Enhancement of STM images and estimation of atomic positions based on maximum entropy deconvolution

S.D. Böhmig *, M. Schmid, H. Störi

Institut für Allgemeine Physik, Technische Universität Wien, A-1040 Wien, Austria

(Received 3 January 1994; accepted for publication 18 February 1994)

Abstract

A new method for restoration and sharpening of scanning tunneling microscopy (STM) data is presented. According to the STM theory of Tersoff and Hamann it is assumed that the response of the STM can be approximated by the convolution of a localized atomic density of states of the sample and a Gaussian, which limits the resolution. Therefore, one must find the solution of an inverse problem, which is done by minimizing the mean square deviation between the measured and the reconstructed image using entropy as a regularization functional. This nonlinear method is shown to be superior to linear filters such as the Wiener filter in that the solution carries as minimal information as is necessary to fit the data and is not constrained to low frequencies. On metals, where atomically resolved STM images show mainly geometrical information, the centers of mass of the resulting peaks are taken as the atomic positions which are compared to those estimated visually from the STM images. The method has been applied to both the periodic Cu(111) surface and to the nonperiodic shifted row reconstruction of Pt_{10}Ni_{90}(100).

1. Introduction

The resolution of scanning tunneling microscopy is limited by the tunneling process itself, which is mainly determined by the overlap of tip and sample electronic waves [1,2]. As the lateral resolution of a STM cannot exceed this limit, further enhancement can be done via processing of the STM data only. This approach has its main applications in atomically resolved STM images of metals, where the data represent mostly geometrical information, unless special tip–sample interaction mechanisms, [3] corrugation reversal [4] or effects of adsorbates [5,6] occur.

Assuming an s-wave tip and Bardeen's approximation, Tersoff and Hamann have shown that the resolution of a scanning tunneling microscope operated in constant height mode can be described by a Gaussian resolution function [1]. This approach is limited to tip–sample distances, where tip and sample are sufficiently far apart to be considered independent, which is certainly not the case in atomically resolved imaging on metals. Nevertheless, due to lack of a more precise analytical description we use a Gaussian resolution function also for closer tip–sample distances, but we cannot employ the width of the Gaussian given by Tersoff and Hamann. We should mention, however, that the method presented in this article is not restricted to Gaussian resolution functions. If a more accurate description of a
convolution kernel describing the imaging process in STM is available, it could be also used in place of the Gaussian assumed here.

We should also note that the STM theory mentioned above applies to constant height measurements, whereas our experimental data are constant current topographs. If the corrugation is sufficiently low (≈ 10 pm), we may assume a linear relationship between current and height and therefore also apply a Gaussian resolution function to constant current topographs. Whereas this condition is not fulfilled in images containing more than one terrace level (i.e. steps) on a single crystal surface, the use of constant current topographs is justified for analysis of reconstructions with low corrugation.

The data acquisition process is then described by the following discretized linear operation

$$d(x, y) = G(x, y) * f(x, y) + b(x, y),$$

(1)

where d are the measured data, f are the unknown parameters which are convolved with the Gaussian kernel G and b denotes the noise term. Eq. (1) can be transformed into a system of linear equations:

$$d = Af + b,$$

(2)

where d, f and b are vectors of size n (i.e. the number of measurement points) containing the pixels in an arbitrary order; matrix A is derived from the Gaussian G. Due to noise and the inaccuracy of the model, the estimation of a unique and stable solution \( \hat{f} \) (or \( \hat{f} \)) is generally a nontrivial task and cannot be obtained directly by inverse filtering with \( \hat{f} = A^{-1}d \).

