Diffusion filtration for the evaluation of MEMs surface

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KEYWORDS : MEMs surface, geometrical feature, diffusion filter, PDE, wavelet shrinkage

MEMs surfaces are one type of typical structured surface. For this type of surfaces the accuracy of the geometrical feature (line width, step height etc.) are generally more important than roughness. For the exaction of these geometrical features, traditional convolution based filtration techniques are lack of the ability to preserve the feature with high accuracy. In this paper, a Partial Differential Equation (PDE) based nonlinear diffusion filter is proposed for the filtration of structured surface. In this model, the filtration procedure can be seen as a nonlinear heat equation, which describes the distribution of heat (or variation in temperature) in a given region over time. By choosing a proper diffusivity function, which is a nonnegative monotonically decreasing function in respect of the gradient of the surface, the diffusion process will take place mainly in the interior regions/feature (line, step, etc.) of the surface, and it will not affect the region boundaries. A wavelet based regularization method is introduced into the diffusion procedure, which can help to decrease the measurement outliers' influence. Experimental work using simulated and practical measurement surface data shows that, the proposed filter can separate the geometrical feature (especially the line and step) from roughness and measurement noise and outliers with ideal edge preserving property.

Manuscript received: January XX, 2011 / Accepted: January XX, 2011

1. Introduction

Surface metrology as a discipline is currently undergoing a huge paradigm shift: from stochastic to structured surfaces [1]. Structured surface can be defined as "surfaces with deterministic pattern of usually high aspect ratio geometric features designed to give a specific function". All structured surfaces are specifically designed to meet a highly defined functional requirement such as the specific optical response of a Fresnel lens. A key common feature of structured surfaces is that they are normally high aspect ratio surfaces where the surface geometry is the critical determination of component function. The scale of structured surfaces ranges from the macro scale down to the nano scale. Specific examples include MEMS/NEMS devices, micro moulding, micro fluidic systems (lab on a chip), defined geometry abrasives (3M Trizac), structured coatings, micro-lenses and optic elements, bio integration coatings, self cleaning coatings and sheet metal products.

The ability to adequately characterise these structured surface geometry is crucial in the optimisation and control of such functional surfaces. However, despite of rapid development of structured surface related products, the suitable metrology theory and practical methodologies are still far behind the requirements, because traditional surface texture parameters, such as roughness, waviness, and statistical descriptions can only be related to the function of such and add little information.

MEMs surfaces are one type of typical structured surface. From the function point of view, the accuracy of the geometrical feature (line width, step height etc.) of this type of surfaces is generally more important than the roughness. Removing noise from the measured surface data is often the first step for the accurate separation of these geometrical features. Its therefore the basic requirement of the denoising techniques is that they should not only reduce the noise, but do so without blurring or changing the location of the features. However, traditional filtration techniques are lack of the ability to preserve the feature boundary with high accuracy. For example, when using the Gaussian filter for the MEMs surface, the boundary of the lines and steps are smoothed. As a consequence, it is very difficult to exactly evaluate the width of lines and heights of steps. In recent years, the Surface Metrology Group (SMG) in Centre for Precision Technologies (CPT), University of Huddersfield (UoH) has investigated several techniques for the analysis of structured surface, including robust filters [2], wavelet filters, morphological filters and pattern analysis. Among them, based on Prof. Scott's fundamental work, new data segmentation method and feature parameters have been successfully used in the characterization of the structured surface [3-5]. Our recent work has included approaches based on non-linear diffusion. These techniques, based on the use of partial differential equations, have been extensively studied since the early work of Perona and Malik in 1987.

In this paper, a Partial Differential Equation (PDE) based nonlinear diffusion filter with the ability of both denoising and edge preserving is introduced for the filtration of structured surface. Section 2 introduces the physical background of the filter; Section 3 gives the detailed description of the diffusion filter for surface characterization; the numerical solution and experimental comparison are demonstrated in the section 4; and finally the conclusion will be given in section 5.

