The powder data are processed with a suite of PDP-11 FORTRAN programs operating in the following stages:

(1) The raw data from a number of parallel scans are presented as an intensity [I] & a standard deviation [DI] for each microdensitometer reading (usually at intervals of 0.05mm, i.e. using a 50 micron aperture).

(2) This output is inspected, and values of line intensities [I] = I(peak) - I(background), peak positions [M(obs)] in mm., and σ-[M(obs)] are selected manually for both specimen and internal standard, and checked against the film itself. At present this procedure seems to be preferable to automatic peak-searching, especially in cases of very strong, very weak, or poorly-resolved patterns.

(3) Values of [M] = M(obs) corrected for the non-linearity of d* vs. sin Θ by comparison with the internal standard, [I] and σ-[M] are given to an exhaustive-search indexing program which supplies possible indices for some or all of the lines.

(4) These indices are supplied to a cell-parameter refinement program, where they are cycled with an appropriate weighting scheme to remove redundant indices and to derive cell parameters and their standard deviations.

(5) Line positions [M(calc)] are generated for comparison with [M(obs)] to see whether a satisfactory match has been achieved.

(6) If accepted, the indexed data are output in any desired format and incorporated in the local databank file for use with the original data, from which information such as peak shapes and integrated intensities can be extracted later.

12.1-04   PODA: AN APPROACH TO MULTI-PURPOSE POWDER DIFFRACTION ANALYSIS, R. A. Coyle, Aeronautical Research Laboratories, Department of Defence, Melbourne, Australia.

For some time punched paper tape has been used for automatic recording of powder diffraction data. In-house computing facilities have then been used for computation and storage of the data. Paper-tape equipment is being replaced by microprocessor interfaces enabling on-line processing of some of the measurements such as searches for peaks, and residual stress. However, in an applied research laboratory, the complexity and changing nature of the tasks can be better accommodated using the capabilites of a large computer. In this context the program PODA was developed for multi-purpose analysis of powder diffraction data on a large computer. This program allows correction for both experimental and geometrical factors, calculation of the required variables, collation with previous tests and final presention of the results in graphical or tabular form.

PODA is structured like many of the DIGITAL utilities and responds to strings of characters as instructions allowing operational flexibility. The program gives simple diagnostic messages for data or instruction errors, has default options for constants and includes a facility for repetitive operators.

Some of the facilities available are to 1) read data in an any format with or without angle readings, 2) archive and retrieve data in binary form on disk or magnetic tape, 3) correct for absorption, background or Lorentz-polarization by reference to tables or by calculation, 4) eliminate alpha 2 reflections,

5) correct for dispersion, 6) calculate Fourier transforms, 7) plot pole figures, 8) fit a curve of best fit, 9) calculate centroid and area of a diffraction line, 10) hand edit data, 11) plot in a choice of formats. The standard data format includes a heading which records the operations performed on the data and the date of last change.

A number of outputs will be shown as examples, together with a copy of the operations manual.

12.1-05   A GUINIER DIFFRACTION CAMERA EMPLOYING A ROTATING ANODE X-RAY SOURCE. By J. D. Oliver and W. B. Broering, Miami Valley Laboratories, The Procter & Gamble Company, Cincinnati, OH 45247.

Rapid and reliable analytical techniques are required for prompt and effective product development. Implementation of these techniques has benefited directly from the decreasing cost and increasing availability of microcomputers.

This presentation describes a method to rapidly characterize solid-state materials at selected temperatures over the range of -100°C to +300°C. Pivotal elements of the method comprise the first successful combination of a Huber Guinier diffraction system with microprocessor-controlled variable temperature fixtures and a Rigaku RU-100 rotating anode X-ray source. Developed films are scanned with a LSI-11 automated Grant microdensitometer. High quality X-ray patterns require exposure times ranging from 5 to 12 minutes. The instrumental design and the precision of data will be described in detail.