16.2-11 NRCCAD, AN ENHANCED CAD-4 DIFFRACTOMETER CONTROL PROGRAM. By P.S. White, Y. Le Page and E.J. Gabe, Chemistry Division, National Research Council of Canada, Ottawa, Canada K1A 0R9 and Chemistry Department, University of New Brunswick, Fredericton, N. B., Canada E3B 6E2.

The control program for the Enraf-Nonius CAD-4 diffractometer has been enhanced. Although the CAD-4 configuration used during this development consists of PDP11/73 and a Nonius 546 interface containing a Falcon SBC-11/21 computer, the software has been tested on the four combinations of PDP11/23 or MicroVAX-II host computers with interfaces equipped with LSI-11/2 or Falcon computers. On a PDP11 host the program will compile under both the DEC FORTRAN-IV and FORTRAN-77 compilers. The current NRCCAD version incorporates all the original Nonius commands plus numerous modifications and additions. The capability to run the diffractometer from a terminal attached to either the host computer or the interface is retained, but the communications code has been modified so that response time at a terminal attached to the host is greatly improved. All dialogue and prompts have been expanded and clarified and a number of checklists have been added. The procedure to start and stop the program has been simplified and the program may now be restarted without reloading the interface programs. A number of modifications have been made to the interface programs to permit scans with up to 512 steps. The system is distributed with a set of command files that will generate the required tasks after the operator answers a few simple questions. The following facilities have been added. The Nonius reflection centering algorithm, to which the criticism of Frevel et al. (Frevel L.K., Emge T.J. and Kistenmacher T.J., 1983, J. Appl. Cryst., 16, 126) applies when monochromatized radiation is used, has been enhanced to overcome this objection in cases where reflections with little or no $\alpha1/\alpha2$ overlap can be used. The list of reflections for cell-parameter refinement has been expanded from 25 to 200 entries. Theta-zero and Kappa-zero errors are experimentally eliminated by an algorithm which uses the results from 4 related centerings at +/- theta angles for each reflection. The use of these facilities gives more accurate and precise cell parameters in an acceptable time. A symmetry-constrained 2Θ least squares routine is also available. The CREDUC cell-reduction algorithm (Le Page Y., 1982, J. Appl. Cryst., 15, 255), based on the identification of 2-fold axes of metric symmetry, has been incorporated as an alternative to the Nonius routine TRANS. A new mode of data collection, DHSETS, is driven by routines that derive symmetry operations from the space group symbol. This segment approach (Le Page Y. and Gabe E.J., 1979, J. Appl. Cryst., 12, 464), permits full spheres of data to be collected as a sequence of unique sets. Index limits, lattice-type and glide-element absences are detected automatically. The only input required is the range of theta and a space group symbol with the correct diffraction aspect, which does not have to be a standard setting. Profile analysis can be performed (Grant D.F. and Gabe E.J., 1978, J. Appl. Cryst. 11, 114) on scans with up to 512 steps, which results in significantly more accurate data without the overhead of storing the profiles for later processing. The system is designed to be operated from a Tektronix-compatible graphics terminal, in which case the profile of the last reflection measured can be displayed by setting a switch on the pocket terminal. This facility works with the terminal connected to either the host or the interface computer. The Nonius routine ALIGN has been modified to correct an error and a routine, SETPHA, has been added to facilitate the correct setting of the counting chain. A number of 'spare' commands are available for the addition of user-written routines.

16.2-12 REVISED SOFTWARE FOR ROUTINE DATA COLLECTIONS OF TWINNED CRYSTALS WITH THE SIEMENS AED2. By Henning Henke, Institut für Anorganische Chemie der Universität (TH), D-7500 Karlsruhe, West Germany.

High-quality diffraction data still form the basis for any serious experimental work in X-ray crystallography. Especially with twinned materials, one faces difficulties during data collection if the aim is to obtain as many reliable reflexion intensities as possible. For a Siemens/Stoe four-circle diffractometer the measuring and plot routines have been adapted to the typical situations which are encountered with twinned crystals. Each reflexion is flagged according to measuring conditions. Prerequisite is a knowledge of the twinning law. The complete chain of data-processing programs is available, including subsequent structure refinement. A reasonable model must be supplied by the user.

Main features of the extended software are as follows:
(1) input of the twin axis or plane is normally sufficient; alternatively the matrix may be fed in that describes the transformation between first and second twin individual;
(2) optional swap of the orienting matrices facilitates the change-over from one individual to the other;
(3) assignment to one of three categories (perfect coincidence, reflexion splitting, sufficient peak separation) according to resolution in reciprocal space;
(4) one of the objectives is to achieve either horizontal or vertical peak separation in front of the detector, all procedures designed for a Eulerian cradle;
(5) for scans over pairs of twin reflexions the coupling factor between ω and θ is computed individually;
(6) minimal or maximal separation of twin pairs in the equatorial plane of the instrument (K. Tichý, J. Beneš, Helv. Phys. Acta, 1977, 50, 459-466);
(7) control of reflexion overlap in critical situations (cf. W.Denner et al., J. Appl. Cryst., 1977, 10, 177-179);
(8) check on intensity being cut off by the apertures.

16.2-13 COMPUTER SIMULATION OF TWO-DIMENSIONAL INTENSITY DISTRIBUTIONS OBTAINED WITH CRYSTAL-MONOCHROMATED X-RADIATION AND A SMALL SPECIMEN CRYSTAL By A.W. Stevenson CSIRO Division of Materials Science and Technology, Locked Bag 33, Clayton, Victoria 3168, Australia

Two-dimensional ($\Delta\omega$, $\Delta2\theta$) intensity distributions are calculated for the case of crystal-monochromated (pyrolytic graphite) X-radiation incident on a small specimen (Si). The calculations are based on ray-tracing and take into account the mosaic spread of the monochromator, depth of penetration into the monochromator, source emissivity distribution, wavelength distribution, broadening due to the detector aperture, and various aspects of the experimental arrangement involved. The calculations are compared with experimental results and reveal excellent agreement.

A full understanding of such intensity distributions can yield detailed information about the nature of the individual components present. The analysis can also provide details essential to carrying out conventional one-dimensional ($\Delta\omega$) profile measurements in a correct and consistent manner.