

which could not be substituted by the oxygen on the hypoxanthine base.

The studies reported here have shown that mixtures of polynucleotides are capable of forming hydrogen-bonded helical structures which are susceptible to crystallographic analysis. Just as the structure of the fibrous proteins was finally solved by working on the simpler synthetic polypeptides, it is hoped that structural analysis of synthetic polyribonucleotides will aid the solution of the structure of ribonucleic acid and facilitate our understanding of its function.

I would like to acknowledge the generous assistance and advice of Dr. D. R. Davies and the technical assistance of Mrs. J. Johnson. I am indebted to Prof. S. Ochoa and Miss P. Ortiz for the supply of polynucleotide phosphorylase, and for information concerning its use.

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THE BAND THEORY OF METALS

A SHORT and valuable conference was held in the Imperial College of Science and Technology, London, on December 19 and 20 on "The Band Theory of Metals and the Structure of the Fermi Surface". It was attended by about 240 members of the Physical Society and visitors, including Prof. Vonsovski from the U.S.S.R. The chief value of the conference must lie in the way in which it has drawn together many aspects of the subject. In the years 1928-35, almost the whole theory of metals was fairly satisfactorily sketched in outline, and we were often reminded of this during the conference. Since then, much work has gone into filling in the many gaps that remained. The different threads have now been drawn together again into a more comprehensive theory of metals and into a united research front. There were several review papers of various experimental techniques and theoretical developments, emphasizing what relevance the results obtained from them had for the theory of metals as a whole. There was also a good mixture of theoretical and experimental papers, and much emphasis on turning all this to good account by trying to understand, in detail, the properties of at least a few individual metals. As a further elaboration of this theme, the following thoughts remained in the mind of one participant after the conference. In some places the remarks go beyond what was actually said in the formal sessions.

Prof. N. F. Mott opened the conference with a paper on "Band Theory and Ferromagnetism", which brought out the distinct types of wave function that we use in different circumstances to describe electrons in metals. In the earliest development of the subject, the wave functions of the individual electrons were taken as waves $\psi_{\mathbf{k}}$ (with wave vector \mathbf{k}) extending throughout the crystal, and the wave function of the whole metal was written as a product or as a single determinant:

$$\Psi_{\text{Bloch}} = (N!)^{-1/2} | \text{determinant of the } \psi_{\mathbf{k}} \text{'s} | \quad (1)$$

where N is the total number of conduction electrons in the metal. This we shall refer to as the Bloch picture. Because of the periodicity of the lattice, \mathbf{k}

is restricted to a certain region in k -space known as the Brillouin zone. The energy $E(\mathbf{k})$ varies continuously with \mathbf{k} in each zone. Because of the exclusion principle, all the states below the Fermi level E_F are occupied by electrons. The surface in k -space:

$$E(\mathbf{k}) = E_F \quad (2)$$

is the boundary between the occupied and unoccupied levels, and it determines many of the properties of the metal. The earliest successes of this theory include the resolution of the classical difficulty that the electrons in a metal seem to be free enough to give a high conductivity and yet contribute very

much less than $\frac{3}{2} kT$ each to the specific heat. It also explains the qualitative difference between a metal and an insulator, and how semi-metals like bismuth can exist with an apparent number of 10^{-5} free electrons per atom. On this sort of picture, most of the present theory of metals is based, and Prof. Mott reminded the audience how it could account for the ferromagnetism of some metals like cobalt and nickel. However, he emphasized that in other cases we are driven to use wave functions of a qualitatively different type, namely, the Heitler-London type of function. In this picture each electron is more or less tightly bound to a particular atom (position \mathbf{R}_n), and moves in an orbital $\psi(\mathbf{r} - \mathbf{R}_n)$ localized around this atom. The whole wave-function is:

$$\Psi_{HL} = (N!)^{-1/2} | \text{determinant of } \psi(\mathbf{r} - \mathbf{R}_n) \text{'s} | \quad (3)$$

