

Blind estimation of general tip shape in AFM imaging

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ARTICLE INFO

Article history:

Received 21 April 2008
Received in revised form
18 July 2008
Accepted 1 August 2008

PACS:

82.20.Wt
83.85.Ns
87.64.Dz

Keywords:

Mathematical morphology
Dexel representation
Dilation
Erosion
Blind tip estimation
Atomic force microscopy

ABSTRACT

The use of flared tip and bi-directional servo control in some recent atomic force microscopes (AFM) has made it possible for these advanced AFMs to image structures of general shapes with undercut surfaces. AFM images are distorted representations of sample surfaces due to the dilation produced by the finite size of the tip. It is necessary to obtain the tip shape in order to correct such tip distortion. This paper presents a noise-tolerant approach that can for the first time estimate a general 3-dimensional (3D) tip shape from its scanned image in such AFMs. It extends an existing blind tip estimation method. With the samples, images, and tips described by dexels, a representation that can describe general 3D shapes, the new approach can estimate general tip shapes, including reentrant features such as undercut lines.

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1. Introduction

An atomic force microscope (AFM) images a structure by scanning a tiny tip over the sample surface. It is capable of measuring topographic features at the nanometer-scale or even at atomic-scale resolution [1]. However, the topographical image in a conventional AFM is necessarily, because of limitations of the imaging mode, a single-valued height map (Fig. 1a). (Such an object is referred to as an “umbra” in mathematical morphology [3,4] and sometimes as a “2.5-dimensional (2.5D)” object because the set of such shapes is a subset of all 3D shapes.) Recently, a new class of SPM instruments, CD-AFMs [2,6–8], is emerging. These new instruments are capable of imaging general 3D structures, including those with vertical sidewalls and undercut features. Within these 3D structures, there are x – y coordinates at which the surface is multivalued. In this new class of instruments, traditional unidirectional servo control and typically pyramidal or conical tip shapes (Fig. 1b) are replaced with bi-directional

servo control and laterally protruded tip shapes to image general 3D structures (Fig. 1c). These instruments have found applications as reference metrology tools at SEMATECH and in a number of semiconductor fabrication facilities [9,10].

An AFM image is a distorted representation of the sample due to the dilation produced by the finite size of the tip. It is necessary to obtain tip shape information in order to remove such distortion and restore the sample surface. Even though various techniques are available for tip shape characterization [11], blind tip estimation is uniquely important since it estimates the tip shape using only its scanned images, without independent knowledge of the sample(s) (hence its name). In contrast, direct tip imaging methods through scanning electron microscopy or transmission electron microscopy require a lengthy tip measurement process with the risk of damaging or contaminating the tip. Further, these methods produce images in the form of an intensity versus x and y . There are only two dimensions of direct geometrical information. An image is thus suitable for a silhouette or cross-section, but a single image does not characterize the full 3D shape required for distortion correction in AFM. Tip characterization through a known characterizer, although useful, requires advance knowledge of characterizer geometry.

A set of blind tip estimation methods has been independently developed [12–15] for tips used in conventional AFMs. These

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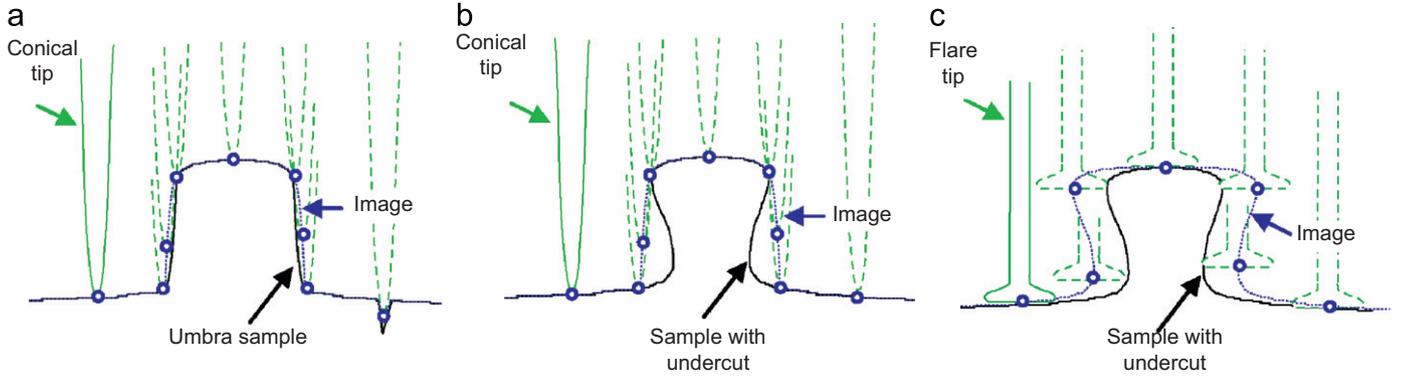


Fig. 1. Conventional 2.5D AFMs cannot access reentrant surface due to their unidirectional servo control and conical tip shape. Newer CD-AFMs under bi-directional servo control with flared tip shapes can access reentrant surfaces (figure based upon Ref. [18]). (a) Umbra on conventional AFM; (b) undercut sample on conventional AFM and (c) undercut on newer CD_AFMs.

methods are based on grayscale mathematical morphology [15], which inherently assumes that samples and tips can be represented by single height functions. Their extension to estimating general tip shapes has been impeded by the lack of a data representation that can represent general 3D shapes.

This paper extends an existing blind tip estimation method [15] and its noise-desensitization procedure to dixel-represented objects in 3D. A dixel representation has recently been adapted for AFM imaging simulation and surface reconstruction for general 3D shapes including undercut surfaces [16,17] and it has been adapted for tip estimation from simulated noise-free images [18]. Upon such extension, this method can for the first time obtain blind estimates of general tip shapes, including those with undercuts or reentrant features, from scanned images with ordinary amounts of noise.

In the remainder of this paper, we briefly describe some notations, operations, and how dexels enable the representation of general shapes (Section 2). Section 3 presents the method for blind tip estimation from general 3D images with noise. Section 4 describes the implementation and the results. We conclude this paper in Section 5.

2. Background

Blind tip estimation is based on set and morphology operations [3,4], the dixel representation, and dixel-represented set and morphology operations [16]. We briefly introduce needed notations, operations, and dixel representation in this section.

2.1. Notation

In this paper, we will use some notations as explained below. A lowercase symbol with an arrow above it (e.g., \vec{x}) denotes a vector.

An uppercase Latin or Greek letter (e.g., A , Δ) denotes a set. We use sets to represent 3D objects. For example, S represents the sample. It is understood to be the set of all points contained within or on the surface of the sample. That is, this set is the set of all points contained within a bounded volume of a particular shape. As is the case in this example, the number of elements in a set may be infinite.

2.2. Set operations

$-A$ is the reflection of set A with respect to the origin (at 0). That is,

$$-A = \{-\vec{a} | \vec{a} \in A\} \quad (1)$$

The translation of a set, A , by a vector, \vec{b} , is determined by adding \vec{b} to every element of A

$$A + \vec{b} = \{\vec{a} + \vec{b} | \vec{a} \in A\} \quad (2)$$

“ \cup ” is called union operation. If A and B are sets, then the union of A and B is the set that contains all elements of A and all elements of B , but no other elements

$$A \cup B = \{\vec{x} | \vec{x} \in A \text{ or } \vec{x} \in B\} \quad (3)$$

“ \cap ” is called intersection operation. If A and B are sets, then the intersection of A and B is the set that contains all elements of A that also belong to B , but no other elements

$$A \cap B = \{\vec{x} | \vec{x} \in A \text{ and } \vec{x} \in B\} \quad (4)$$

Here is a property from set operation [5].

Property 1. If $A \subseteq B$ and $C \subseteq D$, then $A \cup C \subseteq B \cup D$ and $A \cap C \subseteq B \cap D$.

