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Characterization of topography across the scales

ARCNL
ADVANCED RESEARCH CENTER FOR NANOLITHOGRAPHY

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Advanced Research Center for Nanolithography

Internship supervised by
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Advanced Research Center for Nanolithography

The Advanced Research Centre for Nanolithography (ARCNL) founded in 2014 in Amsterdam. The centre belongs to ASML and the Dutch Research Council (NWO). Since the foundation, Joost Frenken is heading ARCNL.

The structure is dedicated to unravelling the physical fundamentals for nanolithography technologies. The research program is bonded to the R&D department program at ASML. The laboratory is divided into three thematics: Source, Metrology and Materials. Each group are thus divided into the subgroup as shown in *Figure 1*.

Thematic into ARCNL
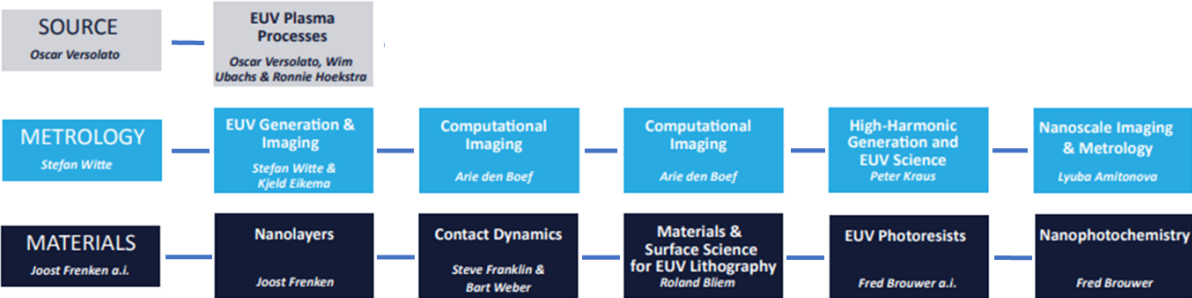

Figure 1 - Group structure in ARCNL

For the internship, I was in Contact dynamic group, co-directed Bart WEBER and Steve FRANKLIN. It is a dynamic team with professor, post-docs, PhD, interns and technicians. On the pathway to provide a friction forecast. The group is focused on the understanding of the phenomena involving during the friction. Thus, how can the interface influence it?

Introduction

In Tribology, the science of interactive surfaces in relative motion, surface topography plays a major role in the determination of the various phenomenon taking place at the interface. In realistic systems, the facing surface profiles set the local contact points. In order to understand and predict tribological phenomenon, it is of paramount interest to find the most relevant method to characterize surfaces. The topography is thus considered as a fractal.

To gather surface information into a set of parameters (Root-mean-square of heights, Correlation length and Hurst exponent), two mathematical tools show promising insights: The Heigh-Height Correlation Function (HHCF) and the Power Spectral Density (PSD). Whereas the HHCF considers the relative height variation with respect to the horizontal distance, the PSD considers the absolute height variation. The HHCF is based on the principle of correlation function which determined the correlation between stochastic variables (variables whose values depend on outcomes of a random phenomenon). Sinha and al. in 1988[1] provide the fitting function containing the characteristic parameters of the surface. The PSD for fractal topography was introduced by P. Ranganath Nayak in 1973[2], where the fitting function (for PSD2D) gathering the three parameters used to qualify surface profiles is still under debate.

In this report, we define and compare the two methods for artificially generated and real measured surfaces. From the surface profiles measured, we perform the HHCF and PSD analysis method and compare the outcome information on the surface characteristics. For this study, measurements were carried out by an Atomic Force Microscopy (AFM) in no contact mode (tapping mode). The real surface analysed are 3mm diameter SiN spheres, manipulated beforehand to exhibit multiple different surface topographies.

Firstly, I will present the AFM measurement as well as the different surface model needed for the analysis, statistical and fractal. From these models, three parameters will be defined. Secondly, the PSD and HHCF concepts will introduce, the definition, the calculation and fitting methods. The fitting function for PSD2D will be proposed. Thereafter, the PSD and HHCF will carry out for SiN and artificial surfaces which lead us to the difference between the two methods. In the last part, the consequences of the resolution upon the surface determination will be discussed

1. Surface Roughness

1.1. Atomic Force Microscopy

For this project, the surface measurement is carried on atomic force microscopy (AFM, Dimension Icon, Bruker). The AFM is a method based on the interaction between a tip located at a cantilever end, and the atoms belonging to the surface. The other cantilever side is attached with a piezoelectric which changes the tip-surface distance. Moreover, a laser beam is reflected on the cantilever back which provides a tip position feedback. The laser reflection is measured by a quadrant photodiode. The AFM diagram in no contact mode is shown in *Figure 2*.

The AFM results shown in this report come from the no contact tapping mode. In this mode, the resonance frequency is applied to the cantilever. The tip-surface interaction is ruled by the Leonard-Jones potential. During the measurement process, the tip-distance change regarding the roughness and the vibration. This variation induces the potential change. The z-position of the piezo element corrects the tip height to keep the potential constant. The computer records the height variation of the tip. The result is called a heightmap.
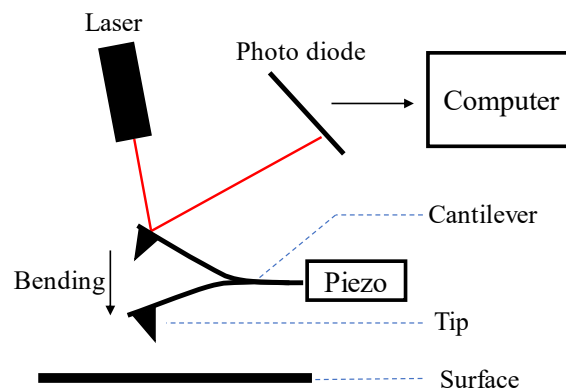
Figure 2 – Atomic force microscopy diagram in no contact mode

The tip motion along the surface follows two axis named: the fast-scanning axis (FSA) and the low-scanning axis (LSA). It means, in an orthonormal plan, that the FSA could be represented by the X-axis and the LSA by the Y-axis. Thus, for each value along the Y-axis, the tip measures possible heights along the X-axis. This method makes the height values more coherent along the X-axis than Y-axis. The data obtained are into a grid shape (or matrix). For the sample studied, the X-axis corresponds to the column and the Y-axis corresponds to the lines. The value corresponds to the heights, thus the Z-axis. As the measurement was favourited along one axis, the matrix is considered as a sum of surfaces cross-section. It is as a surface sliced along the fast-scanning axis. This idea needs to be considered for the correlation method.
The AFM data should be input in a software, named Gwyddion. It allows to read AFM file and to transform the data (seen in HHCF script description).

1.2. Topography structure

The correlation represents a statistical measure that expresses the extent to which two variables are related. It is equivalent to the inter-dependency of two variables. In this context, the data set

forms a correlated structure that depends on its nature and profile. Through their statistical structure, their behaviour could be predicted. However, often in physical science, the relationship will be zero for statistical values above a defined cut-off value. It defines the correlation "limit" for the given statistical structure[3].

