulation and display options:

```

LS    LOW-SPEED PRINTOUT
HS    HIGH-SPEED PRINTOUT
MI    PRINT MOST INTENSE PEAKS
SP    PRINT SELECTED PEAKS
PL    PLOT
NO    NORMALIZE
RA    RATIO
FP    FINISHED PRINTOUT
OUTPUT OPTION?

```

The finished printout (FP) returns to IMMA MAIN; the low speed (LS) outputs to the local teleprinter (Figure 20), and the high speed (HS) outputs to the remote lineprinter. Both options ask:

TITLE FOR PRINTOUT.

These 72 characters (one line) of the header will be outputted with the two columns of mass-number and peak-area information. Most intense (MI), Figure 21, causes a response of:

NUMBER OF PEAKS TO BE
PRINTED?

Area of ith Peak:

$$P_i = (C_i)(\text{total area}) / \sum_{i=1}^n C_i$$

Figure 19. EXAMPLE OF A PROPORTIONAL AMPLITUDE PEAK SEPARATION. (P_i is the ith Peak; C_i is the Counts/Clock for the ith Peak)

The peaks are outputted in descending order of magnitude.

Selected peak (SP) outputs up to 100 data pairs whose mass numbers are inputted following the question shown in Figure 22. Ratio (RA) divides all the peak areas by the square root of the mass number. This process corrects the peak areas for increasing dwell time which increases as the square root of the mass. Normalize (NO) allows the normalization of all peak areas to one particular peak. The information requested is the integer mass number to be the basis of normalization and an assigned area. Figure 23 shows a sample normalization. The "." preceding the "PEAK AREA?" question is a reminder that a floating-point number is needed. This convention is used throughout the IMMA program. Plot (PL), Figure 24, allows the operator to plot log amplitude versus mass number. The numbers entered for a plot are the first and last mass numbers to be plotted, followed by the number of peaks per

0759 NBS GLASS K-489 1/20/78

MASS NO.	PEAK AREA
1.0	3.600000E+01
10.1	2.000000E+01
11.0	1.010000E+02
14.1	3.200000E+01
16.0	2.160000E+02
22.9	2.750000E+02
27.0	1.390000E+03
28.0	4.540700E+04
29.0	2.421000E+03
30.0	1.535000E+03
39.0	5.900000E+01
40.0	1.820000E+02
44.1	2.910000E+02
46.0	1.370000E+02
47.1	1.260000E+02
48.0	1.185000E+03
49.0	6.800000E+01
50.1	8.900000E+01
56.0	7.290000E+02
64.1	1.260000E+02
67.0	1.850000E+02
67.6	4.940000E+02
68.0	6.220000E+02
68.5	6.089000E+03
88.1	1.760000E+02
90.0	8.980000E+02
90.9	2.090000E+02
92.0	2.680000E+02
94.0	2.780000E+02
106.0	2.450000E+02
107.0	4.500000E+01
108.0	8.700000E+01
109.9	6.800000E+01
130.0	3.040000E+02
132.0	3.170000E+02
134.0	7.521585E+03
135.1	2.023248E+04
136.1	2.510110E+04
137.1	3.591702E+04
137.9	2.311284E+05
140.0	2.740422E+03
142.0	3.560000E+02
149.9	5.927523E+02
151.1	1.965442E+03
152.1	2.215022E+03
153.1	3.338132E+03
154.1	1.946724E+04
155.3	2.495799E+02
156.0	2.027837E+03
158.1	2.550000E+02
164.1	3.500000E+01
166.2	1.000000E+02
170.0	4.400000E+01
181.0	4.960000E+02
182.3	6.200000E+01
196.8	4.790000E+02
198.2	9.800000E+01
205.9	5.500000E+01
206.9	6.000000E+01
207.9	9.800000E+01
290.7	7.800000E+01

Figure 20. SAMPLE LOW-SPEED OUTPUT.

PROCESSING OPTION?

MI

NUMBER OF PEAKS TO BE PRINTED?

12

MASS NO.	PEAK AREA
137.9	2.311284E+05
28.0	4.540700E+04
137.1	3.591702E+04
136.1	2.510110E+04
135.1	2.023248E+04
154.1	1.946724E+04
134.0	7.521585E+03
68.5	6.089000E+03
153.1	3.338132E+03
140.0	2.740422E+03
29.0	2.421000E+03
152.1	2.215022E+03

Figure 21. SAMPLE OF THE MOST-INTENSE-PEAKS OUTPUT.

PROCESSING OPTION?

SP

MASS NO. TO PRINT OUT?

A MASS NUMBER =999 TERMINATES LIST.

130
132
134
135
136
137
138
999

MASS NO.	PEAK AREA
130.0	9.709238E-02
132.0	1.004554E-01
134.0	2.366125E+00
135.1	6.337440E+00
136.1	7.835601E+00
137.1	1.116901E+01
137.9	7.166000E+01

Figure 22. SELECTED-PEAKS OUTPUT.

PROCESSING OPTION?

NO

MASS NUMBER TO BE BASIS OF NORMALIZATION?

138

.PEAK AREA?

71.66

PROCESSING OPTION?

Figure 23. SAMPLE NORMALIZATION.

page (for automatic paging). Both automatic and manual scaling are provided. For automatic scaling, the maximum and minimum points are defined as the integer LOG (maximum)+1 and integer LOG (minimum-minimum/10), respectively. The maximum and minimum power of 10 may alternatively be entered manually. Upon completion of the plot, the scaling values are returned to be kept with the plot.

Single Peak and Ratio

Peaks (PKS) is another IMMA main option (Figures 25 and 26). This series of routines allow information from a single peak to be analyzed. This information may either be input from the cassette tape or gathered in real time. If it is a real-time run, the operator may output results to both the teleprinter and X-Y recorder. Analysis and output routines are available that are similar to the mass-scan (SCN) options. The first question asked is:

LIVE RUN? (Y,N).

A run that is not a real-time run asks for a file name like the mass scan. If a real-time run is chosen, two additional questions follow:

LIVE PRINTOUT? (Y,N)

LIVE PLOT? (Y,N)

which must be answered. If a live plot is requested, scaling information is also requested as is the plot type, Figure 25. A live output option decreases the response of the system after the first buffer is filled by delaying the emptying of that buffer. A minimum continuous time of two seconds per reading is required after filling the first buffer.

When the END-OF-TEST button is pushed, or an END-OF-FILE is encountered when reading from tape, the computer asks for a processing option:

```

PROCESSING OPTION?
PL
MASS NO. RANGE TO BE PLOTTED?
80
160
NO. OF PEAKS PER PAGE?
80
AUTOMATIC SCALE? (Y,N)
Y

MASS NUMBERS 80 TO 160.
MAXIMUM AREA =10** 6
MINIMUM AREA= 10** 1

```

Automatic
Scaling

```

PROCESSING OPTION?
PL
MASS NO. RANGE TO BE PLOTTED?
80
160
NO. OF PEAKS PER PAGE?
80
AUTOMATIC SCALE? (Y,N)
N
MAXIMUM POWER OF 10 ON PLOT?
5
MINIMUM POWER OF 10 ON PLOT?
1

MASS NUMBERS 80 TO 160.
MAXIMUM AREA =10** 5
MINIMUM AREA= 10** 1

```

Manual
Scaling

Figure 24. PLOT OPTION, SHOWING AUTOMATIC AND MANUAL SCALING.

