Books Received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

Diffusion data, Vol. 5, No. 1, 1971. Edited by F. H. WÖHLBIER Clausthal-Z, Germany: Trans Tech Publications. Subscription US $ 38,00 (sFr. 162,00) per volume of 4 issues in each calendar year.

This journal covers all new reference information on all aspects of solid state atomic transport in crystalline and amorphous solids. The reproduction is by lithography from typed texts and is very clear. The journal claims that published material is covered within a few weeks of its appearance.

Stereographic projections of the cubic and close-packed hexagonal lattices: Produced by A. T. DAVENPORT and A. R. BOOTH. London: Butterworths, 1970. Price (U.K. only) £3·50.

The volume contains 20 stereographic projections of the cubic and close-packed hexagonal ($c/a = 1{\cdot}633$) lattices. The projections are printed on transparent tracing paper and are designed to be used with the 30 cm equatorial stereographic Wulff net also supplied.

Meeting Report

Second International Conference on Small-Angle Scattering. Graz. 26–29 August, 1970

The 2nd International Conference on Small-Angle X-ray Scattering, under the chairmanship of O. Kratky, brought some 200 participants. Sixty-four papers were presented in two parallel sessions; their common aspect was the experimental method employed, although the problems investigated ranged from biological to metallurgical. In this instance, such a formula for a conference proved quite justified. Among the most interesting results presented, many are a consequence of progress either in the precision and sensitivity of the measurements, or in the sophistication of the methods used to interpret the experimental data. Papers of this kind ought indeed to be discussed by specialists who not only appreciate their value but also the possible uncertainties; subsequently, both specialists and nonspecialists can then make confident use of the results. In this report, we will primarily mention those papers which dealt with innovations in the method; we refer the reader to the collected abstracts for the other very interesting but more 'classical' communications. [The collected abstracts representing the papers actually presented are printed immediately following this report].

Compared to the material presented at the last such conference (Syracuse, U.S.A., 1965), one finds a variety of striking new applications which often combine small-angle scattering with other techniques (*i.e.* wide-angle diffraction, electron microscopy, light-scattering, *etc.*). An example, for instance, was afforded by the study of crystal imperfections in alloys and imperfectly crystallized substances, discussed in a plenary lecture by GUINIER.

Theoretical advances were, in recent years, relatively few. POROD reported investigations of interparticle interference effects in densely packed systems, which are sensitive to details of the particle shape and may consequently show qualitatively different scattering diagrams (*i.e.* 'cluster' and 'liquid' types). TEICHGRÄBER and WALENTA discussed the perenially interesting problem of extracting information on particle diameter distributions $P(D)$ in polydisperse systems from the scattering data. WU and SCHMIDT reported theoretical investigations of the intersect distribution function for a system of identical, independent, randomly oriented particles of uniform electron density.

Some of the reasons for the increased confidence with which experimenters now view SAXS results became evident during the session dealing with experimental methodology. SCHMIDT and PATEL discussed their comparison of the Beeman and Kratky cameras, which yielded good agreement for properly desmeared scattering curves obtained with the two quite different geometries from the same sample. Substantially improved monochromatization was reported with the pyrolytic graphite diffracted-beam monochromator by HENDRICKS, who also discussed critically the various methods of measuring absolute intensities. ZIPPER spoke about a procedure for eliminating the $K\beta$-content of the scattering curves by a mathematical procedure, using the measured $K\alpha/K\beta$ intensity ratio of the primary radiation.

Of great interest were reports on recent developments in small-angle neutron scattering. SCHMATZ and SCHELTEN announced that the new small-angle neutron diffraction apparatus at Jülich was put into service. This is an instrument remarkable for its size (80 meters), its multiple detectors, and its performance (a measurement which would take 3 weeks at the Munich reactor can be made with greater precision in one hour). Soon, a more powerful instrument of the same type will be installed at the Franco-German reactor at Grenoble. These devices will allow the development of neutron scattering methods, and their combination with X-ray scattering, which appear of great promise. For small-angle neutron scattering, it is hoped that the coherent and incoherent contributions can be separated (HOSSFELD and AMADORI).

