A video-based spin-polarized LEED data-acquisition system

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A video-LEED system for rapid measurement of spin-polarized low-energy electron-diffraction (LEED) data is described. The system is based on a special, high-dynamic-range camera but will also support TV-rate cameras for less demanding I/V LEED work. The capabilities of the system include LEED pattern recording, and data acquisition for asymmetry versus energy (A/V), intensity versus energy (I/V), and intensity versus time (I/T). The design and operation of the system is described and illustrated by asymmetry data for W(001). © *1995 American Institute of Physics.*

I. INTRODUCTION

In recent years there has been a growing realization of the strong interplay between magnetic, electronic, and structural properties of surfaces and thin films. Surface reconstruction of the former and epitaxial perfection of the latter have to be understood before other data can be meaningfully analyzed. Electron-diffraction techniques are well suited for that purpose. At energies of 30–300 eV electrons scatter strongly and are therefore inherently surface sensitive. Instrumentation commercially available is well suited for a quick evaluation of low-energy electron-diffraction (LEED) patterns for their symmetry and sharpness. However, the information carried by diffracted electrons is much more extensive: the intensities exhibit Bragg oscillations which are intimately connected with the interplanar spacing. Multiple scattering and strong attenuation complicate a simple Bragg interference picture so that a complete, multiple-scattering theory has to be used for for analysis of experimental data. These calculations yield the information about the structure of the first three to four surface layers. The accuracy of this structural determination to a high degree depends on how large and accurate the experimental data set is. Such data sets are most easily obtained by video-based acquisition systems. Several such systems have been described in the literature; see the references in Ref. 1.

The I/V (intensity versus energy) analysis described above yields structural information about the surface region. It would be equally important to determine the magnetic structure of this region as well. Since electrons carry spin, the desired information is, in principle, contained in the asymmetry data, i.e., in the normalized intensity difference of a LEED spot taken with primary beams of opposite spin polarization and varying energy (A/V spectra).[2] As before, an unambiguous magnetic structure determination requires a large and accurate data sets. The spin asymmetries are rather small (of order 1%), much smaller than can be measured with a normal video-based LEED system. Consequently, all published A/V data have been taken by using mechanically manipulated Faraday cups.[3] Such measurements are obviously very tedious unless restricted to the specular beam. The advantage of a direct-view SPLEED system with an appropriate camera and data-acquisition system lies in its ability to simultaneously acquire data over a large energy span for several diffracted beams. The system described below has the capability to acquire such extensive asymmetry data sets quickly and conveniently.

The system consists of a commercial front/reverse-view LEED instrumentation, an external video camera, and the controlling computer. The system is quite flexible; it supports both the Omicron's and Princeton Research Instruments's LEED instrumentation and can be easily modified to support any LEED system capable of I/V data acquisition. The regular TV-rate video cameras as well as cameras permitting the on-chip integration can be used. Since the experimental asymmetries can be quite low (on the order of a fraction of a percent) normal video systems are inadequate. A high-dynamic-range image acquisition system is required. The Hamamatsu slow-scan C4880 camera is supported by this system for A/V work. Its 12–14 bit dynamic range is sufficient for a reliable A/V data acquisition, as will be demonstrated below. In addition, the system supports the easy acquisition of LEED patterns, medium-energy electron diffraction (MEED), and I/V LEED data.

II. HARDWARE AND SOFTWARE

A. Components and configuration

The system is based on a Macintosh computer. Images are acquired by a Nubus based 8-bit deep frame grabber card QuickCapture 50 Hz.[4] The TV-rate video camera is a Pulnix[5] TM-765E with an infrared cut-out filter and a special long-term integration option. Together, they offer a slightly better resolution (768×512) than a RS-170 standard (*North American black/white system*). With its on-chip integration capability the TM-765 camera has a significant advantage. Most other video-based LEED systems[1] integrate the signal by summing up individually digitized single frames, which adds a high level of frame grabber induced noise to the final image. A solution sometimes offered in other systems[1] is to use image intensified cameras which unfortunately are highly nonlinear, nonuniform, and tend to drift with time. The overall dynamic range of the system is limited to 8 bits per pixel (*256 values*) by a frame grabber board. Note, however, that

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the typical LEED spot size ranges between 100 and 600 pixels which results in a much higher effective dynamic range for spot intensity measurements.