PROCESSING OPTION?

(CR)

OPTIONS ARE:

LS LOW-SPEED PRINTOUT.

HS HIGH-SPEED PRINTOUT.

PL PLOT DATA.

FP FINISHED PROCESSING.

PROCESSING OPTION?

Low speed (LS), high speed (HS), and finished processing (FP) are similar to mass scan (SCN) options. Figure 27 shows an LS output for a ratio test. For the plot (PL) option, the computer asks for the plot type, Figure 28. All other inputs are identical to the mass scan plot option except that:

.MINUTES PER PAGE

is asked rather than mass numbers per page. Figure 29 shows a ratio test plot.

Software Expansion

The IMMA programs can easily be expanded to add additional analysis routines. Not quite as easily, the degree of computer control over the interface can be increased. As can be seen in the two examples of Appendix D, the software utilizes only some of the hardware-implemented capabilities. These unused capabilities were included in the hardware because they will facilitate the secondary magnet field and sample stage control software to be developed later.

CION MICROPROBE MAIN. 16:40:42 27/ 1/78
OPTION?

PKS

NUMBER OF PEAKS?

1

LIVE RUN? (Y,N)

Y

LIVE PRINTOUT? (Y,N)

Y

LIVE PLOT? (Y,N)

Y

FIRST MASS NUMBER?

16

MAXIMUM POWER OF TEN ON PLOT?

4

MINIMUM POWER OF TEN ON PLOT?

1

.MINUTES PER PAGE?

24.

PLOT OPTION?

1

TIME	COUNTS 16
010000	00030438
010000	00030652
010000	00017093
010000	00013275
010000	00013125
010000	00013075
010000	00013165
010000	00012767
010000	00012545
010000	00012248
010000	00012129
010000	00012358
010000	00011660
010000	00011219
010000	00011148
010000	00010483
010000	00010083
010000	00009966
010000	00009864
010000	00009581
010000	00009429
010000	00008836
010000	00008907
010000	00008332
010000	00008180
010000	00007941
010000	00007643
010000	00007730
010000	00007535
010000	00007261
010000	00007224
010000	00006968
010000	00006875
010000	00006467
010000	00006288
010000	00006166
010000	00005957
010000	00005967
010000	00005813
010000	00005859

Figure 25. PEAKS OPTION. (A Real-Time Run)

COMPARISON OF MANUAL AND COMPUTER-ASSISTED DATA AC- QUISITION AND MANIPULATION

Mass Scan

The mass-scan function of the computer-assisted data acquisition system provides a method to rapidly quantitate peaks in a mass spectrum. For greatest accuracy, the center of each peak is located manually and counted for a selected time. However, this method is very slow and is usable only if the composition of the sample does not change significantly with sputtering. For samples in which the composition does change significantly while sputtering, an automatic scan can be made with peak recording using the X-Y recorder. However, this method suffers from the time that is required to measure the peak heights and from a relatively low scan rate necessary to keep from exceeding the recorder's capability for displaying peaks accurately.

The precision and accuracy of peak measurement by the interface operating in the mass-scan mode were compared to that of measuring peak heights generated with the X-Y recorder in both the linear and logarithmic modes at scan speeds of 124 and 52 seconds/decade. Accuracy was determined by comparing the intensities of the zinc isotope peaks at m/e values of 66, 67, 68, and 70,

normalized to the Mass 64 isotope peak, with the values obtained by manually stepping from peak to peak and counting. The manually determined peaks were measured in the

```
ION MICROPROBE MAIN... 13:48:48 30/ 1/78
OPTION?
PKS
NUMBER OF PEAKS?
1
LIVE RUN? (Y,N)
N
FIRST MASS NUMBER?
16
FILE IDENTIFYING NO.?
1797
FILE NAMES:
1797
PROCESSING OPTION?
LS
TITLE FOR PRINTOUT?
1797 0 16 1/30/78
```

```
1797 0 16 1/30/78
```

ELAPSED TIME	COUNT RATE	16
1.000000E+01	3.043800E+03	
2.000000E+01	3.065200E+03	
3.000000E+01	1.709300E+03	
4.000000E+01	1.327500E+03	
5.000000E+01	1.312500E+03	
6.000000E+01	1.307500E+03	
7.000000E+01	1.316500E+03	
8.000000E+01	1.276700E+03	
9.000000E+01	1.254500E+03	
1.000000E+02	1.224800E+03	
1.100000E+02	1.212900E+03	
1.200000E+02	1.235800E+03	
1.300000E+02	1.166000E+03	
1.400000E+02	1.121900E+03	
1.500000E+02	1.114800E+03	
1.600000E+02	1.048300E+03	
1.700000E+02	1.008300E+03	
1.800000E+02	9.966000E+02	
1.900000E+02	9.864000E+02	
2.000000E+02	9.581000E+02	
2.100000E+02	9.429000E+02	
2.200000E+02	8.836000E+02	
2.300000E+02	8.907000E+02	
2.400000E+02	8.332000E+02	
2.500000E+02	8.180000E+02	
2.600000E+02	7.941000E+02	
2.700000E+02	7.643000E+02	
2.800000E+02	7.730000E+02	
2.900000E+02	7.535000E+02	
3.000000E+02	7.261000E+02	
3.100000E+02	7.224000E+02	
3.200000E+02	6.968000E+02	
3.300000E+02	6.875000E+02	
3.400000E+02	6.467000E+02	
3.500000E+02	6.288000E+02	

Figure 26. PEAKS OPTION. (Not a Real-Time Run)

ION MICROPROBE MAIN... 14:59:59 30/ 1/78
 OPTION?
 PKS
 NUMBER OF PEAKS?
 2
 LIVE RUN? (Y,N)
 N
 FIRST MASS NUMBER?
 31
 SECOND MASS NUMBER?
 32
 FILE IDENTIFYING NO.?
 1697
 FILE NAMES:
 1697
 PROCESSING OPTION?
 LS
 TITLE FOR PRINTOUT?
 1697 P AND S ON FRACTURE SN 597 1/27/78