In this picture the concept of a Fermi surface does not arise. Prof. Mott mentioned different kinds of ferromagnetics and anti-ferromagnetics which are thought to correspond to the two types of wave function. In particular, the ferromagnetic $3d$ -electrons in iron, and similarly the $4f$ -electrons in gadolinium metal, should be described by the Heitler-London type of wave function (3), in contrast to cobalt and nickel. This view is supported, for example, by data on the saturation magnetic moment of iron-copper alloys. The moment is just 2.22 Bohr magnetons multiplied by the number of iron atoms, in accordance with the view that each magnetic electron is localized

around an iron atom and is therefore removed when the iron atom is replaced by a non-magnetic copper atom. The behaviour is quite different from that of cobalt-copper and nickel-copper alloys. Later in the conference, these ideas were developed more fully and more experimental evidence was brought forward by the following: W. M. Lomer and W. Marshall, "Electronic Structure of Ferromagnetic Alloys"; Miss Y. Cauchois, "X-ray Spectroscopy of Metals"; B. R. Coles, "Electrical Resistivity and Electronic Structure". There was also ample time on the programme for the lively discussion which recurred throughout the conference, and in which many other people contributed. J. R. Schrieffer outlined how wave functions, which are quite different again from either (1) or (3), are being used in "Recent Developments in the Theory of Superconductivity".

All the rest of the conference was devoted to non-ferromagnetic good metals like the alkalis, and copper, aluminium and lead, and their alloys. Even for a good metal, the Bloch type of wave function (1) cannot be regarded as satisfactory, in spite of its many successes. For a free-electron gas which can be worked out in detail, it gives a zero density of states at the Fermi-level, in contrast to all the experimental evidence, which demands a finite one. As R. S. Leigh pointed out in his paper on "Correlation in the Free Electron Gas", this difficulty can be traced to the long-range ($1/r$) nature of the Coulomb potential. The use of the Bloch wave function (1) implies that each electron moves in its orbital ψ_k independently of all the other electrons. This cannot be correct, for the Coulomb repulsion between two electrons is quite strong and must influence their motion so as to keep them from getting too close to one another. This is called 'correlation'. It is closely allied to the longitudinal plasma oscillations of the electron gas as a whole, for which the Coulomb repulsion is also responsible. By starting from these plasma oscillations, a more complicated theory of the free electron gas can be built up following the work of Bohm and Pines, which gives reasonable agreement with experiment for the alkali metals. Mr. Leigh discussed how these results could also be obtained from a somewhat different point of view.

If this left the conference momentarily stunned by the complication of the theory of even a free-electron gas, dependency was soon dispelled. In spite of the complications of correlation, the wave function for the free-electron gas can be written (to a good degree of approximation):

$$\Psi = (N!)^{-1/2} \chi \left| \text{determinant of } \psi_k \text{'s} \right| \quad (4)$$

This is very similar to (1), while the extra factor χ , called the plasma term, describes the correlation of the electrons. The determinant again describes N particles moving independently of one another through the metal. But these particles are no longer simple electrons. The Coulomb repulsion means that each electron is surrounded by a denuded region in which other electrons are unlikely to be. Because of the positive charge of the ions making up the lattice, this denuded region has on the average a positive charge. The particles now consist of the electrons together with the denuded region around each one. Each particle is therefore electrically neutral, and there is now no long-range Coulomb force between them. Only a weak short-range force remains. For this reason there is little correlation and the particles can be described as moving nearly independently.

