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