PERGAMON

Vacuum 65 (2002) 121–126

VACUUM
SURFACE ENGINEERING, SURFACE INSTRUMENTATION & VACUUM TECHNOLOGY

www.elsevier.com/locate/vacuum

Spot intensity processing in LEED images

R. Roučka, J. Jiruše, T. Šikola*

Faculty of Mechanical Engineering, Institute of Physical Engineering, Brno University of Technology, Technická 2, 616 69 Brno, Czech Republic

Received 31 October 2000; accepted 21 March 2001

Abstract

In the paper, a basic approach to the acquisition and processing of diffraction spot intensities of low energy electron diffraction (LEED) images is described. Major attention is paid to the impact of background subtraction methods on structural parameters of solid surfaces. Comparing the application of several background subtraction methods in the testing series of artificial images and the series of real diffraction images of an Al(1 1 1) structure, the methods of averaging on the border, averaging on the quadrants, and approximation in rows/columns were found to be equivalent and gave realistic results. Due to its simplicity, the approximation in rows/columns is recommended for application in LEED.

Keywords: LEED; Diffraction spots; Image processing; Background

1. Introduction

Low energy electron diffraction (LEED) has been used for several decades as one of the major techniques for surface atomic structure determination. Other techniques such as ion scattering spectroscopy (ISS), surface extended X-ray absorption fine structure analysis (SEXAFS), X-ray photoelectron diffraction (XPD), surface X-ray diffraction (SXRD), scanning tunneling microscopy (STM) and, quite recently, atomic force microscopy (AFM) have become useful techniques for surface atomic structure analysis as well. However, LEED still plays an unavoidable role in resolving exact coordinates and vibration parameters of the atoms occupying several outermost layers of solids. To find these coordinates, it is not sufficient to use only geometrical relations and symmetry of the diffraction spots on the fluorescent screen. The evaluation of the structural parameters from the LEED experiment is based on the knowledge of the diffraction spot intensities as functions of primary electron energy (intensity–voltage curves) [1,2]. It is clear that the precise measurement of the diffraction spot intensities is a prerequisite for the correct determination of surface structures. In contemporary LEED instruments the spot intensities are read from the fluorescent screen by a CCD camera. The extracted data include errors generated both in the CCD camera and resulting from the imperfections of the fluorescent screen. Hence, in addition to the reading of the spot intensities for different electron energies (*I–V* curves), the image processing system must provide compensation for these errors. In this paper the basic approach to

*Corresponding author. Tel.: +420-5-4114-2707; fax: +420-5-4114-2842.

E-mail address: sikola@fyzika.fme.vutbr.cz (T. Šikola).

0042-207X/02/$ - see front matter
PII: S0042-207X(01)00360-8

this problem will be described. In particular, different methods for subtraction of the background intensities of the diffraction spots of the Al(1 1 1) surface structure will be applied and their impact on the surface structural parameters compared.

2. LEED image processing system

A common approach for the extraction of the spot intensities from images taken by a CCD camera includes several steps which can be described as (i) *radiometric corrections and reduction of noise*, (ii) *location of diffraction spots*, (iii) *subtraction of the background*, (iv) *spot intensity evaluation and* (v) *corrections to the experimental conditions*.

To implement this task, digital image acquisition and processing software [3] has been developed. The software is written in Microsoft Visual Basic 5.0, which represents a convenient tool for program interface designs, and the computational routines were compiled as dynamic linked libraries using Digital Visual Fortran 6.0.

The pictures recorded by a CCD camera are expressed as two-dimensional arrays of pixel values (intensities) stored as 16-bit numbers in BMP format. These pictures are, in fact, 2D representations in k-space and not true images but, for convenience, we will use the word "image" in this paper. For the imaging of BMP files of LEED patterns on a computer screen, the pixel values are usually transformed into 256 levels of the grey scale and then shown on the screen. As a consequence of the shape of *I–V* curves, the histogram of the LEED image intensities has its maximum at low values. However, if a linear conversion from 16-bit intensity values to 256 grey scale levels is done, some information from the lower part of the image intensity range can be lost. To avoid this, a variable nonlinear contrast conversion, which enhances the low-level values according to the preferences of the operator, can be used. Thus the background, especially, becomes visible on the screen. Of course, all the data processing is done with the original data.

