

example, one crystal of RNase-A was used to collect data from 1.5 to 1.2-Å resolution at 160K. The temperature was then lowered to 98K and data from ∞ to 1.5-Å resolution were collected on the same crystal. After a total of 28.3 days of X-ray exposure the decay in the intensity standards was about 3%. Data from two other RNase-A crystals have also been collected at 180K and 130K from ∞ to 1.5-Å resolution and, again, the decay in the standards after 13.1 days of X-ray exposure was only about 3% in both cases. Data were also collected from an RNase-A crystal at 220K and no radiation damage was observed over an 8.1 day period of X-ray exposure. The structures at each temperature have been refined to current R values of between 14 and 16%.

The reasons for the large reduction in radiation damage that we have observed for RNase-A crystals mounted on glass fibers are not at all obvious but may possibly be linked in some way to the removal of the glass of the capillary tube from proximity to the crystal, to the lack of excess mother liquor surrounding the crystal, or to the exclusion of oxygen from the crystal during data collection. The large reduction in radiation damage appears to be a combination of both the low temperature and the lack of the capillary tube.

qualitative way, crystal transitions. This has been used by Hajdu et al ((1986) Biochem Soc Trans) to study an order-disorder-reorder process in crystals of phosphorylase b.

The use of Laue diffraction data in a quantitative way, in difference Fourier maps, has necessitated new data processing software and new theory. The strategy for the processing software (Helliwell (1985) J Mol Struct 130, 63) involves the usual steps of sample refinement, prediction and integration. The single wavelength Laue spots and multi-component Laue spots are treated differently. Several reciprocal lattice points (rlps) stimulated in one spot can be unscrambled using differential film absorption (for the case of double and triple reflection spots). The integrated data are currently being used in three ways. Hajdu et al (pers comm) are using the fractional difference intensity in Fourier maps whereby wavelength dependent parameters cancel out, to study enzyme substrate interactions. Helliwell et al (this abstract) are comparing the data derived from Laue geometry with monochromatic data from the source crystals to check for systematic errors and improve the software; wavelength normalisation procedures have been developed (partly in collaboration with K Moffat). Harding et al (pers comm) is using wavelength normalized Laue data to solve small molecule crystal structures.

New theory has been necessary. Cruickshank, Helliwell and Moffat ((1987) submitted to Acta Cryst) have derived the observed multiplicity distribution of energy overlap spots. It has been established that the proportion of single wavelength spots is never less than 73% and depends on  $\lambda_{max}/\lambda_{min}$  and the number of Laue spots depends on  $(\lambda_{max}-\lambda_{min})$ .

#### 01.1-2 USE OF POLYCHROMATIC SYNCHROTRON X-RADIATION IN PROTEIN CRYSTAL LAUE DIFFRACTION.

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The Daresbury SRS wiggler is used to provide an intense, smooth continuum of X-rays between 0.2Å - 2.5Å. Laue patterns can be recorded from protein crystals in approximately 100 milliseconds to 1 second using the SRS wiggler protein crystallography workstation (Helliwell et al (1986) Nucl.Instrum. and Methods A246, 617). On this station (9.6) the vertically diverging beam is collected by a cylindrical focussing mirror set to reflect  $\lambda's > 0.5\text{Å}$ . A new workstation is currently under construction on the wiggler line. The design of the new station involves a toroid mirror to focus the vertically and horizontally diverging beam. Laue patterns are expected to be recorded in 1-10 milliseconds. The new station will also be used for point focussed, rapidly tunable monochromatic experiments.

The advantage of using a broad wavelength band is that a large continuous region of reciprocal space is sampled in a single shot. This "traditional" benefit of Laue geometry, taking advantage of the short exposures now possible, is useful for monitoring, in a

#### 01.2-1 FIBER DIFFRACTION AS AN ALTERNATIVE TO PROTEIN CRYSTALLOGRAPHY.

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Many important biological macromolecules, for example actin, myosin, tubulin, flagellin, and the coat proteins of some viruses, form filamentous assemblies with functions specific to those assemblies. Even in cases where these molecules can be crystallized as monomers or small aggregates, it is important to know the molecular structure of the intact assembly in order to understand the function of the molecule. It is therefore necessary to use the methods of fiber diffraction.

The central problem of fiber diffraction is that the random azimuthal orientations of the diffracting particles cause the data to be cylindrically averaged. Considerable information is thus lost; for example, at 3Å resolution the effective number of observable diffraction data for tobacco mosaic virus (TMV) is reduced by a factor of 2.5, and for the bacteriophage Pfl by 1.7. These factors are much higher for lower symmetry systems such as microtubules.

Multi-dimensional isomorphous replacement, analogous to isomorphous replacement in protein crystallography, can be used to compensate for the loss of information. Large numbers of heavy-atom derivatives are needed, but these numbers can be reduced by taking advantage of the fine splitting present in the diffracted layer lines when, as is usual, the helix in the diffracting system repeats approximately, but not exactly, in a small number of turns. Phases determined by MDIR and layer-line splitting can be refined by density modification (solvent flattening), which provides much more powerful constraints in fiber diffracting systems where the diffracted intensity is continuous along layer