images should be ignored. The effects of damage are likely to be systematic rather than just random, and cannot be totally compensated for by scaling. This remains true even for cryogenically vitrified crystals, especially with ultra-bright synchrotron sources.

Following an earlier recommendation by the IUCr Commission on Biological Molecules (Baker *et al.*, 1996), this tabulated information, as a function of resolution, should be deposited with the data and the final model coordinates in the Protein Data Bank. Only then is it possible to have a true record of the experiment and for users of the database to judge the correctness and information content of a structural analysis.

9.1.16. Strategies for automated data acquisition

Progress in crystal-handling hardware has resulted in the development of sample changers both for synchrotron beamlines and the home laboratory. A sequence of samples contained in a Dewar can be mounted on the goniostat, centred in the beam and exposed to X-rays without user intervention. The gain in efficiency arises from the fact that manual intervention is no longer needed between samples, and at SR sites access to the hutch is avoided.

While this provides the potential for greatly increased throughput, it still requires intelligent decision-making software for evaluation of crystals and for optimal strategies of data collection to be achieved with minimal (ideally zero) user input. The steps required in such a system are:

(1) Automated mounting and dismounting of samples from a Dewar.
(2) Automated centring of the sample (or at least loop) in the beam.
(3) Recording and interpretation of two images preferably 90° apart in crystal orientation.
(4) Repetition of steps (1)–(3) for a number of samples of the same protein and ranking of these samples in terms of diffraction quality.
(5) Selection of the best sample and definition of the optimum strategy for data collection, taking account of information provided by the user with regard to the minimum resolution *etc*.
(6) Collection and integration of complete and ideally redundant data.

Robotic sample changers with at least some elements of the above are now operational at many sites [for example, see Leslie *et al.* (2002); McPhillips *et al.* (2002) and Cipriani *et al.* (2006), and also Chapter 9.2]. Considerable advances are expected in the near future, allowing routine automated screening of samples at major synchrotrons. In addition, remote access to synchrotons, by submission of crystals in Dewars for collection by SR staff (the so-called Fedex procedures) or for direct control by the user from their home laboratory through the Internet, is now possible at a number of synchrotron facilities. All of these moves towards automation require electronic databases for the tracking and transfer of samples and their associated data and parameters.

9.1.17. Final remarks

Optimal strategies for data collection are dependent on a number of factors. The alternative data-collection facilities to which access is potentially available, how long it takes to gain access and the overall time allocated all place restraints on the planning of the experiment. In view of this, it is not possible to provide absolute rules for optimal strategies.

Even after the source and overall time have been allocated or planned, the strategy is still the result of a compromise between several competing requirements. Some are general, others depend on the characteristics of a particular crystal or detector. As seen in the previous section, it is not possible to define protocols relevant for all applications. Rather, it is important to consider the relative importance of the parameters that can be varied to the problem in question and make the appropriate decisions.

Thus, data collection may have become easier from a technical point of view, but several crucial scientific decisions still have to be made by the experimenter. It is always beneficial to sacrifice some beam time and interpret the initial diffraction images, so as to avoid mistakes which may have an adverse effect on data quality and the whole of the subsequent structural analysis.

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