Meetings

Crystallography and Crystal Physics

TWO well planned and well attended meetings this summer attest to the present closeness with which crystallographers and other physical scientists are working and to the continually increasing overlap (and, if I may use the word, "cross fertilization") amongst physicists, chemists, metallurgists, and crystallographers. The first was the "International Conference on Current Problems in Crystal Physics" which was held July 1–5, 1957, at the Massachusetts Institute of Technology. The second was the Fourth General Assembly and Congress of the International Union of Crystallography (July 10–17) and Symposia (July 18–19) held in Montreal, Quebec, Canada.

THE primary aim of the MIT Conference was "to bring together crystallographers and theoretical or solid-state physicists, to discuss some topics of common interest". The time of the conference was chosen so that crystallographers planning to attend the meetings at Montreal could participate conveniently. Attendance was by invitation only and 150 scientists from more than 10 countries were present. The Conference was sponsored by the Commission on the Physics of Solids of the International Union of Pure and Applied Physics, with assistance from IUPAP, the International Union of Crystallography, UNESCO, the National Science Foundation, the Office of Naval Research, and the Air Force Office of Scientific Research.

The twenty-eight invited papers were arranged in nine half-day sessions (none on Wednesday afternoon) so that there was plenty of time for discussion and informal presentation of material bearing on the topics of the Conference. Six papers were read at the first two sessions on electron distributions in atoms and crystals. W. Cochran (Cavendish Laboratory, Cambridge) described x-ray diffraction electron distribution determinations of salicylic acid, NH_4HF_2, LiH, and potassium hydrogen maleate. Debye-Waller temperature factors, structure factors, form factors, and bond lengths were calculated from the data and compared with theoretical values from various models where possible. Electron distribution studies in NaCl, LiF, CaF_2, and Al were described in a paper of H. Witte (Technische Hochschule, Darmstadt) as read by E. Wolfel (one of the collaborators on this work). Spectrometer-ionization chamber experiments on powders and single crystals were made to determine the structure amplitudes. H. Renninger (Marburg-Lahn) dealt with the explanation of the anomalous reflection in diamond.

W. H. Taylor (Cavendish Laboratory, Cambridge) described work done with P. J. Black to determine electron configuration in aluminum-rich alloys of transition metals. These investigations were undertaken to test ideas on electron transfer between atoms in alloys (Mott, Pauling, Raynor). The authors concluded that apparent correlations in e/A are of very doubtful significance and that there is no direct way of obtaining information about electron distributions in the atoms from observations on Brillouin zones. R. J. Weiss and J. DeMarco (Materials Research Laboratory, Watertown Arsenal), in a paper read by W. Cochran, concluded from their x-ray studies of atomic scattering factors and comparison with theoretical values (calculated from Hartree-Fock wave functions) that the close-packed metals Cu, Ni, Co have most of their electrons outside the "argon core" in atomic $3d$ states while Fe and Cr (*bcc*) have most of their electrons (six in each case) quite far out radially. They described in some detail how they met problems encountered in making absolute scattering factor measurements: extinction, surface roughness, dispersion correction, Debye-Waller factor, absolute counting, absorption coefficient. D. R. Hartree (Cavendish Laboratory, Cambridge) described work on a systematic survey of the variation of atomic wave function with atomic number. The interpolations of such functions or fields with respect to atomic number must be done with considerable care since they may be used for the interpolation of other atomic properties, such as x-ray scattering factors, or may be adopted as initial estimations in a self-consistent field calculation. The choice and variation of the screening parameters and the scale radius were described in some detail.

Magnetic scattering of neutrons was treated in three papers. R. D. Lowde (Harwell) described experimental work on critical magnetic scattering of neutrons by an iron crystal. This critical scattering, which is associated with a condensed material in the vicinity of a phase transformation, was observed in the general neighborhood of the 110 Laue reflection. R. J. Elliott (University of Reading) read a paper by himself and W. Marshall (Harwell) on the theory of critical scattering. The effects were calculated directly for the Ising and Heisenberg models using the method of Bethe and Peierls for discussing order-disorder in solids. The results were compared with the work of Van Hove and of Zernike and with experimental observations. Theoretical calculations of the magnetic scattering of neutrons by CoO using Kanomori wave functions, Slater wave functions, and others were reported by T. Nagamiya, who read the paper, and K. Motizuki (Osaka University).

