packed into a large executable programs, except STEP, PEAK, SPRIN and PROPT which are independent executable programs. The packed programs should be separated to be used in a micro computer. The least-squares refinement CRYLSP program can not be executed directly in a micro computer. We noticed that the CRYLSP program has a great array-A. If the array-A is moved out the program and modified as temporary data file, the program can be used on a micro computer with only 640K memory. In addition, the difference between FORTRAN-66 and IBM-FORTRAN-77, especially I/O formats, will be considered. Recently, the Micro computers have more and more functions, specially displaying and drawing graphics. We have written several programs for XRS-82. (1) To display and draw patterns in screen or plotter. The patterns are either observed or calculated as the results of STEPCO or CRYLSP programs. (2) To display and draw the atlas topologies framework structure or the ball-atoms in the unit cells. (3) To display and draw the electronic density of Fourier map and different Fourier map. These programs are necessary to run the XRS-82, written in both FORTRAN-77 and BASICA languages. In addition the MS-DOS can be used for running the system successively by both jobs. So that all input and output files have perpetual names themselves. The results of output file can be remained by copy. In order to check up the rewritten XRS-82 system, we compared the results of refinements for ZSM-39 and ZSM-5 structures on AT-386 computer with one result of the Honywell DPS-8 computer in Aberdeen University of U. K. and in Jilin University. The results of refinements are reasonable and only have a little difference. In AT-386 computer, the calculating time of one step of refinement twice cycles is about 1-1.5 hr. for ZSM-39, having 9 atoms, 64 parameters and 76 reflections, and about 3-5 hr. for ZSM-5, having 38 atoms, 67 parameters and 1666 contributing reflections. I thank Prof. Ch. Baerlocher of Institut fuer Kristallographie, Prof. Ch. Baerlocher of Institut fuer Kristallographie, Prof. Ch. Baerlocher of Institut fuer Kristallographie, Prof. F.P. Glasser, Dr. Dent Glasser and Dr. R. A. Howie of Aberdeen University for many help.

PS-02.08.25 AB-INITIO SOLUTION OF MISFIT LAYER STRUCTURES BY AUTOMATIC PATTERSON AND DIRECT METHODS by Paul T.Beurskens*, Gezina Beurskens, and Erwin J.W.Lam, Crystallogr. Lab., Res. Inst. f. Materials, Univ. of Nijmegen, The Netherlands, Sander van Smaalen, Lab. of Chem. Physics, Materials Science Center, Univ. of Groningen, The Netherlands, and Hai-fu Fan, Inst. of Physics, Chinese Academy of Sciences, Beijing, China

A misfit layer compound is an intergrowth structure consisting of two or more types of layers. Each layers can approximately be described as a three-dimensional periodic structure with, however, mutually induced incommensurate modulations. The composite structure is best described as a periodic structure in higher dimensional space (S.van Smaalen (1992), Materials Sc. Forum 100 & 101, 173). We now consider the case of two layers, and reflection data indexed with 4-dim. indices hklm. Layer 1 is defined by the 'main' reflections hkl0 (3-dim. indices hkl), layer 2 is defined by the 'main' reflections 0klm (3-dim. indices klm), while all other reflections hklm (h,m=0) are the (usually weaker) 'satellite' reflections.

The last step (step4) in the present procedure is the determination of the phases of the satellites from the known phases of the main reflections of both layers by application of the Sayre equation in 4-dimensional superspace (Hao Quan, Lia Yi-wei & Fan Hai-fu (1987), Acta Cryst. A43, 820. Fan Hai-fu, S.van Smaalen, E. Lam & P.T.Beurskens (1993), Acta Cryst. A in press). The phases of the main reflections are determined as follows:

Step 1.Solve the 3-dim structure of layer 1 by routine application of a heavy atom structure solution program,

Step 2.Similarly, solve the 3-dim structure of layer2,

Step 3.Use the common origin, which is easily done by a shift function based on R2-minimalization. The four steps are imbedded in an automatic procedure which is incorporated in the DIRDIF system.

PS-02.08.26 TOWARD RAPID INORGANIC PHASE. IDENTIFICATION FROM ELECTRON DIFFRACTION AND EDS DATA by Y.Le Page*, A.Chenite and J.R.Rodgers, National Research Council of Canada, Ottawa, K1A 0R6, Canada

The potential of electron diffraction for the phase identification of inorganic fine particles, e.g. environmental ones in our case, is considerable. Intense diffraction patterns of 1,000A-size particles can be exposed in about 1 second, and semi-quantitative elemental analysis down to nitrogen obtained by energy-dispersive X-ray spectroscopy (EDS) in a minuter or so, off the same single particle. However, this potential is not fully developed. Measurement and analysis of diffraction patterns is time-consuming and leads to a typical accuracy of about 2% in reciprocal lengths. This accuracy , which can be explained by the accuracy in the length measurements used in the calculation of the reciprocal data, is often critical for successful phase identification by combination of semiquantitative EDS analysis and diffraction data. In addition, there are pitfalls in the search of cell databases with low-accuracy data.

Due to recent developments in the performance and cost of optical scanners, CCD cameras and computers, digitized electrondiffraction patterns can be obtained and processed within minutes for a reasonable cost. The accuracy of measurements obtained by image processing of digitized data is comparable with that obtained manually, but many more positions of diffraction spots can be measured, allowing increased accuracy through least squares.

We have been developing experimental and computational methods for rapid phase identification. We will report on:

- image analysis of zero-level convergent-beam patterns;
- calibration of the camera constant;
- least-squares processing of zero-level data;
- least-squares extraction of 3-d cell from single CBED
- novel database search methods.