2. Heat diffusion equation

PDE based linear/nonlinear diffusion method have proved to be useful in many fields ranging from imaging processing to computer aided quality control and post-processing of noisy data. One typical diffusion method is the model of heat diffusion. The heat equation is an important partial differential equation which describes the distribution of heat (or variation in temperature) in a given region over time. For a function $u(\mathbf{x},t)$ of spatial variables $\mathbf{X}$ and the time variable t, the heat equation is [6,7] :

$$\partial u/\partial t = div\left(c\nabla u\right) \tag{1}$$

Where, div is divergence operator, ∇ is gradient operator, and c is called the conduction coefficient which is a measure of heat conduction speed. c is a function of location. When c is a constant, it is a linear diffusion procedure:

$$\partial u/\partial t = div(\nabla u) = c\Delta u \tag{2}$$

Where, Δ is the Laplacian operator. Solution of the diffusion procedure is given by the convolution integral:

$$u(\mathbf{x},t) = \begin{cases} f(\mathbf{x}), & (t=0) \\ (K_{\sqrt{2t}} * f)(\mathbf{x}), & (t>0) \end{cases} \tag{3}$$

Where, $K_\sigma(\mathbf{x})$ is the Gaussian convolution kernel:

$$K_\sigma(\mathbf{x}) := \frac{1}{2\pi\sigma^2}\exp\left(-\frac{|\mathbf{x}|^2}{2\sigma^2}\right) \tag{4}$$

And $\sigma = \sqrt{2t}$. The linear diffusion procedure can be seen as a filtration procedure by using a Gaussian filter with increasing standard deviation. The idea behind the use of the diffusion equation for signal analysis arose from the use of the Gaussian filter in multi-scale signal analysis.

3. Diffusion filter for surface characterization

3.1 Linear diffusion surface analysis

For surface characterisation, let $f(x)$ being the measured/original profile, with x being the spatial coordinate defined on the domain $(0,lx)$ and lx is the measuring length. The linear diffusion filter for profile surface analysis can be defined as:

$$\frac{\partial u}{\partial t} = div(c\nabla u) = c\Delta u = c\cdot u_{xx}$$
$$u(x,0) = f(x) \tag{5}$$

Where, $u(x,t)$ is the smoothed/filtered profile from original profile $f(x)$, with the time scale t, which is corresponding to the standard deviation σ and can be related with the cutoff wavelength that used in general filtration procedure. For linear diffusion filter, C is a constant.

For areal surface analysis, let the surface domain be an open rectangle $\Omega := (0,lx)\times(0,ly)$, the areal surface be represented by a bounded function $f:\Omega\to\mathbb{R}$. Then, a filtered areal surface $u(x,y,t)$ with a scale parameter $t>0$ may be obtained as the solution of a diffusion equation with the measured surface $f(x,y)$ as initial condition:

$$\frac{\partial u(x,y,t)}{\partial t} = div(c\cdot\nabla u) = c\cdot\Delta u = c(u_{xx}+u_{yy})$$
$$u(x,y,0) = f(x,y) \tag{6}$$

Where, u_{xx}, u_{yy} represent the second derivative at point (x, y) in two orthogonal measurement direction respectively.

Linear diffusion filter can smooth/denoise profile/areal surface very well. However, two disadvantages have limited its use for surface filter: (1) the location of the edge of region on the surface will be dislocated with the time scale increase, so the filter results do not give the right position of the surface feature; (2) due to the fact that the linear diffusion is an Gaussian smoothing procedure, it does not only reduce noise, but also smooth important features such as edges.