Alternatively, the system can be configured to support the Hamamatsu slow-scan camera (dual-mode cooled CCD C4880).[6] In this case the frame grabber board is replaced by the ImageQuest IQ-D100, EIA-RS422A digital interface. The advantage of this configuration is its superior linearity, stability, low noise, and high dynamic range. The particular camera the authors used has the 14-bit dynamic range which was further increased to 16 bits (*65 536 values*) by reducing the original 1000×1000 image size to 500×500. We found this resolution to be sufficient for asymmetry work.

The external devices are digitally controlled via a general purpose I/O board.[7] Its two TTL channels are used to control the integration circuitry of the Pulnix camera; one digital-to-analog 12-bit converter generates a ±2 V signal to control the polarization state of the laser beam used in the spin-polarized beam source. A 16-bit digital–analog converter outputs a 0–10 V signal to an optical 1:1 isolation amplifier which in turn supplies a low-voltage external beam energy control signal to the LEED gun controller.

Three different LEED instrumentations have been used in this system: a reverse-view LEED system from Princeton Research,[8] a similar system from Omicron,[9] and an old front-view Phi/Perkin–Elmer system that has been custom modified for asymmetry work as described below. They use different power supplies that are controlled in a slightly different way. While the Omicron power supply can be driven directly from the I/O board, the Perkin–Elmer 11-020 power supply[10] had to be modified by incorporating a special circuitry to allow the external voltage control of beam energy. The Perkin–Elmer power supply can use an external source of beam voltage but this capability has not been utilized because in this mode the 11-020 cannot control the retardation voltage. The power supplies are relatively slow; they take approximately 0.5 s to stabilize at energy steps larger than 100 V. The software takes that into account when changing the energy by delaying the image acquisition by an amount that is proportional to the energy steps.

For the asymmetry mode of operation we use a custom modified front-view LEED system. The modifications include the removal of the original electron gun and its replacement by a spin-polarized source; see Ref. 11. The source uses a GaAs substrate located in a separately pumped chamber with provisions for a proper sample preparation, i.e., cleaning and Cs/O_2 activation. Electrons photoemitted by a circularly polarized HeNe laser beam are bent 90° to obtain the transverse polarization before they are directed toward the main chamber through the isolation gate valve. The electron beam enters the LEED optics axially and is focused on the sample. The system is relatively compact with the total beam path being only some 50 cm long. The beam has an average spin polarization of 25% and a $1/e$ lifetime of several hours to one day.

B. Data acquisition and processing

In the "live"-video mode the program displays a full image on the computer monitor. The image is shown in 127 grey levels with the two brightest levels displayed in red to indicate a saturation condition. The program can also be instructed to display a fully normalized image (*autocontrast*) at some reduction of the refresh rate. The highest screen refresh rate achievable for TV cameras is approximately three images per second. To reduce the video noise in weak images the integration time can be changed from 1 frame to 200 frames. The latter corresponds to an acquisition time of 8 s. To reduce the effects of stray light the user can request automatic subtraction of the background image (*defined as the image seen at 0 eV beam energy*). The refresh rate for C4880 depends on the digitalization mode selected; it is approximately one frame per second in the fastest mode. The maximum integration time for this camera is software limited to 90 min. There is the option to grab and save the full image to a data file. The file format is a binary byte 768×512 for the TV-rate system and a binary signed integer 500×500 for C4880. It can be read by any general-purpose scientific image processing application. All the other data files written by the program are text files which can be read by any application accepting a straight, tab-delimited text format.

1. Intensity profile mode

Careful I/V LEED work requires the most precise alignment of the crystal surface relative to the direction of the electron beam. Even very small misalignments (*on the order of 0.1°*) may lead to significant errors in structure determination. A classical example of this is the misunderstanding with respect to the determination of the tungsten surface reconstruction.[12] The program offers several intensity profile modes to help the user align the system. All of them can be activated in an automatic mode, whereupon the profile is continuously updated on the screen.

In the *centered* mode the program displays a projection of all pixels contained between two circles. Their size and separation between them can be varied. The primary use of this mode is to help establish normal beam incidence. When everything is perfectly aligned all diffracted beams of a given order will be centered between two circles with their intensities being equal.

