Correction of experimental low-energy electron-diffraction intensities

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For the determination of surface structure by quantitative low-energy electron-diffraction (LEED) analysis the experimental intensities are usually measured on the fluorescent screen of display-type optics and then routinely corrected for normalization to constant incident electron current and for background subtraction. An additional correction, which is not usually applied, corrects for the variation of the transparency of the grids in front of the fluorescent screen, as pointed out in 1974 by Legg, Prutton, and Kinniburgh. We show that this correction can be rather easily implemented on data collected with modern computer-controlled data-acquisition systems. The correction is carried out, as an example, on LEED intensity data from Al{110}.

Quantitative low-energy electron diffraction (QLEED)—to date the most successful technique for the determination of the atomic structure of crystal surfaces and ultrathin films[1]—relies upon the comparison between experimental and theoretical intensities of diffracted beams. The experiment consists in collecting curves of diffracted intensities versus energy of the incident electrons [the so-called $I(V)$ curves or $I(V)$ spectra], while the theory uses the dynamical theory of diffraction to calculate the intensities expected from suitably selected structure models.

The most reliable detector for the measurement of intensities of electron beams is the Faraday box, but it is not a convenient detector to use when one wants to collect very rapidly large sets of data such as required by QLEED. For this reason, the large majority of experimental systems around the world use the display-type optics in which the electrons diffracted from the surface under study are first filtered for reduction of the inelastically scattered electrons (a step required by the Faraday box as well), and then accelerated onto a hemispherical fluorescent screen. The filtering and acceleration are done by means of fine-mesh grids located in front of the fluorescent screen. The diffracted electron intensities are then measured indirectly by measuring the intensities of the light emitted by the screen at the points of impact of the accelerated electrons (the so-called LEED spots). These light intensities can be measured very rapidly by means of electronic systems involving television (TV) cameras and suitable microprocessors and video cards.[2–4]

However, the experimental curves obtained by plotting the *light* intensities in the LEED spots versus incident electron energy cannot be immediately compared with the theoretical curves of backscattered electron flux in the corresponding beams versus incident electron energy. Indeed, the assumption that the light intensity is proportional to the electron current is correct, but the calculations assume a *constant* incident electron current and *only* elastically scattered electrons (i.e., no background), whereas the experiment is usually done with an incident electron current that varies with voltage, and with diffracted beams in which the contribution of some inelastically scattered electrons to the measured intensity is never completely eliminated (the background of the LEED pattern).

For this reason, the measured light-intensity curves must be suitably corrected before they can be used for comparison with calculated curves. Two corrections are routinely applied, namely (1) subtraction of the background, and (3) normalization to constant incident current. With the computer-controlled data-acquisition systems mentioned above, these corrections can be done conveniently and rapidly either on- or off-line.[5]

However, in display-type LEED equipment the intensities of the LEED spots may also be affected by inhomogeneities in the phosphor coating of the fluorescent screen, and are certainly affected by the fine-mesh grids located in front of the fluorescent screen. In this paper, we consider only the latter effect. Owing to the hemispherical shape of both the fluorescent screen and the grids, and to the direction of observation of any given LEED spot through a window in the vacuum chamber, the transparency of the grids varies from a maximum along the direction of the incident electron beam (near the center of the fluorescent screen) to zero when the diffracted electrons and the light emitted by the corresponding LEED spot from the fluorescent screen strike the grids near grazing incidence (near the edge of the screen). This effect was pointed out 20 years ago by Legg, Prutton, and Kinniburgh (LPK),[6] who derived a formula for the optical transparency of the grids as a function of the direction of observation. We call this effect the LPK effect. In front-view LEED equipment the LPK effect involves both the diffracted electron current and the light emitted by the corresponding LEED spot; in rear-view LEED equipment the effect involves only the diffracted electron current (and to a lesser

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extent the absorption of the light in the glass supporting the phosphor).

A correction of diffracted LEED intensities for the LPK effect was never routinely applied, as far as we know, except for the work of LPK cited above. This neglect was understandable in the days when the diffracted intensities were measured manually with a spot photometer, because manual correction required time-consuming and error-ridden calculations, and the determination of the location of each LEED spot on the screen for each energy point was a slow and tedious task.

However, with modern computer-based data-acquisition procedures the correction of LEED intensities for the LPK effect is not very difficult, and can be done very rapidly either on- or off-line. The purpose of this Brief Report is to show how such a correction can be implemented.

We need to know the exact location of each LEED spot on the screen for each energy value measured. The video-LEED data-acquisition scheme that we have been using for several years[3] tracks the LEED spots (which move on the fluorescent screen with varying electron energy) by calculating the trajectories of all spots in a coordinate system defined by the video card. Hence the positions of all spots on the video screen are known for each value of the incident electron energy. These positions can be saved to a computer file in the same step that saves the intensities and the background data in any given run. An additional simple procedure allows the determination of the center and the radius R_0 of the fluorescent screen image on the TV monitor, so that the position R of each LEED spot relative to the screen center and hence the reduced radius R/R_0 can be calculated for each energy point on the $I(V)$ curves.

