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The electrical resistivity of metals and alloys

Cambridge Solid State Science Series

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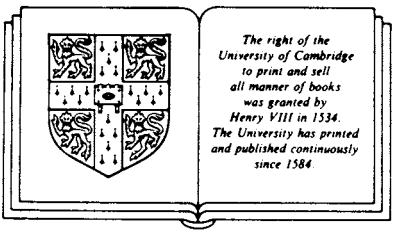

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To my Mother and Father

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Preface

The electrical resistance or resistivity of a conducting solid can be experimentally determined without much difficulty and for many years it has been used as a research tool to investigate various microstructural and physical phenomena. However, unlike conventional diffraction methods which are capable of mapping out scattered intensities in two- or three-dimensional space, an electrical resistivity measurement gives only a single value (at any fixed temperature and structural state) representing an average over all directions of conduction electron scattering. As there is no means of performing the back-transform from this single point, the analysis of resistivity data in terms of microstructure must incorporate calculations of conduction electron scattering based on some model of the structure or microstructure concerned. With the refinement and greater availability of more direct methods, particularly X-ray, neutron or electron diffraction, transmission and analytical electron microscopy (especially atom-probe field ion microscopy which allows an atom-by-atom picture of a material to be established) there has been a declining utilisation of such an indirect method in microstructural investigations. Nevertheless, while a resistivity study may require support from some other technique to allow an unambiguous interpretation of the results, there are many cases where such studies still have particular value, either by virtue of their simplicity or lack of alternative techniques. These include studies of defects, pre-precipitation processes, short and long range ordering or phase separation (particularly with respect to transformation kinetics) and determination of critical transformation compositions and/or temperatures. These studies make use of the sensitivity of the conduction electron scattering process to microstructural details right down to the atomic scale, and the fact that it provides a convenient average over the volume of a specimen.

The electrical properties of metals and alloys are also of great practical importance, especially in applications involving heating, temperature measurement, signal and power transmission, precision resistances, switching devices, semiconducting and thin film devices or simply specification of purity. Development of new methods and materials for such applications will be assisted by a knowledge of the physical processes which determine those properties. On a more fundamental

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level there is the basic need to understand the process of scattering of conduction electrons in solids, particularly in inhomogeneous (i.e. real) solids. In this regard, determination of the resistivity also provides a useful test of some of the elegant electronic band structure determinations that have been carried out over the last few years.

There have been many good texts devoted to the basic aspects of electrons in solids and reviews of specific topics such as electrical properties of pure metals, galvanomagnetic properties of pure metals and deviation from Matthiessen's rule. However, to the author's knowledge there has been no other text devoted to the problem of understanding the electrical properties of concentrated and often inhomogeneous solids. It is hoped that this text will help fill the gap.

This book is thus unashamedly devoted to understanding the electrical properties of real metals and alloys. Because of the complexity of the structures concerned, this often means that some aspects of the work lack the elegance of the more profound theoretical works on ideal materials. Nevertheless, it is hoped that the text will be of use to those interested in such properties and indicate where more research effort is required. Rather than devote space to a formal derivation of basic equations concerning electron states in solids (which is available in many other texts), we will assume that these are known and concentrate more on the aspects of electrical conduction, particularly its dependence upon composition and atomic or magnetic structure.

The general problem is introduced in Chapter 1 in terms of simple diffraction concepts, modified slightly to take band structure effects into account. This has the advantage that those readers who have expertise in the allied fields of X-ray, neutron or electron diffraction but who are less confident in matters concerning electron states will nevertheless be readily able to gain a feeling for the problem. However, it would be wrong to pretend that the electrical properties of alloys which may have complicated electronic, atomic and magnetic structures could be understood quantitively on the basis of a simple theory. In such cases a full understanding of the problem requires facility with complicated and often highly specialised techniques. While it is beyond the scope of this book to give a full tutorial in such techniques, the general models and formalisms will be introduced and related to the problems at hand. Thus, while a reader may not be familiar with ensemble averages or Green's functions, it is hoped that he or she will be able to gain an understanding of the direction taken by modern theoretical approaches, of the problems that have been addressed and to what extent a satisfactory solution has been found. It may then be possible to judge whether efforts should be made to become more familiar with the particular techniques

