Stochastic and fractal properties of silicon and porous silicon rough surfaces

S Hosseinabadi 1 and M Rajabi 2
1 Department of Physics, East Tehran Branch, Islamic Azad University, P. O. Box 163-33955, Tehran, Iran
2 Iranian Research Organization for Science and Technology (IROST), P. O. Box 33535-111, Tehran, Iran
E-mail: hosseinabadi.s@gmail.com

Abstract. In this paper, we investigate the stochastic properties and fractal behavior of Si and porous silicon (PS) rough surfaces to characterize the complexity of their morphology. To this end, height fluctuations of these rough surfaces are determined by Atomic Force Microscopy (AFM) and then roughness and correlation length of the surfaces are calculated. The generalized Hurst exponent, $h(q)$ and singularity spectrum, $f(\alpha)$ are obtained by using two dimensional MF-DFA method for both rough surfaces; Our results show that both mentioned surfaces are multifractal and have different scaling exponents. To investigate the reason of the observed multifractality behavior, we determine height distribution, skewness and kurtosis measures and show that the deviation from the Gaussian distribution for the height fluctuations of the surfaces can be a reason for the observed multifractality behavior.

1. Introduction
In the last decades, exploring and characterization of stochastic surface morphology has been one of the interesting fields of study, because surface roughness has an enormous influence on many important physical phenomena such as optical and optoelectronics properties, surface conductivity, reflection and scattering [1, 2, 3]. One can characterize many natural phenomena by a degree of stochasticity: Seismic recordings, cosmic background radiation [4, 5], turbulent flows [6, 7, 8, 9], stock market [10, 11], earthquakes [12] and the surface roughness during growing of many materials and corrosion [13, 14, 15] are examples of such phenomena and processes. Many random processes in nature generate fractal structures; Fractal structures or scaling properties have been observed in space fluctuations of rough surfaces and such interfaces show self-similar or self-affine properties [16, 17, 18, 19, 20]. Fractal properties have also been studied in the other topic such as biology [21, 22], bacterial colony growth [23], diffusion-limited aggregation [24] and climate indicators [25]. When the structure is uniform and regular, we have a monofractal structure and the system is described only by one scaling exponent named Hurst exponent, $H$; any irregularity in the system can reduce to the multifractality behavior. A multifractal system is combination of different monofractal subsets [17, 18] and various regions of the system have different scaling exponents, named generalized Hurst exponent, $h(q)$; In other words, multifractals should be described by many different numbers of scaling exponents $h(q)$, where $q$ is a real number. Because of infinite scaling exponents, the theoretical and the numerical study of the multifractal surfaces is more complicated than those of monofractal ones. Changing
one of the $h(q)$'s can lead to different feature in the system. Another important feature of the multifractal systems, is the presence of the singularity spectrum, $f(\alpha)$, where $\alpha$ is the H"older exponent. Recently there has been an increasing interest in the notion of multifractality because of its extensive applications in different areas such as complex systems, industrial and natural phenomena. In this paper, we study the statistical and fractal properties of silicon surface and porous silicon (PS) rough surface produced during electrochemical etching of Si. Because of band gap broadening of PS compared to silicon and room temperature visible photoluminescence, more studies make it a promising material for Si based optoelectronic devices [26, 27, 28]. In this study, we determine the height fluctuations of Si and PS surfaces with Atomic Force Microscopy (AFM); Then we investigate the complexity of the height fluctuations and determine the fractal properties of them by two dimensional multifractal detrended fluctuation analysis. We show that the studied rough surfaces are multifractal and investigate the reason of the observed multifractality behavior.

2. Experiment
In this study we use (100) oriented, boron doped p-type silicon films with thickness of 525±20µm. Electrochemical etching of Si surfaces are performed at a constant current density of 20mA/cm$^2$ for 20min in solution of 32%HF($HF : C_2H_5OH = 4 : 1$) and porous silicon (PS) rough surfaces are produced. The surface topography of Si and PS surfaces are characterized by Atomic Force Microscope (AFM; Veeco-Termo Microscopes) in contact mode. Figure 1 shows the AFM images of the Si and PS rough surfaces.

