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M. A. Van Hove (Eds.)

The Structure of Surfaces II

Proceedings of the 2nd International Conference on the Structure of Surfaces (ICSOS II), Amsterdam, The Netherlands, June 22–25, 1987

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Preface

This book collects together selected papers presented at the Second International Conference on the Structure of Surfaces (ICSOS-II). The conference was held at the Royal Tropical Institute in Amsterdam, The Netherlands, June 22–25, 1987. It was held in part to celebrate the 25th anniversary of the NEVAC (Netherlands Vacuum Society). The International Organizing Committee members were:

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The ICSOS meetings serve to assess the status of surface structure determination and the relationship between surface or interface structures and physical or chemical properties of interest. The papers in this book cover: theoretical and experimental structural techniques; structural aspects of metal and semiconductor surfaces, including relaxations and reconstructions, as well as adsorbates and epitaxial layers; phase transitions in two dimensions, roughening and surface melting; defects, disorder and surface morphology.

Amsterdam, Berkeley
October 1987

J.F. van der Veen
M.A. Van Hove

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Particular thanks go to all the individuals who contributed much to the well-being of both the conference and the proceedings, especially Louise Roos, Jan Verhoeven, Dorine Heynert and the members of the Local Organizing Committee: F.H.P.M. Habraken, A.G.J. van Oostrom, G.A. Sawatzky, and W.F. van der Weg. An important element was of course the contribution from the International Advisory Committee members: D. Aberdam, J.C. Bertolini, M. Cardona, G. Comsa, L.C. Feldman, F. Garcia Moliner, D.R. Hamann, D. Haneman, A.A. Lucas, T.E. Madey, K. Müller, S. Nakamura, A.G. Naumovetz, P.R. Norton, G. Rovida, W.E. Spicer, A.G.J. van Oostrom, and R.F. Willis.

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Introduction

In the past years, our knowledge of the structure of solid surfaces has advanced considerably. It now proves possible to make atoms on a surface directly visible and to have their positions theoretically explained in terms of their electronic bonding configuration. These breakthroughs have been realized on the experimental side through the introduction of a variety of novel surface analytical tools and on the theoretical side through the use of new computational techniques. As a result, the data base of solved structures has expanded to the point that common trends among different crystal faces and overlayer systems can be identified. These proceedings cover the latest developments in the field, grouped according to the following scheme.

Part I treats various theoretical and experimental aspects of new analytical techniques. In particular, it focuses on the microscopy of surfaces, based either on electron diffraction or on scanning tunneling microscopy.

Relaxation and reconstruction phenomena in metal surfaces are the subject of Part II. The analyses have been refined to a level where even sub-surface atom displacements can be determined with reasonable accuracy. Not only the static displacements but also the vibrational properties can be measured and calculated.

An important topic in surface crystallography is the characterization of adsorbate overlayers on metals. This subject is extensively covered in Part III. The results are relevant for understanding heterogeneous catalysis and corrosion phenomena. Noteworthy is the progress that is being made with the detection and location of hydrogen atoms at surfaces.

Parts IV and V present recent results that have been obtained on clean and adsorbate-covered semiconductor surfaces. In particular, the atomic geometries of various metal overlayers on silicon are investigated as well as the structural rearrangements induced by the adsorbate.

Part VI provides new information on the structural aspects of epitaxial growth of thin films. A number of articles deal with the influence of lattice strain on various physical properties of the film; other papers focus on the growth process itself.

Phase transitions form the subject of Part VII. For two-dimensional overlayer systems both theory and experimental methods are well developed. Intriguing are the atomic-scale observations of surface melting. In this chapter,

various phenomenological descriptions of surface melting are discussed and a first microscopic theory is presented.

Part VIII discusses various types of surface defects and disorder, which are induced either by the preparation technique or by the surface probe. Attention is also given to near-macroscopic changes in surface morphology that may occur upon heating or exposure to a reactive gas. Results in these areas are significant for understanding the behaviour of surfaces under practical circumstances.

Part I

Techniques

Resolution in Scanning Tunneling Microscopy

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In any microscopy, it is extremely useful to know the resolution (or more precisely the resolution function) of the instrument. Here the present understanding of the resolution of Scanning Tunneling Microscopy (STM) is reviewed.

The principles of STM have been described in detail by the inventors [1], and are not repeated here. Understanding, or even defining, the resolution of STM raises tricky issues for two reasons. First, STM is inherently nonlinear, so the usual definition of resolution in terms of convolution with an instrumental function cannot be applied directly. Second, STM is actually a spectroscopy, in that it is sensitive to the electronic structure of the sample. It is therefore hard to say what is the "ideal" image which one would expect for an arbitrarily sharp resolution.

The resolution of STM has been previously addressed by Tersoff and Hamann [2] and by Stoll [3] in the case of simple metals. More recently, it was pointed out [4] that the resolution may be quite different for semiconducting or semimetallic surfaces. In fact, the resolution of STM is inherently sample-dependent in principle, and often in practice.

Here, a specific convention is described for defining the "ideal" STM image. Then, using this convention, a formal expression is derived for the resolution function. This expression is evaluated for metals, giving a very reasonable instrumental resolution function which is relatively independent of the sample. Then the case of a semiconductor or semimetal surface is briefly discussed. In that case, the resolution function becomes very sample-dependent, with a rather peculiar lineshape.

In general, one defines resolution by assuming that there exists some ideal image $I_0(x)$, which would be seen in the case of perfect instrumental resolution.