The *spot* mode displays the projection of all pixels contained within a given square area. As before, position and size of the square can be adjusted. In addition, the program calculates and displays the total integrated intensity. The background intensity (*calculated from the perimeter intensity*) can be optionally subtracted. This feature is essential to focus the system and to verify that the system is linear in all relevant parameters. For example: it can be used to compensate the response dependence of the system on the location of a diffractive spot on the LEED screen. Such a dependence may be due to several facts: cosinelike distribution of the light emitted by a diffractive spot, lens vignetting properties (*which in turn explicitly depend on the lens aperture*), and geometrical effects when the image is projected onto a flat CCD chip. The best way to deal with such optical effects is to measure an appropriate instrumental function and use it for correcting the raw LEED intensities.

We obtained such an approximation function by simply projecting a He–Ne laser beam (*appropriately attenuated*) from the LEED focal point to different parts of the screen and measuring the spot intensity. It turned out to be to good approximation, a weakly quadratic function of radial distance from the LEED axis. The program uses user-provided parameters describing this function to calculate this correction automatically. As such the correction compensates only for the properties of the optical system; it does not include CCD pixel nonuniformity.

The third mode, i.e., the *line* mode, displays the intensity along any line crossing the CCD center. It is used primarily to verify the proper energy convergence of diffracted beams.

2. *Intensity versus energy (I /V) mode*

The primary consideration for a successful operation in the I/V LEED mode is the ability to precisely follow beam trajectories. This task is complicated by the deep minima sometimes observed in I/V spectra that are indistinguishable from the diffuse background. We chose the simplest possible solution: the beam trajectory is defined by two locations on the screen together with their respective energies. The user enters those locations interactively. The tracking may be linear or autocenter. In the linear mode the program simply assumes that the spot moves linearly as a function of the inverse square root of energy. The tracking function is then determined by defining locations. This mode works best when both camera and electron optics are perfectly aligned with the external magnetic field properly compensated.

The autocenter option uses the same algorithm to find the nominal beam location at each energy step but it will offset it to the maximum intensity pixel within the original integration area. We found this method tracks the beams quite precisely even if the primary beam is not exactly normal. For this mode to work successfully in low intensity, high noise images (*or dirty LEED screens*), it helps to have the camera optics slightly defocused.

The system has the capability to track 50 beams with the energy step and range limited only by the total number of points in the spectrum (2000). The beam integration area can be varied between 10 to 100 pixels. The background intensity is calculated from the perimeter intensity and can be subtracted out. Stray light rejection (*background subtraction*) can be specified either at the beginning of the scan or at each energy step. The program by default displays the raw image at each energy step and superimposes on it the current location of all tracked beams. For faster I/V scans this automatic image updating can be switched off.

After the run is finished the I/V data are automatically displayed on the screen. The raw data can be saved to an annotated text file. Any further data processing, e.g., same-order beam comparison/averaging, primary beam current normalization, etc., may be done using any general-purpose data analysis/presentation software.

Some I/V data-acquisition programs attempt to measure the primary beam current. We felt that the beam current cannot be accurately measured by standard LEED electronics. Such measurements are better done separately and used later to normalize the raw data.

3. *Asymmetry versus energy (A/V) mode*

The asymmetry versus energy mode has been incorporated to facilitate the research into the magnetism and structure of surfaces and ultrathin films. The asymmetry magnitudes expected in SPLEED,[13] $A=(1/P_0)(I_+-I_-)/(I_++I_-)$, can be quite small as the typical spin-polarized sources operate at low polarization (P_0=25%–30%) and both the exchange and spin-orbit induced asymmetries typically average a few percent,[14] usually reaching higher values only in the vicinity of the Bragg minima. It is therefore quite clear that stability and dynamic range of the 8-bit, TV-rate system are insufficient to measure asymmetries of LEED patterns. The C4880 camera offers much higher stability and a significantly better dynamic range (1 part in 16 384) and is therefore well suited for asymmetry measurement. The software measures the raw asymmetry $A_e=(I_+-I_-)/(I_++I_-)$ in a manner similar to that described in the previous section. The only difference is that for each data point two intensities are recorded; one with the spin polarization up (I_+) and another with the spin polarization down (I_-). The polarization is controlled by a ±2 V signal applied to the electro-optical device switching the ellipticity of the laser beam. As an option, instead of the intensity image the asymmetry image of a LEED pattern can be displayed. Though the pertinent intensity changes are rather small (of order 1%) and cannot be seen by eye, they can be made visible on the computer screen. In the authors' experience, the asymmetry images are quite useful in determining the beam quality, as small deviations from the proper convergence will be reflected in the fine structure of the spot much better than in the normal intensity image. Similarly, it is also easier to detect small misalignments of the primary beam (i.e., away from the normal incidence) in the asymmetry image.