1.2.1. Surface roughness

The surface roughness (or roughness) corresponds to the variation heights from a topography. The roughness is composed of hills (asperities) or valleys with a high statistical variation of size[4]. An example of a cross-section of surface roughness is shown in *Figure 3*.
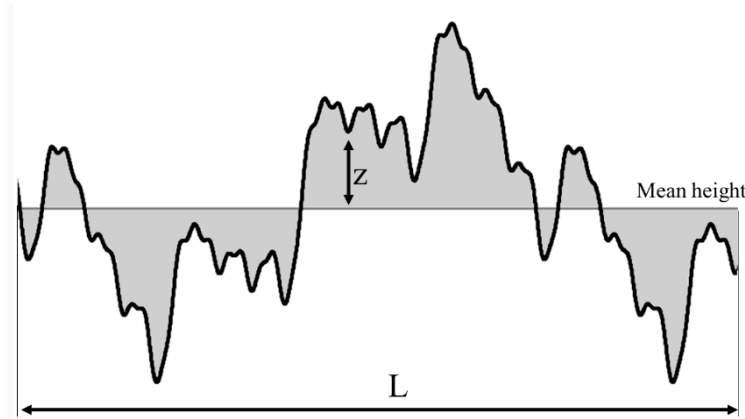
Figure 3 - Example of a surface cross-section

The roughness is mainly characterized by the root-mean-square height, σ. It represents the height deviation from the mean height level (z) along the x-axis[5], it is definite by:

$$\sigma = \left(\frac{1}{L}\int_0^L z^2 dx\right)^2 \tag{1}$$

where L the cross-section length and z the height deviation from the mean height level.

However, this parameter exclusively represents height information. The lateral information as the slope, the width and thus the asperities geometry are unconsidered. This lack of topography details leads to similar roughness value sigma for different surface profiles. In *Figure 4*, Different cross-sections with the same σ but with different shape are plotted.
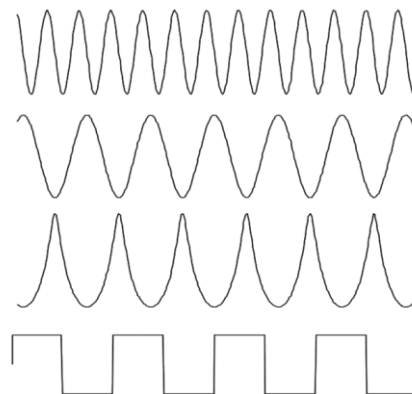
Figure 4 - Surface cross-section with the same root-mean-square of heights[4]

Therefore, additional parameters need to describe the surface profile more accurately. In the friction field, the characterization of the lateral variation of asperities is provided by the fractal model[6].

1.2.2. Fractal roughness

The fractal is a model developed by Mandelbrot in 1969[7]. The fractal model describes the self-similar structure. This property is: through the different magnification, the same structure is found. Consequently, the surface shape of the fractal object is independent of the magnification. It introduces geometry dimension non-integer, called fractal dimension (Df). It represents how your structure fills the space[8].

In the case of fractal roughness, it is the asperities shape that is observed for different magnification. It is like asperities on asperities. However, most of the roughness is not fractal within any scales. The fractal model is only appliable within the distance range bordered by the cut-off lengths $[\lambda_1, \lambda_0]$[6]. The lower cut-off λ_1 represents the smallest size of fractal asperity, and the upper cut-off λ_0 represents the biggest one. The upper cut last distance is also called correlation length (ξ). All the asperities with a size above the λ_0 are not involved in a fractal structure. Inside the fractal range, the asperity size correlated by the scaling factor (S) with :

$$z' \rightarrow zS^{\alpha} \tag{2}$$

Where z is the size (or height); z', the scaled size; S the scaling factor; α, the Hurst exponent

The Hurst exponent is linked to the fractal dimension, $D_f = E - H$ with E the upper Euclidean dimension (line, surface, cube, etc). In case of cross-section, E = 2 and for the surface E = 3.

1.2.3. Roughness structure

The topography variation due to the evolution of one parameter, is presented in *Figure 5*. The figures come from Heusinger and al. paper[9].
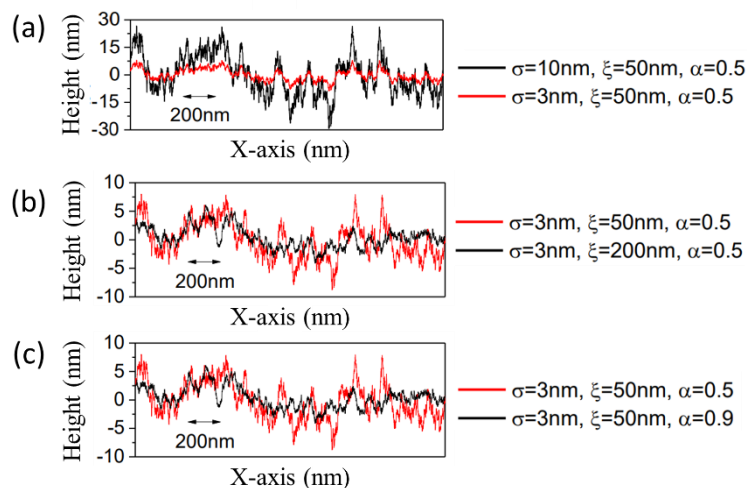
Figure 5 - Parameters influence upon the roughness structure. [9]

The root-mean-square of heights definition is the characterization of the height variation from the mean level of heights. A high value of σ leads to a high amplitude of heigh variation, as

shown in *Figure 5a*. The height distribution along Z-axis is wilder. The σ value represents the asperities stretching along Z-axis (Height).

The correlation length corresponds to the biggest size of fractal asperities (statistically) belonging to the surface. Over the length, the height variation is considered stochastic. As shown in *Figure 5b*, the distance between the two apexes is closer than the other cross-section. For the high value of ξ, the asperities seem to spread upon the surface. The correlation length act as a stretching factor along the X-axis.

The Hurst exponent is connected to the fractal dimension (where $Df = 2 - \alpha$ for surface cross-section). Lower values of α lead to a higher value of Df. For $\alpha = 1$, $Df = 2$; the roughness slopes are smooth in this case. The Hurst exponent corresponds to the jaggedness upon the roughness. In *Figure 5c*, the roughness is noisier for $\alpha = 0.5$ than $\alpha = 0.9$.

As follows, the asperities are characterized by their width and height by ξ and σ respectively. The roughness inside this "box" is characterized by α[10], [11].

In addition to the "regular" model, the fractal model provides a deeper understanding of the roughness structure. The HHCF and the PSD characterize surface topographies by mean of: the root-mean-square of heights, the correlation length and the Hurst exponent (called roughness parameters).

