CCDs are capable of being operated in very flexible ways, flexible CCD controllers are expensive. The consequence is that few commercial CCD X-ray detectors permit use of all the available options.

The detector itself is contained in a cryostat with the low-noise parts of the controller nearby, either in a separate box connected by a short cable or mounted inside the cryostat itself. A longer cable carries the time-multiplexed digitized data to the computer. High-speed serial data technologies are under investigation to simplify this connection and will become imperative for the much larger format detectors that are being developed.

Several installations have constructed a safety shield in front of the detector that opens only when data are being collected. This device helps to protect the delicate front surface of the detector and is highly recommended.

Data acquisition software. There is a wide spectrum of computer configurations surrounding CCD detectors. The major tasks to be performed are operating the detector, controlling the beamline, storing raw data, correcting images and analysing diffraction patterns. In home laboratories, where exposure times are relatively long, a single PC typically handles these tasks. In another arrangement, the detector controller is really an embedded system, mostly unseen by the operator, making the detector a remote image server. The raw data or corrected images come to the user's workstation where subsequent analysis is performed. This circumvents the problem that the detector computer may be running a different operating system from the workstation. At storage-ring sources, where the data volume is very large, the detector is almost always configured as a remote image server; the user's workstation does not even need to be nearby. Clusters of remote computers that can perform tasks in parallel become attractive for streamlined data collection, correction and analysis from large data sets. Remote analysis over the internet is being explored by several storage-ring facilities.

Control software should be easy to use, but flexible and extensible. It should be easy to set up experiments and sequence the individual steps in an experiment: exposure, readout, correction, storage and crystal movement, and wavelength change for MAD experiments. Extensible software would permit a user-written macro to be run at each step in place of the detector primitive that is provided. For instance, if it were desired to collect two images at different exposure times for each position of the crystal, extensible software would make it easier to set up the experiment. Finally, the software should permit access to all of the readout modes of the detector. For instance, a detector may be capable of rapidly scanning a small region of interest for alignment purposes, or it may be capable of streak-mode operation for certain types of time-resolved experiments. Available CCD detector software for macromolecular applications has room for much improvement. Hopefully, software will continue to undergo rapid development. Standardization is especially needed.

7.2.5. Applications to macromolecular crystallography

Storage rings. CCD detectors have gained widespread acceptance for macromolecular crystallography at storage-ring sources, in part because of the high-quality data they give, but more for their speed, convenience and efficiency. Accurate data to high resolution are especially important for MAD phasing, and CCD detectors excel in this application. In the past with film, or even storage phosphors, teams of perhaps ten people were required to perform a synchrotron experiment; today, a single person per shift can perform an experiment. With increasing beam flux, improved X-ray optics and faster CCDs, it is often possible to collect full data sets in little more than an hour. Anticipated improvements in speed for CCD detectors should soon make it feasible to collect fine-sliced rotation data routinely; these data are expected to yield better structure solutions.

Home laboratories. Acceptance of CCD detectors for macromolecular crystallography at home laboratories has been slower, in part because there is not such a premium on speed, and in part because of cost. Diffracted spot sizes are larger than at synchrotrons, so highly accurate data should be obtainable. Fully automatic storage phosphor systems work quite well with conventional sources and at this time are lower in cost than large CCD detectors. However, they have a minimum cycle time, caused by the mechanics of the readout scheme, and the required exposure for a strongly diffracting crystal can best this time by a wide margin. Thus, for strongly diffracting specimens, CCD detectors can be significantly more efficient.

7.2.6. Future of CCD detectors

The basic principles of CCD detector technology are now well developed, but various incremental improvements have already been demonstrated and may be expected in commercial detectors. These include larger detector areas, faster read times (owing to both faster electronics and multiamplifier CCDs), more flexible control electronics, better optimized phosphors and calibrations, and, especially, better software. Lower-cost CCD detectors would certainly be welcome. It is easily predicted that the application of CCD detectors will continue to increase rapidly for at least several more years until displaced by even better technologies, such as pixel array detectors (see Section 7.1.4 in Chapter 7.1).

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