14. X–7 MODERN EXPERIMENTAL METHODS IN LEED*. By A. Ignatiev, Department of Physics and Chemistry, University of Houston-University Park, Houston, Texas U.S.A.

Surface crystallography by low-energy electron-diffraction (LEED) has progressed significantly in the past two decades, encompassing the determination of surface unit cells, exact surface atom positions, and recently the analysis of surface defects and two-dimensional phase transitions. This progress has been accompanied by a recent surge in new instrumentation which is more sensitive, has high data aquistion rates, has high angular resolution, and is less surface destructive. The improvements of the instrumentation lie in new small beam size and low beam divergence electron guns, position sensitive detectors and computer assisted vidicon data aquisition systems. This modern instrumentation will be discussed in light of the major types of surface crystallographic data that can be extracted from LEED measurements.

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14. X–8 A STEP TOWARDS AUTOMATIZED SURFACE STRUCTURE DETERMINATION. By K. Heinz, Lehrstuhl für Festkörperphysik, University of Erlangen-Nürnberg, Erwin-Rommel-Str. 1, D-8520 Erlangen, FRG

Surface structure determination by Low Energy Diffraction (LEED) usually suffers from the tedious experimental task to measure diffraction intensities and on the other hand from the complexity of the computational programs which are necessary to extract the structural data according to a full dynamical scattering theory.

It is shown that the experimental problem has been solved by various modern methods. Especially the use of a TV camera, which views the diffraction pattern and passes the video signal on a processing computer for automatic data evaluation, leaves the measurement to nearly routine work. Not only integral intensities but also intensity profiles can be recorded from which half widths and background levels become available. The speed and accuracy of the method makes an extended field of surface physics accessible to LEED, e.g. time dependent processes.

Computer controlled measurements stimulate the idea to implement the dynamical calculation on the same computer, too. The problems to be overcome are twice, namely that full dynamical programs are too extensive for the limited memory of a laboratory computer and too complex to be routinely managed by an experimentalist. Both problems are solved by using approximative schemes, especially the quasidynamical method. Within this approach the diffraction of an atomic layer is calculated kinematically but multiple diffraction between layers is allowed. Comparison to the full dynamical treatment and theoretical considerations shows that peak positions in the I(E)-spectra are well reproduced, peak heights, however, are less reliable. This holds especially for energies above about 100-200 eV. Using the Pendry-r-factor for theory-experiment comparison, which is sensitive mainly to peak positions, nearly the same structural parameters result as with the full dynamical treatment. This holds at least for some simple and clean surfaces tested so far. Thus the method is believed to yield a rough structure determination.

The computer memory necessary for the quasidynamical calculation allows its implementation on the same computer which is processing the LEED measurement. Results obtained are nearly identical with those using a large scale computer. Moreover, also the r-factor comparison as the third step of structure determination after intensity measurement and calculation is performed on the laboratory computer. Though only rough structural data can be expected in view of the approximations used in the calculation, this is expected to be a step towards automatized structure determination.

14. X–9 THE CALCULATION OF LEED INTENSITIES. By P.M. Marcus, IBM Research Center, Yorktown Heights, N.Y. 10598, U.S.A. and F. Jona, Stony Brook University, Stony Brook, N.Y. 11794, U.S.A.

Structure determination by LEED intensity analysis has two essential parts: 1) calculation of intensities of LEED beams for a given structural model with given conditions of incidence 2) determination of best-fit parameters of the model by systematic variation of the parameters to improve the fit of calculated to observed intensities. The first part is a mathematical and computational problem made difficult by the strong scattering of the incident electron among the atoms of the crystal; the second part is a statistical problem concerned with data handling and criteria of fit, which uses the results of intensity calculations. Unlike bulk X-ray diffraction structure analysis, the first problem dominates LEED structural analysis. Most current methods of handling the intensity calculation are variations of procedures which calculate a scattering matrix for the discrete set of plane waves (beams) incident on and scattered by a slab of crystal periodic in two dimensions, i.e., having translational symmetry only parallel to the slab surface. For any set of incident beams spherical wave properties lead to a set of linear equations which relate the amplitudes of spherical waves around each (translationally) nonequivalent atom in the slab to the incident amplitudes. A matrix inversion is then required to determine the scattering matrix, which contains the desired reflection coefficients. The order of the matrix inversion is given by the product of the number of spherical waves in the expansion and the number of nonequivalent atoms in the slab. However, if the crystal is made up of sufficiently