1.3. Samples

Two kinds of heightmap have been analysed in this work. The heightmap from the real surface and analysed with AFM. Thereby, five surfaces from SiN sphere, with a window size of 10x10μm of 1024x1024pixel, have been taken. The surfaces are designed by their roughness texture, Ultrasmooth, Semi-rough, Rough and Ultra-rough. Various processes have been utilized for the roughness changing:

- Ultrasmooth: Polished by T. Jacobs.

- Semi-rough: Collapsing of two balls at ultrasonic speed.

- Rough: Sandpaper

- Ultra-rough: Sandblast for few seconds.

The pristine SiN sphere surfaces will be also analysed. One surface is sampled in a window size of 10x10μm of 1024x1024pixel named Pristine-10. The second surface was taken with a window size of 90x90μm of 2048x2048 pixel named Pristine-90.

The second kind is the surface generated. This surface is calculated from a theoretical Power Spectral Density curve. Thus, for the example used in the HHCF and PSD presentation, a surface called SIMU is calculated with a root-mean-square of heights of 100nm, a correlation of 500nm and a Hurst exponent of 0.75.

2. Roughness characterization by correlation function

The roughness structure is quantified by the mean of two mathematical tools, namely PSD and HHCF. The two calculation operations express as well as the parameter extraction from the curves. Moreover, a focus is made on the HHCF Matlab script that I wrote during the project. Next, the two methods compare

2.1. Height-height Correlation Function (HHCF)

2.1.1. Definition

The Height-Height Correlation Function (HHCF) allows quantifying the correlation between two heights regarding the distance between them[12]. Thus, the correlation is defined by the square of the height difference. *Figure 6* is a surface cross-section scheme (along the x-axis). The vertical axis showed the height. Two points are at the position x_1 and x_2 with their respective height $z(x_1)$ and $z(x_2)$. Both points are separated by the distance r.
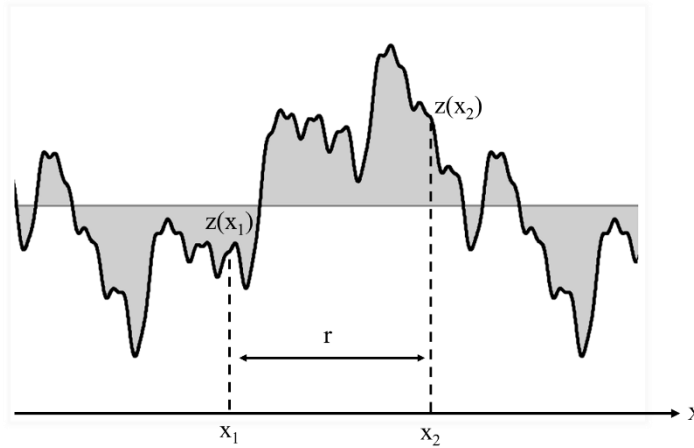
Figure 6 – Surface cross-section – Example of HHCF calculation

The HHCF function (g) between only two points is defined by *Eq. 3*.

$$g(r) = [z(x_1) - z(x_2)]^2 \qquad (3)$$
$$with : r = x_2 - x_1$$

In the case of cross-section, the HHCF considers the average between all the squared height difference for the same distance r. Thereby, the heightmaps from AFM measurement are calculated from *Eq. 4*. The HHCF is determinate over a length scale ranging from the pixel size (10-80nm) to the window size (90um).

$$g(r) = \frac{1}{Y(X-r)} \sum_{y=1}^{Y} \sum_{x=1}^{X-r} [z(x+r, y) - z(x, y)]^2 \qquad (4)$$

With: r the distance in pixel separating the two pixels ; Y the matrix limit along the Y-axis (pixel) ; X the matrix limit along the X-axis (pixel) ; x pixel number on the X-axis ; y pixel number on the Y-axis.

Eq. 4 is the function used by Gwyddion. The function considers the correlation only along the fast-scanning axis. The correlation function obtained correspond to the mean of the HHCF of

all the cross-sections. This calculation method considers the X-axis (fast scanning axis) representing the surface roughness. This consideration is based on an isotropic surface hypothesis where statistically, the roughness is the same along with all the directions.

However, *Eq. 4* does not give any information about the surface. It is only used to plot the HHCF. Thus, Sinha and al.[1] propose an empirical expression for HHCF, represented by the intermediate Gaussian-exponential equation form *Eq. 5*.

$$G(r) = 2\sigma^2 \left\{ 1 - exp\left[-\left(\frac{r}{\xi}\right)^{2\alpha} \right] \right\}$$ (5)

With: G(R) the second form of HHCF, σ the root-mean-square of roughness amplitude, ξ the correlation length and α the Hurst exponent.

2.1.2. Height-Height Correlation Function fit

The HHCF from SIMU surface resulting from the *Eq. 4* is shown in *Figure 7a* (black curve). The HHCF is used to be plotted on a log-log scale. The curve shape is composed of two parts well distinct: a slope and a plateau. The slope corresponds to the distance range where the HHCF increase with the distance r. In the plateau part, the HHCF remains constant with increasing distance r for higher values.

A correlation is the synonym of a dependency of a variable on another one. The HHCF represents the dependency of a height change with respect to their relative distance. This correlation is explained by the fractal structure of the roughness, which is characterized by the fractal parameter: the Hurst exponent. When the HHCF does not evolve with the distance, the heights are no more correlated. In this area, the roughness represents stochastic meaning, represented by on average, the height difference for two points separated by a distance r will be the same as this distance increase. Therefore, for distances above the correlation length (cut-off length), the plateau value is linked to the root-mean-square of the height (σ). The limit between the two parts is given by the cut-off length, namely the correlation length (ξ).
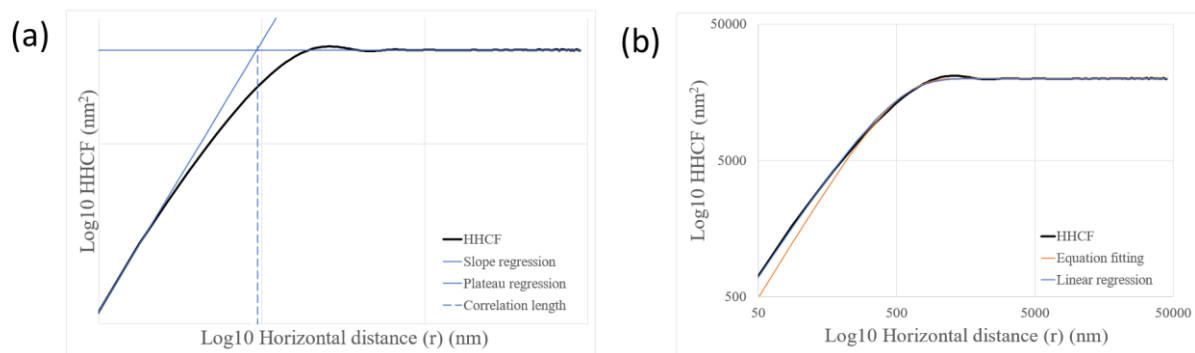

Figure 7 - (a) Linear regressions for HHCF and (b) HHCF fitting functions for SIMU

To achieve the roughness parameters determination, the first idea was to fit with the function (*Eq. 3*). However, in *Figure 7b*, the fitting function lacks accuracy for low distance. This error

cannot be ignored. It is due to the importance of this range for the link between the slope and the Hurst parameter.