1697 P AND S ON FRACTURE SN 597 1/27/78

ELAPSED TIME	COUNT RATE 31	COUNT RATE 32	RATIO
1.000000E+01	8.990000E+01	9.560000E+01	9.403766E-01
2.000000E+01	1.038000E+02	1.819000E+02	5.706432E-01
3.000000E+01	1.015000E+02	1.590000E+02	6.383648E-01
4.000000E+01	9.610000E+01	1.515000E+02	6.343234E-01
5.000000E+01	8.750000E+01	1.396000E+02	6.267908E-01
6.000000E+01	8.230000E+01	1.354000E+02	6.078286E-01
7.000000E+01	7.600000E+01	1.313000E+02	5.788271E-01
8.000000E+01	6.500000E+01	1.246000E+02	5.216693E-01
9.000000E+01	6.270000E+01	1.129000E+02	5.553587E-01
1.000000E+02	6.320000E+01	1.148000E+02	5.505227E-01
1.100000E+02	5.690000E+01	1.029000E+02	5.529640E-01
1.200000E+02	5.790000E+01	9.810000E+01	5.902141E-01
1.300000E+02	5.430000E+01	9.850000E+01	5.512690E-01
1.400000E+02	4.670000E+01	8.920000E+01	5.235426E-01
1.500000E+02	4.610000E+01	8.440000E+01	5.462085E-01
1.600000E+02	4.430000E+01	8.280000E+01	5.350242E-01
1.700000E+02	4.170000E+01	7.440000E+01	5.604839E-01
1.800000E+02	3.940000E+01	7.040000E+01	5.596591E-01
1.900000E+02	4.260000E+01	6.850000E+01	6.218978E-01
2.000000E+02	3.710000E+01	6.180000E+01	6.003236E-01
2.100000E+02	3.810000E+01	6.250000E+01	6.096000E-01
2.200000E+02	3.400000E+01	6.290000E+01	5.405405E-01
2.300000E+02	3.160000E+01	5.780000E+01	5.467128E-01
2.400000E+02	3.470000E+01	4.940000E+01	7.024291E-01
2.500000E+02	3.610000E+01	5.480000E+01	6.587591E-01
2.600000E+02	3.350000E+01	5.180000E+01	6.467181E-01
2.700000E+02	3.370000E+01	4.820000E+01	6.991701E-01
2.800000E+02	2.810000E+01	4.550000E+01	6.175824E-01
2.900000E+02	2.770000E+01	4.380000E+01	6.324201E-01
3.000000E+02	2.810000E+01	4.620000E+01	6.082251E-01
3.100000E+02	2.860000E+01	4.820000E+01	5.933610E-01
3.200000E+02	2.850000E+01	4.500000E+01	6.333333E-01
3.300000E+02	2.980000E+01	4.620000E+01	6.450216E-01
3.400000E+02	2.640000E+01	3.900000E+01	6.769231E-01
3.500000E+02	2.660000E+01	4.050000E+01	6.567901E-01

Figure 27. SAMPLE LOW-SPEED PEAK OUTPUT.

order: 64, 66, 67, 68, and 70, then 70, 68, 67, 66, 64, and averaged. This two-step operation was necessary because significant changes in count rates were evident, even over the time required to measure five peaks and after lengthy presputtering. Measurements were made both before and after the mass-scan measurements and were averaged. All scan peaks were normalized to $m/e = 64$ intensity which was set at the abundance found by the manual method. The interface clock rate was set at slow. Table 1 lists the results for scans made at 52 seconds/decade. With the interface, the error is 1% or less and the standard deviation 3.5% or less, except for $m/e = 70$. In addition to the $^{70}\text{Zn}^+$, a contribution due to Al_2O^+ was found at $m/e = 70$. The result of the Al_2O^+ contribution, which amounted to one half to two thirds of the peak intensity, was a continuous change in relative abundance of this peak. The normalized intensity of $m/e = 70$ was 1.22 about one hour before the interface and chart data were taken, and 1.87 a few minutes after. For this reason, a weighted average is included in the table as well as the average value for the $m/e = 70$ standard. Due to oxide-level fluctuations, the $m/e = 70$ data must be lightly regarded.

The logarithmic and linear chart data had good precision, but very poor accuracy due to an inability of the analog system, electronics, and X-Y recorder to respond rapidly enough to the peaks at 52 seconds/decade. Since

PROCESSING OPTION?

PL

PLOT OPTION?

1 FOR MASS A VS TIME

2 FOR MASS B VS TIME

3 FOR MASS A/MASS B VS TIME

4 FOR MASS B/MASS A VS TIME.

PLOT OPTION?

1

CALCULATE SCALE? (Y,N)

N

MAXIMUM POWER OF TEN ON PLOT?

3

MINIMUM POWER OF TEN ON PLOT?

0

.MINUTES PER PAGE?

24.

.TOTAL MINUTES?

24.

MAXIMUM COUNTS/SECOND 3

MINIMUM COUNTS/SECOND 0

PROCESSING OPTION?

PL

PLOT OPTION?

2

CALCULATE SCALE? (Y,N)

N

MAXIMUM POWER OF TEN ON PLOT?

3

MINIMUM POWER OF TEN ON PLOT?

0

.MINUTES PER PAGE?

24.

.TOTAL MINUTES?

24.

MAXIMUM COUNTS/SECOND 3

MINIMUM COUNTS/SECOND 0

PROCESSING OPTION?

PL

PLOT OPTION?

1

CALCULATE SCALE? (Y,N)

N

MAXIMUM POWER OF TEN ON PLOT?

3

MINIMUM POWER OF TEN ON PLOT?

0

.MINUTES PER PAGE?

24.

.TOTAL MINUTES?

24.

MAXIMUM COUNTS/SECOND 3

MINIMUM COUNTS/SECOND 0

PROCESSING OPTION?

FP

ION MICROPROBE MAIN... 15:33:42 30/ 1/78
OPTION?

Figure 28. PEAK PLOT TYPES.

the smallest errors (least relative reduction in peak size) will occur in the low-intensity peaks, these peaks will be relatively stronger compared to the $m/e = 64$ peak which is the most intense. Thus, the smaller 67 peak appears to have the greater error than the large 66 peak. It is clear that, at this scan rate, the X-Y recorder chart (logarithmic or linear) is totally inadequate for quantitative measurements, but the interface is capable of collecting data with good accuracy and precision.

Figure 29. SAMPLE PLOTS FOR THE RATIO TEST.

Table 1 also reports the results at a scan rate of 124 seconds/decade. Note that the interface data are little changed from the faster rate, but accuracy of the X-Y recorder data has improved greatly. However, the interface data are still clearly superior in precision and accuracy. The linear chart appears to be somewhat better than the logarithmic chart at this speed. To achieve the full accuracy capability of the X-Y recorder, the scan rate would have to be further reduced.

Table 2 summarizes the results obtained with nickel isotopes at scan rates from 380 to 52 seconds/decade, with clock periods of 40 msec (extra slow) to 10 msec (fast). The greatest reproducibility is found at the lowest rate with the longest clock period. There are two reasons for this: (1) the lowest rate gives more counts in each peak to give the best statistics, and (2) the slower clock rate detects the peaks at lower count rates and thus causes less truncation of the peak envelope. In the fastest scan (using the 10-msec clock period) the small peak at Mass 64 was apparently truncated significantly which caused a large error in abundance for this peak. Statistics on this peak were also poor, as only 30 - 50 counts were collected.

Above Mass 75, a peak-and-valley detector separates peaks where the count rate between peaks does not drop enough to detect the end of the first peak in the normal manner. After reading the mass-scan file, a list of these overlapping peaks is printed, as shown in Figure 18. The number of counts in the clock period at the center of the peak, the mass number, and the total counts in the overlapping peak envelope are printed. The counts collected in each peak are automatically calculated by ratioing the total counts according to the counts collected at the center of each peak. The list of selected peaks in Figure 22 is for the barium 130, 132, 134, 135, 136, 137, and 138 isotopes normalized to the natural abundance of 138. Peaks 134 - 138 were overlapping peaks separated by the peak-and-valley detector. A measure of accuracy obtained is indicated in Table 3 which compares the isotope ratios as printed in Figure 22 with the values listed on the KAPL chart of the nuclides.

