IMAGE BASED METROLOGY FOR QUANTITATIVE ANALYSIS OF LOCAL STRUCTURAL SIMILARITY OF NANOSTRUCTURES

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ABSTRACT

The orientation correlation function is a measure of the spatial range over which nanoscale structures maintain their structural (orientational) similarity. In this paper we describe an image processing system that is used to estimate this correlation function from electron microscope images of the chemically patterned nanoscale structures. We describe the estimation of a robust orientation field from the image and the subsequent estimation of the correlation function from the orientation field. We present results that have been obtained using our image metrology system. Sensitivity of the estimated values with respect to the image processing parameters is also presented.

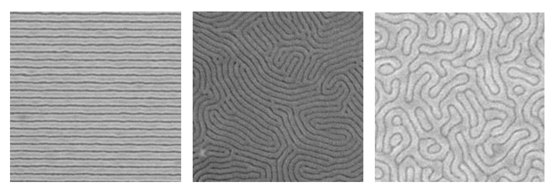
Index Terms— Image based metrology, Image processing for nanoscale, Orientation estimation, Applications.

1. INTRODUCTION

Self assembly [1] of block co-polymers on chemical substrates is a technique that holds great potential for the design of geometric structures at the nanoscale. Quantitative information that measures the degree of local geometric self-similarity will help understand the effect of long-range and short-range interactions on the organization of the nanostructures. In this paper we describe an image based metrology system that calculates the orientation correlation function which is a useful characterization of the local self-similarity of geometric structures.

The orientation correlation function measures the similarity in orientation between a pair of points that are a particular distance apart. A fast decrease in the values of the correlation function with respect to distance suggests dominance of short-range effects, whereas the dominance of long-range effects is implied by a slow decrease in the correlation function. Electron microscope images of the nanostructures can be used to estimate the correlation function and make inferences about the spatial range of the local similarity. Intuitively, the more the "twists and turns" in the structures the greater the rate at which the correlation function decays. In the example images shown in figure 1, obtained by using an electron microscope, it can be expected that the similarity in orientations between two points in the left most image is high over larger distances (the correlation function of the image decays slower) than in the right image. Thus the correlation function captures the information about the local geometric similarity of the nanoscale structures.

The rest of the paper is organized as follows: Section 2 describes the orientation correlation function and explains how the results of standard image processing algorithms must be interpreted and used in the context of the nanoscale structures. The estimation of the local orientation image, a key step in the correlation function calculation, is described in section 3. The estimation of the orientation correlation function and the correlation length is explained in 4. We conclude the paper with a discussion of the results obtained using our system in section 5.



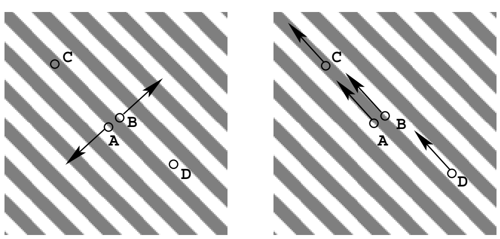
(a) (b) (c)

Fig. 1. Example images of the nanostructures we are studying. Rate of decay of orientation correlation function increases from the left to right image.

2. ORIENTATION CORRELATION FUNCTION

The order parameter at a point, λ, is a quantity that is used to characterize the local geometric structure. It is a function of the angle between the tangent line to the ridge structure at the point of interest and the reference line. The correlation function provides information about the similarity in the order parameter between any two given points that are separated by a particular distance [7]. The order parameter for the nanopatterns that we wish to analyze must thus be related to the local orientation θ of the ridge-like structures [3].

The application of gradient filters [10] to the image gives orientation estimates that are directed normal to the edges or along the direction of maximum intensity change. The orientation estimates at the two edges of the *same* ridge will differ by $180°$ (see figures 2 (a) and (b)). This difference in the estimated orientation at opposite edges of a ridge-like structure must be handled (see section 3) correctly. Another issue that must be addressed is the non-uniqueness in direction of travel along a ridge (there are two possible directions). We handle this degeneracy by defining the order parameter to be twice the local orientation estimate, i.e., $\lambda = 2\theta$. The calculation of the continuous vector and the subsequent use of the order parameter as defined above helps resolve these ambiguities. The correlation function depends on the minimum angle through which the tangent line to the ridge structure at a point must be rotated to make it parallel to the tangent line at any other point and the distance between the two points.



