02- Methods for Structure Determination and Analysis, Computing and Graphics

packed into a large executable programs, except step, peak, spin and prop 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 files, the program can be used in a micro computer with only 64K memory. In addition, the difference between FORTRAN-66 and IBM-677, especially I/O formats, will be considered. Recently, the Micro computers have more and more functions, capable of displaying and drawing graphics. We have written several programs for XRS-82. (1) To display and draw patterns as screen or plotter. The patterns are either observed or calculated as the results of TEKNO or CRYLSP programs. (2) To display and draw the atlas topologies framework structure or the ball-sticks in the unit cell. (3) To display and draw the density map of Fourier map and different Fourier maps. These programs are necessary to the XRS-82, written in both FORTRAN-77 and BASKA 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 managed 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 the result of Honeywell DRS-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 1.1-1.5 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. Dr. Baerlocher of Kristallforschung, Prof. Dr. Baerlocher of Institut fuer Kristallographie, Prof. Dr. Baerlocher of Innsbruck fuer Kristallographie, Prof. Dr. F.P. Glasser, Dr. Denis Glasser and Dr. R.A. Howe of Aberdeen University for many help.

02-02-18 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 1000A-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 matter of 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 semi-quantitative 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 electron-diffraction 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 3-6 cell from single CBED
- novel database search methods.


A misfit layer compound is an intergrowth structure consisting of two or more types of layers. Each layer 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 Smalend (1992), Materials Sci. Forum 103 & 104, 173). We now consider the case of two layers, and reflection data indexed with 4-dim. indices hkl. Layer 1 is defined by the 'main' reflections hkl (4-dim. indices hkl), layer 2 is defined by the 'main' reflections 0klm (4-dim. indices klm), while all other reflections klm (h,m=0) are the (usually weaker) 'satellite' reflections.