Four papers on neutron determination of hydrogen positions in crystals were presented. G. E. Bacon (Harwell) described work, based on two-dimensional projections of neutron scattering density, on several substances in an attempt to further elucidate the role of

hydrogen bonds in solids and other bonds involving hydrogen, such as the C-H bonds. The neutron diffraction C-H bond length differs by more than 15% from the x-ray measurements. R. Pepinsky (Pennsylvania State University and Brookhaven National Laboratory) discussed some new x-ray and neutron studies of hydrogen bonding and the three-dimensional refinement on the IBM 704 machine. Some problems in the stereochemistry of hydrogen bonds were described, as were problems of dielectric anomalies and other transition phenomena involving H-bonds. H. A. Levy and S. W. Perterson (Oak Ridge National Laboratory) in a paper presented by Levy, described neutron diffraction studies of hydrogen containing single crystals (hydrides, hydroxides, acid salts, acids, hydrates). In addition the structural nature of transitions in a number of hydrogen-containing systems including halides and ferroelectric phosphates and arsenates and organic structures such as urea, resorcinol, etc. were also studied. Some of these have been carried through complete least squares refinements yielding parameters of a high degree of precision and providing hitherto unavailable information concerning thermal vibrations in crystals. Helen Megaw's paper (Cavendish Laboratory, Cambridge) on some empirical problems concerning atomic bonds was not intended as a connected account of any problem or piece of research, but rather it was meant to call attention to a number of points where the theories are still not adequate for handling the observed facts. She formulated some of the questions that face a crystallographer in trying to understand and to generalize about actual structures in terms of interatomic bonds. Miss Megaw dealt with the structure of the hydroxyl ion, temperature changes in interatomic bonds with special reference to thermal expansion of the individual bond and coordination number and atomic environment. She emphasized the need for recording experimentally determined scattering factors in order to provide a check on the theoretical curves and perhaps call attention to new phenomena which would otherwise have been overlooked.

One session was devoted to two papers on the theoretical and experimental studies of energy bands in crystals. The theoretical aspects were treated by F. Herman (RCA Laboratories, Princeton) who discussed some of the methods for predicting the possible complexities which may occur in the band structure of crystals. Emphasis was on the symmetry arguments which play such an important role in energy band theory; quantum theory of solids and the various approximations were for the most part dealt with qualitatively. B. Lax (Lincoln Laboratory, Lexington) in his paper reviewed four major methods of investigating the band structure of semiconductors and metals experimentally: (1) the powerful techniques of cyclotron resonance (both microwave and infrared frequencies), (2) the de Haas-van Alphen measurements, (3) the anisotropic galvanomagnetic effects and (4) infrared absorption phenomena (in semiconductors), particularly the newly discovered oscillatory magnetoabsorp-

tion effect. A brief discussion of the experimental techniques was presented and specific models of the energy bands for a number of semiconductors and semimetals were described. The experimental results were presented in the form of graphical data selected from representative publications and recent theoretical interpretation of these results was also given where possible.

The last four sessions were devoted to the thermal vibrations of crystals with the last two emphasizing the determination of the thermal vibrations by thermal diffuse scattering of x-rays and neutron diffraction. In all, 14 papers were given at these sessions, and only brief reference will be made to most of them. J. M. Robertson (Glasgow) reported on the structure of naphthalene and anthracene. E. G. Cox (Leeds) described work on the crystal structure of benzene and the motion of the carbon atoms in the molecule. D. S. J. Cruickshank (Leeds) gave a paper on the lattice vibrations of benzene, naphthalene, and anthracene and presented a mathematical treatment in which he expressed the rigid body vibrations of the molecules in terms of two tensors giving the anisotropic translational and angular vibrations. He discussed the theory of lattice vibrations and emphasized that the three techniques of x-ray diffraction, calorimetry, and Raman spectra are complementary.

Dame Kathleen Lonsdale (University College, London), in her paper on molecular movements in crystals, emphasized the need for getting (and reporting) the physical properties (elastic constants, thermal expansion coefficients, etc.) and x-ray data at one time when the investigator has the crystal at the desired temperature, etc.—even if one cannot interpret the data. The paper by H. J. Grenville-Wells (University College, London) was concerned with the analysis of accurate measurements of electron density distribution in crystals so as to distinguish between (a) bonding anisotropy and zero point energy and (b) thermal vibrations. S. Miyake (Tokyo) read a paper by himself and S. Hoshino on the temperature characteristics of x-ray intensity of reflection from crystals having zincblende and wurtzite type structures. E. Montroll (University of Maryland, College Park) presented a paper on the frequency spectrum of diatomic simple cubic lattices, ordered and disordered. This work, which was done in collaboration with P. Mazur, A. Maradudin, and G. Weiss, made a detailed analysis of the lattice vibrations of a diatomic simple cubic lattice with nearest neighbor interactions, central and noncentral. It was pointed out that many of the problems involved had already been solved by Rayleigh and Lord Kelvin and in recent times by Lifshitz and other Soviet workers.