We also need to know the functional dependence of the grid transparency T upon the distance R from the center of the screen. We assume here that the system has central symmetry, i.e., that the grid transparency depends only on the distance R from the screen center, not on the azimuth. (This assumption is obviously a simplification. Without this assumption the problem would be more complicated, but still soluble.) The function $T(R)$, rather, the function $T(R/R_0)$, can be determined experimentally as follows.

The sample is biased negatively to a sufficiently high voltage to cause the incident electron beam to turn around and land on the fluorescent screen. The light spot thus created can be focused and moved about on the screen by means of the Helmholtz coils, which are always available in experimental systems dedicated to QLEED work. With the beam current kept constant, the intensity of the reflected spot is measured for a number of known positions (R/R_0) on the fluorescent screen. The measurements are repeated for different values of the beam current and for motion of the reflected spot along different azimuths. The intensities are then normalized to unity and plotted as functions of R/R_0.

The results of our measurements on a front-view LEED system are shown in Fig. 1. The curve drawn through the (rather large) scattering of the experimental points represents the function $T(R/R_0)$ of grid transparency versus reduced radius that applied to the particular LEED optics used.

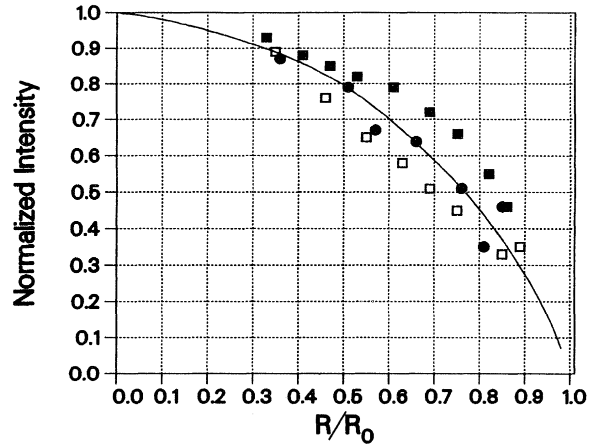

FIG. 1. Transparency of a four-grid front-view LEED optics as a function of reduced radius R/R_0. R_0 is the radius of the screen image on the TV monitor, and R is the distance of a spot from the screen center. Different symbols denote results of measurements with different electron currents (from 0.026 to 0.032 μA). The solid curve is taken as the $T(R/R_0)$ function discussed in the text.

Note that the acquisition of the $T(R/R_0)$ curve needs to be done only once for any given LEED optics (as long as the screen and the grids are not changed), and also that it does not require a single-crystal sample—it can be done with a polycrystalline sample and at chamber pressures which need not be in the ultrahigh-vacuum range (we did our measurements at pressures of about 10^{-7} Torr).

The procedure for the L correction (as we call, for short, the correction of intensity data for the LPK effect) is then the following. For each electron energy and for each beam we subtract the local background from the measured beam intensity, we find the reduced-radius position R/R_0 of the beam and divide its intensity by the value of T at that position as found from the $T(R/R_0)$ curve (Fig. 1). Of course, the normalization correction is still applied. The L-corrected intensities are then saved to a file.

The importance of the L correction is difficult to gauge with confidence for all cases. In general, we expect it to have about the same effect as the normalization to constant incident current. But note that the normalization plays a big role only at low electron energies, whereas the L correction can have significant consequences at all energies, because it depends not on the energy but on the position that a given beam has on the screen. For example, high-index beams appear on the LEED screen at high energies, hence their $I(V)$ spectra are not much affected by the normalization process, because at high energies the incident electron current is nearly constant, but the L correction may change the relative height of intensity peaks quite considerably and possibly their energy positions as well, albeit to a lesser extent. These changes *may* be beneficial, because high-index beams are notoriously more difficult to fit to model calculations than low-index beams. We expect that the L correction will have a large effect in some and hardly any effect in other QLEED analyses. In the future, we plan to apply the L correction to all data used in QLEED analyses, and report both normally corrected and L-corrected data for comparison.

As a first example, we show here the effects of the L correction on intensity data from Al{110}, a well-studied surface in the recent past.[7,8] In this work, the L correction was applied off-line. Figure 2 depicts eight $I(V)$ spectra: in each panel the dotted curve is the normal[9] experimental curve, the solid curve is the L-corrected, and the dashed curve is the theoretical curve optimized as described below for the L-corrected data. We see that differences between normal and L-corrected data are hardly perceptible in the low-index beams [Fig. 2(a)], but very noticeable in the high-index beams [Fig. 2(b)].

