

## Computer Program Abstracts

The category *Computer Program Abstracts* provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Following normal submission, a *Computer Program Abstract* will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 of the June 1985 issue of the *Journal* [*J. Appl. Cryst.* (1985), **18**, 189–190].

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**CPSR – an integrated software package of menu-driven computer programs for X-ray powder-pattern refinement.** By Yu. G. ANDREEV and N. I. SOROKIN, *ONIL KGK Moscow Civil Engineering Institute, Olympiisky prospekt 50, 141019 Mytishchi, Moskovskaya oblast, Russia*, and A. K. CHURAKOV, *MP 'Ekoelektrom', ul. Vyborgskaya 16, 125212 Moscow, Russia*

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**The crystallographic problem:** Currently available software products for profile and Rietveld refinements do not possess handy multi-item input facilities. This means that certain difficulties may arise for some users. Moreover, most of the commonly used least-squares refinement methods require initial and true values to be close. Otherwise refinement of selected parameters is needed in advance of the overall procedure.

**Method of solution:** *CPSR* utilizes a two-stage method: (i) full pattern profile refinement; (ii) crystal-structure parameter adjustment using integrated intensities from the previous stage. The main features are: (1) initial structure-model input in the form of *Structure Reports* information; (2) default setting of initial parameters; (3) menu-driven input and change of parameters; (4) quasi-Newtonian second-derivatives method of variable metric (Fletcher & Powell, 1963) for least-squares refinement, with analytical derivatives calculation, automatic break on procedure conclusion and regularization scheme enabling initial parameters to deviate strongly from the true ones.

**Software environment:** The *CPSR* programs are written in C using the Microsoft QC 2.01 version under MS-DOS 4.01. The package utilizes a menu-making library (Navernjuk, 1989) and data banks of space-group settings,

scattering factors and X-ray wavelengths.

**Hardware environment:** *CPSR* runs on an IBM-compatible PC/AT computer equipped with 640 kbytes of memory, a coprocessor and an EGA(VGA) adaptor.

**Program specification:** The present version of *CPSR* involves single-phase refinement of up to 100 parameters at both stages. All functions are menu driven; menu selections are performed with both the keyboard and the mouse. Screen graphics multipage support is provided for calculation and refinement. The source code contains about 10 000 lines

**Documentation:** Machine-readable files contain a user's guide and a full description of the formulae used in calculation and refinement.

**Availability:** *CPSR* package (including executable files, data banks, test example and documentation) is available from the first two authors, free of charge for noncommercial users, on two 1.2 Mbyte 5.25 in floppy disks supplied by the user along with postage costs.

**Keywords:** X-rays, powder patterns, profile refinement.

### References

- Fletcher, R. & Powell, M. J. D. (1963). *Comput. J.* **6**, 163–168.  
Navernjuk, A. (1989). Personal communication.

## New Commercial Products

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### AxioDoc A: New Digital Image Archives for Microscopes

The **AxioDoc A** digital image archives from Carl Zeiss is far more than just one of many available multimedia systems. It was designed especially for microscopy and marks the beginning of a new era in the handling of photomicrographs.

Slowly but surely, a change has taken place in professional microscopy: video

printers are now increasingly taking over tasks which have been the realm of classical photography until now. Their main benefits are their speed and the cleanness of the method.

To date, the photograph collection or the slide archive were often the end of the line for thousands of pictures. This included a system which allowed the user to search for pictures. The electronic successor to this is the new digital image archives AxioDoc A from Carl Zeiss, linking the microscope, the stored images and the connected data for the first time.

The digital archives system is based on a PC system with a 486 processor and the Windows 3.1 user interface. The archival system consists of an additional card for image acquisition, the MaRS (Magnification Recognition System) system for Zeiss microscopes with ICS (Infinity Color-Corrected System) optics and convenient image-filing software. Stored images can be relocated quickly and reliably.



New digital image archives Zeiss AxioDoc A for microscopes

The archives can contain many different 'boxes', depending on the number of users or subjects. This means that images can be interlinked with external data, such as numbers of specimens. Furthermore, it is possible to perform simple measurements of the images and to store the results, such as lengths and angles.

The digital image archives AxioDoc A will initially be an application-neutral instrument, much like a camera. However, a number of optional special programs already exist at this early stage, such as the analysis of grain sizes using electronic comparison standards or the DDE software (Dynamic Data Exchange): if a user wants to perform measurements of the same kind repeatedly, for example in quality control, the measuring data are continually read into the Excel table calculating program from Microsoft via DDE. This program, again, opens up a wide variety of possibilities for displaying histograms and curves or for statistic evaluation on other PC's.

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