A REALISTIC ESTIMATION OF NANOSURFACES AREA FROM SEM GRAYSCALE IMAGES

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In this paper we present an efficient algorithm for evaluating the surface area of three-dimensional nanostructures by means of their two-dimensional images (SEMmicrographs) in grayscale using linear and non-linear extrusion method to implement it for nanowalls. It is studied a particular case in which the image is performed in a direction perpendicular to the light, and the illumination is diffused (no shadow) in order to allow more precise correlation between the elevation and gray levels.

Keywords: two-dimensional image, three-dimensional visualization, surface topographical analysis, non-linear elevation, non-linear extrusion

1. Introduction

In the computerized analysis of photography, there are already several consecrate definitions and we will present them further. We can say that a grayscale or greyscale digital image is an image, in which the value of each pixel is a single sample, that is, it carries only intensity information. Much more, the images of this category, also known as black-and-white images, are composed exclusively of shades of gray, varying from black at the weakest intensity to white at the strongest [1]. Qualitatively speaking, grayscale images are distinct from one-bit bi-tonal black-and-white images, which in the context of computer imaging are images with only the two colors, black and white (called bi-level or binary images). Grayscale images have many shades of gray in between. Grayscale images are often the result of measuring the intensity of light at each pixel in a single band of the electromagnetic spectrum and in such cases they are properly monochromatic when only a given frequency is captured.

Nanofabrication is a state of the art technology. Various chemical, mechanical, biochemical and semiconductor products have characteristics controlled by the nanostructures of the surface and interphase. Surface microscopic imaging is generally used to capture different surface features. By

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properly analyzing the surface image, valuable information regarding manufacturing process and product performance can be extracted. While microscopy measurements can offer very accurate qualitative information about surface features, for many applications, it is critical to obtain a quantitative description of the surface morphology. Various statistical features can be used to characterize the surface in quantitative way.

Correct principial assessment of the three-dimensional surface area value can be achieved by two mathematical ways. In the first method, the studied surface can be described by means of the precise functions and in the second method by using the Cartesian coordinates for a finite number of points on the surface. In the first case, the area can be calculated exactly while in the second only an approximate estimate is obtained.

2. Theoretical background of surface estimator

A lot of advanced methods including the microscopic technology have revolutionized the way objects can be perceived on the nanoscale. Thus perhaps the most powerful tool such as the scanning electron microscope (SEM) provides the ability to rapidly characterize samples using high magnification, producing two-dimensional (2D) image representation of the samples taken from different structural materials, from metals and alloys to super hard ceramic.Contextually, SEM pictures will be used by us, together with a suitable analytical technique, to obtain very good results.

Often we have only a plane (two-dimensional or 2D image) picture of a spatial (three-dimensional or 3D) image, such as, for example, SEM (Scanning Electron Microscope) micrographs or TEM (Transmission Electron Microscopy) images of nanostructures, terrain satellite images, old photographs of different objects and real-time registration of street traffic [2]. The aim of the present paper is to create 3D models for such pictures using specialized software and calculate the surface area. These techniques are already used by some graphics editing programs like Adobe Photoshop, Corel Bryce, MacDEM, World Construction which are specialized in exploring the 3D world geometrical properties without the possibility to calculate the obtained 3D surface area.

In the next paragraphs, after creating the linear or non-linear elevation model of a two-dimensional space, two numerical methods will be used to estimate the area of the 3D surface, with arbitrary complexity. In the first case, there is used a discrete method, determined by the resolution of the 2D picture and in the second case this digitization is eliminated using interpolation functions $f(x,y)$, where x and y are the picture length and width respectively.

