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QUARTERLY PROGRESS REPORT NO. 3

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,[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 Quarterly Progress Report No. 2 (Q.P.R. No. 2), December, 1953.

During the third quarter sketches were made of the seventh and eighth zones of the face-centered cubic structure. The zones of the face-centered cubic structure are considerably more complicated than those of the body-centered cubic structure. An indication of this is obtained by comparing the following table for the f.c.c. structure with the corresponding one for the b.c.c. structure given in Q.P.R. No. 2.[2]

[1]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.

[2]The table in Q.P.R. No. 2 contains two errors. For the eighth zone there are 288 instead of 312 faces and 456 instead of 480 edges.

FACE-CENTERED CUBIC STRUCTURE

Zone	1	2	3	4	5	6	7	8
Number of Faces	14	72	96	204	104	576	624	912
Number of Edges	36	132	180	336	228	936	1152	1656
Number of Corners	24	62	86	134	126	362	530	746

The model of the fourth zone of the face-centered cubic structure has been completed. We now have models of the first four zones of each of the simple, face-centered, and body-centered structures. Three glass cases are being constructed to house these models, which is necessary partly for the protection of the models, but mainly so that the models can be displayed in their proper relative positions. Details, drawings, and pictures of the zones will be given in a later report when the mounting of the models is nearer completion.

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. A summary of known results and a report of our early work on the nearly-free-electron approximation are given in Q.P.R. No. 1. Our work along this line has been aided by the appearance of a paper in Germany by Dr. J. Homilius[1] which came to our attention in December, 1953. Dr. Homilius has obtained some new theoretical results for the first zones of the s.c., f.c.c., and b.c.c. structures. An evaluation of this and other work of ours based on an application of sodium is under way.

An important difficulty which is being encountered at present is that according to all methods of calculation that seem to come close to reality certain metals, such as Na, behave in a way which suggests that the conduction electrons are nearly free in their motion through the material.

[1] Z. Naturforschg, 8a, 432 (1953).

Even the effective mass is in that case very close to the actual electron mass. Yet, if the nearly-free-electron approximation is directly applied, the Fourier coefficients and energy gaps, obtained are an order of magnitude or more too large. It is clear that this difficulty should be resolved before further energy gaps are calculated.

PLANS FOR FUTURE WORK

The construction of zone models is being continued. It is evident from the greater complexity of the higher zones that the construction of their models will be much more difficult, and other methods may have to be devised. It is hoped that we will soon be able to decide whether useful information can be obtained from the nearly-free-electron approximation if it is used with reasonable care.