(a) (b)

Fig. 2. (a) Gradient directions obtained from image processing techniques are along the edge normal and only at places where the intensity change is large. Points A and B, where the intensity change is large, are at the edges of the *same* ridge but have orientations that differ by $180°$. Points C and D in the interior of the ridge may be assigned incorrect direction estimates. (b) The required orientation estimates at the points A, B, C, D. The low pass filtering (see section 3) provides fairly correct values for the interior points C, D.

3. LOCAL ORIENTATION ESTIMATION

In this section and in the remainder of the paper we will use **bold** capital alphabets (e.g. $\mathbf{\Theta}, \mathbf{\Phi_s}, \mathbf{I}$) to represent images and regular font alphabets (θ, I, ϕ_s resp.) to represent the pixel value at a generic position $\mathbf{p} = (x, y)$.
The horizontal and vertical gradient images $\mathbf{D_x}$ and $\mathbf{D_y}$ are obtained by the convolution (represented as $*$) of a Derivative-of-Gaussian filter with the input image, $\mathbf{I}$,

$$\mathbf{D_x} = \partial_x(\sigma_1) * \mathbf{I}, \text{ and } \mathbf{D_y} = \partial_y(\sigma_1) * \mathbf{I}. \tag{1}$$

The convolution of the image $\mathbf{I}$ with the DoG filter $\partial_x(\sigma_1)$ (resp. $\partial_y(\sigma_1)$) is equivalent to smoothing the image with a zero mean Gaussian filter with variance σ_1^2 and then taking the finite differences of the smoothed image in the horizontal (resp. vertical) direction. The horizontal and vertical gradients are used to calculate the images $\mathbf{\Phi_s}$ and $\mathbf{\Phi_c}$ whose entries are given by

$$\begin{aligned}\phi_s &= \frac{2D_xD_y}{\sqrt{D_xD_y + (D_xD_x - D_yD_y)^2}}\\ \phi_c &= \frac{D_xD_x - D_yD_y}{\sqrt{D_xD_y + (D_xD_x - D_yD_y)^2}}.\end{aligned} \tag{2}$$

The terms D_xD_x, D_yD_y are the variances of the local gradient and D_xD_y is the covariance. The images $\mathbf{\Phi_s}$ and $\mathbf{\Phi_c}$ together are called the continuous vector field equivalent of the orientation image [2] and the pixel entries are equivalent to $\sin(2\theta)$ and $\cos(2\theta)$ respectively To make the extraction of the orientation image robust to noise, corrupted ridge structures, minutiae etc, we low pass filter the continuous vector fields:

$$\mathbf{\Phi'_s} = G(\sigma_2) * \mathbf{\Phi_s}, \quad \mathbf{\Phi'_c} = G(\sigma_2) * \mathbf{\Phi_c}, \tag{3}$$

where, $G(\sigma_2)$ is a zero mean Gaussian filter of variance σ_2^2. The entry at position (x, y) of the orientation image is estimated as:

$$\theta(x, y) = \frac{1}{2}\tan^{-1}\left(\frac{\phi'_s(x, y)}{\phi'_c(x, y)}\right). \tag{4}$$

Note that the low pass filtering facilitates the assignment of sensible values for the orientation even in regions where the edge strength is small, i.e, center of the ridge like structures (as desired). Results show that our method produces orientation fields that are comparable in accuracy to other existing methods [2, 6, 5, 8, 9].