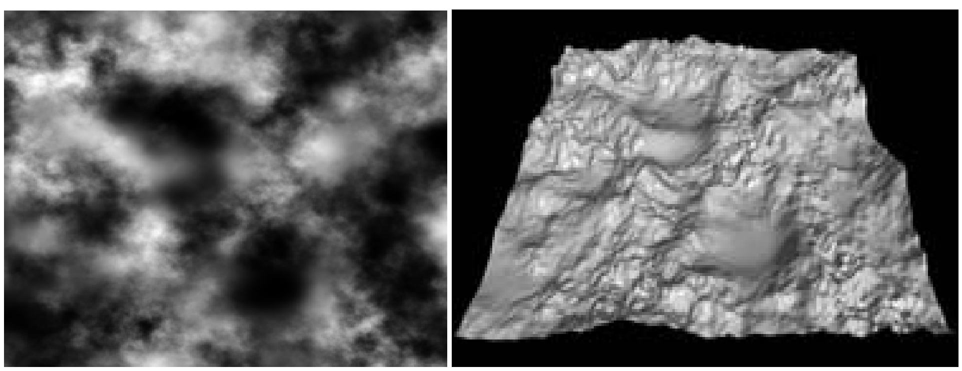
This information, i.e. the 3D surface area, is useful in some special cases such as evaluation of the terrain water absorbance, heat transfer of the electrical circuits into air, specific surface area for complex structures etc. In order to model the 3D elevation (linear or non-linear) and calculate the surface area, the *Mathematica*software is used for the implementation of the algorithm. The specific functions are presented in the following paragraph.

2. 1 Surface area of a 3D image created from 2D image

All samples were initially viewed at lower magnification in order to identify suitable regions of the surface for analysis, prior toanalysis at higher magnification.

In order to create a 3D model from two-dimensional pictures, the *Digital Elevation Model* (DEM) is frequently used. This technique is useful in case of grayscale pictures because in the case of 256 levels there are 256 elevation heights for the 3D image.

In order to show the diversity of the domains of application, an edificatory example is represented in Fig. 1, respectively two images belonging to the public domain, (see http://commons.wikimedia.org/wiki/File:Heightmap.png), recorded in May 2014. We have here, in the clear: in a) there is the grayscale image for a height map model, while in b) a 3D model is created using this method, in perspective view.



a) b)

Fig. 1. a) A heightmap created with Terragen, b) The same heightmap converted to a 3D mesh and rendered with Anim8or.

According to the computer graphics glossary, a heightmap or heightfield is a raster image used to store values, such as surface elevation data, for display in 3D computer graphics.

This method was developed in some cases for the implementation in other imaging software [3-5] without a direct algorithm for estimating the surface area. In *Mathematica*, where line instructions are used step by step, without recalibrations of distances, the algorithm is reduced to a few lines. The case of study is focused on a grayscale SEM image of nanosurfaces (see Fig. 2). As said, grayscale is a range of monochromatic shades from black to white. In other words, a grayscale image contains only shades of gray and no color. Inherently, each pixel has a luminance value, regardless of its color. Luminance can also be described as brightness or intensity, which can be measured on a scale from black (zero intensity) to white (full intensity). The first step is to import and transform the 2D image into a matrix, i.e. *m* in the algorithm (all variables are italic and the functions are bold), with the same size as the picture. This method will be further used to estimate the specific surface of different nanostructures from 2D SEM images. The matrix elements are numerically equal, in the case of the linear elevation method (LEM), with grayscale level numbers 0 for black and 255 for white.

$$m_{ij} = \text{Color}(Grayscale\ level)_{ij} \tag{1}$$

ln[1]:=fin = "1.bmp";

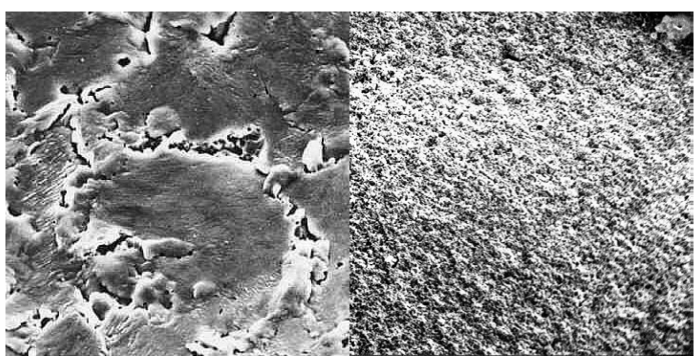
calea = "D:\\ ";

ln[2]:=elem = **Import**[*calea*<>*fin*, "Data"];

es = **Import**[*calea*<>*fin*, "ImageSize"];

m = **N@Map**[255 **-** **Mean**[#] &, *elem*, {2}];

ArrayPlot[*m*];



a) b)

Fig. 2. SEM image of nanosurfacesfrom scaled captures
a) 50 μm (First image) and b) 1 mm (Second image)

In the images of Fig. 2, the scanning electron microscopy of the cavitated surface for the material entitled “45” [6], at two different magnifications, is presented. More precisely, the material “45”, conform to its original denomination, is a carbon steel of high quality, hardened and tempered. This alloy contains C(0.43), Mn(0.63), Si(0.26), P(0.030), S(0.033) and Fe in rest.

