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Cross-correlation method for intensity measurement of transmission electron diffraction patterns

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Abstract

This paper describes a method of intensity measurement of diffraction spots from digitized negatives using cross-correlation. The method is highly robust against noise and diffuse background in the diffraction pattern; therefore intensities of very weak spots such as those due to a reconstructed surface can be measured accurately. The reliability of this method and the implication for a quantitative structure analysis by transmission electron diffraction are discussed.

1. Introduction

In order to solve a surface structure using transmission electron diffraction, accurate measurements of intensity values of surface spots are essential [1,2]. Traditionally, the intensity of a diffraction spot is found by integrating the total counts around the spot. However, this method is no longer accurate when the diffuse scattering in a diffraction pattern cannot be properly modelled and subtracted. The low signal to noise levels of the surface spots also make the measurement difficult, since the intensity levels are of the order of 10^{-4} of the incident beam or smaller [3].

The success of correlation techniques in quantitative analysis of transmission electron microscopy images is well established [4,5]. In this paper, we show that by using a correlation method, individual diffraction spots from a Si(100)-2×1 transmission electron diffraction pattern are well fitted against a motif spot and the peak counts are thereby extracted. We demonstrate that the correlation method is robust for weak spots with a strong diffuse background. The accuracy of the technique is evaluated through test images.

2. Techniques

A clean 2×1 reconstructed surface of silicon (100) was prepared by ion-beam sputtering and annealing in the side chamber of the Hitachi UHV-H9000 microscope [6]. Diffraction patterns were recorded onto negatives with a series of exposures from 4 to 60 s to cover the large dynamic range of the surface as well as bulk spots, e.g. Fig. 1a. The negatives were digitized to 8-bits using an Optronics P-1000 microdensitometer. A calibration experiment was carried out to determine the relationship between the digitized count and the electron dosage on the negative

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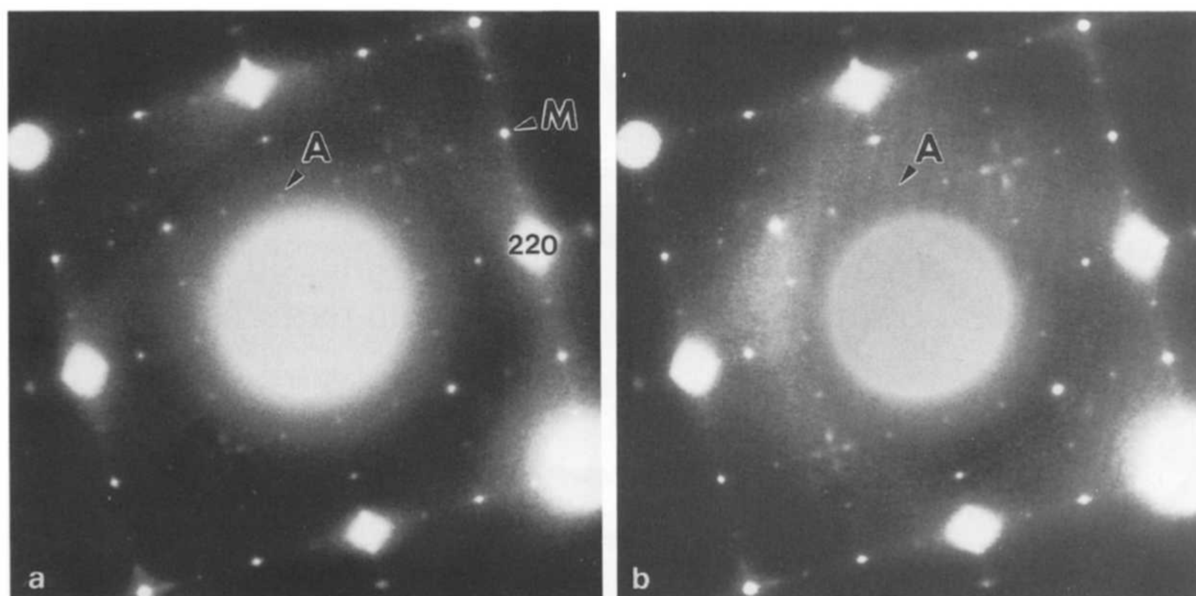

Fig. 1. (a) Selected area diffraction pattern from a Si(100)-2 × 1 reconstructed specimen. (b) The (1 × 1) spot marked "A" in (a) was removed using the correlation method, leaving the background undisturbed. Both images were recorded from the computer screen. They were dodged during printing, so the appearance is slightly different.

using a Faraday cup in the microscope for beam current measurement. The plot in Fig. 2 shows that it is linear, with one count equivalent to 14 electrons. The standard deviations of the digitized counts were also determined and indicated by error bars in the plot.

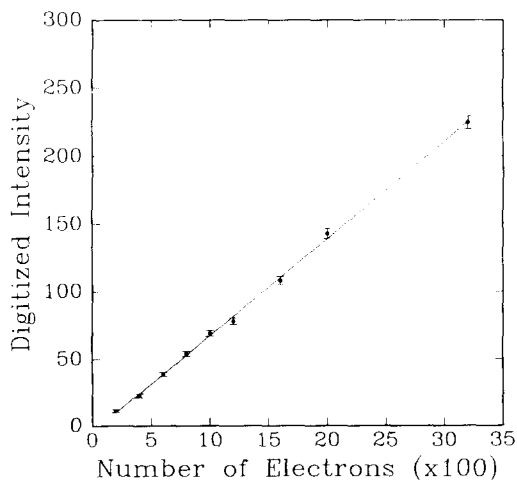

Fig. 2. The digitized intensities by the microdensitometer were calibrated against the electron dosage on the negatives. It is linear in the range used herein with one count equivalent to 14 electrons. Scans were from a 100 × 100 pixel area of the negatives.