2.3. Morphological operations

Mathematical morphology is a branch of set theory that deals with unions and intersections of sets and their translates. Following are some definitions and a property from mathematical morphology [3,4]:

“ \oplus ” denotes dilation. The dilation of object A by object B is defined by

$$A \oplus B = \bigcup_{\vec{b} \in B} A + \vec{b} \quad (5)$$

“ \ominus ” denotes erosion. The erosion of object A by object B is defined by

$$A \ominus B = \{\vec{x} | B + \vec{x} \subset A\} \quad (6)$$

“ \circ ” denotes opening. Opening of object A by object B is defined by

$$A \circ B = (A \ominus B) \oplus B \quad (7)$$

“ \bullet ” denotes closing. Closing of object A by object B is defined by

$$A \bullet B = (A \oplus B) \ominus B \quad (8)$$

Dilation is an increasing function of its arguments. That is [4],

Property 2. If $A \subseteq B$, then $A \oplus C \subseteq B \oplus C$ and $C \oplus A \subseteq C \oplus B$.

2.4. Dixel representation

In order to facilitate subsequent discussion, this subsection reviews the dixel concept and briefly outlines its use in Ref. [16] to implement mathematical morphology for general 3D objects.

This more general implementation is based on a representation in which the usual rectangular array of pixels is replaced by an array of “dexels”. Each dexel may have multiple heights, each of which represents the height of a transition from inside to outside of the object or vice versa. This naturally allows reentrant surfaces and undercut features to be represented by dexels. The dexel approach is a version of volumetric data representation where 3D objects are represented as a set of 1D blocks with depth on a grid.

We may construct a dexel object, A_d , associated with a real object A , as follows. First, choose an origin and orientation for a rectangular coordinate system. Define a grid in the x – y plane of this coordinate system. The x coordinates in this grid are given by $x_i = x_0 + i \times d_x$ for $i = 0, 1, \dots, m_x - 1$ with i an integer index, m_x the number of grid elements in the x direction, x_0 the position of the first such element, and d_x the grid spacing in the x direction. The y coordinates are similarly defined. Now imagine a line, L_{ij} , parallel to the z axis (with z ranging from $-\infty$ to ∞) at x_i, y_i for each i, j in the grid. We can define A_d as

$$A_d = \bigcup_{i,j} (L_{ij} \cap A) \quad (9)$$

A 2D example of this is shown in Fig. 2. The object (shown in gray) has undercut edges. Those intervals of the lines that are enclosed by the object (i.e., the intersection between the object and the vertical lines) are shown darker and thicker (e.g., b_{ijk}). The dexel object representation includes the collection of locations of the end-points of these intervals in an indexed grid. Each column in the object is represented by a single dexel. The entire object is then a 2D array of dexels.

Formal representation properties of dexel, as noted in Ref. [19], include spatial addressability and spatial hashing, directionality, Boolean simplification, rigid motion, discrete translations, null-set representation, and completeness.

With this dexel representation, complex 3D set and morphological operations are simplified to arrays of 1D operations. The details of such dexel-based set and morphological operations are available in Ref. [16].

2.5. Volume of dexel object

Although dexels are defined as lines with no width, we can represent the real 3D object by “dexel blocks”. A dexel block (e.g., B_j in Fig. 3) is defined by dilation of the dexel line with a horizontal rectangular element. The rectangular element has its origin at its center and dimensions r_x and r_y , where r_x and r_y are the grid spacing of dexels in the x – y plane. The volume of block B_j is $V(B_j) = (h_{i+1} - h_i) \times r_x \times r_y$. For an object comprised of n blocks, $B = \bigcup_{j=1}^n B_j$, the volume is simply the sum of the volumes of the individual blocks: $V(B) = \sum_{j=1}^n V(B_j)$.

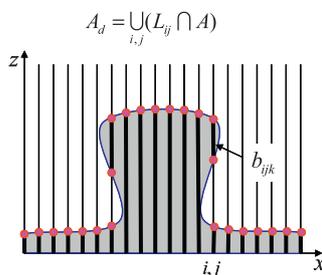


Fig. 2. Dixel representation of an object (figure based upon Ref. [16]).

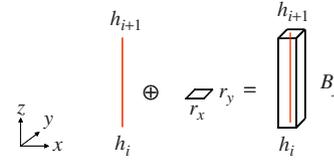


Fig. 3. Dilation of a dexel line segment with a horizontal rectangular element to get a dexel block to represent 3D object.

3. Method of blind tip estimation

Among the blind tip estimation methods available in the literature [12–15], we choose to extend Villarrubia’s method [12,15] since it is based on set theory and can be directly implemented with the dexel representation. Its original implementation was for grayscale (pixel-represented) images. Consequently, it could only be used to estimate similarly represented tips. However, an extension of this method for dexel-represented images can estimate tips of general 3D shape.

The relationship between the sample S , tip T , and image I (apart from ideally small effects due to noise, cantilever twisting, etc.) can be written as

$$I = S \oplus P \quad (10)$$

where $P = -T$, is the reflection of the tip through the origin. (See, e.g., Refs. [12,15] and references therein.) The operator in this equation is dilation. Sample reconstruction is by erosion

$$S_r = I \ominus P \quad (11)$$

A similar equation governs tip reconstruction if a known sample (a tip characterizer) is used. The reconstructed sample, S_r , represents the smallest outer bound on the sample that one is entitled to conclude from a given tip based upon information in the image. It is not, in general, everywhere equal to S because there may be parts of the sample (e.g., a crevice) not entirely accessible to the tip.

The tip and the image were shown [12,15] to satisfy the following relation:

$$(I \ominus P) \oplus P = I \quad (12)$$

The superficially similar statement $(a-b)+b = a$ is true for any b because addition and subtraction are inverse operations. However, erosion and dilation are not strict inverses, and there do exist tip shapes for which Eq. (12) is not satisfied. This forms the basis of the existing blind tip estimation method. If all tips that fail to satisfy Eq. (12) are eliminated, the remaining set must include the actual tip shape.

3.1. Existing blind tip estimation for conventional AFM images

The existing method is an iterative solution of Eq. (12) for a value, P_r , that is an outer bound on the true tip shape, P . This solution can be described as

$$P_{i+1} = \bigcap_{\vec{x} \in I} ((I - \vec{x}) \oplus P'_i(\vec{x}) \cap P_i) \quad (13)$$

Eq. (13) allows the calculation of the $(i+1)$ th iteration result from the i th result. \vec{x} is a point in the image I , $P'_i(\vec{x})$ is a set of points in P_i that can touch I at \vec{x} with the apex point contained in I , which can be defined as

$$P'_i(\vec{x}) = (\vec{x} - I) \cap P_i \quad (14)$$

Upon convergence, the result of estimated tip shape P_r can be defined as

$$P_r = \lim_{i \rightarrow \infty} P_i \quad (15)$$

The limit is shown for $i \rightarrow \infty$, but in practice the series converges in a finite, and generally small, number of iterations. Such an estimated tip is an outer bound of the actual tip. That is,

$$P \subseteq P_r \quad (16)$$

Since blind reconstruction seeks to find the largest tip consistent with all features in an image, small amounts of noise can lead to considerable instability in the algorithm described so far. Features due to random noise or other measurement artifacts need not be consistent with each other. An effort to make them so leads to an overly sharp tip. (A tip can always be made consistent with all features by making it artificially sharp.) This problem was circumvented [15] by the use of a threshold that defines a size below which inconsistencies are not considered significant enough to warrant a change in the estimated tip. This procedure was implemented by comparing scalar heights of objects with a scalar threshold.

