2

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Surface Crystallography by LEED

Theory, Computation and Structural Results

With 19 Figures

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Preface

Surface science has experienced an impressive growth in the last two decades. The attention has focussed mainly on single-crystal surfaces with, on the atomic scale, relatively simple and well-defined structures (for example, clean surfaces and such surfaces with limited amounts of additional foreign atoms and molecules). One of the most fundamental types of information needed about solid surfaces concerns the relative atomic positions. The geometrical arrangement of surface atoms influences most physical and chemical properties of surfaces, the list of which is long and includes a number of important technological applications: electronic surface states, contact potentials, work functions, oxidation, heterogeneous catalysis, friction, adhesion, crystal growth etc.

Surface crystallography - the determination of relative atomic positions at surfaces - has found a successful tool in Low-Energy Electron Diffraction (LEED): this technique has now determined the atomic positions for nearly a hundred surfaces, whether in the clean state or with additional foreign atoms or molecules. The main aim of this book is to publish a set of computer programs that has been specifically designed for and extensively used in surface crystallography by LEED. These programs are based on the dynamical (i.e. multiple-scattering) theory of LEED. They include a number of features reducing the computing time and computer-core requirements. They can be used as they stand for a selected set of surfaces, or they can be slightly modified to handle an unlimited number of other types of surfaces. The computer programs have been conceived in a building-block form to allow the selection in any given situation of the most efficient combination of several theoretical methods. To that end extensive information is supplied about the underlying theory, about the structure of the programs and about the choice of suitable input parameters. The intention is to enable the user, who might be an experimentalist or a graduate student, to perform independently a surface structural analysis by LEED.

Since the LEED theory describes the phenomenon of propagation of slow electrons (energy in the range 0-400 eV) through ordered arrays of atoms, this

description is valid for a variety of other modern surface analysis techniques that also involve the propagation of slow electrons through crystalline lattices: thus the methods and computer programs described in this book would find ready applications to, for example, ultraviolet photoemission spectroscopy, Auger electron spectroscopy and high-resolution inelastic electron energy loss spectroscopy.

To give the reader a better feeling for the LEED process, which is not as complicated as might appear at first sight, we supplement the basic theory with a more phenomenological description of the diffraction of electrons at surfaces. Both to illustrate the capabilities of surface crystallography by LEED and to provide a comprehensive and organized review of its results, a chapter is devoted to describing and referencing all surface structures obtained in this way (and known to the authors).

In writing this book we are mainly indebted to John Pendry, who introduced one of us (MAVH) to the field of LEED and whose influence is felt in particular in this book. We also wish to thank a number of colleagues for their critical and constructive comments arising from the actual use of our programs: we should mention in particular B.J. Mrstik, N.L. Stoner, P.R. Watson, A. Ignatiev, B.W. Lee and S.L. Cunningham. We gratefully acknowledge essential help on the part of Sandie Tong (for the figures) and Joyce Miezin (for the typing). Special thanks to S.-W. Wang are also appropriate. One of us (MAVH) is moreover indebted for hospitality and the availability of computational facilities during the preparation of this book to the groups of Prof. W.H. Weinberg at the California Institute of Technology and of Prof. G. Ertl and Prof. H. Jagodzinski at the University of Munich (Sonderforschungsbereich 128). S.Y. Tong acknowledges the hospitality of the Department of Chemistry and the Lawrence Berkeley Laboratory, University of California, Berkeley, where the manuscript received its finishing touches. And last but not least, our thanks go to Prof. R. Gomer and Dr. H. Lotsch (Springer-Verlag) for making the publication of this book a reality.

M.A. Van Hove

Munich and Berkeley, November 1978 S.Y. Tong

Contents