3.2 Adaptive diffusion filter for surface analysis

By introducing an adaptive conduction coefficient c, the above problem can be partly solved. The c can be designed as a function that has small value at the edge while has large value within the interior region of the feature on the measured surface. An improved linear diffusion filter described in formula (7) use a function of the gradient of the original measured surface f as the conduction coefficient/diffusivity function [6].

$$\frac{\partial u}{\partial t} = div\left(g\left(\|\nabla f\|^2\right)\cdot\nabla u\right) \tag{7}$$

Compared with standard linear diffusion filter, the conduction coefficient in this improved model is substituted with a function that : $c = g(\|\nabla f\|^2)$, where $g(\cdot)$ is a nonnegative monotonically decreasing function in respect of $\|\nabla f\|^2$, with $g(0)=1$. Here $\|\nabla f\|^2$ is chosen to locate the edge of the feature. In this way the diffusion process(smoothing process) will take place mainly in the interior regions (line, step, etc.) of the surface feature, and it will not affect the region boundaries where the magnitude of $\|\nabla f\|$ is large. According to [6], the optimized $g(\cdot)$ can be chosen as:

$$g(x) = e^{\left(-(x/K)^2\right)} \tag{8}$$

$$g(x) = \frac{1}{1+\left(x/K\right)^2} \tag{9}$$

Here, K can be a preset constant that is depend on the distribution of the gradient of surface. It can also be set according to the value of integral of histogram of the absolute values of the gradient throughout the surface [6]. In our work, for simplicity, the K can be preset as the mean absolute value of the gradient of the original surface:

$$K = mean(\|\nabla f\|) \tag{10}$$

Figure 1 gives two types of widely used diffusivity function.

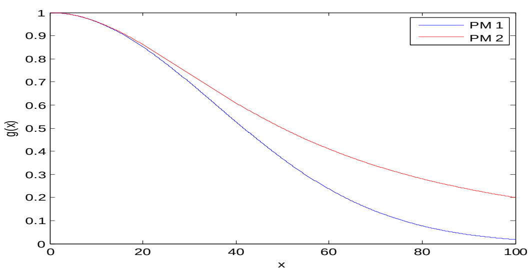

Figure 1 Diffusivity function

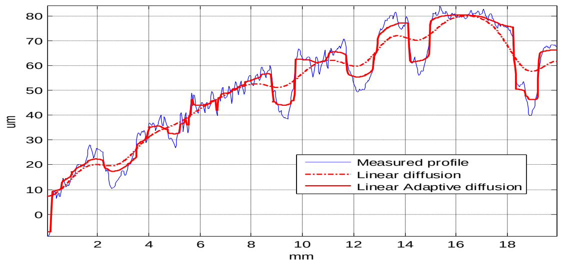

Figure 2 Comparison of the linear diffusion and the linear adaptive diffusion

Figure 2 compares the filtering results of a practical measured profile surface by using linear diffusion and linear adaptive diffusion filter. From these results one clear sees that: The filtering result of the linear diffusion filter is equivalent to a general Gaussian filter. Profile has been smoothed and however, the edge of the feature has also been blurred; by using the adaptive diffusion filter, the profile has been smoothed very well while the edges have been kept very clear.

Formula (7) is still a linear procedure, as $c = g(\|\nabla f\|^2)$ is a function of position, and do not change with the time increasing. A more complex model was proposed by Perona and Malik for image processing and called the nonlinear anisotropic diffusion filter [6]:

$$\frac{\partial u}{\partial t} = div(g(\|\nabla u\|^2)\cdot\nabla u) \tag{11}$$

Different from the linear case that using the gradient of the original surface as the independent variable, the conduction coefficient/diffusivity function of the nonlinear model using the gradient of the smoothed surface as the independent variable, which means that the conduction coefficient varies not only with different location, but also with the time increasing:

$$c = g(\|\nabla u\|^2) \tag{12}$$

And also, the K is set as the mean absolute value of the gradient of the updated surface value.

$$K = mean(\|\nabla u\|) \tag{13}$$

3.3 Wavelet Regularization

The accuracy of the above models is highly dependent on the gradient calculation of the surface. One serious problem is that outliers in the measured surface could often introduce very large oscillations of the gradient ∇u. It is therefore the gradient-based model possibly miscalculate the true edges and outliers, which leads to undesirable diffusion in regions where there is no true edge. A possible way to improve this is to regularize the model.