3.2. New blind tip estimation for general (dixel-represented) images

In this section, we describe our generalization of the just-described method to the more general 3D case. The generalization of equations that involve only set operations, like Eqs. (13)–(15), is in principle straightforward. One simply substitutes the dixel version of these operations. The noise threshold, previously implemented as a scalar addition, requires more consideration.

We begin by observing that the threshold procedure described in the last section as a scalar operation can be alternately described as the substitution of $I \oplus \Delta$ for I in Eq. (13), where Δ is a line segment from 0 to t (t is the “threshold”) along the z direction. Having thus recast the threshold algorithm as a set operation, we further generalize by recognizing that Δ is a tolerance to noise, so in 3D it should be a volume within which the noise will fall. That is, in the general case we must allow Δ to be a set with extent in 3D. For example, Δ could be a small cuboid, and the size along the x , y , and z directions is

$$\Delta = \Delta(\delta_x, \delta_y, \delta_z) \quad (17)$$

The threshold Δ shown in Fig. 4 is represented by a set of dixel blocks from $-\delta_x$ to $+\delta_x$ in the x direction, from $-\delta_y$ to $+\delta_y$ in the y direction, and with the height of each dixel block from $-\delta_z$ to $+\delta_z$ in the z direction, where δ 's are related to the noise levels along the corresponding directions. To make it simple, we denote the above threshold as

$$\Delta = \delta_x \times \delta_y \times \delta_z \quad (18)$$

Although in general Δ is 3D as described here, it may not always be necessary to use the full available generality. We have observed instances in simulations (as in examples to be shown later) where a 2D or 1D approximation has been sufficient.

In simulations we have observed that substitution of $I \oplus \Delta$ for I is best done in Eq. (14) as well as in Eq. (13). (The equivalent scalar version of this could presumably also have been done for the existing method. However, we have observed sensitivity to omission of this only in the case of images with vertical or undercut sidewalls, a situation important to our present purpose but which cannot arise in conventional images.) Motivated as described, we extend blind tip estimation to general 3D dixel-represented objects with a threshold added to noisy images via

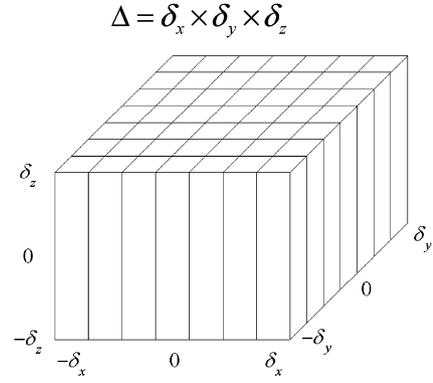


Fig. 4. Dixel representation of a 3D threshold, $\Delta = \delta_x \times \delta_y \times \delta_z$.

the following equations:

$$P_{i+1}(\Delta) = \bigcap_{\vec{x} \in I} ((I \oplus \Delta) - \vec{x}) \oplus P'_i(\vec{x}, \Delta) \cap P_i(\Delta) \quad (19)$$

$$P'_i(\vec{x}, \Delta) = (\vec{x} - (I \oplus \Delta)) \cap P_i(\Delta) \quad (20)$$

$$P_r(\Delta) = \lim_{i \rightarrow \infty} P_i(\Delta) \quad (21)$$

All sets, including the threshold structuring element Δ , are now understood to be full 3D dixel objects.

We illustrate the importance of the finite threshold in a simulation in Figs. 5–7. For simplicity, the illustration is confined to the contribution to the reconstructed tip from a single point on the image, and the threshold is chosen only along the z direction. Fig. 5 shows in the ideal noise-free case as to what tip reconstruction we ought to obtain. After addition of Gaussian noise with standard deviation, $\sigma_z = 1$ nm, along the z direction to the noise-free image, Fig. 6 shows that the method fails if we do not use a threshold. Finally, Fig. 7 illustrates how proper use of a threshold restores the reconstructed shape to close to the ideal result.

We can see that the tip (P_{i+1} , the green mesh area in Fig. 6) estimated from the noisy image without threshold differs from the tip (P_{i+1} , the green area in Fig. 5) estimated from noise-free image by an amount much larger than the 1 nm noise. The resulting tip is overly sharp (much smaller than the tip estimated from noise-free image). In Fig. 7, the corresponding result using a threshold $\Delta = 3$ nm along the z direction is much closer to the estimated tip (P_{i+1} , the green area in Fig. 5) from the noise-free image.

3.3. Discussion of threshold Δ

To find the proper threshold, first we need to understand the relation between the noise, threshold, and estimated tip. Here are some properties of threshold Δ

Property 3. If $\Delta_1 \subseteq \Delta_2$, then $P_r(\Delta_1) \subseteq P_r(\Delta_2)$.

To see this, observe that P' (Eq. (20)) and $(I \oplus \Delta) - \vec{x}$ in Eq. (19) increase in size as Δ increases, owing to the increasing property of dilation (Property 2). Since both are increasing with Δ , so is their dilation, $(I \oplus \Delta - \vec{x}) \oplus P'(\vec{x}, \Delta)$. Thus, every term in Eq. (19)'s intersection is larger, and so therefore is P_{i+1} . P_r is the limit of a series, each term of which is larger than before, so it too will increase with increasing Δ .

Property 4. In the limit of very large Δ , $P_r(\Delta)$ approaches P_0

To see this, consider Eq. (19). If we choose Δ to be a sphere of radius r or a cube of side r , then as $r \rightarrow \infty$, $((I \oplus \Delta) - \vec{x})$ fills all

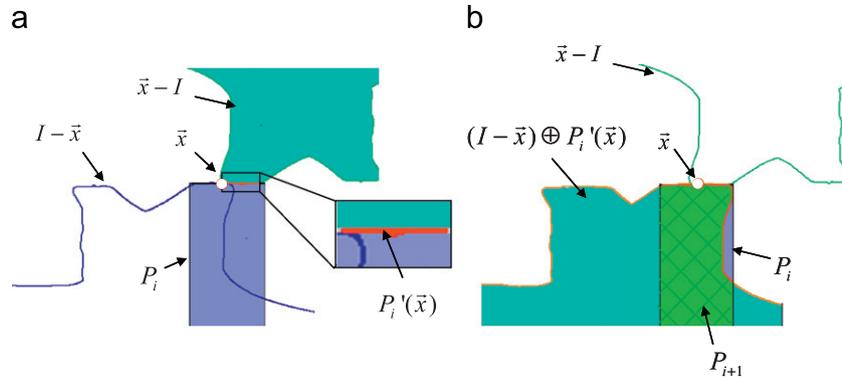


Fig. 5. Blind tip estimation from a noise-free image. (a) $P'_i(\bar{x}) = (\bar{x} - I) \cap P_i$, where $\bar{x} - I, P_i, P'_i(\bar{x})$ are shown in colored background, $P'_i(\bar{x})$ is also shown in zoom in area and (b) $P_{i+1} = ((I - \bar{x}) \oplus P'_i(\bar{x})) \cap P_i$, where $(I - \bar{x}) \oplus P'_i(\bar{x}), P_i$ are shown in colored background, P_{i+1} is shown in green mesh.