A second method is operated for the parameter determination; two linear regressions are plotted in a log-log scale, in *Figure 7a*. The first regression fits the slope where the coefficient is equal to 2α ($G(r) \propto r^{2\alpha}$ for linear scale). The second regression fits the plateau where the ordinate is equal to 2σ². The correlation length which delimits each part, it is calculated from the intersection of both, $\xi = \left(\frac{2\sigma 2}{A}\right)^{\frac{1}{2\alpha}}$.

2.1.3. Height-Height Correlation Function Scipt

Before running the HHCF MatLab script (in *Annexe 1*), the curvature from sphere samples should be subtracted from the surface. The curvature does not belong to the roughness. Thereby, Gwyddion fits each line (cross-section) with a 2nd-degree polynomial, then subtracts them to the actual measurement to flatten the surface profile. Moreover, the AFM measurement involves scanning error like the misaligned row or the apparition of scars due to local defaults. These defaults are corrected with Gwyddion by extrapolation from the surrounding pixels.

Afterwards, the script processes the HHCF as defined with *Eq. 2* and fits with the two linear regressions. However, the distance range where the two linear regression functions are applied still needs to be defined.

The purpose of the slope fit is the number of values considered. The linear regression fits at minimum the six first HHCF values (from the smallest distances on). Under this limit, the correlation is considered too dependent on the resolution. From these six points, fits are calculated considering more and more values, until considering the twenty-first point (15 fits are made in total). The Hurst exponent value is obtained from the fit with the minimum error.

For the plateau regression, the HHCF needs to be cropped in half due to the influence of the picture edge on the average. For the higher distance r, the HHCF calculation (in *Eq. 4*) considers fewer values in the average ("X-r"). Statistically, the high distance r is less representative of the surface. Then, the σ value is given by the intercept of the fit with no slope. It represents the mean value of the plateau. Instead of to fit, the intercept is calculated by the average of the last HHCF values.

2.2. Power Spectral Density (PSD)

2.2.1. Definition

To introduce the power spectral density, the surface line is considered as a continuous function, despite the matrix form of the heightmap. This "surface function" can be represented as the summation of sinusoidal functions, called Fourier Series. The roughness is considered thus as periodic. The Fourier transform (FT) of the sinusoid summation gives a summation of Dirac pics relative to the amplitude and the wave-vectors of the sinus function. An example of a

surface profile composed of two sinusoidal functions in *Figure 8b*. In *Figure 8a*, the two sinuses are plotted apart. Where $S_1(x) = A\sin(\beta_1 x)$ and $S_2(x) = B\sin(\beta_2 x)$ with S1 and S2 the sinusoidal functions, A and B the amplitudes and β1, β2 the frequencies. The wavelengths (λ) are $\lambda_1 = 2\pi/\beta_1$ and $\lambda_2 = 2\pi/\beta_2$ [13].
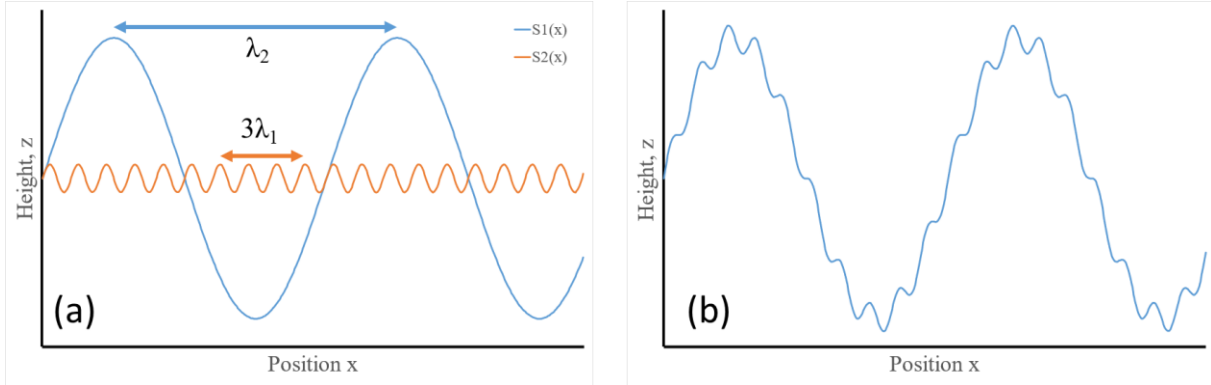
Figure 8 - (a) Sinusoid function S1 and S2 and (b) the sum of both.

The Power Spectral Density (PSD, *Eq. 7*) is the Fourier transform of the Autocorrelation Function (ACF, *Eq. 6*). With the ACF, the correlation is characterized by the factor of two heights. It depends on the distance between two pixels or called wavelength in this case.

$$ACF(r) = \frac{1}{Y(X-r)}\sum_{y=1}^{Y}\sum_{x=1}^{X-r}[z(x+r,y).z(x,y)] = \sigma^{2}e^{-\left(\frac{r}{\xi}\right)^{2\alpha}} \tag{6}$$

$$C(q) = \int_{-\infty}^{+\infty} ACF e^{-2\pi i q r} dr \tag{7}$$

With : σ, the root-mean-square of the roughness amplitude, ξ, the correlation length, α, Hurst exponent, q, the wavevector, r, the horizontal distance

2.2.2. Power Spectral Density fit

For the SIMU surface, the ACF and the PSD^{2D} are represented in *Figure 9*. Show by ACF curve in *Figure 4a*, the correlated part is related to low distances. The ACF depending on the distances. The stochastic part is related to the constant part of the curve for the high distances. For the ACF the constant value represents the mean height level and equal to 0 when this level is subtracted from the heightmap. The correlation length is the distance r when ACF equals 1/e.
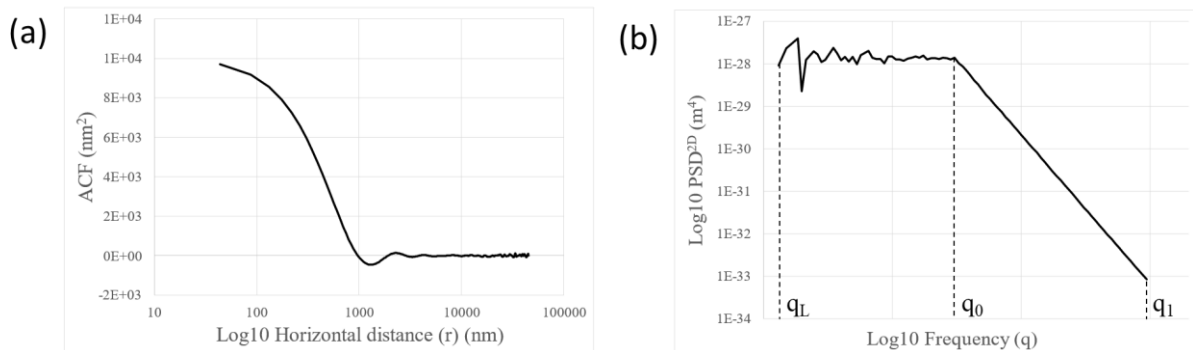
Figure 9 - (a) The ACF and (b) the PSD calculated from the simulated surface

The FT of the ACF brings the correlation in the reciprocal space, in frequency (q) with $q = \frac{2\pi}{r}$ (m^{-1}). If the PSD is calculated over a cross-section of a surface, called PSD^{1D}, its unit is m^3. In this work, the PSD is calculated over a surface, called PSD^{2D}, the unit corresponds to m^4. The PSD is calculated from the centre of the map and thus average the value from the different directions.

