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PowderX: Windows-95-based program for powder X-ray diffraction data processing

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The crystallographic problem: A Windows-95-based program (*PowderX*) has been written for powder X-ray data processing and analysis. It can be used for plotting X-ray patterns, data smoothing, background subtraction, α_2 elimination, peak search, indexing and zero-angle error correction. *PowderX* can also be used for data format conversions to prepare the input data for Rietveld refinement and structure determination programs such as *DBWS*, *FULLPROF*, *GSAS*, *SIMPRO* and *EXPO*.

Method of solution: *PowderX* takes full advantage of the graphical interfaces of Windows 95. Pull-down menus and a mouse are used to control the program executions. *PowderX* provides convenient tools for processing powder X-ray diffraction data. The Savitsky–Golay (Savitsky & Golay, 1964) method or any of another three methods can be used for data smoothing and peak search. Background subtraction can be made either automatically by the Sonnerveld method (Sonneveld & Visser, 1975) or manually by mouse clicking. The α_2 elimination can be performed either using the methods of Rachinger and Ladell (Rachinger, 1948; Ladell *et al.*, 1975), or using a new method developed by the author of the program.

Software environment and hardware environment: *PowderX* is written in Visual Basic and runs under Windows 95 or Windows 98. Minimum hardware specification: a 486 or above processor, a VGA colour monitor, a mouse, 8 Mbytes of RAM, 8 Mbytes of hard disk space.

Program specification: *PowderX* can read 13 data formats, produced by either angular-dispersive or energy-dispersive X-ray diffraction techniques on various diffractometers (manufactured by Mac Science, Philips, Siemens, Rigaku, *etc*). It uses a new and accurate Cu $K\alpha_2$ elimination algorithm (Dong, Chen & Wu, 1999). With *PowderX*, zero-angle shift can be corrected automatically before indexing and no internal standard material is required (Dong, Wu & Chen, 1999). It can produce the input file for *TREOR*90 (Werner *et al.*, 1985) after an automatic peak search, so only minor editing is needed.

Documentation: Online help describes the main features of the program and provides instructions for the user. A user's manual is also available as a Microsoft *Word* document in rich text format.

Availability: The files for standard windows installation of the program and the user's manual are freely available for academic and non-commercial use. The program may be obtained from the author by e-mail (chengdon@aphy.iphy.ac.cn). This program has more than 80 users in the world to date.

Keywords: powder X-ray diffraction; data processing; indexing; peak search; data format conversion.

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DISCUS, a program for diffuse scattering and defect structure simulations – update

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The crystallographic problem: In contrast to the determination of the *average* structure based on Bragg scattering, there is no general procedure to extract information about the disorder of a material from its diffuse scattering. Two years ago, we first published the program *DISCUS* (Proffen & Neder, 1997), which allows the creation of defect structures and the simulation of diffuse scattering. The program can also be successfully used to aid teaching of diffraction physics (Neder & Proffen, 1996). This abstract gives an overview of the changes and enhancements between the published version 2.01 and the current version 3.2.

Method of solution: The program *DISCUS* allows one to create structures from the contents of an asymmetric unit using the space-group symbol. Structures can be modified using the Fortran-style interpreter or built-in functions of the program. Disordered structures can be analyzed, *e.g.* by calculating bond-length distributions, and the Fourier transform can be calculated. *DISCUS* includes a module for reverse Monte Carlo (RMC) simulations. We will focus here on the new features of the program. The Fourier transformation is now calculated about six times faster and allows the subtraction of the average structure factor $\langle F \rangle$. The scat-

tering intensity can optionally be calculated as an average of intensities from small areas of the model crystal chosen at random. This results in smooth diffraction patterns (Butler & Welberry, 1992). *DISCUS* can also simulate powder diffraction patterns. Two new modules were included to create disordered structures: a stacking-fault generator and a Monte Carlo simulation segment allowing the introduction of occupational as well as displacive short-range order. Additional modules allow one to perform general symmetry operations and to transform between different crystallographic systems. The calculation and RMC-style refinement of the atomic pair distribution function (PDF) of a given structure is another new feature of the program. Finally, it should be noted that *DISCUS* now supports the use of rigid molecules. This can only be a very brief listing of features; for details visit the *DISCUS* World Wide Web (WWW) home page (see below).