Deconvolution or deblurring problems with respect to the restoration of STM images have been discussed for a long time [7–11]. Pancorbo et al. [7] model the interaction tip–sample utilizing a point spread function (i.e. the convolution kernel) based on Stokseth [12] in analogy to defocused optical systems with a circular aperture. Deblurring is carried out by means of the Wiener filter, which aims at minimizing the mean square deviation between the real parameters f and the calculated estimation \( \hat{f} \), averaged over the random parameters. Here, parameters f as well as b are considered to be statistically independent, spatially homogeneous random fields. The spectrum of the noise in STM images is generally assumed to be a function of frequency u according to a \( 1/u^\beta \) law, where \( \beta \) denotes a parameter near 1 [13,10]. These works demonstrate a high improvement of the image quality regarding the suppression of noise and the elimination of correlations between consecutively measured pixels. However, two problems arise with this type of filtering: First, not only the noise spectrum but also the spectrum of the true parameters f has to be estimated a priori, which might be difficult. Second, the Wien filter is essentially a low-pass filter thus constraining the amount of sharpening whereby the cut-off frequency decreases with the amount of noise in the higher-frequency portions of the spectrum. Important information in f should therefore mainly be located in the low-frequency part of the spectrum. As a consequence of this, oscillations or “ringing” effects are introduced in the vicinity of sharp changes in the intensity of the images [14]. Summarizing, these characteristics make it unfeasible to deconvolve noisy STM images with Gaussians with width in the range of the depicted atoms, which should result in narrow and thus high-frequency peaks. Nonlinear techniques have been proposed to circumvent similar problems [14–16]. Weisman et al. [9] demonstrate the superiority of the morphological pseudoconvolutions technique over the Wiener filter in suppressing noise and the preservation of edge and texture information inside STM images. It is a local technique operating in the image domain which starts from the mean- or median-filtered image and adds high-frequency portions (edges, texture), calculated by means of morphological operators, to the result [17]. Its drawback is that it is more an enhancement technique than a restoration filter based on a mathematical model of the underlying acquisition process. Similar results were obtained in a comparative study in the case of scanning Auger images [18].

Maximum entropy is a fundamental nonlinear technique for the solution of inverse problems in different fields of research, like image processing, radio astronomy or tomography [19–21]. Two as-
sets make this method very suitable for the problem under discussion: First, it imposes positivity on the resulting image $\hat{f}$, and second it was shown to be the only method to give the result which has theoretically just enough structure to fit the data and no more [22,23].

In this paper we solve the inverse problem of Eq. (1) with the maximum entropy approach [24]. After deconvolving the measured data we extract the maxima of image $f$ and then – starting from these initial positions – calculate the centers of mass of the peaks of $f$. If the selected point-spread function is adequate and our previous assumptions about STM imaging are valid, these positions, which are the maxima of the local density of states, can be taken as atomic core positions in the two-dimensional image plane.

Further processing of these data can be used to determine more detailed information of the atomic structures investigated. Based on the atomic core positions derived from deconvolved STM data, we have measured the distances between rows of atoms on a reconstructed surface by first fitting parallel lines through the atomic positions in the direction of the rows and then estimating their exact positions.

All calculations were performed on a DEC-5000/240 workstation utilizing the public-domain image processing package KHOROS [25,26] and the maximum entropy library MEMSYS-5 [27], which was incorporated into KHOROS to perform the actual deconvolutions. Most of the used algorithms (such as the Hough transform) are part of KHEROS.

2. Theory and computational methods

2.1. Maximum entropy deconvolution

Due to the noise term or incomplete information, Eq. (1) is not solvable exactly by direct mathematical inversion. Instead there will exist a set of feasible solutions $\hat{f}$ all consistent with the observed data (i.e. solutions that fit the data), from which the “best” one has to be selected by taking into account available prior knowledge. The simplest and most convenient choice to measure the misfit between the data and the reconstruction is the chi-squared statistics

$$\chi^2 = \frac{1}{\sigma^2} (d - A\hat{f})^T (d - A\hat{f})$$  \hspace{1cm} (3)

in the case of uncorrelated Gaussian noise with zero mean and variance $\sigma^2$. On average $\chi^2$ may be expected to take a value close to the number of measured data points $n$. The feasible set of solutions is then defined by imposing a constraint $\chi^2 = \chi_0^2$ on the solution from which we select the vector $\hat{f}$ that maximizes a function $S(f)$ [24]. $S(f)$ is a norm defined in the parameter space and should comprise any available a priori knowledge on the solution. Using the method of Lagrange multipliers, the calculation of $\hat{f}$ is carried out by minimizing the functional

$$J_{\alpha}(f) = \frac{1}{2} \chi^2 - \alpha S(f),$$  \hspace{1cm} (4)

where constant $\alpha$ is the regularization parameter.