The large-scale structure of high polymers is a subject of current interest, in particular the long periods (of the

order of 100 Å) which are observed with X-rays and in the electron microscope in many polymers and under a variety of conditions. This is therefore a fundamental aspect of their structure which should be of general significance. At the moment, there is no complete theory which accounts for all these observations from first principles. One is at the stage where new observations are needed to understand this still somewhat mysterious phenomenon. A number of papers clarified certain specific points. Thus, PETERLIN demonstrated the mechanism of plastic deformation, and showed how the structure is modified in the course of drawing a fiber. KELLER and his collaborators showed a relationship between the long periods and the monomer units of the chain for a series of polyamides, and put clearly in evidence the discontinuous change in the number of monomer units in the fold period. This is not, however, valid for polyethylenes. POINT and his collaborators, on the other hand, conclude that it is not possible to account for the macroscopic deformations of a sample with only the data of the small-angle diagrams; one arrives at the somewhat disturbing conclusion that the sample contains matter whose structure is not apparent but whose action determines the change of macroscopic dimensions.

No longer does one measure only the sizes of the long periods, but one also attempts to determine the structure of polymers on this scale. Thus, SADLER, ATKINS, KELLER and WILLMOUTH use the well-known crystallographic methods (the measurements of intensities of successive orders) to investigate well-ordered polyamides. BROWN and FULCHER determine the electron density correlation function (as is done in the study of amorphous materials) for less crystalline polymers. FISCHER and KLOOS are able to detect the glass transition of various polymers by measuring the temperature dependence of the small-angle intensities. The thermal expansion coefficient of the intercrystalline surface layer of polyethylene is obtained from the gradient of the intensity-temperature curve above T_g.

Carbons have been the subject of SAXS investigations from the beginning. RULAND and PERRET have demonstrated just how far our knowledge can be extended today. On the one hand, they were able to determine density fluctuations (which produce deviations from Porod's law) on a very small scale, and on the other, average filament diameters of the order of microns (using the multiple small-angle scattering usually considered an effect to be avoided).

The various sessions devoted to biologically important systems opened with a group of papers on proteins. In an elegant paper by STUHRMANN, a new mathematical approach (based on expanding the electron density distribution in spherical harmonics) for analyzing the experimental scattering functions of dilute mono-disperse proteins in solution was described and applied to myoglobin. The shape scattering was separated from scattering due to the interior structure by measurements in a series of solvent systems of different electron densities. The shape of myoglobin thus determined agreed well with crystallographic results. The remaining papers on biological systems fell into two broad categories – those dealing with macromolecules in solution and those concerned primarily with membranes or fibres. Some highlights only: DURCHSCHLAG, KRATKY, PUCHWEIN, SCHUSTER and KIRSCHNER were able to support an allosteric mechanism for the binding of nicotinamide adenine dinucleotide (NAD) to yeast glyceraldehyde-3-phosphate dehydrogenase; the apo-enzyme contracts about 7% at full saturation, but the observed degree of contraction is not linear in the degree of saturation. This work represents an example of the precision with which small relative volume changes can be determined by SAXS; an absolute determination of volumes cannot be done so exactly, but in relative measurements under strictly constant conditions, various sources of error are eliminated. One would suspect that measurements of effects as small as these would not have been considered even a few short years ago.

PUCHWEIN, KRATKY, GÖLKER and HELMREICH were able to arrive at a prismatic model for both the dimer and tetramer of phosphorylase-*b* in solution. This is the first example where the scattering curve of a paucidisperse solution could be separated into contributions from the two components, one of which (dimer) was known and therefore enabled analysis of the second (tetramer) which was not available in pure form. The very active Graz group and its collaborators also contributed studies of *Helix pomatia* hemocyanine (PILZ, KRATKY and MORING-CLAESSON), bacteriophage *fr* and *R*17 (ZIPPER, KRATKY, HERRMANN and HOHN), DNA-actinomin complexes (on the basis of measurements down to concentrations of 0.045 g/100 ml) (WAWRA, MÜLLER and KRATKY), and phenylalaninespecific *t*-RNA (PILZ, KRATKY, CRAMER, HAAR and SCHLIMME). These very careful experiments, which incorporate absolute intensity determinations in a decisive way (making use of the experimental and theoretical methods developed in the Graz laboratory), represent excellent examples of the way SAXS can be used as a precise tool to obtain biologically significant information – for instance the change in shape of the DNA-molecule upon complexing, or the conformational changes of *t*-RNA as a function of temperature and of the influence of counter ions. The paper of LUZZATI provides still another example of a fundamental result which can be attained by a thorough utilization of the SAXS method. It shows, in effect, that nucleic acids behave like rigid rods in solution; SAXS has also shown that they undergo a transformation from the normal to an intermediate state which corresponds to a separation of the normal double helix. Here again, precise measurements of absolute intensities and of densities were employed, and yielded information not revealed by other methods.