2.1. Radiometric corrections

The background signal generated by the camera itself is reduced by radiometric corrections. Even in the case of a closed objective of the CCD camera (i.e. the CCD detector is in complete darkness) we get some nonzero signal at the camera output. This background signal is called *the dark current* and the image obtained in this way is called *the dark field* [4]. The dark current results from the generation of electric charges due to thermal vibrations of the crystal lattice of the detector. The intensity of the dark field depends on the exposure time and its values are superimposed on the LEED image pixel values. The correction procedure consists of subtracting the dark field from the image intensities. The dark field intensity values are obtained by the averaging of two images taken under the closed objective before and after taking the LEED pattern images.

Additionally, the individual pixels of the CCD arrays are not perfect and may differ from each other in their properties. When taking the image of a uniform white object, we generally get different intensities from pixel to pixel. This is also caused by the defects of a camera objective. The corresponding image is called *the flat field* [4]. The flat field causes nonuniform multiplication of the pixel values in LEED images. Hence, the corrections of these imperfections are made by dividing the image pixel values by the normalised flat field pixel values.

2.2. Localisation of diffraction spots

After these corrections the diffraction spots in a LEED image are to be distinguished from the background. The typical spot sizes range from 15 to 20 pixels (of 512×512 pixels in total). The background is diffuse and it is difficult to characterise it mathematically. In addition, we cannot easily fit the spot profiles by analytical curves and the spot pixel values can extend over the whole range of possible intensity scale. Hence, there is no straightforward procedure for finding the spots without the intervention of the user. This process consists either in denoting each spot manually or, in setting the 2D lattice periodicity, which enables the program to find all the spots automatically. Once the spots are located, their positions can be traced automatically in subsequent pictures of the *I–V* series because the spots "move" in small steps towards the screen centre for increasing electron energies (2 eV- steps).

The position of a diffraction spot is defined by coordinates of the pixel with the highest value within the area of the spot. However, more pixels with this value might actually be found there. Therefore, we determine the position of the spot as the first moment of the area occupied by pixels with these highest values. CCD cameras also produce the spike noise due to bad pixels in the detector array. This noise is apparent from the presence of pixels with very high or very low values and must be filtered out, otherwise the centre of the spot is determined incorrectly. Filtering is done by finding the exceptional values and by replacing them with the average value of the surrounding pixels.

2.3. Subtraction of the background

To remove the background from spot intensities, it is necessary to estimate its intensity profile in each diffraction spot. Therefore, each spot is surrounded by a delimiting square centred to the position of the spot and the background intensity in the spot is approximated from the pixel values on the spot boundary. It is important to make the spot boundaries as small as possible to avoid considerable errors in background subtraction and, consequently, in the evaluation of the spot intensities. One can use several methods for the approximation of background intensities. These methods are briefly described below:

2.3.1. Approximation by average value on the border

The method assumes that the background intensities are constant within the spot area [5]. The value of the background is defined as the arithmetic average of pixel values along the border of the delimiting square. This value is then subtracted from each pixel value within the spot area.

2.3.2. Approximation by average value on the border of the quadrants

This method is used by many authors [2,6]. The spot is delimited by a square of odd width value (in number of pixels). The square is then divided into four quadrants. In each quadrant we again assume a constant background. We calculate the arithmetic average of the pixel values along the outer border of every quadrant. This value is then subtracted from the pixel values within the corresponding quadrant.

2.3.3. Approximation in rows and columns

Here, a background, the intensity of which changes linearly either in rows or columns is assumed. The intensity values of pixels lying in a row (column) connecting two opposite border pixels are then given by linear interpolation between the values of those two pixels [7].

2.3.4. Approximation by a 3D surface

This method interpolates the background values by two-dimensional quadratic forms with boundary conditions given by the border pixel values. In this work two different forms were used:

$$B(i,j) = a_0 + a_1 i + a_2 j + a_3 ij \quad \text{(4-coeff.)}$$

and

$$B(i,j) = a_0 + a_1 i + a_2 j + a_3 ij + a_4 i^2 + a_5 j^2 \quad \text{(6-coeff.)},$$

where $B(i,j)$ is the background value, i and j are pixel coordinates. The coefficients $a_0 \ldots a_5$ in these formulae were evaluated by a least-squares method.

2.3.5. Expansion of minimum

The pixel values on the border of the delimiting square are considered as the background values. Hence, one can let them expand into the area of the diffraction spot. This was done by the convolution filtering of image pixel values. A square of 3×3 pixels was taken as a filter. Within this square around a processed pixel, the minimum pixel value was found and taken as the background value in the processed pixel. This must be done several times to let the values from the border expand to the centre of the spot area. The number of repetitions depends on the width of the square delimiting the diffraction spot [8].