3. Statistical and Fractal Analysis
3.1. Roughness and correlation function
A rough surface is usually studied in terms of its deviation from a smooth surface or roughness, $\sigma$ as $\sigma = \langle [h(\vec{r}) - \bar{h}]^2 \rangle^{1/2}$ in which $h(\vec{r})$ is the height at position $\vec{r}$ and $\bar{h}$ is the mean height [13]. The surfaces with equal $\sigma$ may have different shapes and morphology; Therefore, the correlation function $C(\vec{r},\vec{r}')$ or the correlation length scale , over which the correlation function reaches 1/e of its maximum should be investigated. The correlation function is defined by

$$C(\vec{r},\vec{r}') = \langle [h(\vec{r}) - \bar{h}][h(\vec{r}') - \bar{h}] \rangle$$ (1)
For an isotropic surface, we can define the normalized correlation function as follows:

$$C(|\vec{r} - \vec{r}'|) = \frac{\langle [h(\vec{r} + \vec{l}) - \bar{h}] \cdot [h(\vec{r}) - \bar{h}] \rangle}{\sigma^2}$$  \hspace{1cm} (2)

where $l = |\vec{r} - \vec{r}'|$.

Our calculations show that the roughness of PS rough surface is greater than Si one ($\sigma_{Si} = 7.3 \pm 0.1 \text{nm}$ and $\sigma_{PS} = 14.200 \pm 0.001 \mu\text{m}$); Also the height fluctuations of PS surface are more correlated than Si one. Figure 2 shows the correlation function, $C(l)$ with respect to the separation distance, $l$. This diagram shows that the correlation length of PS is greater than Si or in other words, the correlation length increases when the Si thin film is etched by HF solution.

![Figure 2. Correlation function $C(l)$ for Si and PS surfaces.](image)

### 3.2. Fractal properties

There are different methods to determine the fractal properties of random data sets; These methods are such as spectral analysis [29], fluctuation analysis [30], detrended fluctuation analysis (DFA) [22, 32, 33], wavelet transform module maxima (WTMM) [34, 35] and discrete wavelets [36, 37]. For real and experimental data sets and in the presence of noise, the multifractal DFA (MF-DFA) method gives very reliable results [31, 32]. This algorithm is simpler than WTMM but involves a bit more effort in programming. To analyse the fractal behavior of the height fluctuations of our rough surfaces, we use the two dimensional MF-DFA algorithm and determine the spectrum of the generalized Hurst exponent, $h(q)$. Two dimensional MF-DFA algorithm is as follows: In this method, height fluctuation of the rough surface is represented by $Z(\vec{r})$ at coordinate $\vec{r} = (i, j)$ and has the following steps [31]:

**Step 1**: Consider a two dimensional array $Z(i, j)$ where $i = 1, 2, ..., M$ and $j = 1, 2, ..., N$. Divide the $h(i, j)$ into $M_s \times N_s$ non-overlapping square segments of equal sizes $s \times s$, where $M_s = \lfloor \frac{M}{s} \rfloor$ and $N_s = \lfloor \frac{N}{s} \rfloor$. Each square segment can be denoted by $Z_{\nu,w}$ such that $u_{\nu,w}(i, j) = Z(l_1 + i, l_2 + j)$ for $1 \leq i, j \leq s$, where $l_1 = (\nu - 1)s$ and $l_2 = (w - 1)s$.

**Step 2**: The cumulative sum in each segment is calculated by:

$$u_{\nu,w}(i, j) = \sum_{k_1=1}^{i} \sum_{k_2=1}^{j} Z_{\nu,w}(k_1, k_2);$$  \hspace{1cm} (3)
where $1 \leq i, j \leq s$.

**Step 3:** Local trend in each segments is determined by fitting procedure as follows:

$$\tilde{u}_{\nu,w}(i, j) = ai + bj + c. \hspace{1cm} (4)$$

Variance for each segment is determined as follows:

$$\delta_{\nu,w}(i, j) = u_{\nu,w}(i, j) - \tilde{u}_{\nu,w}(i, j), \hspace{1cm} (5)$$

$$F^2_{\nu,w}(s) = \frac{1}{s^2} \sum_{i=1}^{s} \sum_{j=1}^{s} \delta_{\nu,w}(i, j). \hspace{1cm} (6)$$

**Step 4:** Fluctuation function in $q$’th order is obtained by averaging over all segments:

$$F_q(s) = \left( \frac{1}{M_s \times N_s} \sum_{\nu=1}^{M_s} \sum_{w=1}^{N_s} \left[ F^2_{\nu,w}(s) \right]^{q/2} \right)^{1/q}, \hspace{1cm} (7)$$

$F_q(s)$ increases with increasing $s$ and depends on the order $q$. In the above relation, $q$ can take any real value except zero. For $q = 0$, equation (7) becomes

$$F_0(s) = \exp \left( \frac{1}{2M_s \times N_s} \sum_{\nu=1}^{M_s} \sum_{w=1}^{N_s} \ln F^2_{\nu,w}(s) \right). \hspace{1cm} (8)$$

**Step 5:** Finally, the scaling behavior of the fluctuation functions should be investigated by analyzing log-log plots of $F_q(s)$ versus $s$ for each moment of $q$,

$$F(s) \sim s^{h(q)}. \hspace{1cm} (9)$$

For $q = 2$ the Hurst exponent is obtained by:

$$H \equiv h(q = 2) - 1. \hspace{1cm} (10)$$

If $h(q)$ with respect to $q$ is a constant value, the system will be monofractal and the constant value named Hurst exponent; in other words, a monofractal system can be characterized by a single scaling law with one scaling exponent (Hurst exponent ) in all scales [17, 18]. In multifractal structures, scaling behavior of the system is changing with $q$ and should be described with the whole spectrum of scaling exponents $h(q)$.