Five of the seven papers in the final session were in French and the material treated is indicated by the titles of the papers. J. Laval (Collège de France, Paris): Diffusion des rayons x provoquée par l'agitation thermique des atomes dans les cristaux. D. Cribier (Collège de France, Paris): Etude des oscillations d'agitation thermique dans un cristal de fluorine (CaF_2). Y. LeCorre (Collège de France, Paris): Travaux sur l'agitation thermique. A. Laberrigue (Collège de France, Paris): Diffraction des electrons par des monocristaux influence de la temperature. H. Curien (Paris): Diffusion des rayons x par effet Compton dans les cristaux. E. H. Jacobsen (General Electric Co., Schenectady) presented a paper on lattice dynamics and thermal diffuse scattering of x-rays, particularly on the determination of elastic constants from diffuse scattering near Bragg reflections. Noncentral forces must be taken into account and forces out to third nearest neighbors are important—even in metals. B. N. Brockhouse (Chalk River) reported work in collaboration with A. T. Stewart on lattice dynamics by neutron spectroscopy. Studies were made on neutron energies after diffraction (analogous to Raman effect) in investigating diffusion of spins in ferromagnetic materials, incoherent scattering, etc.

A special informal session following the last paper was called to hear J. Laval (Collège de France, Paris) aided by Y. Le Corre (Collège de France, Paris) explain his multiconstant theory of elasticity. Among those who participated in the discussion were W. A. Wooster (Cambridge), P. P. Ewald (Brooklyn Polytechnic Institute, Brooklyn), I. Waller (Uppsala), P. M. Marcus (Carnegie Institute of Technology, Pittsburgh), M. Lax (Bell Telephone Laboratories, Murray Hill), B. E. Warren (MIT, Cambridge) and A. Guinier (Conservatoire National des Arts et Métiers, Paris) who also served most ably as interpreter.

The conference papers were of a high quality and no attempt has been made here to comment on them critically. The success of the MIT meetings was in a large measure due to the high level, stimulating discussion following each paper (which discussion, regrettably, often had to be cut short because of lack of time). Although most of the 150 scientists attending participated actively at the Conference, mention should be made of a few besides the speakers mentioned earlier (several of whom contributed significantly to the discussion of many of the papers) who made the most worthwhile contributions to the spirited discussions: M. Blackman (Imperial College, London), P. P. Ewald, who also gave the after-dinner speech at the Conference dinner on July 4 with his usual charm and clarity, A. Seeger (Stuttgart), W. A. Wooster, J. Slater (MIT, Cambridge), and especially I. Waller who probably made more important comments than any other single person.

All those attending the Conference (including wives) were housed together in the MIT Baker dormitory which fact materially aided the spirit of scholarly and social companionship which pervaded the meetings. A word of appreciation to Professor J. Slater of MIT and his staff is in order for their attention to the many details which insured a smooth meeting and the comfort of the visiting participants and thus a most successful conference. The proceedings of the Conference will be published in a forthcoming issue of the *Reviews of Modern Physics*.

THE size of the Fourth Congress and Symposia of the International Union of Crystallography (Montreal, July 10–19) can be appreciated from the statistics. There were 742 registrants at Montreal (600 actives and the remainder mostly wives) compared with 630 in Paris in 1954, 340 in Stockholm in 1951, and 310 at the first International Congress and General Assembly of the (then) new Union of Crystallography at Harvard University in 1948; one would rather not extrapolate to the Fifth Congress in Cambridge in 1960. In all, 304 papers (mostly of 15 minutes duration) were given during the Congress and Symposia by representatives from 22 nations. All active registrants had received 133 pages of "long" abstracts in advance of the meetings and these will be published in a forthcoming issue of *Acta Crystallographica*. No attempt will be made here to describe the 1/5 (approximately) of the papers this participant heard even as briefly as for the MIT conference above. The contributed papers were arranged under 17 topic headings: (1) i. apparatus, ii. techniques and methods, (2) recent progress in structure determination, (3) minerals, (4) clay minerals, (5) metals and alloys, (6) inorganic structures, (7) organic structures, (8) proteins and related compounds, (9) fibrous structures, (10) order-disorder phenomena, (11) deformations and imperfections, (12) liquids, liquid crystals, amorphous material, glasses, (13) phase transformation, martensitic transitions, ferroelectrics, λ-point transitions, (14) crystal growth, (15) neutron diffraction, (16) symmetry, morphology, twinning, and (17) teaching of crystallography.