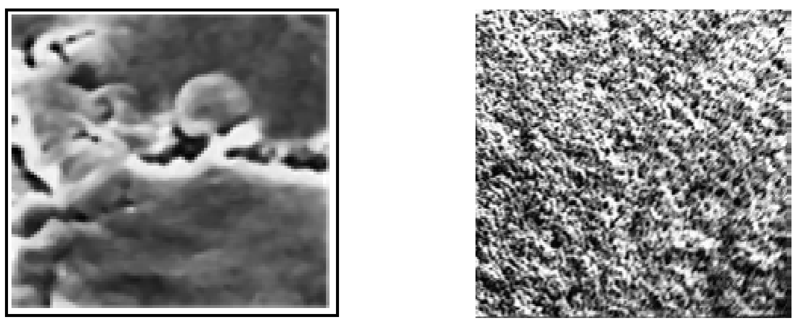
In order to reduce the calculation time we use only a part of this image, cropping only a small dimension (about 150x150 px’s), as presented in Fig. 3.

ln[3]:=nsi[x_, y_, dx_, dy_] := nsiO[[x ;; x + dx, x ;; x + dx]];

ln[4]:=ena = nsi[70, 70, 150, 150];

es = Dimensions[ena];

Line 4 defines the cropped image zone that starts with coordinates {70, 70} and dimensions {150,150}.



a) b)

Fig. 3. SEM image of nanosurfaces after import theme in Mathematica with reduced dimensions a) a cropped rectangle image from Fig. 1 a), vertices coordinates {{70,70}, {220,70}, {70,220}, {220,200}}, b) a cropped rectangle image from Fig. 1 b), vertices coordinates {{70,70}, {220,70}, {70,220}, {220,200}}

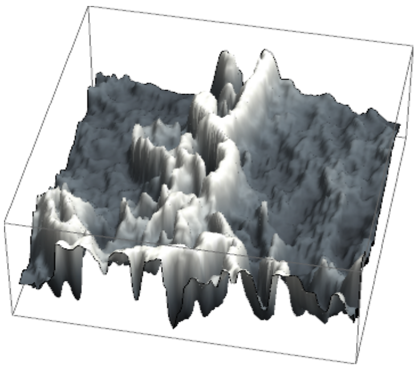
3. Results and discussion

For the best results, we can optimize the initial image using filters or transformation functions for the matrix elements. In the case of non-linear elevation method (NLEM) an additional function $nlf = nlf(x)$ is used where $x \in \{0,1,...,255\}$ and the associated matrix is determined by this function through Equation (1)

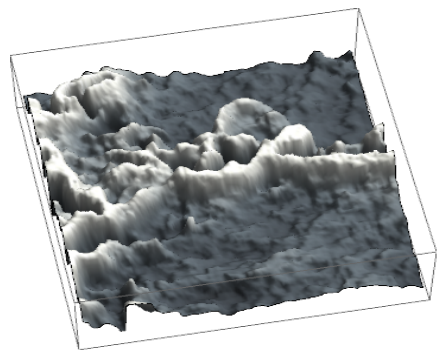
$$m_{ij} = nlf\left(\text{Color}(\textit{Grayscale level})_{ij}\right) \tag{2}$$

This method was tested for a SEM image on the top surfaces of ZnO microcrystals [5, 7].The 3D image can be viewed using the **ListPlot3D** function and for different viewpoints it is represented in Fig. 4.

