Lectures on the application of multiple scattering theory in calculations of the electronic structure of solids

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I. Moertig, E. Mrosan, and P. Ziesche. Multiple Scattering Theory of Point Defects of Metals: Electronic Properties; Teubner, Leipzig (1987) pp. 220 (Teubner Texte zur Physik. Bd. 11).

The book under review is the eleventh volume of the series "Teubner Lectures in Physics" published in the GDR. It has been written by members of the "Dresden group on electron theory" at the Technical University of Dresden who have for a long time and actively carried out calculations of the electron structure and electron properties of solids. This has left its imprint on the book: one feels the practical approach, the authors do not neglect presentation of technical details, methodologies, etc.

It must be said that calculations of the electron structure of disordered bodies and crystals with impurities have been developing very actively recently. The time is now ripe to have a book that presents in a consistent manner the theoretical bases of such calculations. Until very recently there has been only one publication devoted to these problems the well known book of Ehrenreich and Schwarz (1976) translated into Russian in 1979. However in this book the presentation is primarily from the point of view of strong

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coupling theory, and not from the point of view of the now more popular and, probably, more promising multiple scattering theory.

The general structure of the book is as follows. The first two chapters are introductory. In them general concepts of band theory are presented: the density-functional method, the muffin-tin approximation for the potential, supercells, etc. However, it should be noted that in their design these lectures are intended for specialists who are well acquainted with the above topics. Apparently the most valuable for the reader are the following two chapters—the third and the fourth, devoted to the theory of scattering by an isolated potential and by a system of scattering potentials. In spite of their brevity the authors have presented in these chapters quite consistently the most important equations of the theory of multiple scattering.

The fifth, sixth, and seventh chapters form a kind of a separate unit little related to the preceeding part. In them the authors described the methods of calculating concrete physical quantities or effects, specifically the de Haas-van Alfen effect, the residual resistance and the thermo-emf, the magnetoresistance and the Hall constant. Unquestionably, the choice of these particular topics is determined only by the field of scientific interests of the authors—Moertig and Mrosan, and not by their particular importance from the point of view of applying the theory of multiple scattering. However, the presentation of the methods of solving the Boltzmann equation in crystals, in particular the method of Fermi suface harmonics, is of wider interest.

It appears to be somewhat strange to segregate certain technical topics into a separate chapter—the eighth one, which contain only 8 pages. In fact it consists of a description of a model potential of a point defect which would have been more appropriate in the introductory part, and of a presentation of the tetrahedral method of intregration over the Brillouin zone which, it is true, was first developed by the Dresden group, but today is so widespread that it is well known to every physicist engaged in calculations of electron structure. The remaining technical problems (some of them, however, also seem to be superfluous in such a course of lectures) have been relegated to an appendix.

Finally, in the last chapter concrete quantitative results obtained by the Dresden group are presented.

The book is provided with quite a detailed bibliography—more than 300 titles.

On the whole the impression of the book by Moertig, Mrosan, and Ziesche is approximately the following: the book is not devoid of faults, first of all there is an inconsistency in the choice of material. At the same time one can find in it quite good presentation of a number of topics which are not present in monographs available to the Soviet (and, probably, also the foreign) reader. It will be useful to those who are involved in the theory of multiple scattering as applied to disordered solids and impurities and in calculations of the transport properties of solids.