The wave function (4) thus contains a single determinant of extended orbitals, ψ_k . This removes the deficiencies of the simple Bloch theory based on (1), and yet at the same time retains its successes. The concepts of the wave vector k , Brillouin zones and Fermi surfaces remain, and so does our interpretation of physical properties in terms of them. The theme was developed further by J. Hubbard in "Description of the Electron Gas in Terms of the Independent Particle Model". Using this model as a basis for the first time, V. Heine described a "Self-consistent Band Structure Calculation for Aluminium". In this calculation he was also able to overcome some of the mechanical difficulties that have always made calculations of band structure so unreliable, and to obtain reasonable agreement with what is known experimentally about the Fermi surface in this metal. W. M. Lomer presented a paper for Mrs. E. C. Ridley on the energies of the "6s-, 6p-, 7s-, 7p-, 6d-, 5f-Wave Functions of Metallic Uranium". From this the six valence electrons would appear to be predominantly in the 5f-band. Prof. R. Eisenschitz described how one could calculate the "Electronic Levels of Disordered Structures".

We may summarize by saying that for various experimental and theoretical reasons, some of which have been mentioned above, we believe that the concepts of Brillouin zones and Fermi surface have real validity and physical significance, in spite of the complications of electron correlation. Most of the conference was therefore devoted to methods of determining experimentally the shape of the Fermi surface in a given metal (as well as other aspects of the band structure), since this is the key to an understanding of most of the electrical and magnetic properties of the metal. The de Haas-van Alphen effect, discussed by Dr. D. Shoenberg in a paper of that title, would appear to be in principle the most powerful tool for obtaining the shape of the Fermi surface experimentally. The observations give the area of cross-section of the surface normal to the magnetic field, as a function of the field direction, and from this the shape of the surface can be calculated. If the Fermi surface consists of several pieces in different zones, then each piece can be so determined. A. Gold described how "The de Haas-van Alphen Effect in Lead" had enabled him to map out by this method the Fermi surface in lead, which consists of several pieces in the second, third and fourth zones. It is noteworthy how close the band structure is to what one obtains if the Fermi surface is taken as a sphere containing four electrons per atom (free-electron gas model) and the pieces of the sphere are fitted correctly into the zone scheme. This work made us feel that perhaps all other methods could be put in a subsidiary category; but Dr. Shoenberg reminded us that the de Haas-van Alphen effect has its 'blind spots', where it does not at present seem to be applicable. For example, the effect has not yet been detected in any alkali or noble metal. For these metals other methods must be used, and Dr. A. B. Pippard discussed "The Anomalous Skin Effect" with particular reference to determining the Fermi surface of copper. He concluded that the Fermi surface either just touches or just does not touch the zone face in the (111) direction. Circumstantial evidence would favour the former. Dr. R. G. Chambers presented a paper on "Cyclotron Resonance in Metals". The resonance could in principle determine the effective mass at all points on the Fermi surface, as in semiconductors, but some of the differences from

cyclotron resonance in semiconductors were pointed out. So far only bismuth has been studied systematically, but the resonance has also been detected in tin.

This more or less concludes the most powerful tools, in which some quantity is measured as a function of orientation for all directions in space so that much detailed information is obtained. In contrast, the following determinations give a specific piece of information, which may not be obtainable in any other way, but which is an average over the whole band structure or the whole Fermi surface. J. A. Catterall discussed "X-ray Emission from Alkali Metals" with particular reference to lithium. He concluded that the maximum in the emission spectrum definitely came below the Fermi level. Miss R. Coldwell-Horsfall presented a paper on the "Electrical Conductivity Tensor and the Fermi Surface". There was considerable discussion about the density of states at the Fermi-level and related experimental quantities such as the electronic specific heat and the

Knight shift. Papers on this were presented by Prof. H. Jones ("Experimental Data Related to Band Structure"); P. L. Smith ("Electronic Specific Heat of Simple Alloys"); L. E. Drain ("Nuclear Magnetic Resonance in Ag-Cd Alloys"). Prof. Jones pointed out that the electronic specific heat measurements require a density of states about 50 per cent higher than one would expect, and gave a theory of how this might be accounted for. The results presented by P. L. Smith and L. E. Drain showed how much more difficult it is to make sense of the results for alloys, and there was considerable discussion about this.