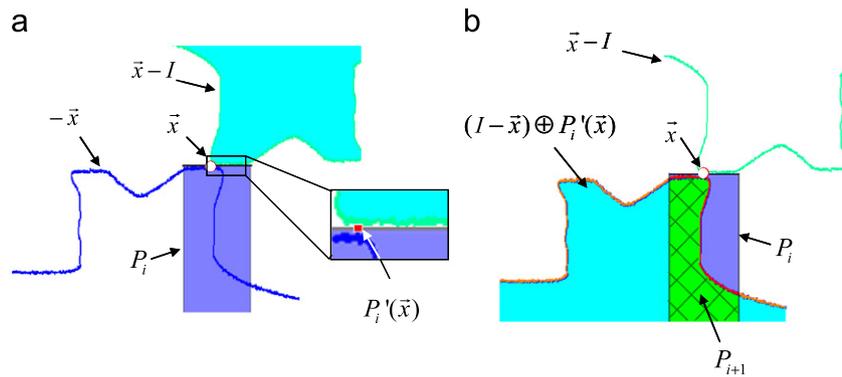


Fig. 6. Blind tip estimation from a noisy image without threshold. (a) $P'_i(\bar{x}) = (\bar{x} - I) \cap P_i$, where $\bar{x} - I, P_i, P'_i(\bar{x})$ are shown in colored background, $P'_i(\bar{x})$ is also shown in zoom in area, $P'_i(\bar{x})$ is smaller than $P'_i(\bar{x})$ in Fig. 5a because of noise and (b) $P_{i+1} = ((I - \bar{x}) \oplus P'_i(\bar{x})) \cap P_i$, where $(I - \bar{x}) \oplus P'_i(\bar{x}), P_i$ are shown in colored background, P_{i+1} (green mesh) is much smaller (differences large compared to noise) than P_{i+1} (green mesh) in Fig. 5b.

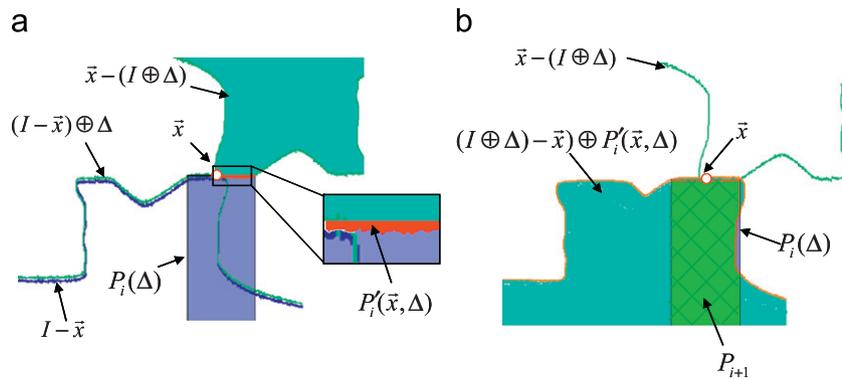


Fig. 7. Blind tip estimation from a noisy image with threshold (a) $P'_i(\bar{x}, \Delta) = (\bar{x} - (I \oplus \Delta)) \cap P_i$, where $\bar{x} - (I \oplus \Delta), P_i, P'_i(\bar{x}, \Delta)$ are shown in colored background, $P'_i(\bar{x}, \Delta)$ is also shown in zoom in area, $P'_i(\bar{x}, \Delta)$ and $(I - \bar{x}) \oplus \Delta$ are outer bounds of their counterparts in Fig. 5a and (b) $P_{i+1} = (((I \oplus \Delta) - \bar{x}) \oplus P'_i(\bar{x}, \Delta)) \cap P_i$, where $((I \oplus \Delta) - \bar{x}) \oplus P'_i(\bar{x}, \Delta), P_i$ are shown in colored background, P_{i+1} (green mesh) is close (differences comparable to the chosen noise level) to P_{i+1} (green mesh) in Fig. 5.

space, as then does $(I \oplus \Delta - \bar{x}) \oplus P'_i(\bar{x}, \Delta)$. The intersection of “all of space” with P_0 is just P_0 .

The importance of these two properties is: on the one hand, we observed in the example that when $\Delta = \{0\}$ noise tends to make the reconstructed tip overly sharp; on the other hand, Property 3 says our result will increase monotonically with increasing Δ . Property 4 says this increase can be continued up to a point where the reconstructed tip contains the true tip shape (since P_0 is chosen to be an extreme outer bound). Thus there are values of Δ that produce results at both extremes, too narrow and too blunt. Between these extremes there is an optimal size for Δ .

For blind reconstruction from conventional images, it was found [15] that with increasing threshold at first the volume of the estimated tip increases slowly. Then over a short threshold interval, the volume increases much faster. Afterwards, the tip volume resumes its slow increase. The location of this rapid volume change was taken to indicate the appropriate threshold value to use. Our experience with the generalized algorithm is similar, as shown in Fig. 8, where there is a fast increase of volume between $\Delta = 0 \times 0 \times 2$ and $0 \times 0 \times 2.1$. (Note that according to our notation introduced in the previous section, the leading zeros here mean our threshold element has only a single dixel, at the 0,0 grid

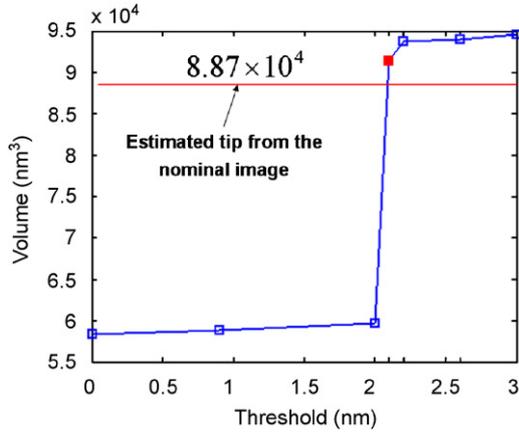


Fig. 8. Example of volume vs. threshold parameter in z axis.

position. The image has Gaussian noise with standard deviation along the x and y directions $\sigma_x = \sigma_y = 1$ nm; details will be shown in Section 4.1.) After the “jump of volume”, the increase becomes slower and smooth again. With the jump of volume, the estimated tip changes from an overly sharp estimated tip to an estimated tip, which is an outer bound on the actual tip.

Hypothesis. Therefore, we hypothesize that the selection of 2D/3D threshold Δ can be made by the jump of estimated tip’s volume with the increasing of δ_x, δ_y , and δ_z .

This hypothesis will be tested in simulation examples in Section 4.

3.4. Algorithm of new blind tip estimation using dixel representation

The procedure of our new blind tip estimation is shown in Fig. 9, in which we define an initial tip, P_0 , typically as a dixel object with its top at

$$\text{Top}(P_0) = \begin{cases} 0 & \text{for } 0 < x < s_x \text{ and } 0 < y < s_y \\ -\infty & \text{otherwise} \end{cases} \quad (22)$$

P_0 is a rectangular tip with size $s_x \times s_y$ and should be an outer boundary of the real tip. Typically, we set the apex of P_0 at $(s_x/2, s_y/2, 0)$. At the outset, uncertainty about the tip shape is large, so a considerable margin of safety can be built in to insure that $s_x \times s_y$ is large enough to contain the tip.

Then the procedure in Fig. 9 describes the determination of P_r , the final estimated tip using a particular value of threshold Δ .

3.5. Algorithm of finding proper threshold Δ

As discussed above, we have observed a jump of volume from underestimated tip to proper-estimated tip as Δ is increased. We need to find the Δ of this change. The proper Δ can be found with the following process. For simplicity, we assume here a 1D $\Delta = 0 \times 0 \times \delta_k$ as we have found to work in the examples we tried. The generalization of this procedure to other forms, e.g., $\Delta = \delta_k \times \delta_k \times \delta_k$, $\Delta = (a \times b \times c)\delta_k$ with a, b , and c fixed constants, or even $\Delta = \delta_x \times \delta_y \times \delta_z$, is straightforward should it prove necessary.

Step 1. Calculate the estimated tips with different thresholds $\Delta = 0 \times 0 \times \delta_k$ using Eqs. (19)–(21), where, $\delta_k = d_\delta \times k$ ($k = 0, 1, 2, \dots$) with d_δ the amount of increase between thresholds.

Step 2. Calculate volumes of the estimated tips, $V(P_r(\Delta_k))$ ($k = 0, 1, 2, \dots$).