2.4. Determination of the spot intensities and corrections to the experimental conditions

When the background is subtracted, the total intensity of the diffraction spot is calculated by the summation of pixel values within the spot area.

After that, the spot intensities have to be corrected to the experimental conditions. This includes corrections to the varying distances of spots on the hemispherical screen from a CCD chip, to the dependence of light emissivity on the angle of observation (Lambert's cosine law) and to the variation of electron beam current with energy. These corrections are not discussed in the paper. More information can be found in the literature [9,10].

3. Testing of the methods and comparison of the results

To compare the different methods of background subtraction, a series of test images was prepared. Each image of size 300×300 pixels consisted of a diffuse background with two superimposed artificial spots of known intensity. The spots had, approximately, a Gaussian intensity distribution and included a noise signal. The position of the spots "moved" on the background from one image to another in steps of two pixels from the margins of the screen to its centre, similarly to a real LEED experiment (see above).

In the test the whole series of images by all the background subtraction methods described above was processed. The test included centering the delimiting squares to the pixels of maximum value in the spots—i.e. finding the spot positions, and comparison of average intensity values of the spots and their dispersions achieved by different background subtraction methods. The influence of the width of the delimiting squares was studied as well.

In Table 1, the average intensity values of two spots and their dispersions in the whole testing series of images processed by different background subtraction methods are compared. As the intensity in each testing spot was 5143, one can see that the method of expansion of the minimum included the biggest error. In this method, the total intensity was shifted to higher values as a result of positive values in the spot pixels after subtraction of the background. Hence, the expansion method needs a very accurate determination of the spot border. The approximation by a 3D surface (6 coefficients) was also rather different from the exact value. The two averaging methods possessed higher dispersions of intensities due to very low negative and very high positive values of pixels on the border and in the corners of the delimiting square. The best results were achieved by the method described above as approximation in rows.

After the test on the artificial series, the background subtraction methods were tested on the

Table 1
Comparison of the results of background subtraction methods applied on a testing series of artificial images

Method	Spot 1		Spot 2	
	Average intensity	Dispersion	Average intensity	Dispersion
Average on the border	5284	86.3	5106	93.0
Average on the quadrants	5023	52.9	5098	34.8
Approximation in rows	5118	30.8	5129	20.6
Approximation in columns	5149	24.9	5057	23.4
Approximation by surface (4 coeff.)	5130	24.5	5089	17.0
Approximation by surface (6 coeff.)	4950	22.4	5041	53.9
Expansion of minimum	6105	49.9	5750	176.9

real diffraction images of an Al(1 1 1) surface structure. The corresponding LEED experiment was carried out in cooperation with the group of D. L. Adams at Aarhus University. The series of 300 images taken for an electron energy interval of 50–350 eV was processed by all the individual background subtraction methods discussed above.

The standard full-dynamical calculations [9] were applied to five *I–V* curves corresponding to five symmetrically non-equivalent spots [(0 1), (0 −1), (−2 1), (0 2), (0 −2)]; each of them was obtained by averaging the *I–V* curves over symmetrically equivalent spots. Electron damping energy V_{im} as well as the *R*-factor (the normalised sum of squares of differences between the calculated and measured intensities) were defined in the same way as published by Adams [9].

In Fig. 1, the individual *I–V* curves for the (0 1) spot obtained by three different background subtraction methods are shown. The highest curve in the figure was achieved by the method of expansion of minimum. The other curves in the figure belong to the approximation by a 3D surface (6 coefficients) and the approximation in rows. Processing the images by the application of the remaining methods (both averaging methods, approximation in columns, and approximation by a 3D-surface—4 coefficients) gave us nearly identical curves to that obtained by the approximation in rows.