Table 1

COMPARISON OF PRECISION AND ACCURACY OF PEAK MEASUREMENT IN MASS SCANS BY INTERFACE COLLECTION AND X-Y RECORDER AT TWO SCAN RATES

Mass/Charge	Standard Abundance (%)	Interface {7 Values}			Logarithmic Chart (3 Values)			Linear Chart (4 Values)		
		Abundance (%)	Standard Deviation (%)	Error (%)	Abundance (%)	Standard Deviation (%)	Error (%)	Abundance (%)	Standard Deviation (%)	Error (%)
At 52 Seconds/Decade										
64	48.70	48.70 ⁽¹⁾			48.70 ⁽¹⁾			48.70 ⁽¹⁾		
66	26.92	27.30 ± 0.25	± 0.9	1.0	33.2 ± 0.29	± 0.9	23.2	41.1 ± 0.26	± 0.6	52.6
67	4.98	4.95 ± 0.17	± 3.5	0.6	10.8 ± 0.25	± 2.3	116	10.4 ± 0.10	± 0.9	109
68	17.86	17.94 ± 0.11	± 0.6	0.4	24.2 ± 0.20	± 0.8	35.5	33.7 ± 0.65	± 1.9	88.5
70	1.54	1.70 ± 0.09	± 5.4	10.4	5.3 ± 0.25	± 4.8	242	4.8 ± 0.30	± 6.2	210
70 ⁽²⁾	1.74	1.70 ± 0.09	± 5.4	2.3	5.3 ± 0.25	± 4.8	203	4.8 ± 0.30	± 6.2	174
At 124 Seconds/Decade										
64	48.70	48.70 ⁽¹⁾			48.70 ⁽¹⁾			48.70 ⁽¹⁾		
66	26.92	27.27 ± 0.46	± 1.7	1.3	28.0 ± 0.59	± 2.1	41	28.1 ± 2.4	± 8.4	4.5
67	4.98	5.00 ± 0.13	± 2.6	0.4	7.0 ± 0.86	± 12.2	41.6	5.2 ± 0.31	± 5.9	3.7
68	17.86	17.88 ± 0.14	± 0.8	0.1	20.7 ± 0.25	± 12.4	15.8	18.4 ± 1.4	± 7.8	3.2
70	1.54	1.79 ± 0.07	± 3.7	16.2	3.5 ± 0.36	± 10.3	126	2.6 ± 0.27	± 10.6	66.0
70 ⁽²⁾	1.74	1.79 ± 0.07	± 3.7	2.9	3.5 ± 0.36	± 10.3	99.7	2.6 ± 0.27	± 10.6	46.9

(1) Normalizing value.

(2) Time weighted average of standard runs.

Table 2
INTERFACE SCAN ON NICKEL ISOTOPES AT VARIOUS SCAN RATES AND CLOCK PERIODS

Mass/Charge	Scan Rate (sec/decade) and Clock Time (msec)				
	380 and 40 (extra slow)	124 and 30 (slow)	75 and 20 (medium)	61 and 20 (medium)	52 and 10 (fast)
58	67.77	67.77	67.77	67.77	67.77
60	25.85 ± 0.04	26.02 ± 0.30	26.52 ± 0.49	26.24 ± 0.84	26.83 ± 0.65
61	1.13 ± 0.03	1.13 ± 0.05	1.14 ± 0.05	1.05 ± 0.14	0.70 ± 0.18
62	3.48 ± 0.03	3.46 ± 0.05	3.69 ± 0.17	3.56 ± 0.11	3.52 ± 0.09
64	0.87 ± 0.03	0.80 ± 0.15	0.89 ± 0.13	0.95 ± 0.05	0.28 ± 0.13

In order for a peak to be detected, ten counts must be totaled in a clock period. Thus, the longer the clock period, the smaller the peak which can be detected. Table 4 provides a summary of the experimentally determined detectability levels. The detection level was not significantly affected by the scan rate.

In choosing a clock rate, it is best to choose a slow rate for the lowest detection limit and a least truncation of the peaks. However, higher clock rates sometimes have to be used to separate strong peaks which are separated by one mass or less below Mass 75; otherwise, the end of the one peak may not be determined before the second starts. Above 75, the peak-and-valley detector operates to separate the overlapping peaks.

An example of the mass-scan data output is given in Figure 20. Other options allow printing of the most intense peaks (MI), as shown in Figure 21, printing selected peaks (SP), normalizing the spectra to any value with respect to any peak (NO), correction of the peak intensities to correct for inequities caused by the scan-rate function (RA), and plotting the mass-scan data (PL). Figure 22 is a printing of selected peaks which have been corrected and normalized.

The plotting option is also flexible, allowing printing of a selected portion of the mass spectrum with X and Y axes scaled as desired or with the Y axis automatically scaled. A plot of the mass-scan data which was printed in Figure 20 is included as Figure 30. Figures 31 - 33 show this same plot spread out and compared to the analog X-Y recorder plot which was made simultaneously with the collection of these data. It can be seen that some of the very small peaks are not detected by the interface. Figure 31 also shows a case where two strong peaks closely separated below Mass 75 were not resolved and thus combined as one peak. These are the doubly charged barium isotope peaks, $^{137}\text{Ba}^{+2}$ and $^{138}\text{Ba}^{+2}$, which occur at $m/e = 68.5$ and 69 , respectively. These peaks could be resolved either by changing to a shorter clock period or by increasing the instrument mass resolution.

Table 3
BARIUM ISOTOPE RATIOS MEASURED WITH THE
INTERFACE MASS SCAN WHERE ISOTOPE PEAKS
134 - 138 WERE SEPARATED BY THE
PEAK-AND-VALLEY DETECTOR

Mass	KAPL Chart	Interface	
		Normalized to 138	Abundance Ratio
130	0.101	0.097	0.098
132	0.097	0.100	0.101
134	2.42	2.37	2.38
135	6.59	6.34	6.37
136	7.81	7.84	7.87
137	11.32	11.17	11.22
138	71.66	71.66	71.97

Table 4
INTERFACE DETECTABILITY
OF PEAKS

Percent Detected	Clock (cts/sec)			
	Extra Slow	Slow	Medium	Fast
50	225	300	400	800
90	300	450	600	1200

Figure 30. PLOT OF MASS-SCAN DATA FOR FILE 0759, NBS GLASS K-489.

(a) Plot of Mass Scan Data.

(b) Plot of X-Y Recorder.

Figure 31. PLOT OF MASS-SCAN DATA AND X-Y RECORDER. (Mass/Charge = 0 - 80)

(a) Plot of Mass Scan Data.

(b) Plot of X-Y Recorder.

Figure 32. PLOT OF MASS-SCAN DATA AND X-Y RECORDER. (Mass/Charge = 80 - 160)

(a) Plot of Mass Scan Data.

(b) Plot of X-Y Recorder.