Selecting $\alpha = 0$ in Eq. (4) we obtain the maximum likelihood solution or the least-squares fit, which results in fitting the noise. Another approach assumes

$$S(\hat{f}) = -\frac{1}{2} \sum_{u,v} |\text{Fou}_f(u, v)|^2 / |\text{Fou}_f(u, v)|^2.$$  \hspace{1cm} (5)

The solution of Eq. (5) can be obtained directly in the Fourier domain and corresponds to the above mentioned Wien filter for $\alpha = 1$ and a constant noise level ($\text{Fou}_f$ and $\text{Fou}_f$ are the Fourier transforms of the estimated and the true parameter images, respectively) [15].

To obtain the maximum entropy solution, $S$ is set to the generalization of the entropy

$$S(\hat{f}) = \sum_i \left[ \hat{f}_i - m_i - \hat{f}_i \log(\hat{f}_i/m_i) \right],$$  \hspace{1cm} (6)

where the indices $i$ denote the cells of the vectors, i.e. the pixels of the image. The maximum of $S$ is at $\hat{f} = m$ (where $S = 0$), which gives $m$ the meaning of an initial model or premodel, to which $\hat{f}$ defaults in the absence of constraining data or if $\alpha = \infty$. The logarithm imposes positivity on the parameters. Skilling et al. [22] demonstrate that maximum entropy is the only method to select a hypothesis from a set of feasible ones which gives
sensible results in simple cases, in that the solution carries as minimal information as necessary to fit the data and without introducing any additional structure or artefacts. A mathematical derivation of the principle based on four axioms is given in Refs. [24,22].

Since the default model $m$ comprises the prior knowledge on the solution, a careful selection seems essential. We can model the image as a superposition of the “interesting” features and an underlying background with e.g. slowly varying intensity representing the gross structure of the image. If the background is homogeneous, a flat premodel with a constant level $m_0$ seems to be justified, otherwise the reconstruction is known to be troublesome [28,29] and “ringing” effects or artefacts near abrupt changes in the background (edges or texture) may result. In the case of the STM images discussed in this work we have already excluded the deconvolution of constant current topographs with large height variation (e.g. steps) for other reasons and, therefore, such artefacts do not occur. The overall structure of these images (after subtraction of a linear background) is essentially flat, allowing to use the least committing flat premodel.

From the probability theory point of view the problem of inversion is viewed as one of seeking to find the hypothesis $\hat{f}$ which maximizes the unknown conditional posterior probability density $Pr(\hat{f} \mid d, \alpha, m)$ (i.e. the inference) of $\hat{f}$ for a given data vector $d$ [30,23]. This function is not known, however, what we do have is the Gaussian likelihood of the data $Pr(d \mid \hat{f})$ given by

$$Pr(d \mid \hat{f}) \propto \exp(-\frac{1}{2} \lambda^2)$$

and the prior probability $Pr(\hat{f} \mid \alpha, m)$ of the hypothesis based on the maximum entropy principle

$$Pr(\hat{f} \mid \alpha, m) \propto \exp(\alpha S(\hat{f})).$$

In order to reverse the conditioning from the likelihood to the required inference, the theorem of Bayes [31] is used to get

$$Pr(d \mid \hat{f}, \alpha, m) = Pr(\hat{f} \mid d, \alpha, m)Pr(d \mid \hat{f}) / Pr(d),$$

where $Pr(d)$ is the prior probability density or evidence of the measurements which is assumed to be uniform in the range of the data. Hence, we get

$$Pr(\hat{f} \mid d, \alpha, m) \propto Pr(\hat{f} \mid \alpha, m)Pr(d \mid \hat{f}).$$