Similar with method of designing diffusivity function, there are two basic types of method to using regularisation: one is applying the regularisation on the original surface only once; the other is applying the regularisation on the diffused surface at each step. The second one has been widely used for nonlinear diffusion.

A typical improved model is based on Gaussian regularisation:

$$\frac{\partial u}{\partial t} = div\left(g\left(\|\nabla(u*G_\sigma)\|\right)\nabla u\right) \tag{14}$$

Where G_σ is a Gaussian kernel with variance σ, and $*$ denotes the convolution operator. It means that in each iteration there are three steps to calculate the updated diffusivity function: (1) using Gaussian filter to regularize the diffused surface; (2) calculate the gradient using the regularized surface; (3) calculate the diffusion function.

A wavelet shrinkage method is introduced as the regularization filter in the following session.

The kth measured signal value can be written as:

$$u = s + n \tag{15}$$

where s represents the true signal and n the noise. The aim of denoising is to estimate s as accurately as possible from u In the wavelet domain, at the ith decomposition level:

$$w_{u,i} = w_{s,i} + w_{n,i} \tag{16}$$

where $w_{u,i}$ is the noisy wavelet coefficient, $w_{s,i}$ is the true coefficient and $w_{n,i}$ is the noise wavelet coefficient. The denoising problem is then to estimate $w_{s,i}$ as accurately as possible from $w_{u,i}$, and then reconstruct the signal from the denoised wavelet coefficients $w_{s,i}$. Simple denoising algorithms that use the wavelet transform consist of three steps: (1) Calculate the wavelet transform of the noisy signal; (2) Modify the noisy wavelet coefficients according to some rules; (3) Compute the inverse wavelet transform using the modified coefficients to reconstruct the denoised signal. One of the well-known rules for the second step is thresholding analysis, which includes soft and hard thresholding. The basic procedure of the improved diffusion filter is described in formulae (17), (18).

$$\frac{\partial u}{\partial t} = div\left(g\left(\|\nabla(u_T)\|\right)\nabla u\right) \tag{17}$$

$$u_T = IWT(ST(WT(u))) \tag{18}$$

Where u_T represent the shrinked version of u, WT and IWT represent the forward and inverse wavelet respectively, and ST represent the shrinkage operator.

The selection of the threshold value T is the key issue for the denoising problem. The simplest way is to use the variance of the wavelet coefficients on each level as the threshold value. In this paper, the widely used MAP (Maximum a posteriori) method is chosen to estimate the thresholding value. The MAP estimates the signal in terms of the Probability Density Function (PDF) of the noise and the PDF of the signal coefficient.

4. Numerical solution and experiments

To make the model practical for the measured surface analysis, the above model needs to be discretised.

4.1 Profile analysis

For profile surface analysis, let z_i be the height of the measured profile surface at position $(i\Delta x)$, u_i^t and u_i^{t+1} be the filtered profile data at time scale t and $t+1$ respectively, i be the index of the surface co-ordinate in x and y direction, and $i = 0,\ldots,M-1$, M be the number of points in x and y direction respectively, and the lateral sample spacing is Δx. The treatment of the diffusion process can be simplified as [6,7]:

$$u_i^{t+1} = u_i^t + \tau\left[g(\|\nabla_L u\|)\cdot\nabla_L u + g(\|\nabla_R u\|)\cdot\nabla_R u\right]_i^t$$
$$u_i^0 = z_i \tag{19}$$

Where τ is the time spacing, ∇_L and ∇_R represent the forward and backward difference of the neighbor points which are defined as:

$$\nabla_L u_{i,j} = u_{i-1} - u_i \qquad \nabla_R u_i = u_{i+1} - u_i \tag{20}$$

