THE ORNL ATOM PROBE SOFTWARE PACKAGE

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Abstract - An atom probe software package for on-line control of the instrument and analysis of atom probe and imaging atom probe data has been developed. The package was written to provide the maximum information to the operator and has the flexibility to view the data in the most appropriate mode for the type of analysis being undertaken. The data may be displayed in real time, either individually or in combination, as raw masses or times, ion-by-ion element identification, mass or time spectra, multi-element composition profiles, ladder diagrams, cumulative plots and composition. The data may also be analysed immediately with autocorrelations, cross correlations, Fast Fourier Transforms, and frequency distributions or compared to previously stored data. A built in data base containing isotope abundances and normal charge states of all elements is available for element identification.

INTRODUCTION

The ORNL atom probe software package provides a complete self-contained system for atom probe control and data analysis. The design objective for the software package was to produce a comprehensive yet flexible and easily used set of programs for collecting and analyzing atom probe data for both the specialist and inexperienced user. The package provides control of the energy-compensated time-of-flight mass spectrometer, the imaging atom probe (IAP) timing system and mass digitizer, and the pulsed laser systems.

The package was designed to operate on an IBM PC-AT microcomputer under the MS-DOS operating system. The majority of the package is written in C with some specialized routines, such as the interface to the CAMAC timing system, written in 80286 assembly language for speed. However, as the software conforms to a strict Kernighan and Ritchie standard [1] transporting to other computers and operating systems should require little modification other than graphics statements and the low level CAMAC Input/Output interface functions. As an example of this flexibility the examples presented in this paper were obtained with a prototype version of this program running either a straight TOF atom probe or an energy compensated atom probe at the University of Pittsburgh using a Columbia Data Products 1600-4 microcomputer.

ON-LINE CONTROL PROGRAM

The main functions of the on-line control program are to control and monitor the atom probe hardware [2], to collect the data from the

time-of-flight timing system and the IAP transient waveform digitizer, to display the data to the operator in a format suitable for the type of analysis being undertaken, and to analyze the data. The same program is also capable of reanalysing previously collected data.

The interactive program is menu driven and prompts the user with a list of options for all information required. The reassignable function keys are used to interrupt the analysis to change options. Full use is made of color to permit multiple plots on the same display.

The raw and processed data may be output to a dot-matrix graphics printer or to a digital plotter for hard copy. The screen display may also be saved in a disk file at any time for later comparison. In addition, the program permits data collected previously to be analysed during the course of the experiment so that comparisons may be made with other specimens or analyses. Data is stored on a hard disk during the experiment and may be transferred to either 360kB or high capacity 1.2 MB floppy disks for archival storage and reanalysis. The format chosen to store the data on disk is suitable for transfer to other computers and for incorporation without modification into other software packages such as spreadsheets etc.

During the experiment the time-of-flight atom probe ion-by-ion data may be displayed in real time in the following formats for different types of analyses:

- 1) Linear or semilogarithmic mass spectra
- 2) Time spectra
- 3) Multi-element composition profiles - either block or plane format
- 4) Ladder diagrams of one selected species against a second species
- 5) Cumulative profiles of a selected species against total ions
- 6) Sequential ion-by-ion element identification and composition
- 7) Sequential mass-to-charge ratios and number of pulses
- 8) Status, composition and raw data display.

Examples of screen dumps to the printer during accumulation of data for a mass spectrum, a time spectrum, a ladder diagram, and a cumulative plot are shown in figures 1 to 4 respectively. The composition profiles and sequential element identification may be displayed in either a depth-monitored plane format or in blocks of a fixed number of ions. The identity of an ion is determined from a set of ranges which are input either manually or from the data base. Compositions may be determined from the spectra using these same ranges.

When sufficient ions have been collected the data may be further analysed on-line by one or more of the following statistical procedures: autocorrelations, cross correlations, Fast Fourier Transforms, or frequency distributions. These statistical procedures provide information on parameters such as clustering, cluster or precipitate size, characteristic distance measurements, and segregation. These analyses enable the data to be checked prior to removal of the specimen. Examples of a smoothed composition profile and an autocorrelation analysis of a composition profile are shown in figures 5 and 6.

The program also has a FIM and an IAP mode. The FIM mode displays the current specimen voltages and also monitors the alignment of the

DC Voltage = 13500 V Pulse Voltage = 2150 V Total Number of Ions = 2487

Figure 1. Example of a screen dump of a Mass Spectrum to the printer.

DC Voltage = 13900 V Pulse Voltage = 2195 V Total Number of Ions = 2447

Figure 2. Example of a screen dump of a Time spectrum.

Figure 3. Example of a Ladder Diagram.

Figure 4. Example of a Cumulative Profile.

Figure 5. Example of a Composition Profile output on the plotter.

Figure 6. Example of an Autocorrelation analysis of a Composition Profile output to the plotter.

mass spectrometer and permits adjustment of the energy-compensating lens voltage ratio constants. The IAP mode allows the operator to set a dynamically adjusted time delay in order to image a given species for an elemental map and transfer mass spectra from the transient waveform digitizer [2] for analysis.

DATA BASE

With the mass resolution afforded by the new generation of energy compensating mass spectrometers it has become feasible to use a data base for automatic element identification. The system therefore has access to a data base containing the abundances of all naturally occurring isotopes of the elements, their observed charge states, and their atomic number and weight. The data base also indicates whether the element forms molecular ions. A set of simulated field ion micrographs for the usual orientations of the common crystal structures is also available for recall by the control program to assist in interpretation of micrographs.

OTHER SOFTWARE

In addition to the on-line control program the software package contains programs for simulation of field-ion micrographs, for simulation of composition profiles, a conversion program from atomic to weight percent, and for interactive testing of the CAMAC modules of the timing system and the computer. The package also contains a full complement of editors, word processors, spreadsheets, C, BASIC, Fortran and Pascal compilers, C and BASIC interpreters and associated utility programs for a self-contained environment.

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