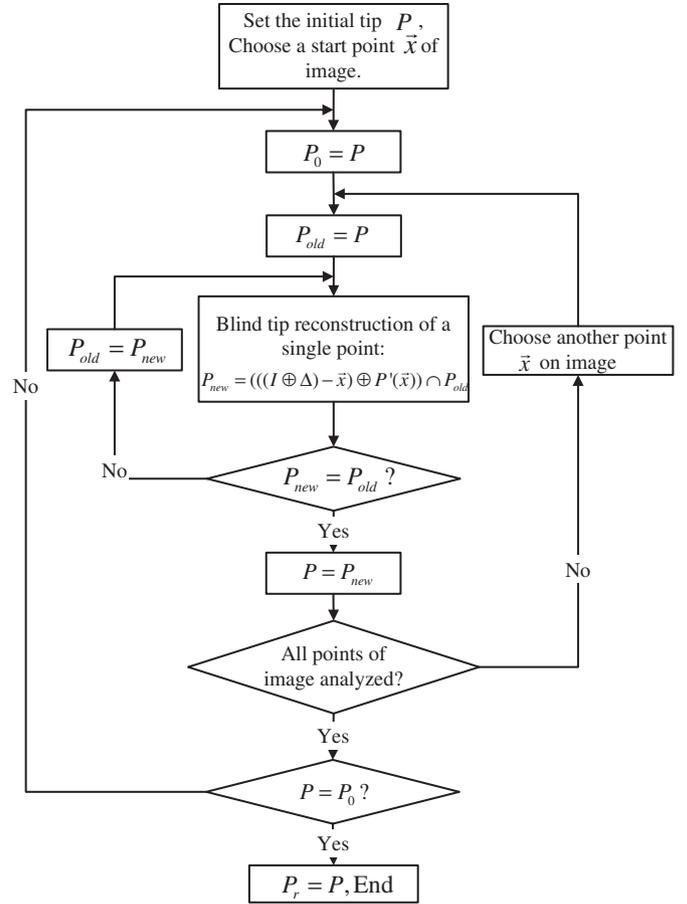


Fig. 9. Flowchart of blind tip estimation with dixel implementation.

Step 3. Calculate the slope of volume with respect to the δ parameter

$$m(\Delta_k) = \frac{d(V(P_r(\Delta_k)))}{d\delta_k} \approx \frac{V(P_r(\Delta_k)) - V(P_r(\Delta_{k-1}))}{\delta_k - \delta_{k-1}} \quad (23)$$

Step 4. Find the δ_k at which the slope of volume change is largest. $\Delta = 0 \times 0 \times \delta_k$ is the threshold we choose, or we can use a more conservative criterion by using $\Delta = 0 \times 0 \times \delta_{k+n}$ ($n = 0, 1, 2, \dots$) where the slope has more or less made a plateau at a smaller value. Then $P_r(\Delta_{k+n})$ is the result for tip estimation from noisy data.

4. Implementation and examples

In this section, we present the implementation and simulation results. We have implemented this method based on the algorithm in Sections 3.4 and 3.5. In order to validate the correctness of our implementation, we perform simulations in which we compare the tip estimated from a noisy image to the ideal tip estimated from the noise-free image, which is an outer bound of the actual tip.

4.1. Example 1

Figs. 10 and 11 show a 2D example of blind estimation of tip shape from a noisy image with undercut features. We simulated a 2D surface with two sharp corners. The width of surface in the x direction is 1200 nm, represented as 1200 dexels (Fig. 10a). The tip (Fig. 10b) is digitized from an image of an actual tip. We used it to

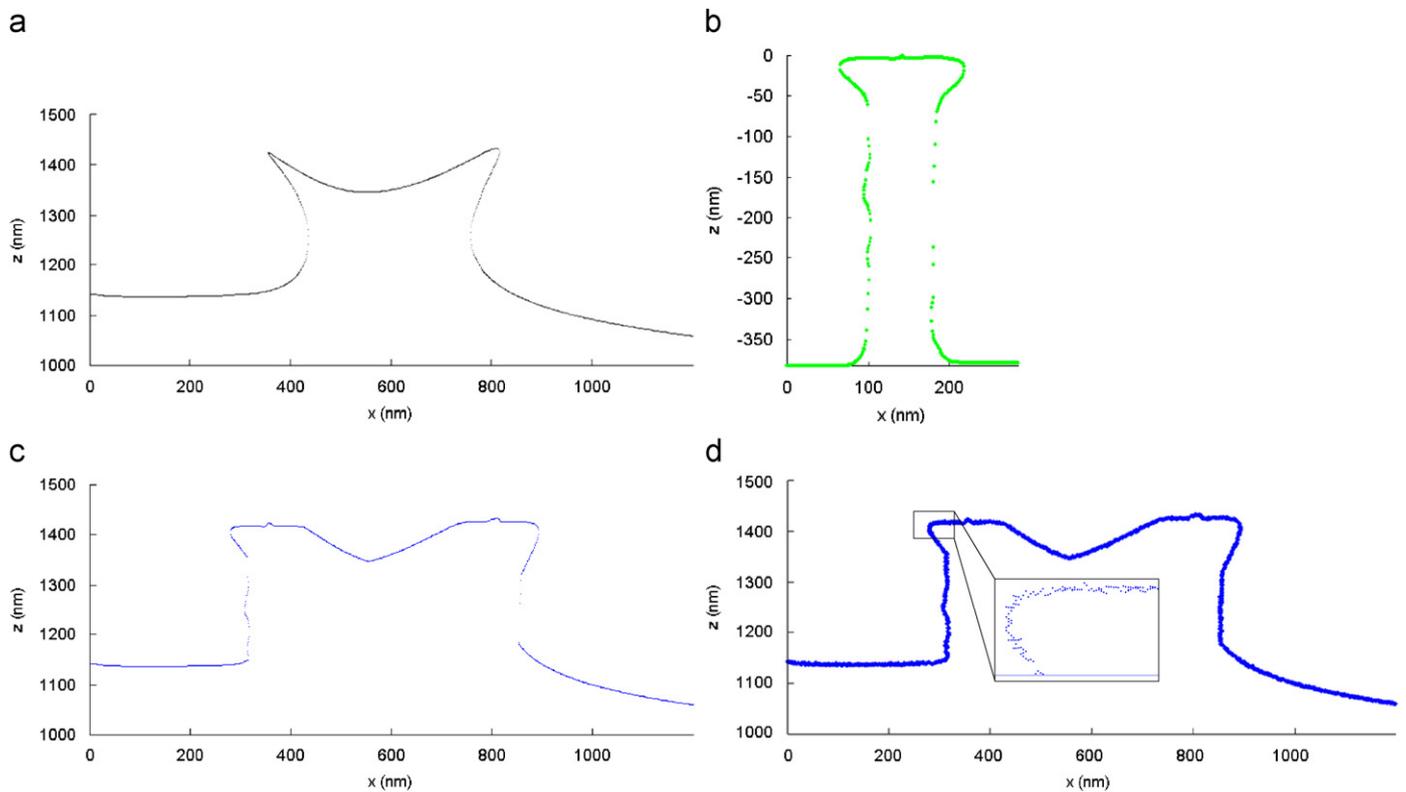


Fig. 10. Two-dimensional example of blind reconstruction, all objects are shown in dixel boundary point mode (a) the surface S ; (b) the tip P ; (c) the noise-free image $I = S \oplus P$; and (d) the noisy image, generated by adding Gaussian noise to the noise-free image. (Note that dexels are uniformly separated along the x direction. The spacing between dixel end-points therefore depends upon the surface slope. It may be large, particularly where the object surface is nearly vertical. This explains the apparent gaps visible in figures (b) and (c).)