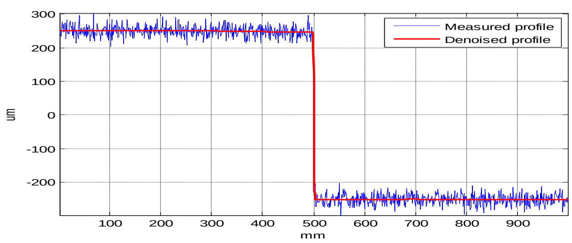

Figure 3 Diffusion filter on a simulated single-side step height

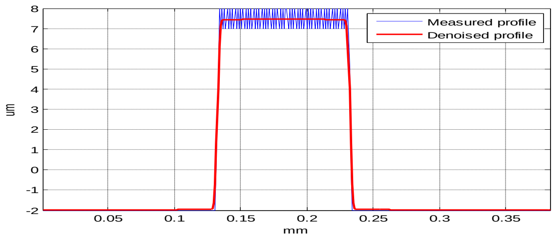

Figure 4 Diffusion filter on a simulated double-sided step height

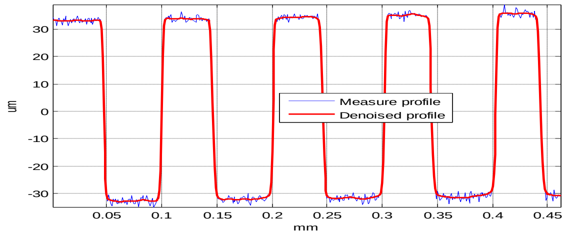

Figure 5 Diffusion filter on a measured multi step height

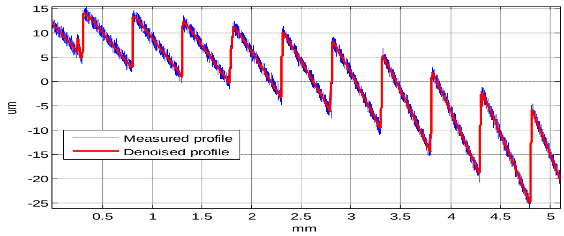

Figure 6 Diffusion filter on a aspheric diffractive lens

As the steps are typical types of featutre in MEMs surface, Figure 3 and figure 4 using two simulated steps to evaluate the performance of the introduced diffusion filter. Figure 3 is a single-sided step and figure 4 is a double-sided step. Gauss distributed noise and also some heavy noises have been added on the test data. From these examples it is very clear that the profiles have been smoothed very well and also the most important feature, edge of the step are well preserved and not distorted at all.

Figure 5 and figure 6 use two practical measured profile surfaces to demonstrate the ability of the diffusion filter for processing surfaced with multiple feature regions. Figure 5 is a standard calibration gauge with multi-steps, and figure 6 is the aspheric diffractive lens profile.

4.2 Areal surface analysis

For areal surface analysis, Let $z_{i,j}$ be the height of the measured surface data at position $(i\Delta x, j\Delta y)$, $u_{i,j}^{t}$ and $u_{i,j}^{t+1}$ be the filter surface data at time scale t and $t+1$ respectively, i, j be the index of the surface co-ordinate in x and y direction, and $i = 0,...,M-1; j = 0,...N-1$, M, N be the number of points in x and y direction respectively, and the lateral sample spacing are $\Delta x, \Delta y$. The model can be numerically described as the following by using a 4-neareset neighbour discretisation scheme of the Laplacian operator [6,7]:

$$u_{i,j}^{t+1} = u_{i,j}^{t} + \tau\left[c_N \cdot \nabla_N u + c_S \cdot \nabla_S u + c_E \cdot \nabla_E u + c_W \cdot \nabla_W u\right]_{i,j}^{t}$$
$$u_{i,j}^{0} = z_{i,j} \qquad (21)$$

The symbol ∇ indicates nearest neighbour difference:

$$\nabla_N u_{i,j} = u_{i-1,j} - u_{i,j} \qquad \nabla_S u_{i,j} = u_{i+1,j} - u_{i,j}$$
$$\nabla_E u_{i,j} = u_{i,j+1} - u_{i,j} \qquad \nabla_W u_{i,j} = u_{i,j-1} - u_{i,j} \qquad (22)$$