The PSD^{2D} displayed in the log-log scale is composed of two parts: a plateau and a slope. As well as the HHCF, the PSD depends on the frequency linearly. Their meaning is physically equivalent to the HHCF, the plateau representing the non-correlated features where the slope represents the correlated features. The curve shape is the same for PSD^{1D}. The frequency range of the two parts is edged by three frequencies. The smallest frequency corresponds to the larger feature into the surface, so $q_L = 2\pi/L$ with L the length of the cross-section. The higher frequency corresponds to the smallest distance, so the resolution $q_1 = 2\pi/\text{resolution}$. The third frequency is the transition frequency between the plateau and the slope, called "knee". It is bonded with the correlation length and equal to: $q_0 = 2\pi/\lambda_0$.

Relative to the Yuxuan Gong and al.[14] and the Fourier transform of an exponential, the PSD function shape is defined by :

$$PSD(q) = \frac{A}{(1 + (Bq)^2)^{C+0,5}} \qquad (8)$$

With A, a constant ; B, the correlation length ; C, corresponds to a roughness exponent different to the Hurst exponent.

The parameter A is different according to the PSD dimension (PSD^{1D} or PSD^{2D}). Thereby, Heusinger and al. based on the work of Palasantzas[15], give *Eq. 9* for the PSD^{1D} :

$$PSD^{1D}(q) = \frac{2\sigma^2\xi}{(1 + (\xi q)^2)^{C+0.5}} \qquad (9)$$

However, this equation has no meaning for the PSD^{2D}. In that way, different equations are proposed by Giorgio Franceschetti and Daniele Riccio[10]. The equivalent of the HHCF equation (*Eq. 5*) in reciprocal space does not exist. However, among the equations, the power spectrum exponential equation is the closest form than the *Eq. 10*, and definite by :

$$PSD^{2D}(q) = \frac{2\pi\sigma^2\xi^2}{(1 + (\xi q)^2)^{\frac{3}{2}}} \qquad (10)$$

By analogy to the previous equations, the 3/2 exponent could be a result of C+0.5 with C=1. Thereby, the proposed PSD^{2D} equation is :

$$PSD^{2D}(q) = \frac{2\pi\sigma^2\xi^2}{(1 + (\xi q)^2)^{C+0.5}} \qquad (11)$$

The proposed equation does not establish a direct link with the Hurst exponent, the α is calculated from a linear regression define by $PSD \propto q^{-2(\alpha+1)}$. The frequency range considered

during the fit is determined by the cut-off wavevector q_ξ $(= 2\pi/\xi)$ from Eq. 9 and the high cut-off wavevector q_{res}.

The root-mean-square, σ is represented by the area under the curve.

$$\sigma^m = 2\pi \int_{q_L}^{q_1} q \times PSD(q)dq \tag{12}$$

Where m is equal to 2 for PSD^{1D} and equal to 3 for PSD^{2D}.

The slope of the PSD curve (in log-log scale) represents the fractal part, as explained in the previous subpart. The range is delimited by q_1 and q_0. Within his range, the Hurst exponent can be extracted by slope$_{PSD}$ = -2(α+1). Thereby in the normal scale, $PSD \propto q_0^{-2(\alpha+1)}$. The link between the correlation length and wavevector have been shown by Palasantzas, where $\lambda_0 = 4\xi$. Thus, the "knee" position is defined by :

$$q_0 = \frac{2\pi}{\lambda_0} = \frac{\pi}{2\xi} \tag{13}$$

Through the two descriptions of HHCF and PSD, the two methods introduce different ways for the roughness structure understanding. The HHCF determines the dependency of the variation height according to the horizontal distance. On the other hand, the variation in the reciprocal space. Nevertheless, both methods show a linear relationship (in log-log scale) with the heights and the relative distance for fractal structure. When the distance between the heights, the curves (from HHCF and PSD) reach a plateau. The heights are not in the same fractal structure.

3. Comparison of the PSD and HHCF.

In the previous part (2.), the PSD and HHCF have been introduced. The two methods determine two mathematical methods to obtain the roughness parameters. In this part, we will see the consequences of the calculation ways.

3.1. Contribution of surface profile

The first analysis between the PSD and the HHCF is carried on all the SiN samples. The roughness parameters in *Table 1* come from the PSD and HHCF curves are represented respectively, in *Figure 10a* and *Figure 10b*.

Table 1 - Roughness parameters obtained by PSD and HHCF

Parameter	Method	Pristine-90	Pristine-10	Ultra-smooth	Semi-rough	Rough	Ultra-rough
σ (nm)	PSD	1,74	1,19	0,92	1,11	7,30	47,07
	New PSD	10,93	7,55	5,79	6,22	46,10	295,72
	HHCF	11,60	7,39	5,18	6,63	40,54	187,50
	Reference	11,62	7,23	4,83	6,56	41,05	167,79
α	PSD	0,80	0,86	0,87	0,74	0,89	0,93
	HHCf	0,76	0,74	0,76	0,60	0,81	0,87
ξ (nm)	PSD	568,36	273,58	270,94	424,98	735,71	1457,97
	HHCF	580,98	260,63	256,03	326,31	521,75	773,11
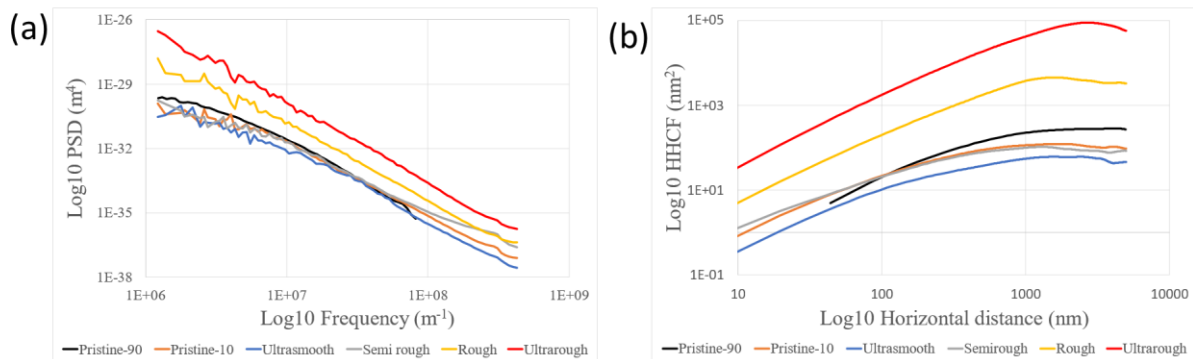
Figure 10 - PSD (a) and HHCF (b) from the SiN surfaces