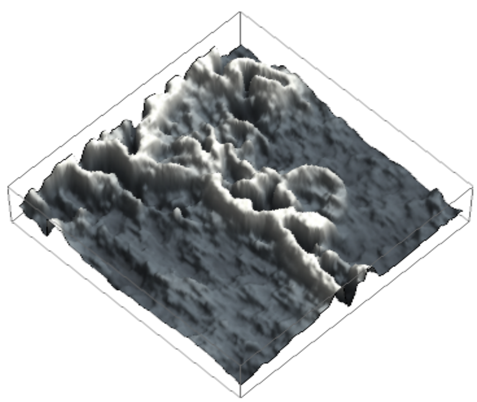
*ln[5]:=***ListPlot3D**[**Transpose**[255 - *m*], Mesh→None, ColorFunction→"GrayTones", Axes→False, Boxed→True, ViewPoint→{5, -1, 10}, AspectRatio→1, PlotRange→{0, 300}];



a) ViewPoint→{1, -5, 5}



b) ViewPoint→{5, -1, 10}



c) ViewPoint→{5, 5, 20}

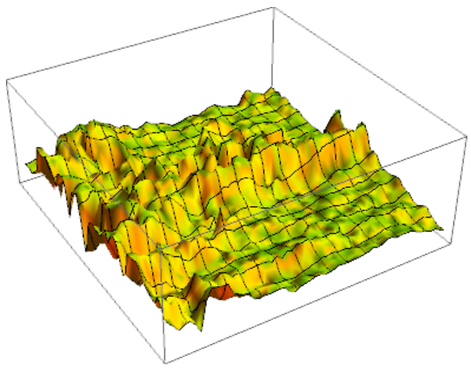
Fig. 4. 3D image of nanosurfacesobtained using DEM for different viewpoints
a) ViewPoint→{1, -5, 5}, b) ViewPoint→{5, -1, 10}, c) ViewPoint→{5, 5, 20}

Using this data we can evaluate in analytical form the expression of a 2D surface area [8], defined by $f(x, y)$ as

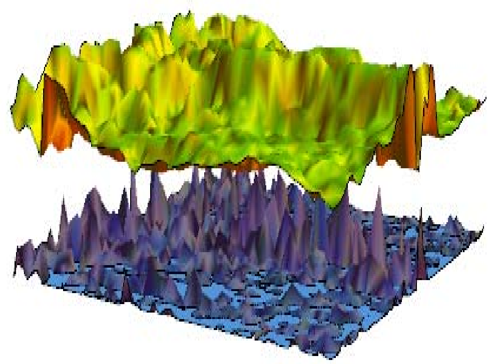
$$S = \iint_{x\,y} \sqrt{1 + \left(\frac{\partial \mathrm{f}(x, y)}{\partial x}\right)^2 + \left(\frac{\partial \mathrm{f}(x, y)}{\partial y}\right)^2}\, \mathrm{d}x\mathrm{d}y \qquad (3)$$

In order to estimate analytically the surface area using formula (3), the interpolation function is created using the function **Interpolation**.

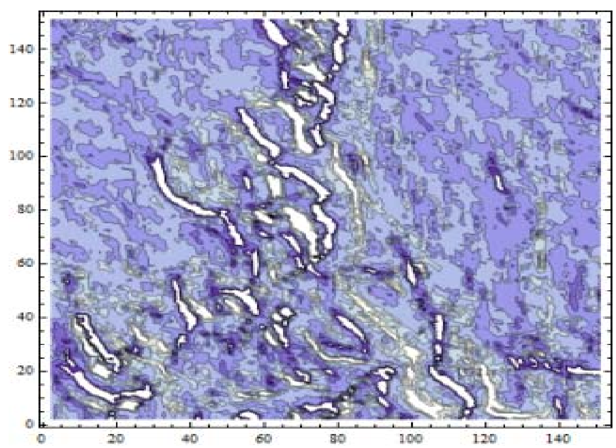
ln[6]:=ptInterpolare = **Flatten**[**Table**[{{i, j}, *m*[[i]][[j]]}, {i, 1, es[[2]]}, {j, 1,*es*[[1]]}], 1]; *fint* = **Interpolation**[*ptInterpolare*];



a) the 3D surface



b) both the 3D surface above and the derivative under – the darker surface



c) contour plot of derivative where the white colors indicate the zones with high variations of the surface heights

Fig. 5. 3D graphics using interpolating function with two variables and its derivative

In order to compare the solution with the original image, the surface and its derivative are represented in Fig. 5.