As can be seen, maximizing $Pr(\hat{f} \mid d, \alpha, m)$ with respect to $\hat{f}$ is equivalent to minimizing Eq. (4). To obtain the value of level $m_0$ of a flat premodel $m$, the maximum of the posterior distribution $Pr(m_0 \mid d)$ is derived at the mean of the hypothesis (which is at average equal to the mean of the data, since $G$ is normalized to one and the noise has zero mean) in the Gaussian approximation of $\hat{f}$ [24]. The remaining parameter $\alpha$ can either be adjusted manually so that the solution seems best from the optical point of view, or the theoretically best value is selected by maximizing the posterior probability density $Pr(\alpha \mid d, m)$ of $\alpha$ as described in Ref. [24]. In our work, the latter method has been employed.

As already mentioned, the hypothesis $\hat{f}$ is constrained to positive values, which is certainly a meaningful assumption if the deconvolution should result in an electronic density. With the assumptions already mentioned in the introduction, the tunneling current in constant height mode can be directly used as input of the deconvolution. Our experimental data, however, are constant current images, which have an arbitrary offset. Assuming a dependence of the tunneling current $I$ on tip height $z$ according to [1,2]

$$I = I_0 e^{-2\kappa d}$$

with

$$\kappa = \sqrt{\frac{2m_e \Phi}{\hbar^2}},$$

one can easily show that the tunneling current in constant height mode is approximately proportional to the height $z$ in constant height mode for small corrugations as long as the height is near

$$z_0 = \frac{1}{2\kappa} = \sqrt{\frac{\hbar^2}{8m_e \Phi}}.$$

In practice, the apparent barrier height $\Phi$ and, hence, the offset $z_0$ cannot be easily determined: At close tunneling distances, $\Phi$ is substantially
lower than the work function of the tip and sample [32] and cannot be easily estimated theoretically, furthermore, experimental determination of \( \Phi \) by measuring \( dI/dz \) would add additional problems to the already difficult task of obtaining good atomically resolved STM images on a metal. Fortunately, our results show that the maximum entropy deconvolution is not sensitive to the offset and works well as long as \( z_0 \) is chosen somewhere in the range between a value somewhat larger than the corrugation of the image and an upper limit in the order of 100 pm.

### 2.2. Estimation of the atomic positions

The resulting hypothesis \( \hat{f} \) will presumably not exhibit perfect peaks at the centers of the atoms but broadened or weak ones with locally varying intensity. Therefore, the positions cannot be extracted by means of a simple thresholding technique which classifies all pixels above a certain threshold as an atomic position. We have developed a simple but robust method, which comprises two steps: First, all local maxima of \( \hat{f} \) are extracted. This is done by applying a gray-scale morphological operation [17], namely a dilation, with a disc-like structuring element of diameter \( l \). If \( D(x, y) \) is the support or domain region

\[
D(x, y) = \begin{cases} 
1, & x^2 + y^2 \leq l^2 / 4, \\
0, & \text{else},
\end{cases}
\]

(14)

dilation of image \( \hat{f} \) is the operation

\[
(\hat{f} \oplus D)(x, y) = \max_{D(i,j) \neq 0} \{ \hat{f}(x + i, y + j) \}.
\]

(15)

Correspondingly, each pixel \( \hat{f}(x, y) \) is set to the maximum gray-level in a neighbourhood specified by the support \( D \). Only peaks with no stronger peak nearer than \( l \) pixels are expanded to the size of \( D \), whereas the remaining peaks are not fully expanded and can accordingly be identified and excluded from further processing. This gives the parameter \( l \) the natural interpretation of the minimal distance between two atomic positions present in the measured data. The centers of all fully expanded peaks serve as a first estimate of the required positions. In a second refinement step the final locations are determined by calculating the centers of mass in a neighbourhood equal to or smaller than \( l/2 \) of these positions on the gray-levels of \( \hat{f} \).