At the end of the first day of the conference, Prof. L. C. Jackson helped to take our minds off metals when he delivered the Duddell Lecture of the Physical Society on "Measurements of the Thickness of the Helium Film". The subject of this very interesting lecture was particularly appropriate to the conference since many of the experimental methods discussed involve low-temperature techniques. V. HEINE

OBITUARY

Prof. R. W. Whytlaw-Gray, O.B.E., F.R.S.

THE death of Robert Whytlaw-Gray on January 21 at the age of eighty removes one more link with the days when the Curies and Ramsay were rejuvenating inorganic chemistry. He was a student of Lord Kelvin and then a research worker in Ramsay's laboratories, where he developed a life-long interest in the physical properties of gases and great experimental skill in their manipulation. This led him to work on molecular and atomic weights, and in 1906 while in Bonn he re-determined the atomic weight of nitrogen by gravimetric analysis of liquefied and fractionated nitric oxide and by density determination. Whytlaw-Gray then returned to University College, London, and in collaboration with Ramsay, determined the atomic weight of niton. This was an outstanding achievement. The density was determined with a modified Steel-Grant micro-balance and about 0.1 mm.³ of niton.

In 1914 he became senior chemistry master at Eton, where his steadiness of purpose enabled him to carry out a considerable amount of research. In 1915 and for long afterwards he engaged in confidential work on toxic and other smokes, their physical properties and the methods by which their effects could be countered. In the fifth Liversidge Lecture, entitled "The Process of Coagulation in Smokes", delivered before the Chemical Society in 1935, he discussed his own and other work on this subject, and in 1936, with H. S. Patterson, published a book entitled "Smokes". His expert knowledge was again utilized by the Ministry of Supply in 1939 and he formed a group of about twelve workers at the University of Leeds to study problems connected with chemical warfare.

Whytlaw-Gray had been appointed to the chair of chemistry at Leeds in 1922 in succession to Arthur Smithells. His research activity there was intense and he developed a buoyancy micro-balance of high accuracy and employed it in the determination of the atomic weights of carbon, fluorine, nitrogen, sulphur and silicon by the use of gaseous compounds of these elements. He was elected to fellowship of

the Royal Society in 1928. After ten years in laboratories designed by T. E. Thorpe, he entered the new building which he, Dawson and Ingold had so successfully planned.

His regime was marked by tact, by careful consideration of the views of others (especially when he differed from them), by an informed appreciation of the needs of other scientific and technological departments and by a firm adherence to those principles which guided his personal and scientific life. On his retirement the Senate was "happy to learn that he is to continue his investigations in the Chemistry Department of which the spirit no less than the fabric owes so much to his unselfish devotion". One of his colleagues said of him: "It may be that some aspects of his character are derived from, or at least, related to the quiet detachment of the exact experimentalist—his unruffled calm to the poise and exactness of his own micro-balances".

When Whytlaw-Gray left Leeds in 1950 the University conferred upon him the degree of D.Sc. *honoris causa*. In recent years he worked at the Imperial Chemical Industries' Akers Laboratory, Welwyn, on the isothermals of xenon at low pressures and also on the normal density of the gas. The communication, with Dr. G. A. Bottomley, published in *Nature* as recently as December 7, 1957, is characteristic of his life-long struggle towards perfection in measurements of the properties of gases and vapours. Some earlier work on the deviation from ideality of vapours at low pressures was shown to be subject to significant error due to adsorption. This he reduced to a constant minimum in a re-designed differential compressibility apparatus, mainly by avoiding passage of mercury through greased stop-cocks. The PV/P graphs for benzene vapour, after correction for adsorption, then deviated from straight lines by less than two parts in 10⁵.

His colleagues and friends will be happy to think that he was able to continue in active work to the end of his long life. He rarely spoke about himself, but it was clear to those who knew him well that he served God 'with a quiet mind'.

FREDERICK CHALLENGER