For the σ, the parameters from method are compared with the root-mean-square calculated by the *Eq. 1* and it used as reference. For the σ_{PSD}, a ratio of 2π is observed, except for Ultra-rough surface, with the reference. According to the *Eq. 12*, σ_{PSD} curve represents the area under the curve multiplicated by 2π. It means that the σ_{PSD} is only equal to the area and not to the real root-mean-square of heights. Then, the new values of PSD are calculated and are called "New PSD" and the new PSD^{2D} formula *Eq. 14* proposed is:

$$PSD^{2D}(q) = \frac{2\pi \left(\frac{\sigma}{2\pi}\right)^2 \xi^2}{[1 + q^2\xi^2]^{C+0.5}} = \frac{\sigma^2\xi^2}{2\pi[1 + q^2\xi^2]^{C+0.5}} \tag{14}$$

Eq. 14 will be the equation used all the next PSD analysis in this report.

For the PSD^{2D}, an artefact appears at the high frequencies. As well as the correlation length, the biggest frequency takes to fit is correspond to 4 times the resolution size. With this size

estimation of the smallest feature in the heightmap allow better fit. These changeset are thus considered for the following analysis.

Between the surface Pristine-10, Ultra-smooth and Semi-rough, the parameters σ and ξ do not change between both method and between the sample. Indeed, from the reference value, the σ difference goes from 0.09 nm to 0.93nm, with the closest value obtained by HHCF. Regarding to the PSD and HHCF curves, the order is hard to determine for PSD ones notably for the low frequencies. However, for HHCF the plateau levels are relevant from the values. The roughest of three Pristine-10, it has a higher level than the Semi-rough and the Ultra-smooth which is the smoother. In case of the correlation length, no references could be determinate, but the difference is slight, from 16nm to 19nm between both methods. Their determination is considered good in both cases. In case of the Hurst parameter, as well as the correlation length, no reference is calculated. The PSD and HHCF find quite the value, where the difference are between 0.4 and 0.14. The parameters keep the same trend, where the lower value belong to the Semi-rough surface for both figures (PSD and HHCF). Then, these surfaces are well characterized by the two methods.

The second comparison corresponds to the analyse between both Pristine surfaces, token from different spheres (but technically with the same properties) and with different window size, 90μm and 10μm. Moreover, in the figures, the curves from the large window size surface have been cut out to fit in the diagram. As well as the three previous surfaces, the σ values do not change between the method and are equal to the reference. Nevertheless, as the heightmaps do not come from the same surface, their σ are different. A higher σ is calculated for Pristine-90 (11.62nm) regarding Pristine-10 (7.23nm). This difference is also visible through the plateau level in both cases. For the correlation length, both methods agreed on the value for the surface Pristine-90 and slightly the same for the second surface. However, $\xi_{Pristine-90}$ is twice higher than the $\xi_{Pristine-10}$, supporting the difference between the two structures. On the other hand, the Hurst exponent represents a common point through the HHCF with 0.76 and 0.80 for Pristine-90 and Pristine-10 respectively.

With the samples, Rough and Ultra-rough, the limits are reached. The difference (δ) between σ_{PSD} and the reference is low for the Rough surface ($\delta \sim 5nm$) but high for the Ultra-rough surface ($\delta \sim 130nm$). A difference of 30nm is noticeable for the σ_{HHCF} from Ultra-rough surface. The differences are explained by the presence or not the plateau. Only the Rough surface through HHCF analysis belong to a plateau. The σ_{PSD} for Rough surface and σ_{HHCF} Ultra-rough contains an error with respect to the reference. The plateau shape does not appear for both cases. Thus, this lack of accuracy around the plateau leads to a drift of the σ value but the error induced is low. The PSD curve from Ultra-rough shows only a line without "knee". The fractality of the roughness structure is higher than the window size. The same trend is observed with the correlation length. A difference of value between both methods is about 200nm for Rough surface and twice high for Ultra-rough surface ($\delta \sim 700nm$). Knowing that the "knee" frequency is corresponding to 4ξ one. The frequency is higher than the lower one.

The method comparison shows similarities in the correlation function. However, when the correlation length is too close to the window size, the σ, ξ values drift. This effect is less important for HHCF than the PSD.

Moreover, for the two Pristine surfaces, the difference comes from the roughness structure the non-isometry of the surface (see in 3.2.2).

3.2. Variation of window size

In this subpart, the influence of the window is focused. The set of samples are analysed. Firstly, the PSD and the HHCF are calculated from the artificial surface and thus the real surface in second. These samples allow bringing to light the surface anisotropy.

3.2.1. Artificial surface

Five surfaces have been generated on the same roughness parameter, σ = 11.6nm, ξ = 580nm, α = 0.75. Each surface has a different window size and the same number of pixels (2048x2048). The resolution changes regarding the window size: 4.39 ; 43.95 ; 439.45 ; 580.00 ; 634.77 nm.pixel^{-1}. The surfaces have been called with respect to their resolution. The PSD and HHCF curves are shown in *Figure 11*. The parameters obtained by both correlation functions are shown in *Table 2*.

Table 2 - Roughness parameter of simulated surfaces

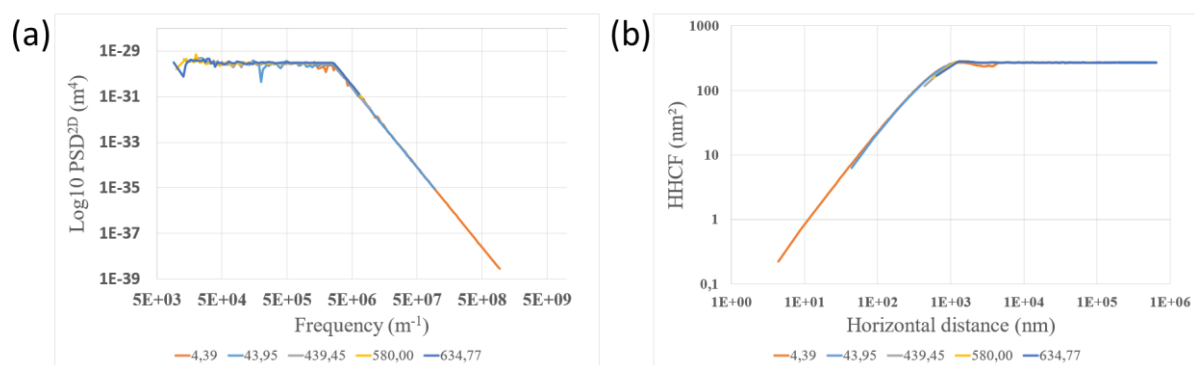| Parameter	Method	4,39	43,95	439,45	580	634,77
σ (nm)	PSD	14,0	13,5	26,0	53,3	66,9
	HHCF	11,6	11,6	11,6	11,6	11,6
α	PSD	0,75	0,75	0,75	0,75	0,75
	HHCF	0,76	0,77	0,51	0,41	0,37
ξ (nm)	PSD	474,4	374,8	171,6	84,1	67,7
	HHCF	447,4	511,4	988,4	1135,9	1191,5

Figure 11 - PSD (a) and HHCF (b) of simulated surfaces – Window size variation

For each method, all the curves obtained overlapping each other. For isotropic and periodic surfaces, the window size and the resolution do not influence the shape. However, the

parameters calculated from the curves depend on the window size, the resolution, and the correlation method.

