Spin Polarization in Double Diffraction of Low-Energy Electrons from W(001): Experiment and Theory

J. Kirschner
Institut für Grenzflächenforschung und Vakuumphysik, Kernforschungsanlage Jülich GmbH, 5170 Jülich, West Germany

and

R. Feder
Institut für Festkörperforschung, Kernforschungsanlage Jülich GmbH, 5170 Jülich, West Germany

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We report on the first successful double-scattering low-energy electron diffraction experiment, which clearly reveals spin-polarization effects. Polarization and intensity of the specular beam from W(001) have been measured as functions of the azimuthal angle of incidence ("rotation diagrams"). The agreement of the data with their theoretical counterparts is quite satisfactory. High polarization sensitivity and detector efficiency in the present experiment demonstrate the feasibility of a new type of spin-polarization detector.

Experiments on double diffraction of low-energy electrons from two crystal surfaces, aimed at observing spin-polarization effects, have a long history of failure. Davisson and Germer, shortly after their discovery of electron diffraction, carried out a double-scattering experiment with two Ni(111) surfaces.[1] They found no polarization to within their experimental accuracy of 0.5%. A reanalysis of their data, correcting an analysis error made originally, resulted in polarization values up to 27%, but with a large er error margin.[2] Theoretical low-energy electron diffraction (LEED) calculations[3] for the geometry of the experiment[1] did not, however, confirm these large-spin-polarization findings, but suggested that the intensity asymmetries could have been generated by alignment errors (as small as 0.5°). Other workers in the 1930's also reported negative results for their spin-polarization experiments (even for high-Z materials) and the double-scattering LEED approach was not pursued any further.[4]

In this paper we report on the first double-scattering LEED experiment in which spin polarization is successfully observed. We compare experimental rotation diagrams of intensity and spin polarization to theoretical results obtained by relativistic calculations. The efficiency of the present experiment with respect to the detection of electron spin polarization is considered very promising, both in sensitivity and intensity.

The experimental setup is shown schematically in Fig. 1.[5] Unpolarized electrons from an electron gun impinge on the (001) surface of the first W crystal, called polarizer in the following. The angle of incidence with respect to the surface normal is $\theta = 47.5° \pm 1°$. The specularly reflected (0, 0) beam passed through a hole in the LEED screen. The intensity of the quasielastically scattered electrons is measured by a movable Faraday cup. When the collector is retracted, the electron beam enters an acceleration-deceleration stage, where the kinetic energy of the electrons is adjusted to the desired scattering energy E_0 at the second crystal. After energy analysis in a cylindrical mirror analyzer (second-order focusing; deflection angle 90°), the beam is focused onto the second W crystal, called analyzer. The angle of incidence is $0° \pm 0.5°$, the kinetic energy is set to 105 eV. The (2, 0) beam and the ($\bar{2}$, 0) beam diffracted from the analyzer crystal are detected by two Channeltrons, operating in the pulse-counting mode. Thus the polarization detector does not require any mechanical manipulation of the analyzer crystal (as was the case in

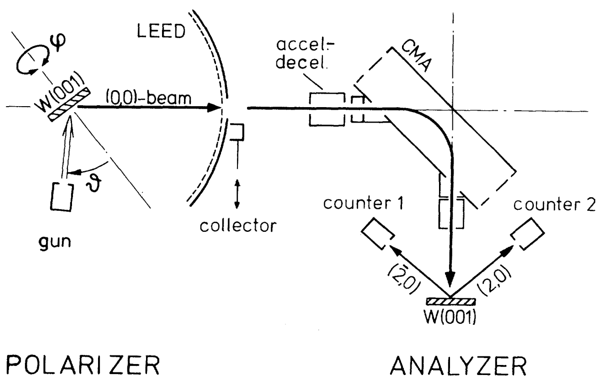

FIG. 1. Schematic of the experimental setup of the double-scattering LEED experiment.