Figure 33. PLOT OF MASS-SCAN DATA AND X-Y RECORDER. (Mass/Charge = 160 - 240)

The CARISMA analysis program is a main option in the data acquisition-and-analysis system (Appendix C). Two of the options are primarily used: Option 1 requires entry of electron

NBS GLASS K-489

ASSIGNED SUM= 37.000

12 ELEMENTS.

BACKGROUND= 0.00C/S

PLASMA CONDITIONS--TEMPERATURE= 9020.00, LOG P(E)= 5.9340

NE= 0.689870E+18 DELTA E= 0.1761

N(0) = 0.2369E+20

MASS	ELEMENT	AT.PCT. RAW C/S	ALPHA CORR. C/S	BETA K(N)	ZI/ZA K(NN)
11	B	0.5306 7.700E+01	2.817E-02 9.599E+01	5.097E-04 1.242E+20	1.664E-01 4.973E+41
27	AL	0.5219 1.360E+03	3.426E-01 1.360E+03	6.342E-04 3.611E+21	1.528E-01 0.000E-01
28	SI	67.3204 4.357E+04	1.007E-01 4.722E+04	2.606E-03 2.454E+20	5.321E-01 5.501E+42
44	SIO	0.0000 PPM. 2.230E+02	5.339E-03 2.417E+02	2.606E-03 3.036E+20	5.321E-01 8.542E+42
48	TI	0.2813 8.690E+02	5.583E-01 1.183E+03	5.505E-04 1.473E+21	1.101E+00 2.435E+42
56	FE	0.3793 4.950E+02	1.862E-01 5.400E+02	7.029E-04 3.161E+22	7.892E-01 0.000E-01
64	ZN	3.5252 9.600E+02	7.299E-02 1.964E+03	3.743E-04 7.449E+21	1.850E+00 0.000E-01
90	ZR	0.6109 1.203E+03	5.044E-01 2.338E+03	5.947E-04 2.577E+21	8.921E-01 1.613E+43
138	BA	25.4731 1.000E+05	7.209E-01 1.395E+05	1.798E-04 3.052E+21	6.056E-01 0.000E-01
140	CE	0.4678 1.766E+03	6.109E-01 1.996E+03	4.482E-04 2.459E+20	9.417E-01 0.000E-01
181	TA	0.4301 7.480E+02	3.094E-01 7.480E+02	4.043E-04 6.733E+19	1.195E+00 5.571E+40
206	PB	0.4594 2.340E+02	2.827E-01 9.915E+02	1.253E-03 1.098E+22	7.285E-01 0.000E-01

OPTION 3 USED. GRID SEARCHED FOR BEST FIT OF 3 INTERNAL STANDARDS.

AL = 0.1821 SI = 24.9100 FE = 0.1844

ANALYSIS RECALCULATED TO 37.000 PERCENT, EXCLUDING OXYGEN.

11	B	1.96339E-01
27	AL	1.93116E-01
28	SI	2.49085E+01
44	SIO	0.00000E-01
48	TI	1.04078E-01
56	FE	1.40343E-01
64	ZN	1.30431E+00
90	ZR	2.26050E-01
138	BA	9.42506E+00
140	CE	1.73072E-01
181	TA	1.59122E-01
206	PB	1.69977E-01

Figure 34. CARISMA OPTION 3 OUTPUT FROM THE TELEPRINTER.

temperature and pressure and requires only a few seconds of computer time, while Option 3 requires two standards and will accept up to six. In the PDP-15/35, with the program broken into small segments, an Option 3 computation may take 1.5 hours or more. Thus, the system is designed to run CARISMA Option 3 in the background, while allowing use of the other IMMA options. The mass-scan data of Figure 20 were used with appropriate elemental corrections for calculation of composition by CARISMA. The printout is included as Figure 34.

In summary it can be stated that the mass-scan function of the data-acquisition system quantitates mass-scan data more rapidly and with better accuracy and precision than the analog X-Y recorder system, and nearly as accurately as manually stepping peaks. When conditions and peak intensities are changing, it provides a capability for quantifying peaks which would be impossible otherwise. Flexibility for data manipulation and plotting is provided. Its biggest drawback is failure to detect the small peaks below 300 counts/second.

A possible addition to the system would be the capability for stepping from peak to peak and dwelling for a preselected time. This capacity would allow detection of smaller peaks, but would require a much more accurate mass determination.

Single-Peak Profiling

Figure 35 shows a profile of $^{90}\text{Zr}^+$ obtained in the usual manner on the X-Y recorder compared to the profile plotted by using the computer. The manually obtained plot is not electronically apertured since the electronic aperture will not handle the analog ion-current signal. The data-system-acquired plot does reflect use of the electronic aperture which accepts counts only from a central portion of the raster to avoid edge effects and give better depth resolution. Apertured data can be obtained automatically on the teleprinter without using the computer or data system. However, it has the drawback that there is a three-second delay between counting periods for printing of each line of data compared to a few milliseconds for the data-acquisition system to read the scalars. This relatively long time limits the recording of fast events to point taking every 3 - 4 seconds (using 0.1 - 1-second recording periods), whereas the data-acquisition system can record data every 0.1 second if desired, with little loss between recording periods. A second drawback of the unaided system is that the apertured data would have to be manually plotted, a very time-consuming process. Figure 36 compares the normally setup teleprinter output and the output from the computer. The record from the computer gives total elapsed time in the profile and the count rate unless the teleprinter

Figure 35. PROFILES OF THE $^{90}\text{Zr}^+$ ON MULBERRY ALLOY WITH A 150-nm (1500-Å) OXIDE FILM.

Normal Operation			Computerized System		
			ELAPSED TIME	COUNT RATE	90
001.000	00036673	090.2	1.000000E+00	3.648200E+04	
001.000	00016836	090.2	2.000000E+00	3.230100E+04	
001.000	00010111	090.1	3.000000E+00	2.518400E+04	
001.000	00005980	090.2	4.000000E+00	2.120100E+04	
001.000	00003819	090.3	5.000000E+00	1.669100E+04	
001.000	00002906	090.2	6.000000E+00	1.364200E+04	
001.000	00002549	090.3	7.000000E+00	1.238400E+04	
001.000	00001979	090.1	8.000000E+00	1.005700E+04	
001.000	00001776	090.1	9.000000E+00	8.874000E+03	
001.000	00001793	090.1	1.000000E+01	7.871000E+03	
010.000	00015905	090.1	1.100000E+01	6.539000E+03	
010.000	00014789	090.2	1.200000E+01	5.583000E+03	
010.000	00014654	090.1	1.300000E+01	5.331000E+03	
010.000	00015061	090.2	1.400000E+01	4.323000E+03	
010.000	00014451	090.1	1.500000E+01	3.899000E+03	
010.000	00013774	090.2	1.600000E+01	3.780000E+03	
010.000	00013059	090.2	1.700000E+01	3.304000E+03	
010.000	00012133	090.2	1.800000E+01	2.770000E+03	
010.000	00011407	090.1	1.900000E+01	2.737000E+03	
010.000	00010970	090.2	2.000000E+01	2.484000E+03	
010.000	00010803	090.1	2.100000E+01	2.281000E+03	
010.000	00010504	090.1	2.200000E+01	2.261000E+03	
010.000	00010118	090.2	2.300000E+01	2.010000E+03	
010.000	00009031	090.2	2.400000E+01	1.887000E+03	
010.000	00006153	090.2	2.500000E+01	1.960000E+03	
010.000	00003586	090.2	2.600000E+01	1.893000E+03	
010.000	00002266	090.6	2.700000E+01	1.703000E+03	
010.000	00001784	090.2	2.800000E+01	1.727000E+03	
010.000	00001475	090.1	2.900000E+01	1.637000E+03	
010.000	00001478	090.1	3.000000E+01	1.610000E+03	
010.000	00001444	090.2	3.089100E+01	1.516274E+03	
010.000	00001410	090.1	4.089100E+01	1.435700E+03	
010.000	00001347	090.2	5.089100E+01	1.380100E+03	
010.000	00001327	090.2	6.089100E+01	1.334300E+03	
010.000	00001247	090.1	7.089100E+01	1.283900E+03	
010.000	00001253	090.2	8.089100E+01	1.298600E+03	
010.000	00001260	090.2	9.089100E+01	1.311700E+03	
010.000	00001285	090.2	1.008910E+02	1.319500E+03	
010.000	00001180	090.2	1.108910E+02	1.294600E+03	
010.000	00001132	090.1	1.208910E+02	1.252000E+03	
010.000	00001102	090.2	1.308910E+02	1.197500E+03	
010.000	00001119	090.1	1.408910E+02	1.122200E+03	
010.000	00001058	090.1	1.508910E+02	1.079800E+03	
010.000	00001068	090.2	1.608910E+02	1.061200E+03	
010.000	00001030	090.1	1.708910E+02	1.046100E+03	
010.000	00001022	090.6	1.808910E+02	9.997000E+02	
010.000	00001015	090.1	1.908910E+02	9.982000E+02	
010.000	00001008	090.2	2.008910E+02	9.904000E+02	
010.000	00000969	090.2	2.108910E+02	9.511000E+02	
010.000	00001000	090.1	2.208910E+02	9.161000E+02	
010.000	00000996	090.2	2.308910E+02	7.598000E+02	
010.000	00001003	090.1	2.408910E+02	5.440000E+02	
010.000	00001028	090.2	2.508910E+02	3.517000E+02	
010.000	00000965	090.1	2.608910E+02	2.452000E+02	
010.000	00000984	090.2	2.708910E+02	1.920000E+02	
010.000	00001015	090.2	2.808910E+02	1.510000E+02	
010.000	00000973	090.1	2.908910E+02	1.462000E+02	