separated slabs, between which a beam expansion of the electron wavefunction is adequate, then a separate smaller matrix inversion can be carried out for each slab. The reflection coefficients are then found by combining the scattering matrices into a single set of linear equations for the beam amplitudes produced by the incident beam. Such methods have given good quantitative structural results for about 100 clean and adsorbate-covered ordered surfaces, but all the structures are rather simple. The computational problem grows with the cube of the number of nonequivalent atoms in a slab, as is characteristic of matrix inversion or eigenvalue problems. Accordingly the size of the computation quickly becomes prohibitive for structures with more than about 10 nonequivalent atoms in a slab. To overcome this limitation on complexity of structure, a reformulation of the multiple scattering problem has been developed which depends on the strong attenuation (of the coherent part of the electron wavefunction) that accompanies the strong scattering. Starting from scattering of the incident beam at an atom, a complete but finite set of scattering paths can be found which are less than a critical length l_c; these paths involve a small cluster of atoms around the initial atom. The complete scattered wave from the cluster can be found by direct summation over the paths; rapid convergence of the scattered wave as l_c increases can be shown. In typical cases the cluster involves about 100 atoms, l_c is 10 or 12Å and at most an electron is scattered 4 times. The calculation is then repeated for each nonequivalent atom. This multistage-scattering finite-cluster method avoids matrix inversion and the calculation of scattering matrices for infinite slabs. The size of the calculation grows only linearly with the number of nonequivalent atoms, thereby making practicable the analysis of much more complex structures than are now studied.

14. X–10 ACCURACY AND RELIABILITY OF SURFACE STRUCTURE DETERMINED BY LEED. H. L. Davis and J. R. Noonan, Solid State Division, Oak Ridge National Laboratory,* Oak Ridge, Tennessee 37830, USA.

In a LEED analysis surface structural information is obtained using a trial and error process in which several experimental I-V profiles (diffracted current vs. energy) are compared with various sets of calculated I-V profiles. Each set of calculated profiles is obtained by first proposing a specific atomic structure for the surface under investigation, that set is then compared with the experimental profiles, another structure is assumed and its corresponding calculated profiles compared with the experimental ones, etc. So the surface structure determined in an analysis is that one model structure for which the calculated profiles have the "best" agreement with the experimental profiles. Thus, as will be discussed and illustrated with specific examples, the accuracy and reliability of a surface structure determined by LEED is related to the quality of agreement achieved between the calculated and experimental I-V profiles, to experimental and theoretical (calculational) factors which improve or degrade the quality of the agreement, to the specific techniques (e.g., R-factors) used to compare the several different experimental profiles with the corresponding calculated ones in order to determine the "best" agreement, to the sensitivity of the comparison with variations of the assumed structure, etc. Then, results from several recent analyses will be used to demonstrate that LEED structural analyses of clean metallic surfaces can be performed with a precision of better than 0.02 Å in the atomic spacings of the near-surface region, with the precision degrading for the deeper atomic layers. Also, some of the procedures which have enabled this improved LEED precision to be obtained will be highlighted.

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14. X–11 QUANTITATIVE ANALYSIS OF LEED DATA. By David L.Adams, Institute of Physics, University of Aarhus, DK-8000 Aarhus C, Denmark.

The determination of surface structure using low-energy electron diffraction (LEED) is carried out by means of comparison of experimental LEED intensities with intensities calculated for trial model structures. This process of structural *refinement* is constrained by the length of the model calculations, which require the use of multiple-scattering theory. The importance of multiple-scattering contributions to the diffracted intensities appears to preclude the prior use of *direct* methods for obtaining a first approximation to the surface structure.

The present work is concerned with attempts to develop systematic procedures for structural refinement, based on the use of a simple r-factor, similar to that used in x-ray crystallography. Surface structure determination is carried out by minimization of the r-factor as a function of both the structural and nonstructural variables of the calculations. Since an unconstrained minimization is ruled out by the length of the calculations, emphasis is placed on procedures which exploit the relative sensitivity of the r-factor to variations of the different variables, the extent of correlations between the variables, and the systematic re-use of partial results of the intensity calculations. A simple, iterative minimization procedure is described, and illustrated by its application to the determination of multilayer relaxations of some metal surfaces.

14. X–12 PRESENT STATUS AND FUTURE TRENDS IN CONVERGENT BEAM ELECTRON DIFFRACTION. By J.W. Steeds, H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol, U.K.

Convergent beam electron diffraction has become established as a singularly powerful technique. It is widely used for accurate thickness determination of thin specimens, for investigation of local lattice parameter variations, for space group determinations and for aspects of microanalysis which derive from these powers. It has recently proved itself unrivalled in discovering the existence of broken symmetry when low temperature phase transitions occur and in identifying borides, carbides, nitrides or oxides in complex alloys. Although no rigorous method of structure determination by electron diffraction has yet been worked out, except when weak scattering can be assumed, ab initio determinations of reasonably complex structures have now been performed by methods which seem to be capable of quite widespread application. Now that it is possible to perform high quality experiments with electron microscopes operating at 300 keV or above, exciting prospects exist for extending the technique to more complex problems, and for more radical developments which seem rich with promise.

References

Vincent R, Bird, D.M. and Steeds, J.W. 1984 in "Electron Microscopy and Analysis 1983" Institute of Physics Conference Publication No. 68 p.37.

Vincent R., Bird, D.M. and Steeds, J.W. Structure of AuGeAs by Convergent Beam Electron Diffraction
I. Derivation of Basic Structure
II. Refinement of Structural Parameters
submitted to Acta Cryst.