From HHCF, σ is equal to the inputted value. For any window (or distance range) the plateau is considered allowing the measure of σ. The Hurst exponent is considered equal to the reference for the two surfaces, with the most limited resolutions. When the resolution becomes closer to the correlation length inputted, α decreases until it reaches 0.37 with a resolution of 634.8 nm.pixel^{-1}. The correlation length maintains similar trends. It is slightly underestimated for the surface with a resolution under ξ/10. It ends with a value overestimated for the low-resolution surfaces.

For the PSD, the changing of the parameter is due to the curve shape. The rupture between the slope and the plateau is discontinuous, so does not match with the PSD formula. The misfit induces a bad estimation of the correlation length. For a resolution of 44 nm.pixel^{-1} and more, the correlation length is calculated to be inferior to the resolution. Due to this wrong estimation, the Hurst exponent is considered meaningless for the surface with ξ < resolution. Otherwise, α is equal to the reference. The fit does not match the curve. The areas under the curves do not correspond. The root-mean-square of heights is overestimated for the same surfaces as α and ξ.

Thereby, the surfaces with the same parameters have PSD and HHCF curves overlapping each other. The resolution or the window size do not influence the curve shape. However, the parameter determination by HHCF is influenced. When the resolution and the correlation length are close, the fractal parameters (α and ξ) do not correspond to the input parameters. This influence is unseen with the PSD determination. The PSD curve misfit induces wrong values for all the roughness parameter determination. The abrupt change with the fractality and the stochastic properties of the roughness does not represent the concrete cases.

3.2.2. Real surface

The PSD and HHCF have been calculated for five SiN sphere surfaces with different window sizes, presented in *Figure 12*. The different surface analyses correspond to a cropped version of the Pristine-90 surface. For each surface, the pixel number was reduced to decrease the window size: 90μm ; 45μm ; 22.5μm ; 11.3μm ; 5.1μm. The window size decreasing keeps the resolution equal for all the surfaces. The surfaces are designated regarding their window size.
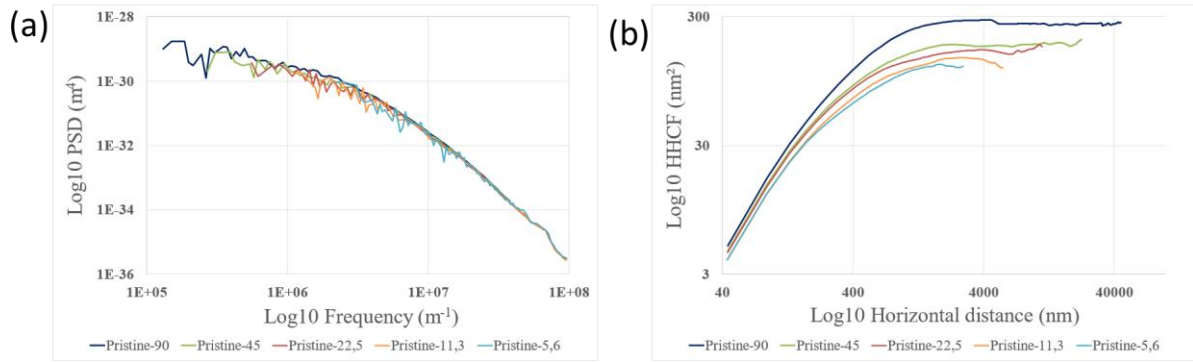
Figure 12 - PSD (a) and HHCF (b) of the real surfaces.

In the case of a concrete surface, the PSD curves are still overlapping (in *Figure 12a*). Although the curves include differences. From a smaller window size, the PSD amplitude is lower than Pristine-90. As the window has decreased with respect to the sample, the lower frequency as well. The PSD at low frequencies is noisy regarding the high frequency. All the PSD curves match in the high-frequency range. The HHCF (in *Figure 12b*) describes an evolution of the plateau level with the various surfaces. It seems to start on lower distance r with lower window size. On the first distance r, the slopes are similar but with an offset between.

The parameters obtained by both correlation functions are presented in *Table 3*. For each surface, the root-mean-square of heights of reference is calculated.

Table 3 - Roughness parameters of real surfaces, from PSD and HHCF

Parameter	Method	Pristine-90	Pristine-45	Pristine-22.5	Pristine-11.3	Pristine-5.1
σ (nm)	PSD	11.1	10.1	9.8	8.9	9.2
	HHCF	11.6	10,0	9.4	7.8	8.1
	Reference	11.6	9.7	9,0	7.9	7.5
α	PSD	0.58	0.61	0.64	0.64	0.63
	HHCF	0.76	0.73	0.72	0.71	0.7
ξ (nm)	PSD	556.71	440.22	382.18	312.26	318.54
	HHCF	581.1	554,00	534,00	460.3	486.6

For the PSD, HHCF and the reference, σ decreasing as expected by the fall of the HHCF plateaus. However, the σ_{PSD} decreases with a lower than the $\sigma_{Reference}$ and σ_{HHCF}. The σ_{PSD} and σ_{HHCF} values increase for Pristine-5.1 surface. For other surfaces, the difference with $\sigma_{Reference}$ and σ_{HHCF} does not exceed 0.4 (showing a proper fit on the plateau). About Hurst parameters, both methods do not describe the same change. The α_{PSD} increase whereas α_{HHCF} decrease. Nevertheless, the variations are small and thus considered constant. The differences are more significant for the correlation length. The HHCF describe a maximum loss of 121nm regarding a maximum loss of 241nm. For both methods, the σ from Pristine-5.1 is higher than the Pristine-11.3 one.

The root-mean-square of heights and the correlation length variation according to the window size shows the non-isotropy of the surface. However, the HHCF and PSD are based on an

isotropic surface model as they are calculated by average. The window size changes the statistical distribution of the height and width of the roughness. The window size influences the results obtained by HHCF and PSD. Moreover, the jaggedness from the low frequencies could be the cause of the difference of σ. For both methods, the fractal structure is considered as low influenced by the window size.

3.3. The differences

We have analysed different surfaces with different window size and different roughness amplitudes. The anisotropy of the surface thus induces a statistical shift of σ and ξ. In this subpart, the curve overlapping is explained by the phenomenological equations for PSD and not for the HHCF. In a second time, how a σ shift can influence the PSD curve.