4. *Intensity versus time (I /T) mode*

Two diffraction techniques are frequently used to monitor film growth. In reflection high-energy electron diffraction (RHEED) a 5–50 keV electron beam is directed toward the sample at extreme grazing incidence with the intensity of the diffracted beams being monitored. Another technique, viz. medium-energy electron diffraction (MEED), utilizes a less energetic beam (1–3 keV) at less grazing incidence and the variation in intensity of several diffracted spots is recorded. Both allow the relatively precise determination of film thickness (*intensity oscillates with layer periodicity*) when film growth proceeds in the Frank–Van der Merve (i.e., layer by layer) or Stranski–Krastonov mode (i.e., layer by layer followed by clustering).

The program supports the I/T mode by allowing the definition of up to ten arbitrary RHEED/MEED/LEED spots the intensity of which are to be monitored. Once the collection mode is entered a reduced (50%) constantly updated image is placed on the monitor together with a chart-recorder-like window showing the intensity of selected spots as a function of time. The vertical scale is automatically readjusted, with the total time elapsed and the number of time samples being displayed. The user can define the time interval and can stop/restart the scan at any time. The mini-

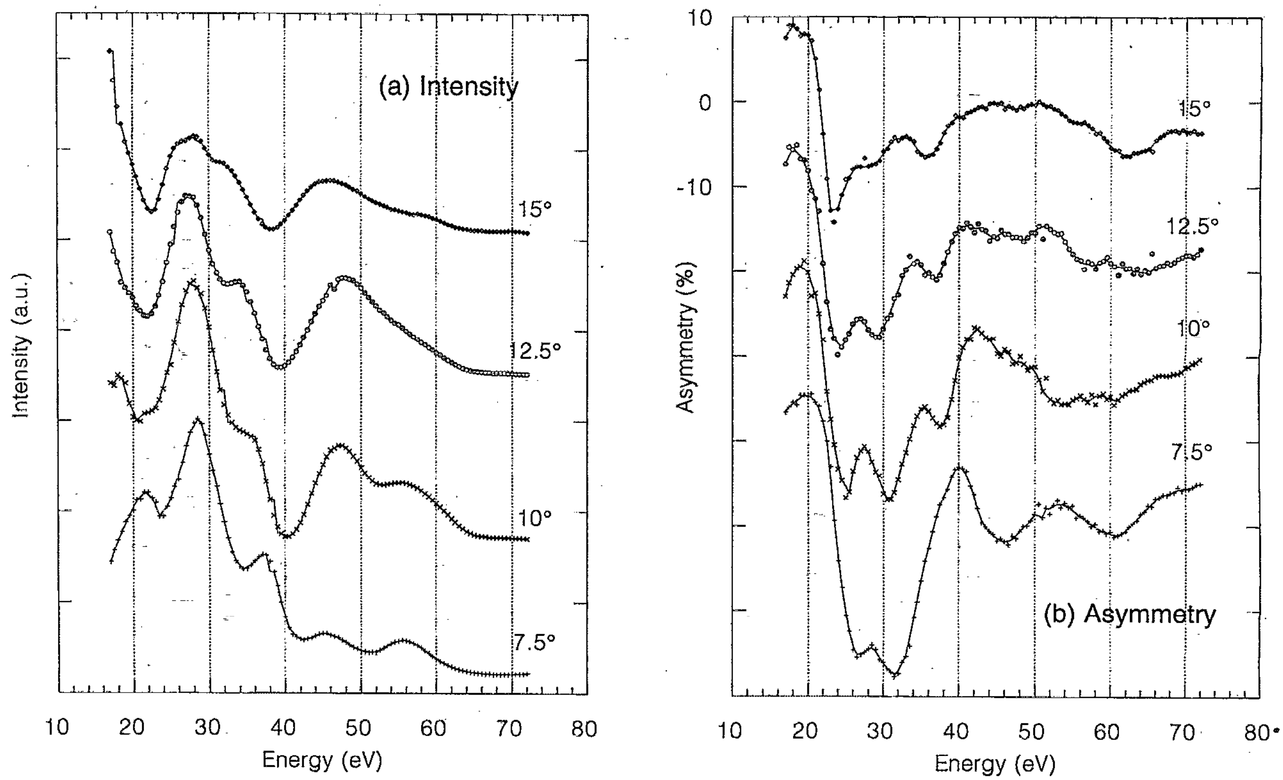

FIG. 1. (a) Spin-averaged scattering intensity for specular diffraction from W(100) at several angles of incidence as a function of the primary beam energy. The angles are given relative to the surface normal. For clarity the data are offset vertically. (b) Spin asymmetry as a function of beam energy. Again for clarity, apart from the 15° data each trace is shifted downward by 15%. The solid lines are guides to the eye only. The data were obtained with the beam polarization normal to the (010) scattering plane.

mum time interval is approximately 0.4 s (1.5 s for C4880) and the maximum number of time steps is 2000. As above, once the data are collected, an annotated text file can be created to store the data. Note that the I/T capability can also be used to determine temperature characteristics of the LEED intensities.

III. PERFORMANCE