Figure 36. SINGLE-PEAK PROFILE DATA THAT WERE COLLECTED BY THE COMPUTER-DATA-ACQUISITION SYSTEM AND BY THE NORMAL AUTOMATIC TELEPRINTER.

output is "live", in which case the output is in terms of time and counts similar to the normal output. After live printing, the recorded data in the elapsed time/count rate format may be requested. Another advantage of the computerized system is the ability to replot

and rescale the data quickly and as many times as desired. In the normal operation, the X and Y scales are set before the runs, and only one copy is made. The X-axis scale is a time scale which is difficult and time consuming to set up manually with accuracy. Then, if the profile takes longer than expected, it may have to be completed on a second sheet. For report copy, the test may have to be rerun with a new scale setup. Thus, in single-peak profiling, the computer-assisted data-acquisition system provides for:

Improved plotting capability by:

- Apertured plots, and
- Reduced dead time in the digital scaler reading.

Time saving by:

- Plotting the parameters setup quickly,
- Plot copies made quickly with scales set as needed,
- No loss of plot due to improper scaling, and
- No need for hand plotting of apertured data.

Peak Switching or Ratio Profiling

In peak switching or ratio profiling, using the standard mode of operation, direct plots on the X-Y recorder are an average of the signal from the two peaks being detected. To get the individual plots, the data from the teleprinter must be manually plotted. With the computer system, apertured data from each peak are stored, and each peak or the ratio of the peaks (A/B or B/A) is readily plotted. For monitoring purposes, one peak or ratio can be plotted live. Figure 37 shows the profiles of Nb^+ , Zr^+ , and Nb^+/Zr^+ from a single-ratio profile. The Nb^+/Zr^+ ratio plot shows a thin layer of niobium enrichment on the surface of the oxidized Mulberry^(d) which would not be readily apparent from the individual element profile. Figure 38 compares the teleprinter output from a standard or normal run and one made with the computer. Use of the computer-assisted data-acquisition system for peak switching or ratio profiling has all the advantages provided for single-peak profiling plus the capability of plotting each peak and calculation, and plotting the peak ratios.

Figure 37. RATIO PROFILES OF $^{90}\text{Zr}^+$ AND Nb^+ ON MULBERRY WITH A 150-nm (1500-Å) OXIDE FILM.

(d) Mulberry is a ternary alloy of depleted uranium, containing 7.5 wt % niobium and 2.5 wt % zirconium.

Normal Operation				Computerized System			
				ELAPSED TIME	COUNT RATE 90	COUNT RATE 93	RATIO
001.000	00019163	00097641	1.000000E+00	1.838500E+04	9.437400E+04	1.948100E-01	
001.000	00008893	00030084	2.000000E+00	1.567300E+04	6.502900E+04	2.410155E-01	
001.000	00004628	00014552	3.000000E+00	1.204700E+04	4.649100E+04	2.591254E-01	
001.000	00002802	00007538	4.000000E+00	9.410000E+03	3.543100E+04	2.655866E-01	
001.000	00001794	00004838	5.000000E+00	7.690000E+03	2.717300E+04	2.830015E-01	
001.000	00001365	00003582	6.000000E+00	6.515000E+03	2.154800E+04	3.023482E-01	
001.000	00001168	00002590	7.000000E+00	5.443000E+03	1.775800E+04	3.065097E-01	
001.000	00001039	00002571	8.000000E+00	4.604000E+03	1.440000E+04	3.197222E-01	
001.000	00000885	00002306	9.000000E+00	3.843000E+03	1.214100E+04	3.165308E-01	
010.000	00008245	00020792	1.000000E+01	3.232000E+03	1.015300E+04	3.183296E-01	
010.000	00007739	00019963	1.100000E+01	2.808000E+03	8.663000E+03	3.241371E-01	
010.000	00007574	00020380	1.200000E+01	2.428000E+03	7.332000E+03	3.311511E-01	
010.000	00007326	00018899	1.300000E+01	2.182000E+03	6.497000E+03	3.358473E-01	
010.000	00007707	00020007	1.400000E+01	1.934000E+03	5.598000E+03	3.454805E-01	
010.000	00007342	00019263	1.500000E+01	1.634000E+03	4.956000E+03	3.297014E-01	
010.000	00007011	00017890	1.600000E+01	1.468000E+03	4.456000E+03	3.294434E-01	
010.000	00006448	00016560	1.700000E+01	1.356000E+03	3.880000E+03	3.494845E-01	
010.000	00006364	00015630	1.800000E+01	1.310000E+03	3.598000E+03	3.640912E-01	
010.000	00006067	00015541	1.900000E+01	1.131000E+03	3.370000E+03	3.356083E-01	
010.000	00006061	00014983	2.000000E+01	1.152000E+03	3.110000E+03	3.704180E-01	
010.000	00005947	00014749	2.100000E+01	1.067000E+03	2.898000E+03	3.681850E-01	
010.000	00005688	00013717	2.200000E+01	1.001000E+03	2.628000E+03	3.808980E-01	
010.000	00004438	00010191	2.300000E+01	9.680000E+02	2.619000E+03	3.696067E-01	
010.000	00002600	00005477	2.400000E+01	8.470000E+02	2.502000E+03	3.385292E-01	
010.000	00001790	00003152	2.500000E+01	9.390000E+02	2.445000E+03	3.840491E-01	
010.000	00001291	00002355	2.600000E+01	8.770000E+02	2.401000E+03	3.652645E-01	
010.000	00001196	00001920	2.700000E+01	8.610000E+02	2.206000E+03	3.902992E-01	
010.000	00001067	00001846	2.800000E+01	7.430000E+02	2.210000E+03	3.361991E-01	
010.000	00001034	00001754	2.900000E+01	7.940000E+02	2.245000E+03	3.536748E-01	
010.000	00001012	00001680	3.000000E+01	7.760000E+02	2.075000E+03	3.739759E-01	
010.000	00000995	00001685	3.100000E+01	7.690000E+02	2.063000E+03	3.727581E-01	
010.000	00000897	00001652	3.200000E+01	6.930000E+02	2.019000E+03	3.432392E-01	
010.000	00000918	00001603	3.300000E+01	7.430000E+02	2.062000E+03	3.603298E-01	
010.000	00000827	00001603	3.400000E+01	6.790000E+02	2.010000E+03	3.378109E-01	
010.000	00000816	00001640	3.500000E+01	7.120000E+02	2.022000E+03	3.521266E-01	
010.000	00000840	00001647	3.600000E+01	6.540000E+02	1.974000E+03	3.313070E-01	
010.000	00000765	00001549	3.699000E+01	7.626263E+02	2.001010E+03	3.811206E-01	
010.000	00000758	00001517	4.699000E+01	6.692000E+02	1.887000E+03	3.546370E-01	
010.000	00000727	00001509	5.699000E+01	6.641000E+02	1.841100E+03	3.607083E-01	
010.000	00000746	00001583	6.699000E+01	6.433000E+02	1.853600E+03	3.470544E-01	
010.000	00000752	00001454	7.699000E+01	6.658000E+02	1.838100E+03	3.622219E-01	
010.000	00000723	00001548	8.699000E+01	6.698000E+02	1.916600E+03	3.494730E-01	
010.000	00000684	00001480	9.699000E+01	6.554000E+02	1.847400E+03	3.547689E-01	
010.000	00000738	00001504	1.069900E+02	6.370000E+02	1.795900E+03	3.546968E-01	
010.000	00000811	00001543	1.169900E+02	6.038000E+02	1.662200E+03	3.632535E-01	
010.000	00000788	00001391	1.269900E+02	5.656000E+02	1.600200E+03	3.534558E-01	
010.000	00000794	00001386	1.369900E+02	5.595000E+02	1.531100E+03	3.654236E-01	
010.000	00000792	00001466	1.469900E+02	5.227000E+02	1.463300E+03	3.572063E-01	
010.000	00000800	00001503	1.569900E+02	5.387000E+02	1.412600E+03	3.813535E-01	
010.000	00000887	00001490	1.669900E+02	5.102000E+02	1.408800E+03	3.621522E-01	
010.000	00000880	00001444	1.769900E+02	5.019000E+02	1.385200E+03	3.623303E-01	