4. CORRELATION FUNCTION ESTIMATION

The correlation function is measure of similarity of the order parameter between pixels that are separated by a distance r. At each pixel in the image we calculate the "average" similarity of pixels at certain predetermined distances. The similarity values are averaged over all the pixels in the image and an exponential decay function is fit to the average-similarity values versus separation distance data. The correlation length (defined below) is calculated from the fitted exponential decay function.
Given the orientation image $\mathbf{\Theta}$ we can calculate the order image $\mathbf{\Lambda}$ using the mapping $\lambda(x, y) = 2\theta(x, y)$. Let $r_i = i\delta_r, \quad i = 1, \ldots, N_r$ be a set of predetermined distances. Consider an arbitrary pixel $\mathbf{p}$ with the order parameter value λ. We sample the order image at N_a equally spaced points that are a distance r_i from $\mathbf{p}$ (see 4). The similarity measure $s_i(\mathbf{p})$ of pixels that are a distance r_i from $\mathbf{p}$ is given by

$$s_i(\mathbf{p}) = \frac{1}{N_\theta}\sum_{j=1}^{j=N_a}\langle \mathbf{v}(\lambda), \mathbf{v}(\lambda_j^i)\rangle, \tag{5}$$

where, λ_j^i is the order parameter value at the j-th sample at a distance r_i from $\mathbf{p}$, $\mathbf{v}(\lambda)$ is the unit vector $(\cos(\lambda), \sin(\lambda))$. $\langle \mathbf{a}, \mathbf{b} \rangle$ represents the dot product between the vectors $\mathbf{a}$ and $\mathbf{b}$. The dot product is 1 when the order values λ and λ_j^i are the same and it is -1 when they differ by 180. Thus the summation in equation 5 measures the average similarity of pixels that are a distance r_i from the pixel $\mathbf{p}$. The similarity metric $s_i(\mathbf{p})$ is calculated for each r_i at all the pixels. We calculate the average of the similarity values (S_i) over the entire image:

$$S_i = \frac{1}{N} \sum_{\mathbf{p} \in \mathbf{I}} s_i(\mathbf{p}), \quad i = 1, \cdots, N_r. \tag{6}$$

We perform a least squares fit of an exponential decay function $S = e^{-r/C}$ to the coordinates $(r_i, S_i) \quad i = 1, \cdots, N_r$. The correlation length is the value of r for which $S = 1/e$. The orientation correlation has been used in the context of

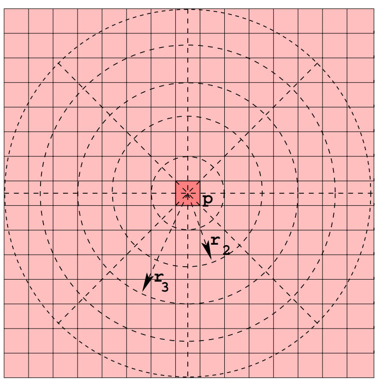


Fig. 3. Sampling grid for estimation of s_i. Shown here is the case for which $\delta r = 1.5$ pixels, $N_r = 5$, $N_a = 8$

image registration in [11]. Related work in the nanoscience community that lead to the identification of exponential decay as the model for the correlation length function is described in [4].

5. RESULTS AND DISCUSSION

In figure 4 we show the correlation function that has been estimated from the input images. We used the following parameters for our sampling grid: $N_a = 72$, $\delta_r = 1.5\ pixels$, $N_r = 50$. We sample the order image only up to a distance of 75 pixels from any given pixel because the correlation function is affected by sampling effects for larger distances. It needs to be noted that our correlation plots are very similar to what we would qualitatively expect.
The variation in the estimate of the correlation length with respect to the two parameters σ_1 and σ_2 are shown in Table 1. The estimated value of the correlation length was not significantly affected in the range of parameters shown in the table. The pixel values translate to a change in physical length of $\pm 2\ nm$.

	$\sigma_1 = 2.0$	$\sigma_1 = 2.5$	$\sigma_1 = 3.0$
$\sigma_2 = 2.0$	8.0933	8.163	8.181
$\sigma_2 = 2.5$	8.061	8.1708	8.179
$\sigma_2 = 3.0$	8.0826	8.1838	8.2

Table 1. Estimated correlation lengths, in pixels, for various image processing parameters for third image in row 1 of figure 4

In summary we have developed an image metrology system that can be used to estimate the orientation correlation function from images. The orientation estimation stage is critical to the success of the method. The estimation of the local orientation especially through the incorporation of geometric information is currently being pursued. Another avenue of research that we are currently investigating is the segmentation of the electron microscope images into regions based on the correlation function.

