16.3-3 IMAGE PROCESSING OF DIFFRACTION PATTERNS INVOLVING SHARP AND/OR DIFFUSE SCATTERING. By H.J. Milledge, M.J. Mendelssohn and P.A. Woods, Crystallography Unit, Department of Geological Sciences, University College London, Gower Street, London WC1E 6BT, U.K.

TV images of diffraction maxima may be obtained either in real time, using a low-light TV camera and a suitable fluorescent screen, or by accumulating a number of frames (say 50) in a frame store, in which case a less noisy image is obtained. (Milledge H.J., Rood A.P.,Nave E. & Woods P.A. IUCr.XI (Warsaw) 14.1-2) These images approach the clarity of that obtainable on X-ray films, from which computer-controlled densitometry now enables high-quality intensities to be obtained provided that suitable software is available to process the raw data.
Such raw data consists of grey-level values for contiguous areas of, say, 50 u x 50 u, which is exactly analagous to information contained in the individual pixels handled by image processing systems, for which increasing amounts of sophisticated software are becoming available.
This poster compares the results obtainable using a Sight Systems VIP (Video interface peripheral) [512 x 512 pixels each having 64 grey levels, and currently available software] from:-
a) Real-time low-light TV images.
b) The corresponding accumulated framestore images.
c) SCANDIG densitometer transmission & absorption data transferred directly to the VIP via a BBC micro.
d) TV images read directly into the VIP from X-ray films and prints.

16.4-1 IMPACT OF THE CDROM ON THE USE OF THE POWDER DIFFRACTION FILE. By R. Jenkins, M. Hojomany and R. Anderson, International Centre for Diffraction Data, U.S.A.

The Powder Diffraction File (PDF) is a collection of approximately 46,000 single phase x-ray powder patterns, maintained and distributed by the JCPDS-International Centre for Diffraction Data. Over the past 10 years there has been increasing use of the PDF in computer readable form, but the limited amount of available disk space on most commercial powder diffractometer systems (typically 5-10 Mbytes) has limited use to a small subset of the total PDF. The current size of the PDF is around 110 Mbytes and, until now, only lists of d/I values have been used.

The recent availability of low cost Compact Disk Read Only Memory (CDROM) systems seems to offer an attractive alternative to conventional disk media. We have recently installed the PDF, plus the Crystal Data File (CDF), on a $1200 CDROM system, having a total available storage of 550 Mbytes. The CDROM system is attached to an IBM XT personal computer with 640K bytes of memory. While seek times are relatively slow--typically 0.5 seconds are required to traverse the complete PDF by use of search indices located on an associated firm disk--search strategies based on PDF numbers, chemistry, strongest d, etc., operate at a speed causing no great inconvenience to the user.

This paper briefly describes this system and our experiences to date, and looks at the likely impact that this product will have on the powder diffraction community.

16.5-1 X-RAY DIFFRACTIOMETRY OF LOW-MASS SAMPLES By L.S. Zevin and I.M. Zevin, Materials Engineering Department and Institutes for Applied Research, Ben-Gurion University of the Negev, Beer-Sheva, Israel.

The need for X-ray diffractometry of low-mass samples often arises in modern technology and research. Applications include thin films in microelectronic devices, airborne dust collected on membrane filters, separated micrograins, includions in rocks and ceramics, samples in forensic analysis, etc. In this study we try to develop a general approach to the diffractometry of low-mass samples of two types: a. powder samples; b. thin films. The intensity diffracted by a low-mass sample with negligible absorption may be expressed as $I_G = I_\omega G/(B/2\mu^*)$ where I_ω = intensity diffracted by a bulk sample, B = cross section of the primary beam, μ^* = mass absorption coefficient and G = mass of the sample. The detection limit is determined by fluctuations of the background created mainly by the irradiated volume of the sample support. Minimizing of this volume by proper collimation and optimal spreading of the powder sample may decrease the detection limit to at least 0.1 μg. The optimal sprading of the sample is expressed as $S \approx 10\ \mu^*/\sin\theta$. The performance of Seeman-Bohlin and Bragg-Bretano diffractometers with thin-film samples are compared on the basis of equal instrumental aberrations. It appears that, for flat specimens, the S-B arrangement has only a marginal advantage in the intensity and that both types of diffractometer may be successfully employed for charazterization of thin films. Numerous examples of low-mass diffractometry are given. These include samples of calcite, quartz and alumina, separated grains of phosphate rock, drug polymorphs, thin films of silicides and nitrides of transition metals.

16.5-2 HIGH RESOLUTION X-RAY POWDER DIFFRACTOMETER. By M. Ahtee and P. Suortti, Department of Physics, University of Helsinki, Finland.

A high resolution version of a conventional Bragg-Brentano diffractometer is built. The take-off angle of radiation is 3°, so that the projected width of the source is 50 μm. A quartz (10.1) primary beam monochromator of the Johansson type is used for $CuK\alpha$ radiation; the radius of the focussing circle is 250 mm. A narrow slit (200 μm) is placed at the focus of the monochromator. The aperture before the sample is ± 6 mrad (equatorial) and ± 30 mrad (axial). The sample is spun about the surface normal. The receiving slit is 0.1 mm or 0.5 mm (0.6 mrad or 0.3 mrad) wide in most measurements, and the axial divergence of the diffracted beam is ± 60 mrad. Beam tunnels are used between the monochromator and the sample as well as between the sample and the receiving slit. A NaI(Tl) scintillation detector with a pulse height discriminator is used, and the measurement is controlled by a micro-computer. High angle reflections show no trace of the $CuK\alpha_2$ component. The resolution, as measured from an annealed Ni sample, is 0.075° (FWHM) at 2θ = 45°, 0.085° at 76°, 0.095° at 93°, and 0.20° at 145°. The values measured from the same sample with a synchrotron radiation instrument are 0.04° at 45° and 0.09° at 76°. The background is mostly due to the detector noise and inelastic scattering from the sample. The peak of the strongest reflection with the 0.05 mm slit is 240 cps and the background less than 0.5 cps, when the tube ratings are 35 kV and 14 mA. The performance of the instrument was tested with good results by a measurement on the room-temperature phase of $NaTaO_3$, where the average density of reflections is 3 per 1 degree of 2θ.

The intensity is increased by a factor of 5 when the X-ray tube is replaced by an 1.5 kW tube, where the projected width of the source is only 20 μm.