

16.2-14 GENERALIZATION OF THE CLASSICAL "PARALLEL" CONDITION.

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In the classical two-crystal system with monochromator (M) and specimen (c) crystal axes parallel, measurement with zero-wavelength-dispersion (zwd) is possible in respect of the "counter" one-dimensional profile at only one value of scattering angle, $\theta = \theta_c$, the so-called "parallel" condition. The procedure is highly selective and therefore of limited applicability. If one examines in $\Delta\omega$, $\Delta 2\theta$ space the situation where the ω rotation axis of c is rotatable (ϕ) about the monochromator beam incident on c, the condition can be generalized so that appropriate choice of ϕ will allow zwd "counter" profile measurement anywhere between $0^\circ \leq \theta \leq \theta_M$, thus releasing this valuable procedure from its earlier severe constraints. The setting condition for ϕ is $\cos\phi = -(\tan\theta_c / \tan\theta_M)$.

simultaneously to detect the intensities of the luminescence with different sensitivities. The second PMT receives roughly 1% of the total amount of the luminescence and covers a higher intensity range where the first one is saturated. (e) In order to decrease the image distortion (about 1% in the conventional system), a drum-type film densitometer is utilized which provides more precise scanning pitches than the flat-type one of the conventional system. (f) Arbitrary sizes of IPs are available simply by taping an IP around the drum. (g) The non-uniformity of response is reduced. (h) A high resolution graphic display system (1280 × 1024 pixels, 8-bit depth, 19") is available in addition to a system for imprinting the image on film. A 32-bit minicomputer, ECLIPSE MV/4000, is used. The digital image data are dumped in magnetic tape (6250/1600 bpi) for further data processing by another computers. The performance of the system will be described.

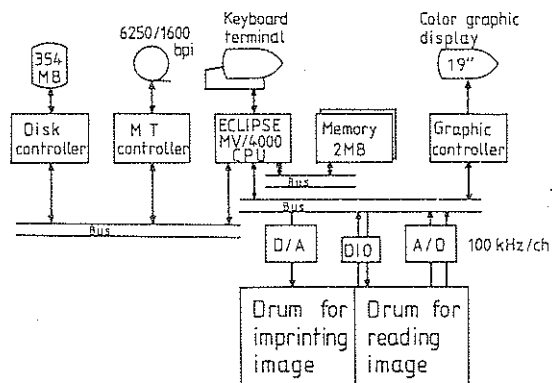


Fig. 1 Block diagram of imaging plate system.

16.3-1 DESIGN AND PERFORMANCE OF IMAGING PLATE SYSTEM FOR X-RAY DIFFRACTION STUDY.

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An imaging plate (IP) is a storage phosphor (BaFBr:Eu^{2+}) screen having a high quantum efficiency and a wide dynamic range (J. Miyahara, K. Takahashi, Y. Amemiya, N. Kamiya and Y. Satow, Nucl. Instrum. Methods 1986, A246 572-577). The IP stores an X-ray image without any substantial fading for several hours, and then the stored image is read out by a photomultiplier tube via luminescence ($\lambda \sim 390\text{nm}$) which is emitted by stimulation with a laser beam ($\lambda \sim 633\text{nm}$) scanning the phosphor screen. The IP was originally developed for diagnostic radiography and is also useful for X-ray diffraction experiments (Y. Amemiya, N. Kamiya, Y. Satow, T. Matsushita, J. Chikawa, K. Wakabayashi, H. Tanaka and J. Miyahara, Biophysics and Synchrotron Radiation (Springer Verlag) in press.). We designed a new readout system for the IP particularly suitable for X-ray diffraction studies. In this system, the following points are improved in comparison with the conventional system designed for diagnostic radiography: (a) Detector quantum efficiency is increased by the use of a special device which efficiently collects the photostimulated luminescence. (b) The pixel sizes of $25 \times 25 \mu\text{m}^2$ and $50 \times 50 \mu\text{m}^2$ in addition to $100 \times 100 \mu\text{m}^2$ are available by adjusting both the focus size and scanning pitch of the laser beam. (c) The output signals from a photomultiplier tube are digitized by a 12-bit A/D in place of a 8-bit A/D converter to improve the precision in X-ray intensity measurement. (d) In order to fully utilize a wide dynamic range ($1 : 10^5$) of the photostimulated luminescence, two photomultiplier tubes (PMTs) are used

16.3-2 SMALL MOLECULE DATA COLLECTION WITH A NICOLET (XENTRONICS) AREA DETECTOR.

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The use of area detectors for the collection of intensity data on protein crystals has received considerable attention the last few years. Several groups have reported the collection of such data and the comparison of this data with data collected on the same protein by either conventional diffractometer methods or by film methods. The merging Rsyms for some of these data collections have been surprisingly high. Inherent problems in protein data collection, such as absorption due to mother liquor used to mount the crystal in the capillary, or sample decomposition in the x-ray beam may be partially responsible for these results.

Small molecule experiments generally do not suffer from the aforementioned problems. Stable crystals with low absorption coefficients, which can be ground to a spherical shape, are easily obtainable. We will report comparisons of data collected on a standard Nicolet P3/F diffractometer equipped with the standard scintillation counter detector with data collected on the same P3/F diffractometer equipped with a Nicolet X-100A area detector system. Comparisons will be made for data collected on very stable small molecule crystals. The data sets to be compared are collected back-to-back on the same crystal without removing the crystal from the diffractometer.