Two examples will demonstrate the performance of this video-based spin-polarized LEED system. The sample was single tungsten crystal cut to expose the (110) face. The standard cleaning procedure for W[15] consisting of heating (2500 °C) in O_2 atmosphere was used to prepare the crystal. There was still some residual contamination as was evidenced by a weak $p(4\times1)$ superstructure. Figure 1 shows the intensity $I=(I_+ + I_-)/2$ and asymmetry $A=(1/P_0)(I_+ - I_-)/(I_+ + I_-)$ for the beam specularly diffracted from the W(001) surface at several angles of incidence. The beam polarization was normal to the (010) scattering plane. For each angle of incidence the data were accumulated in a single 6-min run over the energy range of 17–72 eV in steps of 0.5 eV. The image integration time was 0.25 s.

As evident in the Fig. 1, this strong spin-orbit, high-Z element has relatively large diffraction asymmetries which can easily be resolved with the present apparatus. At low angles of incidence the raw asymmetry A_e can be as high as ±3%–5%, while the estimated root-mean-square noise in the spectra is not higher than 0.1%. These raw data correspond to an asymmetry of ±12%–20% asymmetry and 0.3% of estimated noise if they are corrected for the 25% polarization of the primary beam. Overall the quality of the data is comparable with that obtained by measuring the diffracted intensity directly with the Faraday cup.[13]

A much more stringent test of a video-based SPLEED system is provided by the experiment in which the asymmetry of nonspecular beams is measured. Here, the additional noise may come from the inhomogeneity of the phosphor coating and screen grids as well as to unavoidable dust contamination of the grids. These are, *per se*, not present in SPLEED systems that use the Faraday-cup detection scheme. The representative data obtained with our system are shown in Fig. 2. The panels display the spin-averaged intensity (left panel) and asymmetry (right panel) for two first-order [10] and [$\bar{1}$0] beams. The beams were tracked simultaneously in a single 6-min-long run.

With the primary beam incident along the normal to the surface, the intensity spectra should be identical. The differences seen in Fig. 2(a) are due to a small misalignment of the primary electron beam (our current experimental setup does not allow for sample tilt). Still, the primary beam is relatively close to the normal as it can be judged from the similarity of major features in both spectra. The corresponding asymmetry data are shown on the right of Fig. 2. The overall symmetry of the scattering geometry requires the asymmetry of these two beams to be identical but of opposite sign. Such symmetry is clearly present in the data of Fig. 2(b). All the