Figure 38. RATIO-PROFILE DATA THAT WERE COLLECTED NORMALLY WITH THE TELEPRINTER AND BY THE COMPUTER-DATA-ACQUISITION SYSTEM.

X-Line Profile

In the X-line profile, the X axis is driven synchronously with the ion-beam sweep in a line over the sample. In the normal mode, the pen must be dropped and lifted manually at the start and end of each sweep which is to be recorded. The data-acquisition system controls the pen on the recorder such that a chosen number of sweeps may be recorded with a chosen number of sweeps not recorded between. Five X-line sweeps are shown in Figure 39

Figure 39. X-LINE INTENSITY PROFILES OF FLUORINE, USING THE DATA-ACQUISITION SYSTEM FOR PEN CONTROL.

in which the F^- secondary-ion intensity was recorded as a function of position on a fluoride-exposed Mulberry sample. The system was set to make two sweeps at each location before recording the F^- secondary-ion current. This procedure was carried out to equalize the ion-beam effect on the sample for each trace. As shown, the pen was accurately dropped and picked up at the same point on each of these 65-second sweeps. Manually, the pen pickups and drops are somewhat erratic on rapid sweeps.

This part of the system was primarily designed for use with computer control of the sample stage, such that a series of X-line profiles could be made automatically on a sample. The chart is automatically advanced after each recorded trace when using fanfold paper.

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APPENDIX B

MANUAL TEST CONTROL PROCEDURE

The manual interface controls are essentially self explanatory. Switch positions for the various tests are listed in Table B-1. The sequence for all tests except the X line is:

Table B-1

SWITCH POSITIONS FOR THE VARIOUS TESTS

Test Mode	Interface Switches		Timer Scaler Switches			
	Scan Range	Operation Select	Display Time	Stop Select	Preset Time	Ratio/Normal
X Line	Off	Manual				
Scan	Extra Slow, Slow, Medium, Fast	Auto	Hold	Manual		Normal
Single Peak	Off	Semiautomatic	Hold	Time	(Select Time)	Normal
Ratio	Off	Semiautomatic	Hold	Time	(Select Time)	Ratio

1. Mount the cassette (see Table B-2).

Table B-2

INSTRUCTIONS FOR CASSETTE OPERATION

1. Open door, place cassette (tape side down) into holder, close door.
2. Hold initialize button until tape stops. If this tape is to be written on, press "fast forward" for several seconds.
3. Press reset.
4. Always push "rewind" before removing tape, always erase a tape before first writing on it. It is suggested that the "write lock" tab (on left side) be broken to permanently preserve data.
5. Should it be necessary to position the tape, JOG, FORWARD/REVERSE, and FAST can be used. Push "reset" after changing directions. File sample number and run number are displayed in the forward direction. FILE MARKERS are displayed in the forward and reverse directions.

2. Push the COMPUTER RESET button.^(e)
3. Position the switches as given in Table B-2.
4. Push the scaler RESET button.^(f)

(e) Located on the IMMA front panel (Figure 15).

(f) Located on the timer/scaler front panel (Figure 8).

5. Dial SAMPLE ID, RUN #.(e)
6. Push the EXECUTE button.(e)

The X-line test is initiated by depressing the "computer reset", "X-line execute", and "test mode execute" buttons in sequence. The "delta record" controls which sweep will be recorded. Each nth X-line sweep (where n is the delta record number plus the first sweep) is recorded. The total number of sweeps recorded is equal to the number of records recorded plus the first sweep unless the delta record equals 1. When the delta record equals 1, every sweep is recorded up to the number of records. The X-Y recorder is switched to the "computer" position for pen-lift and paper-advance control. The X-line indicator light is on for the duration of the test.

There are three different methods for actually starting the four tests. The mass-scan test starts when the mass-scan control (Figure B-1) resets (either automatically or manually) and ends at the end of the scan. The single-peak and ratio tests are started and stopped from the IMMA interface, utilizing the "start test" and "end test" push buttons. The X-line test is started automatically by the raster sweep control.

163374
Figure B-1. DISPLAY PANEL OF THE MASS-SCAN CONTROLLER.

APPENDIX C

CARISMA OPERATOR'S GUIDE

Computer operation of IMMA includes a routine to calculate the elemental composition. IMMA outputs a mass number and intensity for each point above background. The intensity is dependent upon the concentration of the material and the response of the mass analyzer. These data are not readily amenable to absolute analysis. Qualitative or comparative data are the best that can be managed without intensive data analysis. One of these data analysis programs, CARISMA (corrections to Applied Research ion sputtering mass analyzers), uses some 7000 constants in tables of element information and the appropriate theoretical equations^(g) to calculate the atomic percent of elements in a sample.^(h) Option 1 yields a quick answer to the problem if the plasma conditions are known; ie, temperature and electron pressure. Option 3 will calculate percentages and plasma conditions when two to six elements and their abundances are entered as internal standards. Unfortunately, this option usually takes 1 - 2 hours.