6. ACKNOWLEDGEMENT

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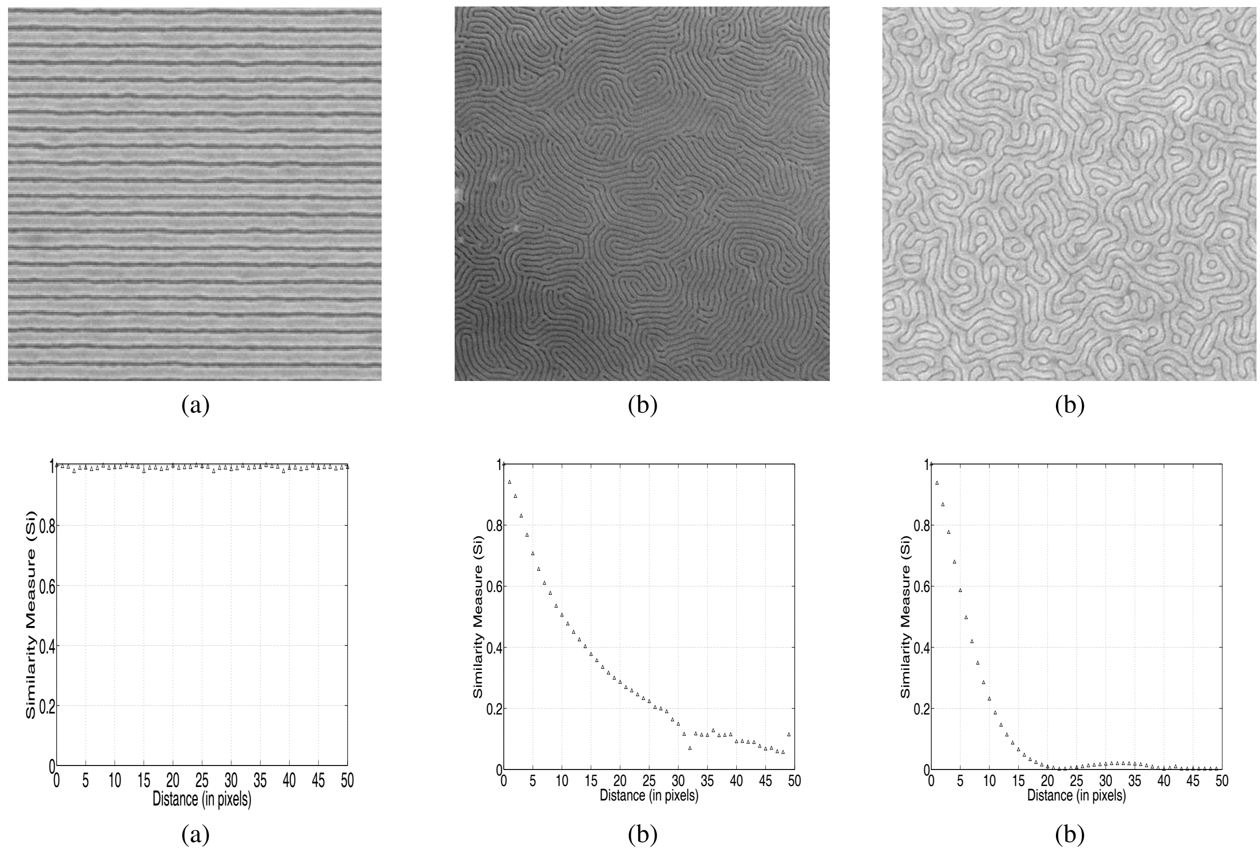

Fig. 4. Row 1: The example images for which correlation lengths are presented. Row 2: The corresponding correlation function plots. For the first image the correlation length is infinite as a constant structure extends throughout the image. For the second and third images the correlation length can be read from the plots as (approximately) 15 pixels and 8 pixels respectively.

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