### 2.3. Estimation of row distances

If the distances between rows of atoms in STM images, which exhibit an ordered structure, are of interest, a consistent and robust method for their estimation seems essential. It is a straightforward approach to first fit straight parallel lines through the atomic positions of each row and then measuring the distance between such lines. The Hough transform is a common tool in the field of image processing to detect parametrized geometric features such as lines, circles etc. in images [14]. Through each location \( (x, y) \) in the image an infinite number of lines can be fitted. If these lines are for example represented in their normal form, the possible sets of parameters form a curve in the two-dimensional parameter space \((\Theta, \rho)\) given by

\[
x \cos \Theta + y \sin \Theta = \rho.
\]

(16)

The corresponding curves in parameter space of locations, which are all positioned on the same line, will cross at a single point or at least very close depending on the discretization of the parameters. The Hough space is then defined as the accumulation over all curves into so-called accumulator cells \((\Theta_i, \rho_i)\). Since we are only interested in lines in a certain direction, all cells in the Hough space except those corresponding to the direction of the rows \( \Theta_r \) are set to zero. Applying the inverse Hough transform we get an image consisting of parallel lines through the atomic positions. Next, we draw a cut through this image orthogonal to the resultant lines and for each peak calculate the center of mass as a measure of the row position.

### 3. Results

Fig. 1 shows an atomically resolved constant current topograph of a Cu(111) surface of size \( 256 \times 256 \) pixels. Due to a change in tip structure, the upper part exhibits less corrugation than the
lower part, therefore, we can use this image to study the results of our enhancement technique with different signal-to-noise ratio.

The best results of the maximum entropy deconvolution were obtained with an elongated Gaussian ($\sigma_x = 134$ pm, $\sigma_y = 90$ pm) and are shown in Fig. 2. Sharp peaks can be discerned at most of the atomic positions, however the sharpness significantly decreases in the upper part of the image as a consequence of less contrast. Nevertheless, there is a good coincidence of the atoms and the estimated atomic positions even in these areas from the optical point of view (see Fig. 1). In the region where the tip changes some stronger deviations regarding the atomic positions can be discerned for the part in the image with less corrugation. This results from the fact that the model of Eq. (1) does not properly cover such effects. Another consequence of the tip change can be seen. If one looks along the rows from upper left to lower right, the points line up very well. However, if one looks along a different direction, the rows in the upper and the lower parts of the image are misaligned. In other words, the tip change did not only reduce the corrugation but it also leads to some offset between the two half images, which may be due to lateral displacement of the foremost (imaging) tip atom.

It should be noted that the border areas of the processed images are subject to errors inherent to implementation details of the maximum entropy method. A close inspection of the positions superimposed on the raw data reveals that the calculated positions are – at average – slightly shifted up relative to the centers of the atoms (~ 1 pixel). This is due to an asymmetric form of the atoms (areas with somewhat lower intensity below each atom) caused by asymmetric tip shape. One solution to this problem is to select a more proper point-spread function which accounts for the asymmetry, another is to uniformly add an offset to the calculated positions. As we are only interested in the random errors of atomic positions as caused by noise in STM data, the shift was eliminated by an offset.