CARISMA, as implemented on the PDP-15/35 under RSX executive, consists of Options 1 and 3 and is called "CAR" as an Ion Microprobe Mass Analyzer Program (IMMAP) option. In general, each line of input is terminated by a carriage return (CR or $\rightarrow$), a $\uparrow$ U (control U) erases the current line (continue as if starting in column one), and rubout (echoed \) erases the preceding character.

The first input shown in Figure C-1 is the identification line, ①. This title (up to 70 alphanumeric characters) is outputted with the calculated answers. The next question, ②, asks for the SUM (default value, 100), TYPE (Option 1 or 3), and ELEMENT (oxide).

The following line, ③, explains the format. A format description may be:

- FFF...F indicates a floating-point format. The number may appear anywhere in the field (positionally independent). The decimal point defaults to the far right of the field (Ex 62.3).
- III...I indicates an integer format (no decimal point). The number should be right justified (position dependent). Blanks are interpreted as zeros. A CR terminates the field (Ex 15).
- AAA...A indicates an alphanumeric field which is position dependent (blanks have a value). The characters should be left justified.

(g) CARISMA is a trademark of the Applied Research Laboratories.

(h) CARISMA has two options that are accepted as "debugged" from both a theoretical and software point of view.

The next question, ④, has a dual purpose. For Option 1, the last two floating-point values are the plasma temperature (K) and log of the electron pressure, respectively. For Option 3, the inputs are used for internal standards (up to six).

The next question, ⑤, asks for the mass number of any element to be removed in the final normalization. (Oxygen is automatically removed.)

The next question, ⑥, asks for the OPTION/OXIDE, mass number, and number of counts (RAW DATA).

The data are to be inputted under the appropriate field descriptor. The options are:

BKGD - The count rate in this line is to be subtracted from all other count rates as a background.

SUM - The count rate is interpreted as the total atomic percentage of the preceding elements.

END - Terminates the data input.

The last question "Did you make a mistake?, (Y,N)" gives the operator the opportunity to repeat the question/answer routine.

At this point, Option 1 calculates for several seconds before outputting data. After everything is printed, CARISMA returns to IMMAP. Option 3, on the other hand, returns immediately to IMMAP, and a CARISMA status indicator is outputted every time IMMAP identifies itself. The status letter ("C" for calculating; "P" for ready to print results) is cleared by typing CAP which waits for CARISMA to finish and then outputs the answers. Option 3 can, therefore, operate interleaved with any IMMAP option without significantly affecting either its execution time or the response time in IMMAP. This is one way to temper the long execution time.

Another way is to batch process from paper tape during an off shift. All the IMMA programs may be batch executed, but CARISMA is particularly suited to this mode of operation because it requires no operator intervention. To create a batch tape, the operator uses paper tape instead of a direct input from the TTY. The tape format is shown in Figure C-2. Essentially, the operator types on tape the answers to all of the questions encountered. A carriage return, line feed, and rubout rather than the normal carriage return must also be typed at the end of each line.

The tape is input via the high-speed paper tape reader at the computer. The output may be to any nonfile-oriented device including the lineprinter. To start batch processing, the computer operator types:

REA 17 PRØ TT8,

```

[LEADER]                                "HERE IS"
CAR)                                     ( ) = CR,LF, rubout)
[TITLE])
[SUM, TYPE, ELEMENT])

N)                                       (in answer to "DID YOU MAKE A
CAP)                                   MISTAKE? (Y,N)")
CAR)                                   (immediately calls output programs
[TITLE])                               which will wait for CARISMA to finish)
                                         NEXT RUN

CAP)
EXT)                                   (exits after last CARISMA data run)

```

Figure C-2. DATA TAPE FORMAT.

then requests the program.

To change the output device to the high-speed lineprinter, he types:

```
REA 13 LA0 TT8.
```

The output device defaults to the IMMA teleprinter. Pagination is included in the lineprinter. For the operator's convenience, if the input and output devices are not the same (ie, batch operation), then the CARISMA inputs will be echoed on the output device so the answer follows the questions visibly.

Technically, CARISMA operates in the first-user partition. This partition consists of only 4K words of memory, so extensive overlaying is used in each task (a task is a logically independent unit of work—a job step). CARISMA consists of four tasks:

- CAR1 - creates the data base on the disk and scratch-pad memory, normally the entry point of CARISMA.
- CAR2 - gets and checks all input.
- CAR3 - performs calculations.
- CAR4 - outputs the answers and erases the data base.

An externally named common area of 512 words (COM5) is used for intertask communication, primarily data-base pointers. To store frequently used constants, 6K of scratch-pad memory is used. The input logical unit number (LUN) is 17; the output LUN is 14.

APPENDIX D

FIRMWARE

The computer communicates with the IMMA interface via IOTs [I/O (input/output) transfers], some of which utilize an 18-bit register to transfer data to or from the interface (see Tables D-1 and D-2). Since the computer must occasionally wait on the result of these IOTs, the IMMA interface is tied into the automatic priority interrupt system (API). This connection allows IMMA to usurp the central processor unit (CPU) and operate at a priority higher than normal software. Associated with an API channel is a unique memory location (vector) containing the address of the inter-

Table D-1

CONTROLLING INTERFACE FOR FIRMWARE INSTRUCTIONS

IOT (Input/Output Transfer Instruction)			
(1)	705402	Execute Register Held	Subcommand (Table E-2)
(2)	705302	Load Data	
(3)	705401	Skip on Data Ready (buffer 1)	
(4)	705421	Skip on Data Ready (buffer 2)	
(5)	705441	Skip on Computer Reset Command	
(6)	705461	Skip on Data Ready (tape)	
(7)	705301	Skip if Interface is On Line	
(8)	705321	Skip on Plotter Paper Advance Complete	
(9)	705341	Skip on End of File (tape)	
(10)	705361	Skip on Buffer Full	
(11)	705404	Clear 3	
(12)	705424	Clear 4	
(13)	705444	Clear 5	
(14)	705464	Clear 6	
(15)	705304	Clear 7	
(16)	705324	Clear 8	
(17)	705344	Clear 9	
(18)	705364	Clear 10	

Table D-2

INTERFACE SUBCOMMANDS

Subcommand	
014000	ON-LINE
010000	OFF-LINE
110000	Select X-LINE Test
310000	Select SCAN Test
410000	Select Single Peak Test
510000	Select Ratio Test
610000	START Test
710000	END Test
120XXX	Load Sample-Run Number (XXX)
220000	Read DATUM from Buffer 1
320000	Read DATUM from Buffer 2
42XXYY	X-Line Load Records (XX) and Skips (YY)
520000	Read DATUM from Tape
62XXXX	Load DAC 1
72XXXX	Load DAC 2

rupt servicing routine. Only a higher priority interrupt can defer the execution of this routine. IMMA operates at the lowest hardware priority, and the worst-case delay is about 2 msec. This much delay is an extremely rare event (normally about 1.8 μ sec), and much larger delays can be tolerated.

To avoid additional operating system overhead, the vector is valid only under program control. Therefore, to prevent crashing the operating system because of an unexpected interrupt, the capability of disconnecting IMMA from the API system was implemented. IMMA is turned on line only when the program is prepared for

interrupts. The interrupt servicing routine saves the status of the system and then proceeds to determine the precise cause of the interrupt by utilizing the skip-if-true series of instructions.

After determining the cause of the interrupt, the appropriate action is taken, the interrupt is cleared, and the routine restores the system to its original status; that is, returns to the interrupted program.

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