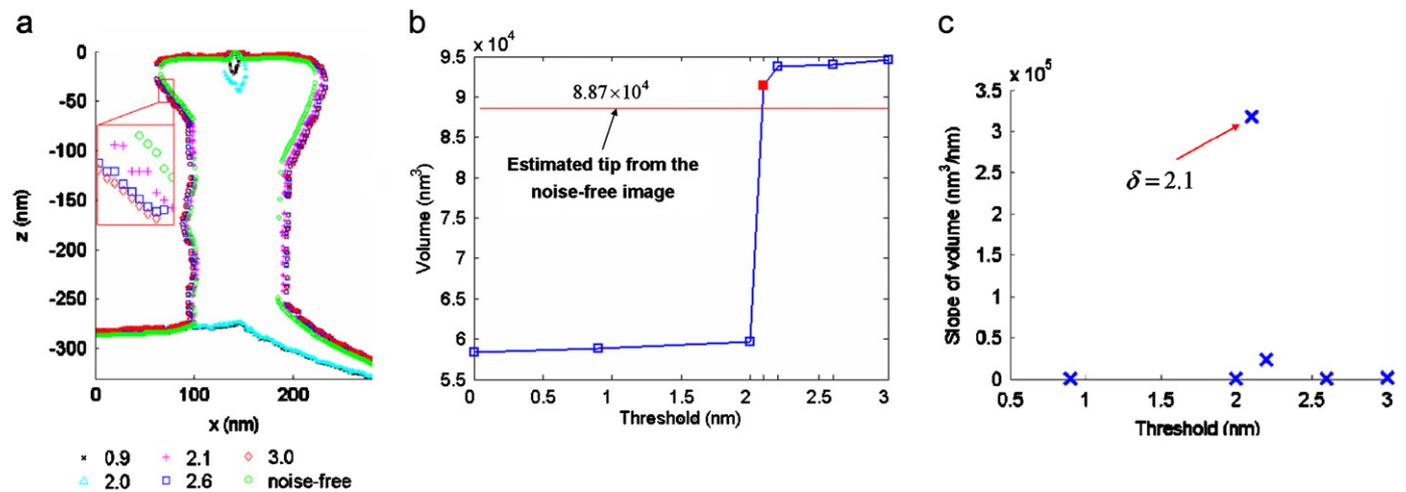


Fig. 11. Blind tip estimation using inputs from Fig. 10, (a) Estimated tips from noisy image for various thresholds, Δ ; (b) volume of those estimated tips vs. threshold parameter; and (c) the slope of volume with respect to δ_z , showing the δ_z that corresponds to the maximum slope.

dilate the surface and obtain the noise-free image (Fig. 10c). Then we added Gaussian noise with standard deviation in the x and z directions $\sigma_x = \sigma_z = 1$ nm to the noise-free image to obtain a simulated noisy image (Fig. 10d). We will try $\Delta = 0 \times \delta_z$.

First we made an initial estimation of the tip's outer bound. The size along the x direction is 285 nm, represented as 285 dexels, all with their tops at $z = 0$. We set the apex point at (142, 0). With the procedure of Section 3, we obtained the estimated tip with varying values of δ_z (Fig. 11a). The volume and slope of the

volume with varying δ_z are shown in Fig. 11b and c. (In 3D it is a volume that is relevant. For this 2D case, our "volume" assumes a 1 nm thickness.) We get a maximum slope at $\delta_z = 2.1$ nm (Fig. 11c). The estimated tip at this value or slightly higher is the tip we want.

To make a quantitative statement of the closeness of this result to the ideal one (obtained from the noiseless image) we need to compare differences between tips. Here is how we compare them.

We use the estimated tip, B , from the noiseless image as our standard. Then we can compare each estimated tip A from a noisy

image with threshold with the tip B to get their difference. We will represent the difference between A and B by difference between their boundaries ∂A and ∂B . As we know, the minimum boundary

along the z direction of estimated tip is always $-\infty$, and the original of A and B are the same when they have the same size $s_x \times s_y$, so when we estimate with same size $s_x \times s_y$ for A and B , we only need to compare the finite-valued boundary ∂A_f and ∂B_f , which can be represented by all the finite-valued height end-points of all dexels in each object. Assume that all those finite-valued height end-points of all dexels of A is $\{\bar{a}_i | i = 0, 1, 2, \dots, m\}$ and all those finite-valued height end-points of all dexels of B is $\{\bar{b}_j | j = 0, 1, 2, \dots, n\}$, then $\partial A_f = \{\bar{a}_i | i = 0, 1, 2, \dots, m\}$ and $\partial B_f = \{\bar{b}_j | j = 0, 1, 2, \dots, n\}$. We define the discrepancy between any single point \bar{x} and ∂B_f as

$$\text{error}(\bar{x}, \partial B_f) = \min\{|\bar{x} - \bar{b}_j| | j = 0, 1, 2, \dots, n\}.$$

Table 1
Difference between estimated tip with threshold and nominal estimated tip for Example 1

$\Delta = \delta_z$ (nm)	0.9	2	2.1	2.2	2.6	3
Minimum error (nm)	0	0	0	0	0	0
Maximum error (nm)	44.7	44.0	7.5	11.8	12.0	12.4
Standard deviation (nm)	13.5	12.9	1.7	2.5	2.4	2.3
Time (s)	56.3	256.5	72.8	82.7	62.75	46.2