Fig. 2. Deconvolution of Fig. 1 by means of maximum entropy with an elongated Gaussian kernel ($\sigma^2_x = 38$, $\sigma^2_y = 17$). Note the decrease in accuracy in the upper part of the image due to the lower signal-to-noise ratio in comparison to the lower part. White (black) corresponds to a high (low) pixel value in the image.
For comparison with maximum entropy results we have used an ideal lattice with the same atomic distances as in the STM image. Due to nonlinearity and drift of the tube scanner of the STM, the image is slightly distorted, especially in the lower parts. For further processing, this systematic error has been eliminated by transforming the extracted pixel positions with a second-order bi-polynomial based on reference points set manually, which then allows us to quantify the accuracy of the proposed method. The standard deviations $\sigma_\Delta$ (averaged over the standard deviations along the x- and the y-axis) of the shifts between the estimated and corrected positions $p_e$ and the non-discretized theoretical lattice points $p_t$ are approximately 0.66 and 0.96 pixels for the lower and the upper part of the image, respectively, corresponding to 6.1% and 8.9% of the surface lattice constant. Fig. 3 shows the superposition of the positions $p_e$ and $p_t$, the latter of which being marked by circles, for the upper and the lower part of the Cu image. From the upper left atoms of the lower image part a systematic displacement can be discerned which is due to drift of the STM not properly covered by the selected geometric transformation. We have intentionally excluded the region where the tip changes from these calculations, since we were interested in the accuracy of the method for different signal-to-noise ratios in undistorted areas only.

Due to the projection of the calculated positions $p_e$ on the image grid, the obtained distances are subject to discretization errors. The distance along any axis can be written as

$$\Delta = p_e - p_t = (p_e' + q_e) - p_t,$$

(17)

where $p_e'$ denotes the undiscretized position. $q_e$ is its distance to the next pixel center in the image and can take any value in the range of $-0.5$ and $0.5$ pixels with equal probability. We are interested in $\sigma^2(p_e' - p_t)$, which is the theoretical accuracy of the method if we had compared the estimated positions and the lattice points in the continuum. According to Eq. (17) this variance is given by

$$\sigma^2(p_e' - p_t) = \sigma^2(p_e - p_t) - \sigma^2(q_e)$$

(18)

and the variance of error $q_e$ is (operator $E$ gives the expected value of the expression)

$$\sigma^2(q_e) = E(q_e^2) = \int_{-0.5}^{0.5} x^2 \, dx = 0.08 \text{ (pixels}^2).$$

(19)

Subsequently, the standard deviations of the displacements in the upper and the lower region reduce to 0.59 pixels (5.4%) and 0.92 pixels (8.6%), respectively. The obtained accuracies seem to be very good if we consider that the atoms cover only approximately $12 \times 10$ pixels at this resolution and there are several distortions present in the image.

Fig. 4 is a constant current topograph of size $256 \times 256$ pixels of the (100) surface of a Pt$_{10}$Ni$_{90}$ alloy single crystal. This image was created from 128 $\times$ 128 pixels raw data by interpolating the added pixel values with cubic polynomials in a neighbourhood of 4 $\times$ 4 pixels (in the original data) in order to improve the accuracy of pixel locations in further processing steps. On this surface, a “shifted row” reconstruction is observed after sputtering and annealing around 800 K [33,34]. Several rows of atoms, which are shifted $\frac{1}{2}(110)$ along the direction of the rows into a
be discerned even in areas where the surface is contaminated by carbon [6] (dark areas in Fig. 4). Fig. 6 shows the 3D representation of a 128 × 128 pixel wide subregion of the raw data and of the corresponding maximum entropy deconvolution as an illuminated surface.

We have also experimented with Gaussians that are elongated in horizontal direction ($\sigma_x^2 = 70$, $\sigma_y^2 = 50$) and rotated by $4^\circ$, which seem to be more in accordance with the shape of the depicted atoms in some areas. In this case structures appearing smooth in Fig. 5 (e.g. next to the shifted rows) are now very sharp, and vice versa. To enhance the overall sharpness, we have therefore pixel-wise added these two images prior to the estimation of the atomic positions.

For comparative reasons we have also filtered the image by means of a Wien filter with a 1/μ noise spectrum (see Fig. 7). As expected the amount of deblurring is significantly less compared to the maximum entropy solution due to the limiting low-pass characteristic of this filter.

bridge position and slightly outward of the surface can be seen. As the difference in corrugation between the shifted row atoms and the other atoms is only between 10 and 20 pm, the use of a constant current topograph for deconvolution is justified. In contrast to the previous example, the shifted row reconstruction is a nonperiodic structure, where the exact atomic positions can be hardly determined by conventional techniques of surface crystallography, such as low-energy electron diffraction.

