

SOFTWARE NOTICE

PRSUPR: Automation and analysis software for wavelength dispersive electron-beam microanalysis on a PC

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ABSTRACT

PRSUPR, an integrated program to acquire data from multiple fixed or scanning spectrometer electron microprobes, is described. X-ray count and coordinate data are automatically stored to random-access disk files for on-line or off-line data processing using the CITZAF sample matrix correction library. A complete set of unknown and standard sample automation features is fully integrated into the program. Extensive documentation and a simple installation program are provided for the nonprogrammer. The program operates on a standard IBM PC or compatible and supports automation, acquisition, and quantitative analysis for a wide variety of microprobe hardware configurations.

INTRODUCTION

Accurate and timely microanalysis requires a powerful yet easy-to-use computer program that includes state-of-the-art matrix corrections and integrated quantitative corrections for spectral interferences. Also essential is the ability to operate on a powerful microcomputer in order to provide on-line graphics and fast data processing of large volumes of data.

In order to meet these demands, we have developed a software program called PRSUPR (Donovan and Rivers, 1990) with a complete automation, acquisition, and quantitative analysis package. The software provides a wide range of features for wavelength dispersive electron-beam microanalysis.

PRSUPR operates under DOS on any IBM PC or compatible with a 286, 386, or 486 processor with 640K RAM, a hard disk, and a math coprocessor. Real-time multitasking for running automated analyses in background is supported with a 386 or 486 processor under a suitable multitasking environment.

PROGRAM FEATURES

PRSUPR accommodates up to 24 matrix-corrected elements in a single run. Up to 250 samples each with up to 50 analyses may be acquired (for a maximum of 10000 data points per run). Each analyzed element may be automatically corrected for up to two interfering elements. Both nonlinear mean atomic number and automated off-peak background corrections are available. The program automatically corrects for standard count drift in real time.

Extensive quantitative matrix corrections for ZAF, $\phi(\rho Z)$, and modern nonlinear-fit Bence-Albee methods (Armstrong, 1988a) using the Citzaf library (Armstrong, 1988b) are totally integrated in PRSUPR using simple multiple choice menus. Both the traditional Frame (Philibert, 1963) and original empirical Bence-

Albee (Bence and Albee, 1968) corrections are included for comparison.

Full-featured stage automation includes automated standard data acquisition using predigitized standard samples referenced to calibrated fiducial marks or user-defined locations from a previous standardization. Automation for unknown sample specimens includes random selected points, line traverses, and x - y stage step scanning from user-defined Cartesian grids with rectangular or irregular polygon boundaries using mouse, trackball, or keyboard input. In addition, the program can operate unattended for days using any combination of the above standard and unknown automation procedures.

Spectrometer automation includes multiple element analysis by spectrometer, automated off-peak measurements, automatic wavelength scanning, and peak intensity alignments at user-defined analysis intervals.

Hardware configuration for PRSUPR is easily accomplished by editing a simple text file containing the various hardware-dependent parameters such as take-off angle, number of spectrometers, stage and spectrometer limits, etc. and is completely documented for the nonprogrammer. The hardware supported by PRSUPR is completely documented for easy installation. Supported hardware includes DC servo or stepper motor controllers using optical quadrature encoder feedback for motion control and also high speed 32-bit digital pulse counters or standard RS-232 serial hardware for X-ray and beam count input. In addition, source code outlines are provided for modification by programmers interfacing to other unsupported hardware.

PRSUPR supports VGA, EGA, CGA, and Hercules graphics display adapters for various data plotting functions such as automated peak scanning and peaking, digitized polygon boundary display, and on-line or off-line analysis display of weight, atomic, and mole percent, formula coefficients, stage coordinates, and beam drift. Mouse or trackball support is offered for manual stage and spectrometer control and various graphics display functions.

Included with PRSUPR are several companion programs. All data files created by any of these companion programs are completely compatible with one another and PRSUPR. Among these programs are the following:

1. PRSMAL, a version of PRSUPR without automation and acquisition capabilities for off-line processing of X-ray data. Although PRSUPR will also operate off line on a PC, PRSMAL requires less free memory.

2. PRTASK (Donovan and Kress, 1991), a version of PRSUPR that interfaces to a Tracor TASK automation system using a

standard serial connection for accurate quantitative analysis in real time. PRTASK also includes the capability to import microprobe X-ray data as simple text files for reprocessing previously acquired data from older probes. It also allows keyboard input of raw k ratios or counts for interactive reprocessing of small amounts of data.

3. STDINP, a program to create and maintain a library of up to 300 standard compositions for quantitative microanalysis. Standard compositions may be entered in either oxide or elemental abundances.

4. PRSCAN, a program containing a subset of the spectrometer automation routines from PRSUPR for wavelength scanning and calibration only.

5. STCORD, a simple program to digitize any standard sample mount in three dimensions relative to physical fiducial marks for use with the PRSUPR standard automation routines. Up to 100 standards may be digitized per mount, with up to 50 points per standard stored to disk.

All programs utilize a simple yet versatile user interface making extensive use of multiple choice menus and defaulted experimental parameters for ease of use. The analysis programs have the ability to save analytical setups on disk for use in setting up new analyses. All software includes complete documentation for users and for programmers who wish to modify the hardware interface.

AVAILABILITY

The entire source code (compiling under Microsoft Fortran and Macro Assembler) is available free as shareware for distri-

bution to individuals and institutions. The program may be registered; registration includes free updates and telephone consultation. To receive the complete source code (executables and documentation), please send five double-sided, high-density 5¼-in. or 3½-in. floppy disks to the first author.

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