Software environment: *DISCUS* is written in standard Fortran77 with the exception of the command-line interface which is written in C. The program is distributed as source code and a Fortran and C compiler are required for the installation. However, executable files may be obtained from the authors.

Hardware environment: The program has been successfully used on various UNIX platforms, including LINUX, and under VMS. Although DOS binaries may be obtained from the authors, a UNIX-type platform is recommended. The memory requirements strongly depend on the needs of individual cases, such as the model crystal size. A typical setup requires about 10–16 MByte of memory. The necessary hard-disk space for the installation is about 10 MByte.

Program specification: Performance of *DISCUS* depends strongly on the computer used. The calculation of a 121 $\times$ 121 point array in reciprocal space from a crystal containing 32 000 atoms takes about 45 s on a Pentium II computer running LINUX.

Documentation: The program is distributed with a detailed users guide explaining the basic concept of the program and with a command reference containing information about every command. Furthermore, *DISCUS* has an online help function, allowing the user to obtain information about a specific command while running the program.

Availability: *DISCUS* is available *via* the WWW at http://www.pa.msu.edu/cmp/billinge-group/discus/discus.html or at http://www.uni-wuerzburg.de/mineralogie/crystal/discus/discus.html.

The program can be used free of charge.

Keywords: automatic structure determination; Patterson methods.

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*XFPA*98: a program for automatic structure determination and automatic refinement

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The crystallographic problem: The distant goal of automatic structure determination is the development of a reliable computer program that is able to solve, refine and interpret crystal structures in a single run.

The project of automatic structure determination was born in 1986 when, under the name *XFPS*, a program for automated Fourier, Patterson and superposition methods was published (Pavelcik, 1986). The program was later supplemented by graphics routines and released as a program for automatic structure determination (Pavelcik *et al.*, 1992) of heavy-atom structures. Recently, the program has been divided into a specialized program for Patterson interpretation, including the macromolecular Patterson [difference, anomalous, *etc.* (Pavelcik & Dodson, 1998)], and a user-oriented 'black-box' program for automatic structure determination and refinement, presented here.

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The principal update of the program includes structure determination of organic molecules (equal-atom structures) by Patterson multisolution (Pavelcik, 1998).

Method of solution: The most relevant changes with respect to the 1992 version of *XFPS* are as follows.

(i) Original Patterson multisolution methods for organic molecules (Pavelcik, 1998).

(ii) New or improved techniques as follows. (*a*) Symmetry minimum function for atoms in special positions (Pavelcik, in preparation) with optional sorting of symmetry minimum function peaks by individual *R* factor or correlation coefficient. (*b*) New Patterson techniques, described by Pavelcik (1994*a*), *e.g.* cross-vector superposition and its automatic interpretation, structure determination in *P*1 space groups with subsequent search for the conventional cell origin, *etc.* (*c*) Modified and more powerful Patterson multisolution based on fragment generators and cross-vector function (Pavelcik, 1988). Atomic types are permuted for a fragment of heavy atoms; the best solution is selected by a combined figure of merit [*R* factors, correlation coefficients, *R*(Patterson), consistency among self and cross-vectors]. Pseudosymmetry of atomic minimum superposition is tested using the method of Andrushewskii *et al.* (1988). (*d*) Automatic Fourier recycling in the crystal space group, and Fourier recycling in *P*1 space group (reflection data and symmetry given for the crystal space group). (*e*) Pseudo-Gaussian peak integrals for sorting electron-density peaks (Pavelcik, 1994*b*). (*f*) Automatic building of hydrogen atoms for a hydrocarbon chain. (*g*) Automatic naming of atoms. An atom name is composed of its chemical symbol and number derived from the fragment number and chemical connectivity. (*h*) Block-diagonal least squares for preliminary refinement.

(iii) Expert routines, including four new expert routines for the automatic structure determination, an improved standard routine as described by Pavelcik (1988), and a new expert routine for structure refinement.

(iv) User-oriented interfaces: graphical input for PC; conversational input for Linux (Unix) workstations; simple input of symmetry (*e.g.* symmetry by space-group number or by a limited number of symmetry instructions related to the space-group generators).

(v) *SHELX* (Sheldrick, 1997) interface: a complete `*.ins` file is produced by *XFPA* for final full-matrix refinement, as well as a CIF. Eventually more