*ln[7]:=***Plot3D**[256 - *fint*[x, y], {x, 1, *es*[[2]]}, {y, 1, *es*[[1]]}, Mesh→None, ColorFunction→"GrayTones", Axes→False, Boxed→False, PlotRange→{0, 255}];

The same images can be obtained replacing in first line the variable fint with the actual name of the bitmap file of the second image (information about the characteristic surface ratio is presented in Table 1). Similar to line "*ln[6]:=*" one may create the 3D graphics in Fig. 5.b, "*ln[7]:=*". Using formula (3) through line 7 (*ln[8]:=*), the surface area is calculated.

*ln[8]:=*S=**NIntegrate**[**Evaluate**[**Sqrt**[1 + (\!\(***SubscriptBox**[\(\[PartialD]\), \(x\)]\(*fint*[x, y]\)\))^2 + (\!\(***SubscriptBox**[\(\[PartialD]\), \(y\)]\(*fint*[x, y]\)\))^2]], {x, 1, *es*[[2]] - 1}, {y, 1, *es*[[1]] - 1}, Method→"MonteCarlo"];

The contour plot is created as follows:

*ln[9]:=***ContourPlot**[**Evaluate**[(\!\(***SubscriptBox**[\(\[PartialD]\), \(x\)]\(*fint*[x, y]\)\)) + (\!\(
***SubscriptBox**[\(\[PartialD]\), \(y\)]\(*fint*[x, y]\)\))], {x, 2, *es*[[2]]}, {y, 2, *es*[[1]]}];

The result in this case is a number with area units determined by a rescaled picture (eventually $\text{pixel}^2 = \text{px}^2$, if one unit for grayscale level is considered as 1 pixel), $S_0 = 150\text{px}150\text{px} = 22500(\text{px}^2)$.

Using information from line "*ln[8]:=*", we obtain a characteristic surface ratio of $r = 11.56$, a dimensionless number that characterizes the size of the 3D surface related to the projected 2D surface.

We calculate the characteristic surface ratio from the relation,

$$r = \frac{S}{S_0} \tag{4}$$

This value is statistically independent of the location of the cropped area. In Table 1, there are indicated some values of r function of the cropped area.

Table 1

No	Position (x)	Position (y)	Dimension (x)	Dimension(y)	Characteristic surface ratio	
					First image	Second image
1	70	70	150	150	11.56	19.61
2	80	80	200	200	11.07	20.01
3	100	100	150	150	11.26	19.94
4	120	120	230	230	11.50	19.46
5	70	150	200	150	11.32	19.95
				Average	**11.34**	**19.79**

Undoubtedly, the quality of the three-dimensional image reconstruction will be dependent on the quality of the input micrograph [9, 10]. Today, working with performance apparatus and SEM software allows for the manipulation of the brightness and contrast prior to the capture of the image. As a professional recommendation, the contrast should be set to the maximum level possible without losing the topological detail [11], in the upper and lower extremities of the surface.

The elegance and efficiency of our algorithm to produce three-dimensional displacement maps based on two-dimensional data have been proved. From now on**,** it will honor and extend the group of analytical techniques that can be applied for the 3D structure visualization and assessment of surface topography. As seen above, it is easily applicable to scanning electron micrographs, when calibrated appropriately using data collected perhaps in the future, from AFM **(**Atomic Force Microscope**)** scans.

4. Conclusions

An efficient algorithm for evaluating the surface area of three-dimensional nanostructures by means of their two-dimensional images in grayscale, using linear and nonlinear extrusion method, has been developed.

The proposed algorithm may be used (with recalibrations, correlation between 2D picture dimensions, grayscale deep and real dimensions), in order to obtain numerical results with units about complex surface areas in a large variety of research fields.

Essentially, the ability to produce three-dimensional realistic images based on two-dimensional data widens the range of analytical techniques that can be applied for the visualization and assessment of surface topography. This technique is particularly dedicated to nanosurfaces images analysis and undoubtedly easily applicable to scanning electron micrographs.

Evidently, without major changes, the authors will further use this algorithm in order to estimate the specific surface area for nanowalls using SEM images and the specific volume of nanostructures, by data corroboration from AFM (Atomic Force Microscope) imaging.

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