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QUARTERLY PROGRESS REPORT NO. 4

THEORY OF CERTAIN ENERGY SURFACES AND BRILLOUIN ZONES

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INTRODUCTION

The general purpose of this project is the investigation of the relations between the shapes of energy surfaces and of Brillouin zones in solids. The reasons why this investigation is important and the proposed methods for carrying out the investigation are discussed in detail in the introduction to Quarterly Progress Report No. 1,* hereafter referred to as Q.P.R. No. 1.

BRILLOUIN ZONES

The first phase of this project is the derivation of the shape of the higher Brillouin zones for the more common crystal structures. The definition and theory of Brillouin zones are outlined in Q.P.R. No. 2, December, 1953.

During the fourth quarter, the model of the seventh zone of the body-centered cubic system has been completed. The seventh zone was done before the fifth or sixth because it is relatively simpler. Work has been started on the fifth zone of the body-centered cubic system. Work on photographing the completed models is in progress.

*Air Research and Development Command Contract AF(600)-750, Project No. R-355-40-10, September, 1953. This report was erroneously labeled No. V instead of No. 1.

NEARLY-FREE-ELECTRON APPROXIMATION

The second phase of this project is an investigation of the shape of certain critical energy contours. One proposed method for doing this is to extend the nearly-free-electron approximation, as explained in Q.P.R. No. 1. Work on this phase during the fourth quarter has been greatly aided by several conferences with Professor H. Jones of Imperial College, London, while he was visiting professor of physics at the Carnegie Institute of Technology.

It is well known that the wave function of an electron in a crystal has atomic-like character in the immediate vicinity of each nucleus and hence can not be accurately approximated by any linear combination of a small number of plane waves.* Furthermore, the complete solution of the secular determinant obtained by expanding the crystalline wave function in plane waves must give the low-lying energy levels of the core electrons as well as those of the valence electrons. It is not feasible to correlate the set of free-electron energy levels with the complete set of core- and valence-electron energy levels. Furthermore, the energy gap between the first and second valence bands, is not given accurately by the simple formula of twice the Fourier coefficient of the crystal potential. This formula generally gives much too large energy gaps. However, Professor Jones has discovered a method (as yet unpublished) for calculating the energy bands of the valence electrons which, with a certain approximation, leads to a secular equation for the energy which is identical in form with that obtained by the nearly-free-electron approximation. The symbols $V_{\vec{m}}$ now have a different physical interpretation and their absolute values are small compared with the corresponding free electron energies. The first valence band can be identified as the perturbed free-electron energies of the first Brillouin zone. Thus, Professor Jones' work provides a theoretical justification for using the nearly-free-electron approximation with the modification that the strong crystal potential is to be replaced by a small, much more uniform potential. All of this, of course, applies only to electrons in actual metals which act as if they are "nearly free."

APPLICATIONS TO METALS AND ALLOYS

One problem which is particularly suitable for analysis by the nearly-free-electron approximation is the detailed investigation of the large metal and alloy Brillouin zones, for example, the zones of bismuth and gamma

*See, for example, J. C. Slater, Rev. Mod. Phys., 6, 209 (1934)

brass. These zones were called "practical zones" in Q.P.R. No. 2. It is usually assumed that there is a large energy gap across the entire surface of such zones, although it is known that this is not true for a practical zone of the hexagonal close-packed structure.* Moreover, for substances which can be treated by the nearly-free-electron approximation, our preliminary investigation indicates that there are many cases for which there is a degeneracy of the energy along certain lines in the surface of the practical zone, but that usually this has a negligible effect on the density-of-states curve. The major objective of this phase of the project is to determine first when degeneracies occur on the surface of practical zones, and second what effect such degeneracies have on the density-of-states curve.

It appears that all the phenomena we wish to investigate in the actual three-dimensional zones occur also in two-dimensional zones, which are very much simpler to analyze. Consequently, several zones of the two-dimensional square structure are being investigated in detail to illustrate certain types of phenomena which occur in important three-dimensional zones. This work is not sufficiently completed to justify detailed reporting at the present time.

PLANS FOR FUTURE WORK

The construction of the zone models and the photographing of the completed models is being continued. The analysis of the large metal and alloy zones will require a geometrical study to determine what planes of the reciprocal lattice intersect the surface of the zone.

The study of the two-dimensional square lattice must be generalized to give the principles to be used in investigating the large metal and alloy zones. Then the more important of these zones will be analyzed to see if there are degeneracies which affect the density of states.

*Jones, H., Proc. Roy. Soc. A147 396 (1934).