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Note on a reflecting optical diffraction spectrometer.

By A. Elliott and P. Robertson, *Research Laboratory, Courtaulds Limited, Lower Cookham Road, Maidenhead, Berkshire, England*

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The optical diffraction spectrometer used for observing 'optical transforms' of the projection of a trial structure is generally constructed with corrected lenses, one being employed to produce a parallel beam of light, with a second lens to focus the Fraunhofer diffraction pattern (Hughes & Taylor, 1953). The difficulties which arise in the application to large molecules, using punched masks, have been referred to by Hooper, Seeds & Stokes (1955), who found that slight imperfections in the lens system introduced distortions. In consequence, these authors make use of a photographic method for preparing masks, and work with very small masks. This reduces distortion caused by optical imperfections.

We have produced satisfactory transforms of polypeptide structures with large-scale drilled masks by replacing the two lenses by a single mirror, working at the centre of curvature, as shown in Fig. 1. For large units, mirrors are generally more satisfactory than lenses and very much cheaper. In the arrangement shown, a single optical surface does the work which is performed by eight in the conventional arrangement, and no errors are introduced by inhomogeneities in the optical glass. The geometric accuracy of surface required in a mirror is, however, higher than that needed in a single lens surface, for a given tolerance of optical path length.

Fig. 1. Illustrating the use of a concave mirror for producing Fraunhofer diffraction patterns.

The mirror has a surface of 17 cm. diameter with a radius of curvature of 10 metres. The departure from sphericity was difficult to measure by the Foucault knife-edge test and the error in path length is probably not more than $\lambda/50$ for light of wave-length 5780 Å. A fairly sensitive test is afforded by observing the diffraction pattern of an unsymmetrical arrangement of holes, such as the projection of a portion of a helix. The diffraction pattern, if undistorted, must have a centre of symmetry. A large optical unit such as this can only be used to advantage in good atmospheric conditions, and we have found the vertical arrangement to be very advantageous. The greater part of the path, including the mirror, is enclosed in a hardboard tube, covered with aluminium foil to lessen radiation effects.

The advantages of working with a large-scale mask are fairly obvious. Drilling or punching (the former is conveniently carried out on a Taylor–Hobson engraving machine) is a rapid method and it is easy to ensure that all holes are of the same size or, alternatively, they may readily be made to any required size by means of small taper broaches. In addition, a mechanical arrangement for altering one coordinate of each atomic species is in some cases practicable; we have made use of this facility in some current work on the structure of β-poly-L-alanine.

As an example of a diffraction pattern produced by the apparatus, and without any implications as to the correctness of the structure on which the mask was based, we reproduce in Fig. 2 the pattern of the helical arrangement of atoms proposed by Huggins (1952) for the α form of poly-L-alanine. The projection is on a plane parallel to the helix axis; there are 90 atoms in each repeating unit and a helix length containing two such units has been employed. The scale of the mask was 1 cm. = 5 Å.

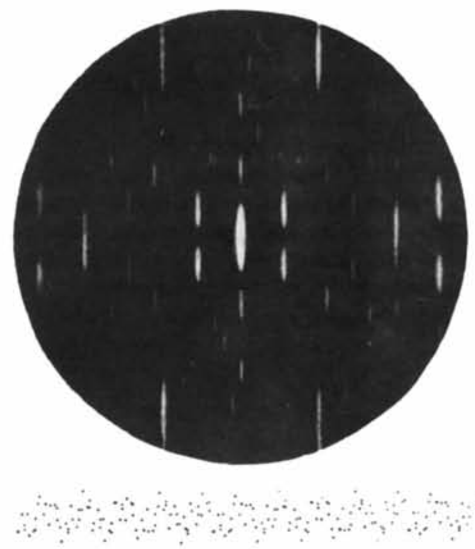

Fig. 2. Example of Fraunhofer diffraction pattern ('optical transform'): $3{\cdot}7_{11}$ helix of poly-L-alanine (Huggins, 1952). Mask shown on one-quarter scale actually employed; atoms projected on plane parallel to helix axis.

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