Ref. 1) and the detection efficiency is increased. The alignment of the angle of incidence at the analyzer crystal is made by means of a laser beam and an optical beam splitter. The choice of the scattering conditions for the analyzer crystal is based on theoretical calculations which predict sizable polarization together with high scattered intensity for the parameters specified above.[6] The polarizer and analyzer are placed in two separately pumped vacuum systems (base pressure $<5\times10^{-9}$ Pa) which are connected by a gate value between the LEED screen and the cylindrical mirror analyzer. The cleanliness of the polarizer crystal is controlled by means of Auger-electron spectroscopy with the LEED system. In addition, the well-known sensitivity of H_2 adsorption on W(001) to traces of coadsorbed impurities[7] is used to check the cleanliness of the crystal. The analyzer crystal is identical in size and shape to the polarizer crystal and was cut from the same ingot. It is treated according to the same procedures as established during cleaning the polarizer crystal. The temperature of the crystals was between 40°C and 80°C during the measurements, i.e., the unreconstructed surface phase of W(001) only was present. Measurements are made with fixed primary energy and fixed angle of incidence by rotating the polarizer crystal azimuthally about its surface normal (rotation diagrams). This mode has been chosen in view of the recent successful application of intensity rotation diagrams to surface structure analysis.[8] In addition, rotation diagrams allow a good experimental accuracy which is even more important in spin-polarization studies than in conventional LEED studies. Finally, in this mode multiple-scattering effects are separated from kinematical (single-scattering) effects, which may provide additional insight into the role of multiple scattering in spin-polarized LEED. The polarization data are calculated from the detector counting rates by means of an on-line calculator according to the formula $P=(1/B)\cdot[(N-A)/(1-NA)]$, where $N=(N_1-N_2)/(N_1+N_2)$ is the measured intensity asymmetry of the two detectors, A is the apparatus asymmetry, and B is the detector sensitivity. B corresponds to the Sherman function in Mott scattering and is the intensity asymmetry that would be obtained from the analyzer for a totally polarized incident beam. The apparatus asymmetry was determined in two ways: (1) A second movable electron gun (not shown in Fig. 1) replaced the polarizer crystal, providing a beam of unpolarized electrons of the same primary energy as those impinging on the polarizer crystal. After adjustment of the electron gun beam to the scattered (0, 0)-beam geometry, an apparatus asymmetry $A\leq 2\%$ can be obtained. (2) As this procedure might not perfectly simulate the final scattering conditions, we checked the asymmetry in the double-scattering setup by covering the polarizer crystal with large quantities of gas (O_2 or CO). With increasing dose, the polarization features in the rotation diagrams vanish, converging to some constant value A'. Both values A amd A' can be made to agree within ±0.5% after careful alignment. An important feature of the double-scattering experiment is its capability of self-calibration. This is achieved by establishing identical scattering conditions for the polarizer and the analyzer with respect to the incident beam and the scattered beams. The movable electron gun and the polarizer crystal are positioned in such a way that the primary beam, with energy E_0, impinges normally onto the polarizer, and that the scattered (2, 0) beam passes into the analyzer section. The measured polarization, corrected for the apparatus asymmetry, is the square of the detector sensitivity B at that particular energy E_0. In this way, we determined the detector sensitivity to be $B_{\text{exp}}=0.28\pm0.05$ (energy $E_0=105$ eV). This value is close to, but somewhat less than, the theoretical prediction of $B_{\text{th}}=0.33$. This experimental detector sensitivity was used for the evaluation of the polarization data shown in Fig. 2. With a primary beam intensity of the order of 10^{-7} A, the total counting rate reached up to 10^6 counts/sec for the (0, 0) beam at energies around 100 eV. Such high counting rates allowed a $P(\varphi)$ rotation diagram to be obtained in 5 to 10 min, with a collection time of 0.6 sec per datum point. As the azimuthal rotation angle φ was measured electrically[9] the intensity and polarization diagrams could be recorded directly on an x-y plotter. Because of the low residual gas pressure and the short measuring time, the crystals needed not to be flashed during a measurement run. Thus small alignment errors of the crystals and the electron beams resulting from thermal movements of the sample holders and residual magnetic fields induced by the heating current could be avoided. This point is of importance as polarization data are known to be more sensitive to small variations of the scattering conditions than intensity data.[10]

The theoretical calculations were made accord-

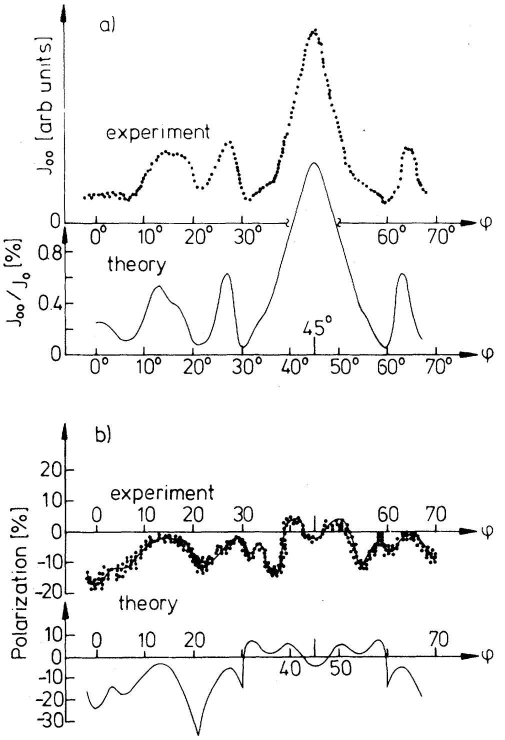

FIG. 2. Comparison of experimental and theoretical rotation diagrams for the (0,0) beam from W(001), Primary energy 100 eV, polar angle of incidence $\theta = 47.5°$. (a) Intensity rotation diagrams. The curves have been normalized at $\varphi = 45°$. (b) Polarization rotation diagrams. The experimental curve represents an original x-y plotter output. The polarization axis has been obtained by self-calibration of the experiment.