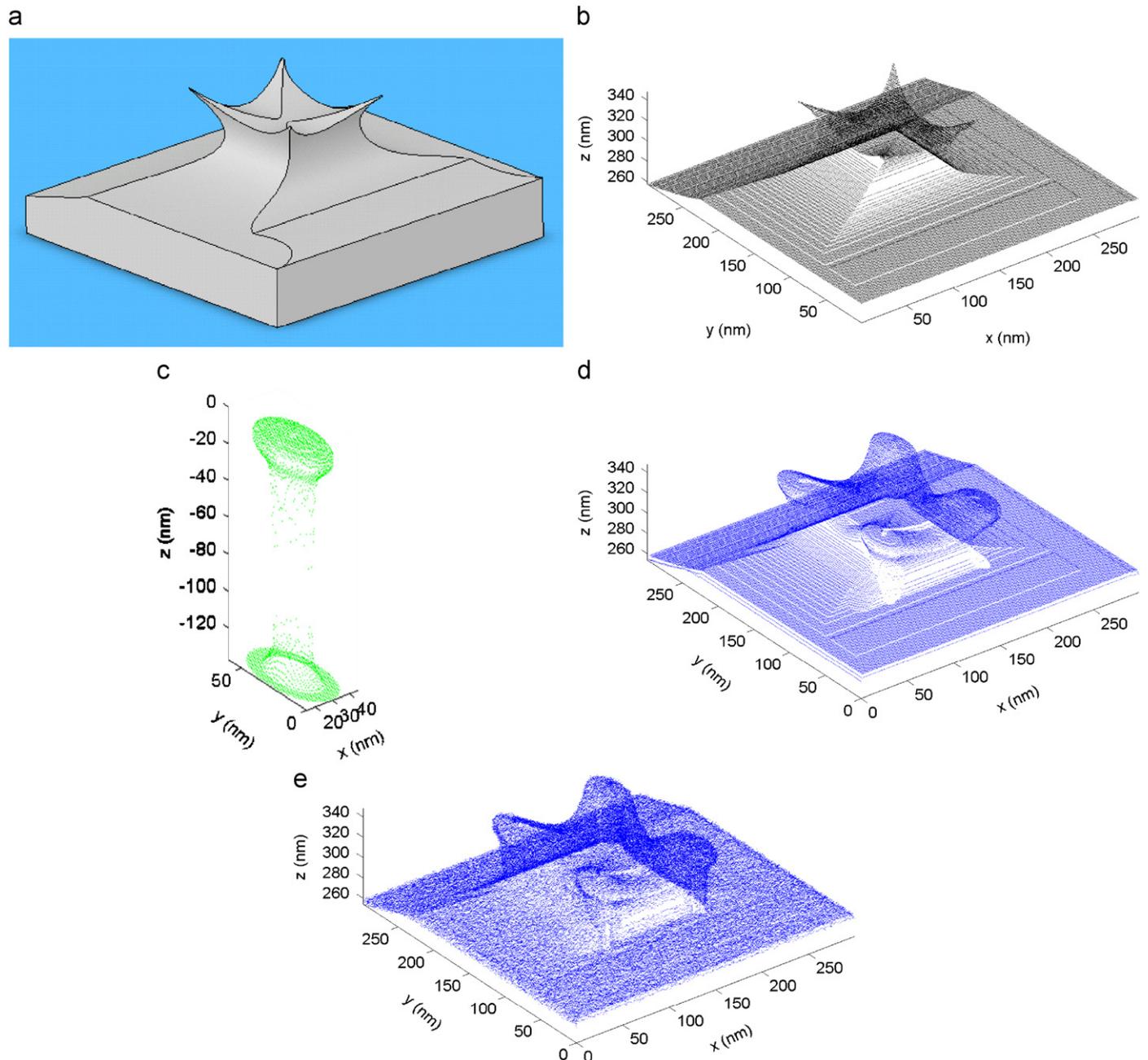


Fig. 12. Three-dimensional example of blind reconstruction. (a) Simulated sample surface, S , with four 1 nm radius corners, shown in the 3D rendering mode; (b) sample surface, S , shown in dexel boundary point mode; (c) tip P (d) noise-free image, $I = S \oplus P$; and (e) simulated noisy image generated by adding Gaussian noise to the noise-free image.

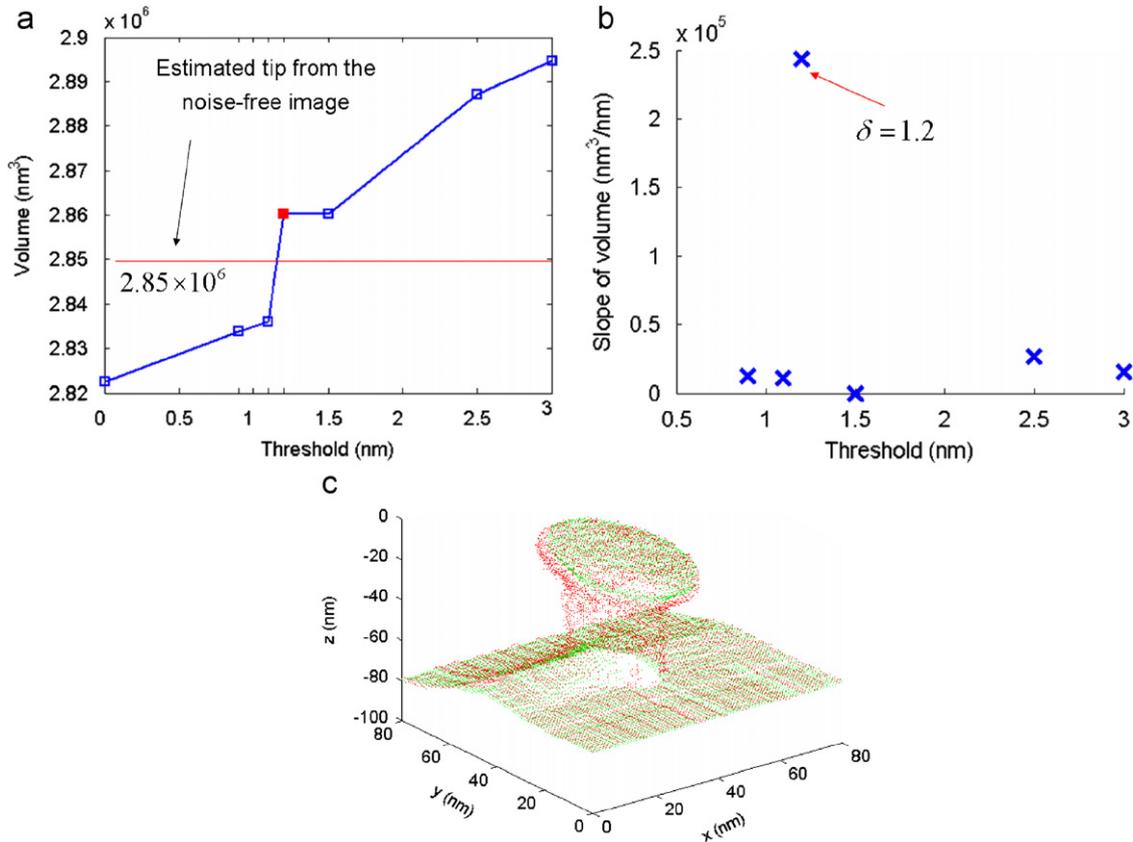


Fig. 13. Blind tip estimation from a 3D image. (a) Volume of estimated tips as a function of threshold parameter; (b) the slope of the volume and location of the δ_z corresponding to the maximum slope; and (c) comparison of the tip (red) estimated from the noisy image with threshold to the tip (green) estimated from noise-free image with $\delta_z = 1.2$ nm.

Then we compare A and B by minimum discrepancy, maximum discrepancy, and standard deviation, defined as

$$\min_error(A, B) = \min\{\text{error}(\vec{a}_i, \partial B_f) | i = 0, 1, 2, \dots, m\};$$

$$\max_error(A, B) = \max\{\text{error}(\vec{a}_i, \partial B_f) | i = 0, 1, 2, \dots, m\};$$

$$\text{stdev}(A, B) = \sqrt{\frac{1}{m} \sum_{i=1}^m (\text{error}(\vec{a}_i, \partial B_f) - \overline{\text{error}})^2},$$

$$\text{where } \overline{\text{error}} = \frac{1}{m} \sum_{i=1}^m \text{error}(\vec{a}_i, \partial B_f).$$

If ∂A_f and ∂B_f are dense enough, those will represent the difference of A and B very well; if ∂A_f and ∂B_f are not dense enough (usually along the z direction), we can upsample the point by interpolation on dixel contours [20].

With the definitions above, we compare those estimated tips $P_r(\delta_z)$ with the estimated tip P_r from the noise-free image in Table 1 by $\min_error(P_r(\delta_z), P_r)$, $\max_error(P_r(\delta_z), P_r)$, and $\text{stdev}(P_r(\delta_z), P_r)$. We find that the estimated tip with $\Delta = 2.1$ nm is closest to the noise-free result. Using a more conservative criterion, we might choose $\Delta = 2.2$ nm. The corresponding tip is still close to the noise-free result (Table 1). The running time in seconds (on a PC equipped with a Pentium[®] D 3.40 GHz × 2 CPU with 2 G RAM²) is also presented in the table. This example demonstrates that we can get a good estimate of a tip from the noisy image with undercut features by using the proper threshold, Δ , and this

Table 2

Difference between estimated tip with threshold and nominal estimated tip for Example 2

δ_z (nm)	0.9	1.1	1.2	1.5	2.5	3.0
Minimum error (nm)	0	0	0	0	0	0
Maximum error (nm)	9.1	8.9	5.8	5.8	7.8	8.6
Standard deviation (nm)	1.18	1.18	1.01	1.01	1.42	1.38
Time (s)	1429	1231	1380	1515	5167	3113

proper threshold can be found by the slope of the volume of the estimated tip.

4.2. Example 2

Figs. 12 and 13 show a 3D example of blind estimation of tip shape with undercut features. We simulate a 3D surface with four sharp corners (radius 1 nm). The lateral size of the surface is 300 nm × 300 nm, represented by a 300 × 300 array of dexels. The tip is simulated with a 41 × 61 dixel array, with the dixel at (20, 30) chosen as the origin point (Fig. 12c). The tip was used to dilate the surface and obtain the noise-free image (Fig. 12d), to which Gaussian noise with $\sigma_x = \sigma_z = 1$ nm was added to obtain the simulated noisy image of Fig. 12e. We used $\Delta = 0 \times 0 \times \delta_z$.