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concerned. However, it is necessary to have a good grounding in quantum mechanics in order to achieve mastery of many of the advanced techniques and readers are so warned. The first chapter also introduces the problems associated with anisotropy of scattering over the Fermi surface and finite conduction electron mean free path, and a working definition of 'short' and 'long' range effects is given. The similarity between replacive disorder (i.e. that to do with atom type) and displacive disorder (i.e. that to do with atomic position) is also briefly discussed and Matthiessen's rule is introduced. The foundation of the Boltzmann equation is also considered as are some of the methods of solution and alternative approaches.

The second chapter is entirely concerned with a discussion of microstructure and definition of parameters which are required for the description of atomic positions and correlations in crystalline or amorphous solids. These concepts are extended to magnetic structures in Chapter 3 and some of the dynamic aspects of isolated spins and spin systems are also discussed. Nearly free electron theory and the pseudopotential approximations are discussed in Chapter 4.

The concepts developed in Chapters 1, 2 and 4 are brought to bear on the determination of the electrical resistivity in Chapter 5, allowing formulation of equations relating this to a variety of structures containing short and long range atomic correlations. The effects of static and dynamic atomic displacements are also considered. Some of the methods appropriate to non-simple metals and alloys are introduced in Chapter 6. The resistivity of the magnetic and nearly magnetic structures discussed in Chapter 3 is considered in Chapter 7. However, the situation here is much less satisfactory as it appears that the assumption of independent electrons made explicit in the earlier chapters is not adequate to determine the magnetic spin–spin correlations. There is still much work to be done in deriving a realistic first principles calculation of the resistivity of such materials. The particular problems associated with the critical point, high resistivity materials and amorphous metals are considered in the final chapter.

In order to allow for an uninterrupted development of the theory, particularly in Chapters 5 and 6, examples and applications of the concepts and equations derived are generally given in separate sections following those devoted to the presentation and development of that theory. Thus, if a reader is interested in a specific problem, he or she should be able to follow almost from first principles and without too much interruption the development of the theory relating to that problem, but will need to turn to the appropriate later section to find the examples and applications.

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The symbols used throughout this book are generally the same as widely employed in the literature. However, as the range of topics covered is quite broad, this often means that the same symbol is used in a different context in relation to different problems. For example, the symbol α is initially used as an atomic correlation parameter but is also used to indicate the ratio of sub-band resistivities in a two-band model of conduction as well as a critical exponent. This problem could be avoided by the invention of a new set of symbols but only at the risk of greater confusion. Where practical a distinction is made with the aid of sub- and superscripts and in all cases the parameters are redefined when they take on a new meaning. Similarly, this work draws on the results of many different fields and, despite efforts to promote the acceptance of SI units, many of these fields have evolved their own 'preferred' units such as Rydbergs or electron-volts for energies associated with electron states and still the micro-ohm cm as the unit of resistivity. Thus, while the formulas derived in this text are correct within the SI system of units, again in order to avoid confusion at the interface between this work and the majority of other published results, the input data and results will generally be given in terms of these preferred units. The conversion factors necessary to obtain SI units are given in Appendix A.

Finally, it is with much pleasure that I acknowledge the valuable discussions that I have had with many colleagues throughout the world and which have been invaluable in moulding the contents of this book. Rather than offend anybody by my forgetfulness which could lead to unintentional omissions from a list of names, I would simply like to thank them all for their interest and helpfulness. With regard to the actual production of this text the situation is much more straightforward as most of the work has fallen on comparatively few shoulders. In this regard I would especially like to thank my wife Kathy for word-processing my scratchy handwriting and for putting up with a rather obsessed author for the past twelve months, Mrs L. Lyons for producing the bulk of the artwork and Ms J. Fraser for photographic assistance. Much of the work was completed while I was on study leave from the Department of Materials Engineering and I would like to thank that Department and Monash University for the opportunity of taking the leave and the members of the Physics Department at Monash for their hospitality during this period.

P. L. Rossiter
1986

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