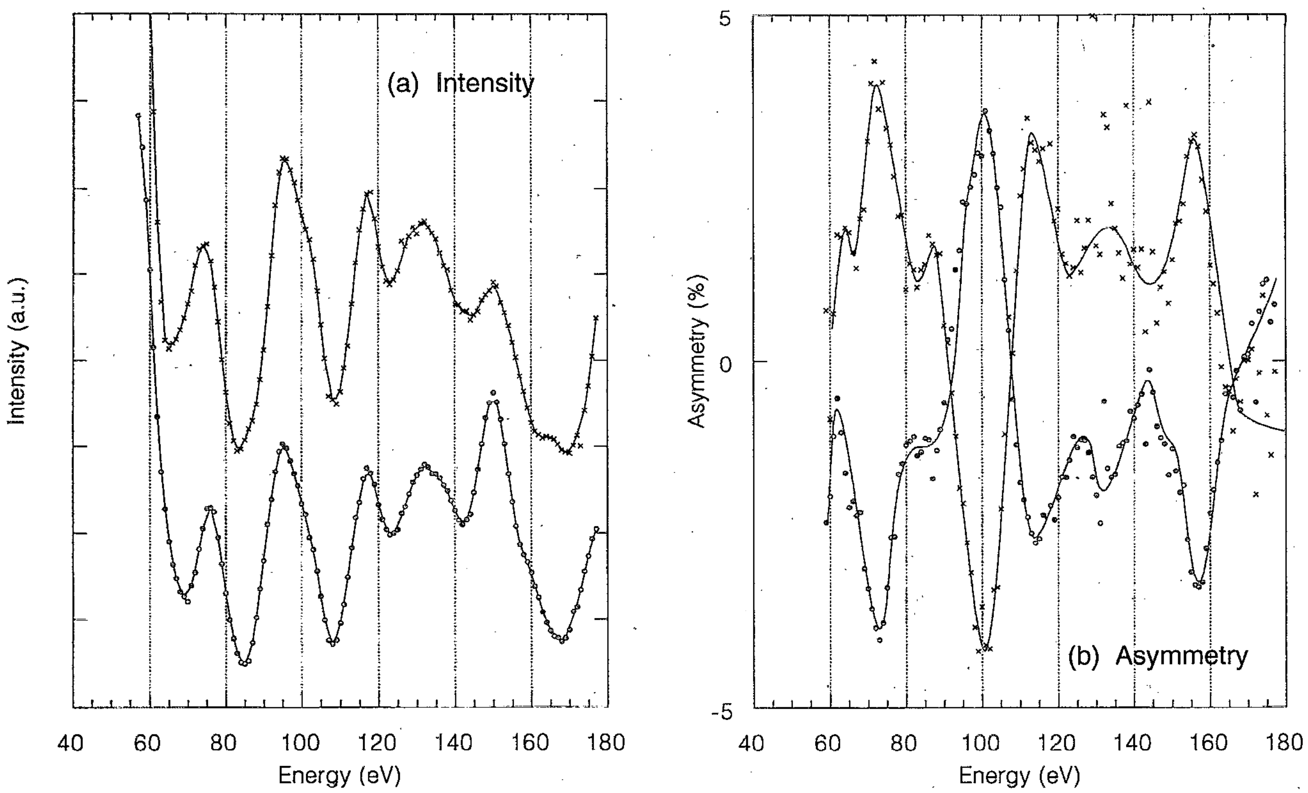

FIG. 2. (a) Spin-averaged intensity and (b) asymmetry for two diffracted beams [10] and [$\bar{1}$0] as a function of the primary beam energy. The small asymmetry apparent in the intensity data is due to tilt misalignment of the primary beam. The solid lines in both (a) and (b) are guides to the eye only.

major features in the spectra are disposed symmetrically around the line of zero asymmetry. Small deviations from the exact symmetry are due to misalignment which has a much stronger effect on asymmetry then on intensity. Some of these deviations are due to occasional problems with beam quality. These problems are expected to be corrected in the next generation of SPLEED optics currently under construction. The overall quality of the data seems poorer than that obtained with the stationary specular beam (see Fig. 1). The number of data points (outliers) that are clearly outside the range of majority of data is much higher. This is due to imperfections in the LEED screen optics as discussed above. Ignoring drastic outliers, the root-mean-square noise estimation is still comparable to that obtained with the specular beam (0.3%). This result is not very surprising in view of the fact that the asymmetry is the absolute ratio of two numbers. The instrument response function, which appears in both numerator and denumerator, cancels out. The reduced signal to noise apparent in Fig. 2 is due to the magnitude of asymmetry lower than that in Fig. 1.

In summary, we have demonstrated here a system capable of quick acquisition of LEED data including for the first time the capability to acquire asymmetry data. Even with the first generation of the SPLEED optics we were able to easily resolve spin asymmetries expected in the diffraction from both magnetic and nonmagnetic surfaces. The primary advantage of the system lies in its ability to record the data for many diffracted beams simultaneously without any mechanical manipulations. It is expected that the easier availability of larger A/V data sets will facilitate further research into the magnetism and structure of surfaces and thin films.

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