Figure 3 shows the generalized Hurst exponent, $h(q)$ as a function of $q$ for Si and PS rough surfaces. The $q$ dependence of the $h(q)$ spectrum represents that these rough surfaces have a multifractal structure. Using standard multifractal formalism [32] we have

$$\tau(q) = qh(q) - 2. \hspace{1cm} (11)$$

Figure 4 shows the $\tau(q)$ as a function of $q$ for Si and PS surfaces. Slope of this diagram is changing with $q$ and shows the multifractality behavior in the height fluctuations of the studied rough surfaces. The singularity spectrum, $f(\alpha)$ of a multifractal rough surface is given by the Legendre transformation of $\tau(q)$ as

$$f(\alpha) = q\alpha - \tau(q), \hspace{1cm} (12)$$

where $\alpha = \frac{\partial \tau(q)}{\partial q}$. For a multifractal surface, various parts of the height fluctuations are characterized by different values of $\alpha$, causing a set of Hölder exponents instead of a single $\alpha$. Figure 5 shows $f(\alpha)$ versus $\alpha$ and confirms the multifractality nature of studied rough surfaces.
4. Height distribution
The multifractality behavior in a system can have different reasons such as the appearance of different correlations in the system or data distribution deviation from the Gaussian one. To investigate the cause of multifractality in the Si and PS rough surfaces, we study the height distribution and higher moments of height fluctuations in these surfaces.

To analyze symmetry of the height under the transformation \( h \rightarrow -h \), we can determine the skewness measure as follows:

\[
S \equiv \frac{\langle (h - \bar{h})^3 \rangle}{\langle (h - \bar{h})^2 \rangle^{3/2}}.
\]

Figure 3. Diagram of \( h(q) \) for Si and PS surfaces.

Figure 4. Diagram of \( \tau(q) \) for Si and PS surfaces.

Figure 5. Diagram of \( f(\alpha) \) for Si and PS surfaces.

This parameter is a measure of the asymmetry of the distribution. Skewness can come in the form of positive skewness or negative skewness, depending on whether data points are skewed to the right or to the left of the data average. Another measure which is based on the fourth moment of the data is kurtosis. This measure compares the weight of distribution tails with...
Gaussian and is a measure of the fatness of the probability distribution compared to the Gaussian distribution as follows:

$$Q \equiv \frac{\langle (h - \overline{h})^4 \rangle}{\langle (h - \overline{h})^2 \rangle^2} - 3. \quad (14)$$

For the Gaussian distribution this measure is zero. In Figure 6, the normalized height distributions $P(h)$ for Si and PS rough surfaces are shown. Regarding to these diagrams, we can see the height distributions of the rough surfaces have been deviated from the Gaussian distribution. Utilizing 13 and 14, we calculated the skewness and kurtosis measures for our surfaces; For the Si, skewness is positive, $S = +7.58 \times 10^{-4}$ and kurtosis is $Q = 6.91 \pm 0.02$ which indicates a peaked distribution compared to the Gaussian (as seen in the Figure 6) and for the PS rough surfaces, skewness is negative, $S = -1.12 \times 10^{-2}$ and $Q = 0.71 \pm 0.02$. As our results show, the height distribution of the Si and PS rough surfaces are deviated from the Gaussian one and it can be a reason for the multifractality behavior in these rough surfaces.

5. Conclusion

In this paper, we have studied the stochastic and fractal properties of silicon and porous silicon (PS) rough surfaces. To this end, we determined the roughness parameter and correlation length of the mentioned surfaces and showed that the height fluctuations in PS rough surface are more correlated than Si one. Also to investigate the fractal nature of the surfaces, we determined the $h(q)$, $\tau(q)$ and $f(\alpha)$ spectra, utilizing the two-dimensional MF-DFA method and showed that the surfaces are multifractal. To find out the observed multifractality behavior reason, we studied the distribution function of the height fluctuations, skewness and kurtosis measures; Our results showed that the height distribution deviation from the Gaussian one can be a reason for the observed multifractality behavior in the Si and etched Si (PS) rough surfaces.

![Figure 6. Normalized height distributions $P(h)$ for Si (left) and PS (right) surfaces.](image)

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7. References

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