Using a similar procedure as for Example 1, the tip's initial outer bound is simulated with a 81 × 81 dixel array, with the dixel at (40, 40) chosen as the origin point. We calculated the volume (Fig. 13a) and slope of volume (Fig. 13b) of the varying estimated tips. The maximum slope was obtained at $\delta_z = 1.2$ nm. The corresponding tip is shown in Fig. 13c. Estimated tips at

² Certain commercial equipment is identified in this report in order to specify the measurement procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the equipment identified is necessarily the best available for the purpose.

varying \cong_z are compared to the noise-free result in Table 2. The estimated tip with $\Delta = 1.2$ nm is closest to the noise-free result. A more conservative criterion, $\Delta = 1.5$ nm, also produces a result close to the right one (Table 2). This demonstrates that the method described in Section 3 also works for a fully 3D example.

5. Discussion and conclusions

In this paper, we have used dexels to represent images, surfaces, and tips of general shape. We have described a generalization of blind reconstruction that applies to such dixel-represented objects. The method enables the blind tip estimation method for the first time to estimate tips of general shape from both noise-free and noisy images. We have used simulations to demonstrate that this generalization of blind reconstruction works. The estimated tips are found to be the outer bounds of and close to the tip estimated from the noise-free image, which is itself an outer bound and close to the actual tip. The advantage of a simulation for a demonstration of this kind is that the right answer is unambiguously known. This makes it a good test of the algorithm. It is not, of course, a test of the model; for example, it does not prove that imaging in the AFM is actually a dilation. For this reason, it will be desirable in future work to validate this blind reconstruction procedure experimentally. However, experiments have already validated blind reconstruction applied to ordinary grayscale images [21] and tip reconstruction using erosion of known tip characterizers [22–25], even for flared tips. These procedures rely upon the same dilation tip-sample interaction model that we have assumed.

An advantage of blind reconstruction is that it combines relevant information about the tip from many different locations on the image and it does not require independent calibration of the sample. As has been pointed out [11,15], this can be extended even to multiple images and it can be combined with the use of a known tip characterizer when one is available. One possible application of this kind is suggested by the following problem: single crystal critical dimension reference materials (SCCDRM) have been used to ascertain the widths of flared tips like those in Fig. 10b [26]. The advantage of the SCCDRM is that it has a calibrated width. However, dimensions other than the width (e.g., corner radii) are not calibrated, and these characterizers are lines with rectangular cross-sections, i.e., vertical (not undercut or flared) sidewalls; they do not touch and therefore cannot characterize the reentrant parts of the tip. On the other hand, there are commercial tip characterizers that are constructed to access these parts of the tip. Unfortunately, these have unknown widths. No single tip characterizer embodies all of the desirable features. The availability of a full suite of mathematical morphology tools, with blind reconstruction in addition to erosion, should

allow the strengths of the various characterizers to be optimally combined.

Acknowledgment

We are grateful for the support from NSF Awards #0800912 and #0529165.

References

- [1] G. Binnig, C.F. Quate, C. Gerber, *Phys. Rev. Lett.* 56 (9) (1986) 930.
- [2] G. Dahlen, M. Osborn, N. Okulan, W. Foreman, A. Chand, J. Foucher, *J. Vac. Sci. Technol. B* 23 (6) (2005) 2297.
- [3] J. Serra, *Image Analysis and Mathematical Morphology*, Academic Press, New York, 1982.
- [4] E.R. Dougherty, R.A. Lotufo, *Hands-on Morphological Image Processing*, SPIE Press, 2003.
- [5] K. Kazimierz, *Introduction to Set Theory and Topology*, Pergamon Press, Oxford, 1962, pp. 27–37.
- [6] D. Nyyssonen, L. Landstein, E. Coombs, *J. Vac. Sci. Technol. B* 9 (6) (1991) 3612.
- [7] Y. Martin, H.K. Wickramasinghe, *Appl. Phys. Lett.* 64 (19) (1994) 2498.
- [8] T. Morrison, C. Marotta, *Micro Mag.* (2005).
- [9] R.G. Dixon, R.A. Allen, W.F. Guthrie, M.W. Cresswell, *J. Vac. Sci. Technol. B* 23 (2005) 3028.
- [10] N.G. Orji, R.G. Dixon, A. Martinez, B.D. Bunday, J.A. Allgair, T.V. Vorburger, *J. Micro/Nanolith. MEMS MOEMS* 6 (2007) 023002-1.
- [11] J.S. Villarrubia, Tip characterization for dimensional nanometrology, in: B. Bhushan, H. Fuchs, S. Hosaka (Eds.), *Applied Scanning Probe Methods*, Springer, Berlin Heidelberg, 2004.
- [12] J.S. Villarrubia, *Surf. Sci.* 321 (1994) 287.
- [13] S. Dongmo, M. Troyon, P. Vautrot, E. Delain, N. Bonnet, *J. Vac. Sci. Technol.* 14 (1996) 1552.
- [14] P.M. Williams, K.M. Shakesheff, M.C. Davies, D.E. Jackson, C.J. Roberts, S.J.B. Tendler, *J. Vac. Sci. Technol.* 14 (1996) 1557.
- [15] J.S. Villarrubia, *J. Res. Natl. Inst. Stand. Technol.* 102 (4) (1997) 425.
- [16] X. Qian, J. Villarrubia, *Ultramicroscopy* 108 (2007) 29.
- [17] X. Qian, J. Villarrubia, F. Tian, R. Dixon, Image simulation and surface reconstruction of undercut features in atomic force microscopy, in: C. N. Archie (Ed.), vol. 6518, SPIE, 2007, p. 651811.
- [18] F. Tian, X. Qian, Blind estimation of general tip shape in atomic force microscopy, in: *Proceedings of the ASME 2007 International Design Engineering Technical Conferences & Computers & Information in Engineering Conference*, Las Vegas, Nevada, 2007.
- [19] E.E. Hartquist, J.P. Menon, K. Suresh, H.B. Voelcker, J. Zagajac, *Comput. Aided Design* 31 (3) (1999) 175–183.
- [20] W. Zhang, X. Peng, M.C. Leu, *ASME J. Comput. Inf. Sci. Eng.* 7 (3) (2007) 203.
- [21] S. Dongmo, J.S. Villarrubia, S.N. Jones, T.B. Renegar, M.T. Postek, J.F. Song, *Ultramicroscopy* 85 (3) (2000) 141.
- [22] G. Dahlen, M. Osborn, H.-C. Liu, R. Jain, W. Foreman, J.R. Osborne, Critical dimension AFM tip characterization and image reconstruction applied to the 45 nm node, in: *Proc. SPIE*, vol. 6152, 2006, p. 61522R.
- [23] H.-C. Liu, J.R. Osborne, M. Osborn, G.A. Dahlen, Advanced CD-AFM probe tip shape characterization for metrology accuracy and throughput, in: *Proc. SPIE*, vol. 6518, 2007, p. 65183K.
- [24] G.A. Dahlen, L. Mininni, M. Osborn, H.-C. Liu, J.R. Osborne, TEM validation of CD AFM image reconstruction, in: *Proc. SPIE*, vol. 6518, 2007, p. 651818R.
- [25] G.A. Dahlen, H.-C. Liu, M. Osborn, J.R. Osborne, B. Tracy, TEM validation of CD AFM image reconstruction: part II, in: *Proc. SPIE*, vol. 6922, 2008.
- [26] R.G. Dixon, R.A. Allen, W.F. Guthrie, M.W. Cresswell, *J. Vac. Sci. Technol. B* 23 (2005) 3028.