In Table 2 the calculated structural parameters (d_1, d_2, d_3—inter-planar spacing between first, second and third layer, resp.; u_1,u_{bulk}—1st layer- and bulk-vibrational amplitude, resp.), inelastic damping energy V_{im}, and the total *R*-factor are compared. One can see here that, in accordance with expectations (resulting from their very similar *I–V* curves), the first four background subtraction methods lead to equivalent results which are in agreement with those published by Nielsen et al. [10]. Contrary to that, the approximation by expansion of minimum (the highest curve in

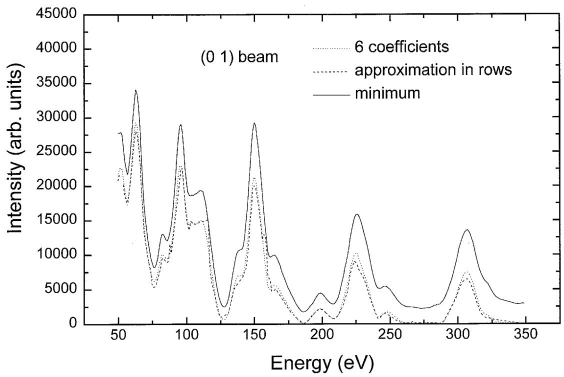

Fig. 1. *I–V* curves for the (0 1) diffraction beam of the Al (1 1 1) surface structure obtained by three different background subtraction methods.

Table 2
Comparison of the structural parameters of Al(1 1 1) surface structure calculated from *I–V* curves obtained for 6 different background subtraction methods

	Border	Quadrant	Rows/columns	4 coefficients	6 coefficients	Minimum
d_1^a	2.36	2.36	2.36	2.36	2.36	2.34
d_2^a	2.32	2.32	2.32	2.32	2.33	2.28
d_3^a	2.35	2.35	2.35	2.35	2.34	2.39
u_1^b	0.16	0.16	0.16	0.16	0.17	0.02
u_{bulk}^c	0.08	0.08	0.08	0.08	0.09	0.002
V_{im}^d	5.3	5.2	5.2	5.1	4.9	5.7
R^e	0.024	0.023	0.023	0.022	0.036	0.059

[a] d_1, d_2, d_3—the interlayer spacings.
[b] u_1—vibrational amplitude of the first layer.
[c] u_{bulk}—bulk vibrational amplitude.
[d] V_{im}—electron damping.
[e] *R*—the total *R* factor (normalised sum of squares).

Fig. 1) gives unacceptable values of the vibrational amplitudes and a higher *R*-factor. The approximation by a 3D surface (6 coefficients) gives us values which differ from those obtained by the first four methods and by Nielsen et al. [10] within the accuracy limits. By comparison of these results with those achieved on the series of artificial images one can say that the expansion of minimum does not give reasonable results and the approximation by a 3D surface (6 coefficients) is too complicated. Hence, they are not recommended for application in LEED. The other methods all give approximately the same results. Therefore, it is recommended to choose as simple a method as possible, i.e. the approximation in rows or in columns.

4. Conclusions

Comparing the application of several background subtraction methods in the test series of artificial images and a series of real diffraction images of an Al(1 1 1) structure, the methods of averaging on the border, averaging on the quadrants, and approximation in rows/columns were found to be equivalent and gave realistic results. Due to its simplicity, the approximation in rows/columns is recommended for application in LEED. On the other hand, the approximation by expansion of minimum provided unacceptable results for vibrational amplitudes, as well as a higher *R*-factor.

Acknowledgements

This work was supported by GAČR under Grant No. GA390781 and GA39K009, by the Grant No. ME 334 (MSMT ČR) within the Czech-US exchange programme, and by the programme TEMPUS. We would also like to express many thanks to Dr. D.L. Adams for permitting us to carry out the experiments in his lab and for lending us his computer code for dynamical LEED calculations.

References

[1] Pendry JB. Low energy electron diffraction. London: Academic, 1974.
[2] Van Hove MA, Weinberg WH, Chan CM. Low-energy electron diffraction. Berlin: Springer, 1986.
[3] Roučka R. Determination of solid surface structure—experimental, diploma thesis. Brno: Brno University of Technology, 1998 [in Czech].
[4] Buil Ch. CCD astronomy: construction and use of an astronomical CCD camera. Richmond: Willmann-Bell, 1991.
[5] Guo T, Atkins RE, Ford WK. Rev Sci Instrum 1990;61:968.
[6] Toofan J, Watson PR. Rev Sci Instrum 1994;61:3382.
[7] Lang E, Heilmann P, Heinz K, Müller K. Appl Phys 1976;9:247.
[8] Russ JC. The Image Processing Handbook. Boca Raton: CRC Press Inc., 1995. p. 187.
[9] Adams DL. Appl Phys 1996;A 62:123.
[10] Nielsen MM, Burchhardt J, Adams DL, Lundgren E, Andersen JN. Phys Rev 1994;B 50:4718.