ing to a relativistic LEED theory described previously.[11] The model specifications entering the present calculations are the following: The scattering phase shifts (up to $l = 7$) were obtained from muffin-tin potentials due to Mattheiss,[12] which were corrected for temperature using a bulk Debye temperature of 380 K. The surface reciprocal lattice vectors were selected by the computer program such as to ensure convergence (up to 40 beams). The inclusion of between seven and nine monatomic layers was sufficient to describe the semi-infinite crystal. The real part of the inner potential was chosen as 10 eV, the imaginary part as 4 eV. The surface barrier was represented by a smooth exponential-type function. The spacing between the top layer and the adjacent layer was taken as contracted by 5% relative to the bulk interlayer distance, according to the results of our recent intensity rotation diagram study.[8]

A comparison of experimental and theoretical intensity and polarization rotation diagrams for the (0, 0) beam at a primary energy of 100 eV (±1 eV) is shown in Fig. 2. The intensity curves [Fig. 2(a)] are normalized at $\varphi = 45°$, the measured intensity being lower than the calculated one by approximately a factor of 3. The overall agreement of shape and relative intensities of the structures in the intensity rotation diagram is considered fairly good, except for some subtle discrepancies near intensity minima and shoulders. In particular, the width of the peak around $\varphi = 45°$ is smaller in the experiment than in theory, with a more pronounced shoulder at $\varphi = 36°$. The slight asymmetry of the experimental curve is an outcome of the small misalignment of the target surface normal and the rotation axis, which leads to small changes of the angle of incidence within the rotation diagram. The agreement of theory and experiment seems to be slightly better on the right-hand side of Fig. 2(a). The experimental polarization rotation diagram in Fig. 2(b) shows significant structure, with polarization values up to 16%. An original x-y plotter output is reproduced in this figure, with no averaging of the data points. The curve through the data points is drawn only to guide the eye. The relatively small scatter of points demonstrates the high efficiency of the present experiment as a spin-polarization detector.

With respect to the sign and position of maxima and minima in the polarization rotation diagram, theory and experiment generally show good agreement. The structure in the polarization rotation diagram is entirely due to multiple-scattering effects, as with single scattering a rotation diagram for the (0, 0) beam would exhibit some constant value only. Because of multiple-scattering effects, the theory predicts that, different from in atomic scattering,[13] polarization maxima are not necessarily coupled to intensity minima. Indeed, our results show large polarization values also at high intensities, e.g., around $\varphi = 0$ where high polarization is found at a relative maximum of the intensity. The partial decoupling of polarization maxima from intensity minima in electron diffraction from single crystals is in contrast to elastic scattering from polycrystalline surfaces, where the general rule of atomic scattering has been shown to hold.[14] The gross features of the polarization rotation diagram have been observed also at elevated temperatures (1300°K). The measured absolute polarization values are close to, but smaller than the theoretical predictions.

This might be due in part to the detector sensitivity B being too small (using the upper limit of our error margin would improve the agreement), or due to the presence of incoherently scattered background which is likely to have a depolarizing effect. An indication for the latter cause might be seen in the intensity minima being less pronounced in the experimental curve than in the theoretical one.

There is only one major exception to the good agreement of experiment and theory, in a small angular range around $\varphi = 36°$. Though the experimental and theoretical curves are similar in shape, the negative excursion is much more pronounced in the experimental curve than in the theoretical one. We note that this discrepancy of polarization data parallels that of the intensities over this same angular range. In order to investigate this problem further, we slightly modified the accessible experimental conditions and theoretical parameters within physically reasonable limits. The primary energy was varied by ±2 eV, and the angle of incidence by ±1°. The real and imaginary parts of the inner potential were varied by a few eV, the surface layer contraction was changed by a few percent, and several different ion-core potentials were tried. All these attempts, however, did not significantly improve the agreement. Possibly the key to an understanding of the present discrepancy is to be found in the rotation of the polarization vector out of the normal to the scattering plane due to multiple-scattering effects. The calculations showed that in this particular range of azimuthal angle the nonnormal components of the polarization vector are large, being of the same order as the normal component. Thus a small change of orientation of the polarization vector or misalignment of the scattering planes might have relatively large effects on the measured normal component. At present, this point has to be left open to further experimental and theoretical investigations.

In conclusion we wish to make the following points: (1) The present experiment clearly demonstrates the feasibility of studying electron-spin–polarization effects in double-scattering LEED. (2) The level of agreement between theory and experiment obtained in this study of the (0, 0) beam from W(001) can be considered quite satisfactory, though not complete. (3) The prospects for an improved electron-spin–polarization detector based on LEED appear very promising.

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