It is also interesting to see what effect the L correction has on a QLEED analysis in the present case. Published reports[7,8] on the structure of Al{110} include determinations of the first, second, third, and fourth interlayer spacings (one set of published results[7] is, in terms of the *change* Δ_{ik} of the spacing between layers i and k, in Å: $\Delta d_{12}=-0.123$, $\Delta d_{23}=+0.071$, $\Delta d_{34}=-0.02$, and $\Delta d_{45}=+0.001$). Here we have carried out a partial intensity analysis of both the normal and L-corrected data independently of one another. By partial analysis we mean that we have investigated only the first and second interlayer spacings, keeping all deeper spacings at the bulk value (the purpose of the present work is not to repeat a full QLEED analysis of Al{110}, but merely to test the effect of the L correction). We have used, as usual, three R factors to quantity the fit of theory to experiment, namely, the Van Hove–Tong R_{VHT},[10] the Zanazzi-Jona r_{ZJ},[11] and the Pendry R_P (Ref. 12) factor. As usual, we find that each of these R factors has a minimum at somewhat different values of the structural parameters for both sets of data. The minima are, for the normal data,

$$R_{\mathrm{VHT}}=0.197, \quad r_{\mathrm{ZJ}}=0.107, \quad R_P=0.315 ,$$

and, for the L-corrected data,

$$R_{\mathrm{VHT}}=0.172, \quad r_{\mathrm{ZJ}}=0.094, \quad R_P=0.288 .$$

Thus, in the present case the L correction produces an improvement in the R-factor minimum by about 13%, 12%, and 9% for R_{VHT}, r_{ZJ}, and R_P, respectively. The averages of the structural parameters investigated here (the changes Δd_{12} and Δd_{23} of the first and second interlayer spacings, respectively, with respect to the bulk value 1.43175 Å) are, for the normal data (in Å),

$$\Delta d_{12}=-0.139\pm0.025, \quad \Delta d_{23}=+0.021\pm0.01 ;$$

and, for the L-corrected data,

$$\Delta d_{12}=-0.127\pm0.020, \quad \Delta d_{23}=+0.037\pm0.01 .$$

The error bars given here are the *maximum* differences among the three results, *not* the estimated accuracy. Thus in the present case the L correction affects the best-fit parameters notably, although this conclusion may not necessarily be true in general.

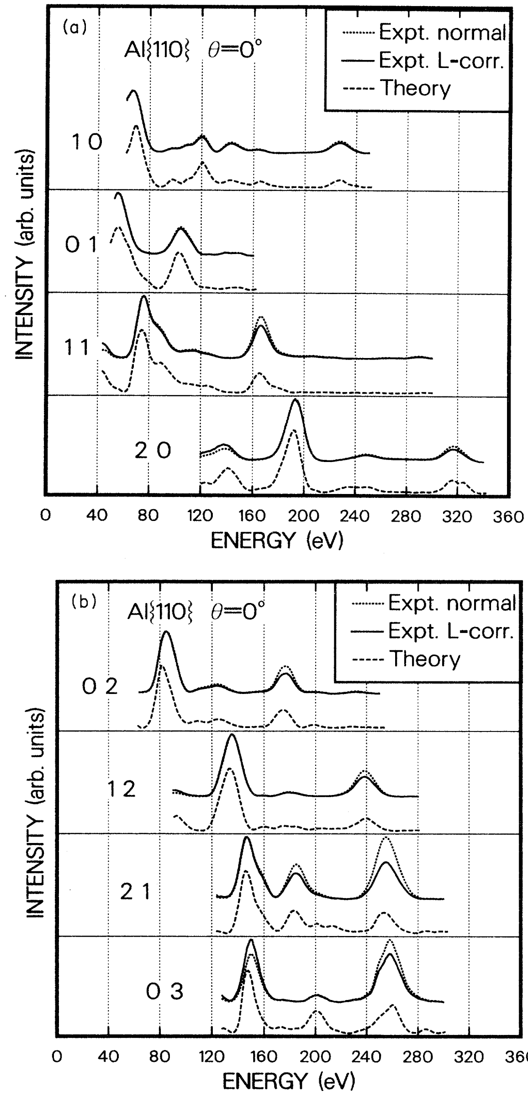

FIG. 2. (a) and (b) Experimental and theoretical $I(V)$ spectra from Al{110}. In each panel the dotted curve is the experimental normal curve (corrected for background and normalization only), the solid curve is the experimental L-corrected curve, and the dashed curve is the theoretical curve optimized for the L-corrected data.

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[1]See, e.g., *Determination of Surface Structure by LEED,* edited by P. M. Marcus and F. Jona (Plenum, New York, 1984), and more recently many articles in the 30th anniversary issue of Surf. Sci. **299/300** (1994), and references therein.

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[5]Another correction, which is often neglected, corrects the energy scale for the contact-potential difference between the sample and the cathode of the electron gun. This correction may amount to 2 or 3 V and affects the experimental value of the inner potential, but does not change the structural parameters.

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[9]By normal here we mean data which have not been L corrected, but have been normalized and background subtracted as usual in QLEED work.

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