The digitized patterns were processed using Semper software. To build a motif image for cross-correlation, a number of diffraction spots (eight in this case), such as those marked "M" in Fig. 1a, with relatively strong intensity and low background were selected. They were cross-correlated, averaged and normalized to form the final motif, which has a total integrated intensity of unity. The motif image was then correlated locally with the spot of interest and the intensity of the spot was evaluated accordingly from the match. In fig. 1b, the (1 × 1) spot marked "A" was removed by subtracting the matched peak from the original (Fig. 1a). The background intensity around the spot is seen to be undisturbed, as is also shown clearly in the line scans of Fig. 3.

Numerical calculations were performed to determine the error in the peak intensity value using cross-correlation technique when noise (assuming a Poisson counting noise) is present in an image. Gaussian peaks were used as a test and

Poisson noise was added to the images. They were correlated with a standard Gaussian (no noise), and the intensity values were obtained. This process was repeated several hundred times to establish a statistical distribution. The square of the standard deviation of the intensity was found to be linear with the peak intensity, $\sigma^2 = 0.025I$, as shown in Fig. 4. (Tests done with peak shapes other than a Gaussian, for example a Lorentzian, showed the same relationship.) The result is significant because when this error estimate was used for the intensity values in silicon (100)2×1 surface structure minimizations, a χ^2 of ~ 1 was obtained which indicated that the error estimate was appropriate [6].

The correlation technique is limited to the case where a diffraction spot is adequately sampled, i.e. at least 4 pixels are required to sample the half peak width. We are currently limited by the lateral scan resolution of 25 μm on the microdensitometer. This implies that a diffraction pattern with a well defocused illumination may need to be avoided, although it contains sharper spots [7] and is aesthetically appealing. An alternative is to use a larger camera length, but the information from the large angle scattering (which is critical for structure determination [6]) will be lost from the negative.

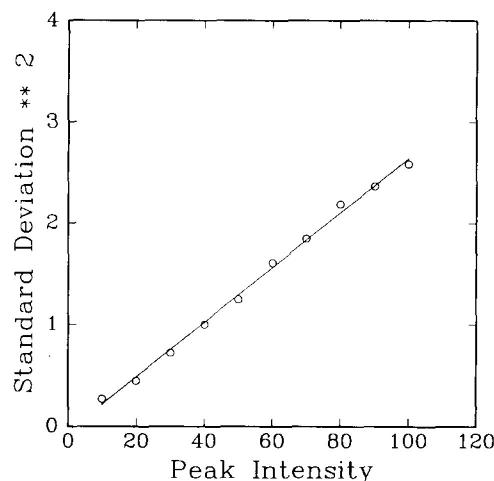

Fig. 4. This plot shows that the square of the standard deviation for the peak count is linear with the peak count, when a clean Gaussian peak is correlated with Gaussians with Poisson noise.

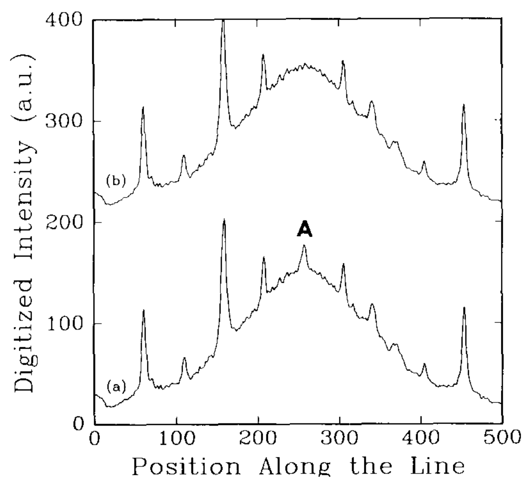

Fig. 3. Line scans from Figs. 1a and 1b showing the clean removal of the (1 × 1) spot marked "A".

One point is worth making with regards to the sensitivity of the negative recording/digitizing method; in this experiment, a conversion of 14 electrons to a count was obtained when an optical density of 2 was selected as the range for the microdensitometer. If instead an optical density of 1 is used, a digitized count will correspond to about 7 electrons; further improvement can also be achieved with the use of faster film. It would appear then that the sensitivity of this technique would be comparable with that of a slow-scan CCD (2 electrons/count) [8].

3. Conclusions

A cross-correlation method was used for obtaining intensity values for surface diffraction in a transmission electron diffraction pattern. The method is robust against the streaking and diffuse scattering and is able to extract intensity values for very weak spots. (While the diffuse scattering due to the plasmons can be removed through the use of an energy filter, the thermal diffuse scattering which is most significant at higher angles [9] cannot be removed.) With a set of multiply

exposed diffraction patterns, intensity values of weak spots can be evaluated from a long exposure negative, the strong spots from a short exposure, and a range of intensity of at least three orders of magnitude can be determined accurately. Coupled with the absolute intensity measurement using electron energy loss spectrometry [3], this can provide a large and accurate data set for quantitative structure determination.

4. Acknowledgement

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5. References

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