The variance $\sigma^2$ of the Gaussian point-spread function was selected in a range between 30 and 70 in order to test the dependence and stability of the results regarding this parameter. From the optical point of view setting $\sigma^2 = 50$ appeared to give the best i.e. most sharp or deblurred result, which is shown in Fig. 5. It did not change much when varying $\sigma^2$ and in a range of approximately 20% around the optimal value. Sharp peaks can
Fig. 4 shows the calculated atomic positions superimposed on the measured data, with minimum atomic distance \( l \) set to 9 pixels (i.e. 150 pm), which is far below the interatomic distance in the bulk (252 pm). Due to the strong decline in gray-level when moving away from the maximum of a peak in the deconvolution (approximately a factor 8–10 at 3 pixels off), parameter \( l \) can be decreased by several pixels without affecting the locations on the pixel scale. The distance between the shifted rows and their neighbouring rows, obtained with the Hough transform, is 0.98 ± 0.04 (standard deviation) of the surface lattice constant \( a_s \). To test the significance of this result we manually displaced the calculated positions by 7% of \( a_s \), corresponding to 1 pixel towards the shifted rows. It appeared that these positions do not match the STM image as well as those calculated. Thus it seems certain that the atoms between the shifted rows are close to the unreconstructed positions, which has interesting implications for the interpretation of the shifted row reconstruction [33].

An interesting question is whether the height information calculated from the original STM data can also be obtained from the deconvolution. Taking the model of the acquisition process (Eq. (1)) with a normalized Gaussian kernel and zero-mean noise the volume covered by single atoms is unaffected by the deconvolution process.

Fig. 6. (a) 3D-representation of a 128×128 pixel wide subregion of Fig. 4 and (b) the corresponding maximum entropy deconvolution. A shifted row can be seen in the middle of the images.

Fig. 7. Deconvolution of the atomically resolved image (Fig. 4) by means of a Wien filter with a \( 1/u \) noise spectrum (\( u \) denotes the frequency). As a consequence of the low-pass behaviour of this filter, the degree of deconvolution or deblurring is minimal and structures are only little sharpened.
This does not necessarily mean that the peak heights after deconvolution represent the height of the atoms. From the optical point of view, the relative heights among the atoms and among the deconvolved peaks seem to be in accordance (see Fig. 6), except in regions where the widths of the peaks are not uniform. Therefore, only integral information taken from a neighbourhood, which can easily be calculated automatically, should be used for further analysis.

4. Conclusions

Scanning tunneling microscopy images have been deconvolved using point-symmetric Gaussian kernels with halfwidth in the range of the size of the depicted atoms by means of the maximum entropy approach. The maximum entropy results exhibit sharp peaks at the atomic positions and are further processed to give an estimation of the corresponding coordinates. This very robust approach turned out to be significantly superior over the linear Wien filter with respect to the amount of deblurring. Experiments demonstrate that the results highly coincide with visually estimated positions in case of a point-symmetric shape of the measured atoms. An asymmetric shape causes the locations to be slightly displaced uniformly throughout the whole image which can easily be corrected manually. For a quantitative evaluation the maximum entropy solution was compared to an ideal lattice in the case of a Cu(111) surface. The achieved accuracy ranges between 6% and 10% of the surface lattice constant depending on the quality of the measurement. In contrast to many other methods of processing STM images (e.g. bandpass filtering), these results are obtained without any assumption of periodicity of the atomic arrangement. The main drawback of the maximum entropy approach is the high amount of processing time necessary (typically 40 min or more in case of 256 x 256 pixel images on a DEC-5000/240).

The resultant atomic positions can be used for further analysis of atomic structures. As an example, a Hough transform was employed to quickly and consistently estimate distances between rows of atoms in STM images of an ordered, but nonperiodic structure.

References