The division of material in the five simultaneous sessions followed approximately that in the five invited general hour lectures which began each of the first five days of the Congress. L. E. Sutton (Oxford University) presented a paper written in collaboration with J. S. Taylor and D. G. Jenkin on our present knowledge of interatomic distances and molecular configurations. P. B. Hirsch (Cavendish Laboratory, Cambridge) talked on imperfect structures, particularly in metals. Part of his paper was a moving picture of actual dislocation motions in stainless steel using transmission electron microscopy. The paper of G. S. Zhdanoz (Institute of Crystallography, Moscow) on crystal chemistry was primarily a historical review although it did include some comments on the application of the crystallochemical rules for the creation of new substances with definite physical properties. G. W. Brindley (The Pennsylvania State University, University Park) dealt with clay minerals and described the main objectives in the diffraction studies of clay: structure analysis, analysis of imperfections, identification of clay minerals, and structural studies of clay mineral reactions. In a paper on the x-ray analysis of proteins, D. C. Hodgkin (University Museum, Oxford) described some of the striking advances made in the last few years. She discussed how best the different lines of approach can meet in the evaluation of the electron distribution in three dimensions in any protein and its interpretation in chemical terms.

The two Symposia, at which 25 papers were read, were conducted in six alternating half-day sessions at the conclusion of the Congress. Symposium 1, "Physical Techniques of Crystallographic Interest", was organized by G. A. Jeffrey (University of Pittsburgh) and the introductory lecture was given by C. J. Gorter (Kamerlingh Onnes Laboratory, Leiden) on magnetic resonance in crystalline solids. Symposium 2, "Electron Diffraction Studies of Solids and Gases", was organized by J. M. Cowley (CSIRO, Melbourne), Z. G. Pinsker (Institute of Crystallography, Moscow), and S. Miyake (Tokyo Institute of Technology).* The introductory paper by Z. G. Pinsker and B. K. Vainstein (Institute of Crystallography, Moscow) dealt with structure analysis by electron diffraction. Pinsker, who read the paper, discussed conditions when the kinematical theory is applicable and recent Soviet theoretical and experimental work. In addition there were open sessions of the Union's Commissions on crystallographic data, crystallographic teaching, and powder diffraction methods as well as exhibits of various commercial and non-commercial devices such as apparatus, charts, new materials, and books of crystallographic interest.

These meetings, although well organized and made most pleasant by the many fine activities and the general hospitality of the Canadian, Quebec Province, and Montreal governments, suffered from the same difficulties of other large professional society meetings. It is certainly not surprising that the size and need for five simultaneous sessions (designed as far as humanely possible for minimum conflict) and short papers with inadequate discussion time contributed to make these meetings less satisfactory than the smaller MIT conference described above. It is the nature of the beastie and Professor W. N. Lipscomb (University of Minnesota) and his program committee and Dr. W. H. Barnes (National Research Council, Canada) and the local committee deserve a vote of thanks for a splendid job under conditions which at best were difficult.

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Nuclear Structure

SOME 500 physicists and chemists from the United States and abroad are expected to attend a Conference on The Structure of the Nucleus which is to be held November 20–22 at the Rice Hotel in Houston, Texas. The meeting is planned as the first of a projected series of conferences inaugurated by The Robert A. Welch Foundation "with the object of stimulating and encouraging chemical research within the State of Texas". Invited addresses will be given by P. J. W. Debye (Cornell), Glenn T. Seaborg (Berkeley), D. H. Wilkinson (Oxford), Eugene P. Wigner (Princeton), J. Hans Jensen (Heidelberg), Ernest O. Lawrence (Berkeley), L. Van Hove (Utrecht), and W. F. Libby

* For a more detailed account of this symposium, see the report by J. A. Ibers, *Physics Today*, October 1957, p. 26.