The conduction coefficients are updated at each iteration as a function of the gradient:

$$c_{N_{i,j}}^{t} = g\left(\left|\nabla_N u_{i,j}^{t}\right|\right) \qquad c_{S_{i,j}}^{t} = g\left(\left|\nabla_S u_{i,j}^{t}\right|\right)$$
$$c_{E_{i,j}}^{t} = g\left(\left|\nabla_E u_{i,j}^{t}\right|\right) \qquad c_{W_{i,j}}^{t} = g\left(\left|\nabla_W u_{i,j}^{t}\right|\right) \qquad (23)$$

Figure 7 gives an example of the diffusion filter on a practical measure MEMs surface. To make it easy to see, figure 8 is the section profiles from figure 7. From this example, one can clearly see that the most important feature on the surface: lines, steps and even very small stairs are preserved very well.

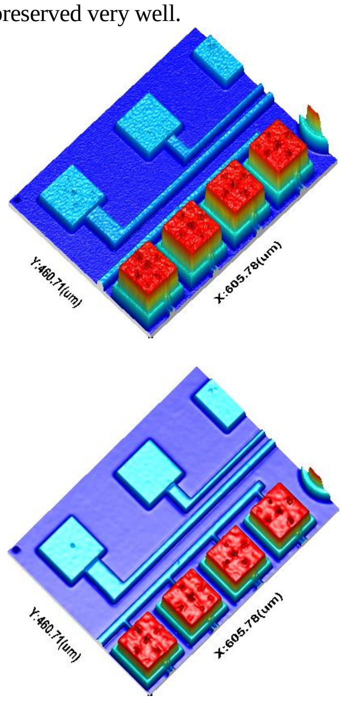

Figure 7 diffusion on a measured Mems surface (Up: measured; down: denoised result)

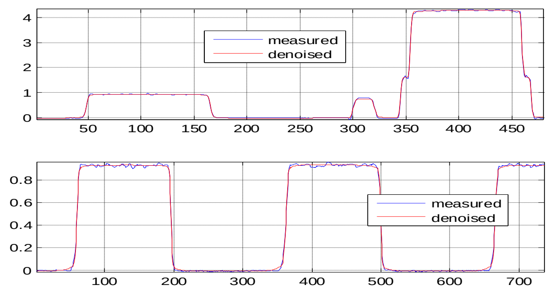

Figure 8 Section profile form figure 7

4. Conclusions

In this paper, a Partial Differential Equation (PDE) based nonlinear diffusion filter that combined with the wavelet domain shrinkage is introduced to denoise the MEMs surface, for which the accuracy of the geometrical feature (line width, step height etc.) are generally more important than the traditional roughness. In this model, the filtration procedure can be seen as a nonlinear heat equation, which describes the distribution of heat (or variation in temperature) in a given region over time. The diffusivity function based on the gradient of the surface can help to separate the internal region area of boundary area of the measured feature. In this way the diffusion process will take place mainly in the interior regions (line, step, etc.) of the surface, and it will not affect the region boundaries where the magnitude of gradient is large. The model proposed here has been coded with Matlab R13. Experimental work shows that the proposed filter can separate the geometrical feature (especially the line and step) from roughness and measurement noise and outliers with ideal edge preserving property. However, the introduced diffusion filters still have some defects which hamper its more general practical application: (1) Staircase phenomena will arise when surfaces have big curvature; (2) It needs much iteration to reach the ideal result, which leads to a time-consuming algorithm. Consequently, our further will focus on the solutions of these problems.

ACKNOWLEDGEMENT

The authors would like to thank the European Research Council under its programme ERC-2008-AdG 228117-Surfund. The author X. Jiang would also like to gratefully acknowledge the Royal Society under Wolfson Research Merit Award.

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