SHIPLEY and ATKINSON discussed SAXS of multilamellar and single bilayer lipid–water dispersions on the basis of various electron density models. BURGE described the SAXS of bacterial flagellae from salmonella. AKERS and PARSONS reported on the structure of the myelin membrane, HALBOTH, HEINEMANN and ZAHN on the structure of α-keratin fibers. Other papers in the general polymer area dealt with the determination of stiff-chain parameters from such molecules as amylose and cellulose (BURCHARD and KAJIWARA), of long- and short-range order in bromine-marked polystyrenes (DURCHSCHLAG, PUCHWEIN, KRATKY, BREITENBACH, OLAJ and WOLF) and with the introduction of new parameters characterizing the curvature and mean torsion of the coil into the theoretical analysis of polymer scattering (KIRSTE).

Other areas of application have continued, though they have not expanded as much. Under this heading would come critical opalescence [liquid Na–Li (BRUMBERGER and ALEXANDROPOULOS), CO_2 (CHU and LIN), argon (BALE, DOBBS and SCHMIDT)], and the metastable miscibility gap in alloys (Al–Zn–Mg, DÜNKELOH and GEROLD). Among inorganic substances, alloys have been among the most intensively studied.

HÖHLER and STEEB employ an apparatus which allows measurement of liquid metal scattering to 1000°C. In Al–Sn, for which there is miscibility in the liquid state and complete immiscibility in the solid state, one finds that the atomic distribution in the liquid is not uniform. SAXS shows the existence of concentration fluctuations with a spatial extent of the order of 10 Å. Heterogeneities in Ti–Nb alloys were studied by HENDRICKS, KOCH and LOVE as a function of heat treatment, and the importance of double Bragg scattering in polycrystalline metallic samples was emphasized. BONFIGLIOLI and ACUÑA have tested Cahn's and Cook's theories of spinodal decomposition by a very detailed study of Al–Zn alloy. There is no doubt that the disparities between predictions and measurements exceed experimental error.

It is of great interest to apply SAXS to liquid crystals in the neighborhood of their transition points. GRAVATT and BRADY have demonstrated the existence of scattering near these points, but the phenomenon is affected by the presence of impurities. Besides, the results could not be interpreted by applying either the theory of first- or second-order transitions.

Extremely weak effects due to very low defect concentrations were measured by the group of WAIDELICH on γ-irradiated LiF crystals. WOHOFSKY measured SAXS intensity distributions, and SPALT and PEISL those in the neighborhood of Bragg reflections. They concluded that there are clusters of about 100 atoms, near F-centers, due to agglomeration of neutral fluorine atoms.

There remains a group of interesting papers which are difficult to classify For instance, a general theory of diffraction by matter in any state of aggregation was presented by BAGCHI, based on the concept of a statistically homogeneous lattice. TCHOUBAR and MÉRING introduced an absolute intensity, based on unit mass of scatterer, which appeared to offer certain practical advantages in the determination of the average intercept length $\bar{l}$ and of the porosity. OELSCHLAEGER reported on the estimation of association constants and heats of association, size, shape and size distribution of associated dye molecules (sodium copper-phthalocyanine tetrasulfonate).

A significant by-product of the conference was the initiation of an absolute intensity project by HENDRICKS; secondary standards will be measured in several laboratories by different techniques and results compared.*

Thus, we see that the 2nd SAXS Conference was of great scientific interest. It must be added that the congress was made very pleasant for the participants by the gracious hospitality of its organizer, Professor Kratky, and of the city of Graz and the province of Styria.

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* See *J. Appl. Cryst.* Vol. 4, part 3, page 268.