3.3.1. Phenomenological equations

The difference could be explained by the phenological expression *Eq. 5* (2.1.1) and *Eq. 7* (2.2.1) for HHCF and PSD, respectively. In *Table 1* and *3*, the window size decreases σ and ξ. It corresponds to a statistical decrease. With α is considered constant. In *Eq. 5*, the decreasing of σ and ξ induce a reduction of the function value. For low distance r, the exponential part has an inferior influence. The HHCF solely depends on σ due to the small shift of the slope (so same α). For higher distance, the exponential importance increase. The ξ decreasing according to the curve induces a decrease of the exponential. However, this effect is not enough to balance the σ decreasing.

On the opposite, the ξ plays a second role in PSD. At the denominator, ξ increase the PSD value and to the numerator, it decreases the PSD value. The two trends have barely the same weight on the PSD curve. Thus, only σ induces variation. However, the weight of the frequency (10^{+5} ~ 10^{+8} nm) in the formula reduces the amplitude of the σ fluctuation.

3.3.2. Mean height level

The HHCF operation is based on the difference between two heights squared and the ACF is a factor of two heights. The two methods are calculated from the Gwyddion method, *Eq. 4* (2.1.1) and *Eq. 6*.

The difference between ACF and HHCF is the surface information kept after the calculation. With the subtraction, the HHCF does not consider the common height. The ACF considers all the values as the raw information to input in the calculation. For example, we consider a non-isotropic surface, with the mean height subtracted. So, the mean height corresponds to zero. The surface is now cropped. As the surface is non-isotropic, the height distribution is different. The mean height in the new window size has drifter form 0 level. The drift is similar to a height offset.

For example, a scheme is presented in *Figure 13*. Three heights (p_1, p_2, p_3) have been measured equidistantly (distance h) from each other over the "Cropped Surface". The offset height is

represented by the distance H. The heights are equal to: $p_1 = H - h$; $p_2 = H$; $p_3 = H + h$. *Table 4* shows the results after the HHCF and ACF have been carried out on the 3 heights.
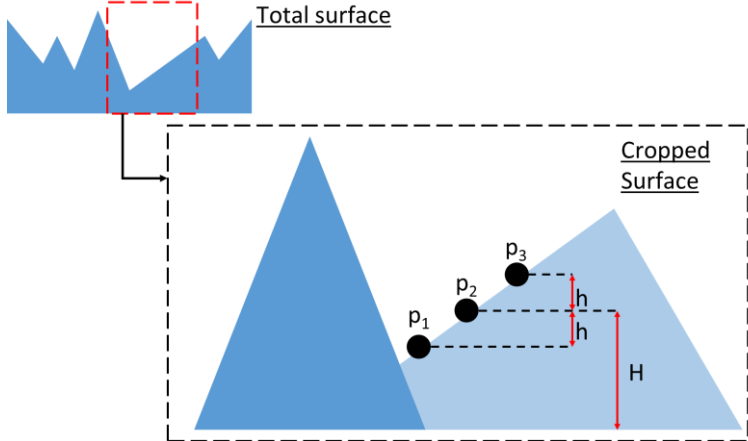
Figure 13 - Downward, the cropped surface from "Total surface", upward. H and h are respectively the off-set height and the distance between two following points.

Table 4 - Correlation values from HHCF and ACF calculation

Compared heights	HHCF	ACF
p1 / p2	h²	H(H-h)
p2 / p3	h²	H(H+h)
p1 / p3	4h²	H² - h²

The HHCF results do not contain the offset value. Thereby, for each height difference calculated, the HHCF does not induce the reference. It solely characterises the height variation. The ACF includes the offset value in the correlation result. As the root-mean-square of heights is defined as the height variation from the mean height. The offset value does not belong to the variation, thus does not belong to the σ. Then, an error is induced on σ when the offset represents a significant part of the total height.

In the pathway to developing the idea, several off-set has been applied over the Pristine-90. Their HHCF and PSD is shown in *Figure 14*. As predicted, the HHCF (*Figure 14b*) does not detect any difference regarding the surfaces, they are equal. However, the PSD curves show differences for low frequency, between qL and qξ. Gradually, the plateau will be substituted by a slope regarding the offset. Knowing the area under the curve is characteristic of σ. As the area increases with respect to offset, σ will drift from the genuine value.
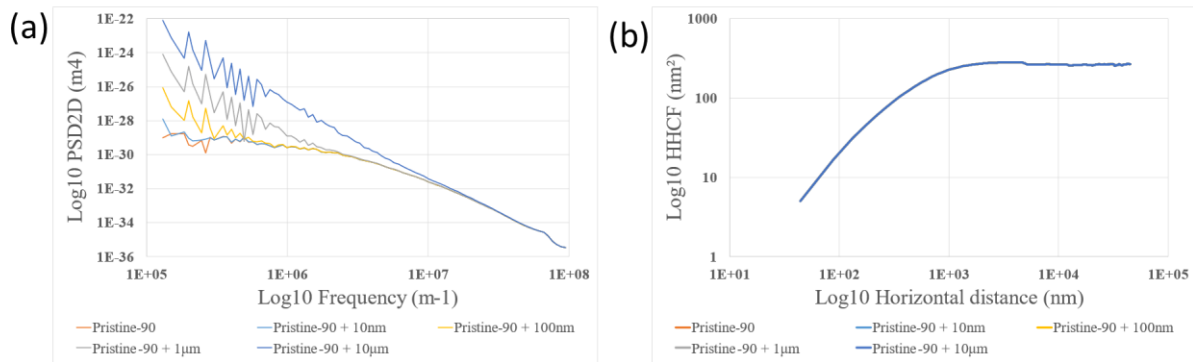
Figure 14 - The PSD (a) and the HHCF of Pristine-90 with several off-sets

The geometry changing of the plateau part induces a shift of the correlation length too. The "knee" underlines the start of the plateau. As the plateau is substituted with height, the "knee" is less and less important until it disappears for an offset of 10µm.

The HHCF and the PSD show similar properties to describe the corresponding surface. The roughness parameters correspond. However, even across the several window size and for real surface, the PSD curve overlapped whereas is not the case for the HHCF. It is justified by the lack of isotropy on the surface and the influence within the fitting equation. The second effect represents a drift of the mean height level that can be only visible for the drifts over 10nm for Pristine-90.

For Pristine-90 and Pristine-10, their difference is solely unexplained by the structure difference. The variation of ξ and σ could also be induced by the window size, as seen formerly. Moreover, in the case of several measurements as for the work of T. Jacob and al.[16], The anisotropy is strongly represented is relevant to the overlapping of shift. Thus, as said in the article, more than 100 measurements should be made to have a good result on the PSD.

For assembling several PSD curves, the loss of information regarding the resolution should be considering.

4. Resolution and roughness structure

Previously, the resolution issue was introduced. It was due to the statistic shift with the different surfaces. However, the roughness structure was unmodified.

In this part, the issue is to investigate the structure changing regarding the resolution. Between the roughness parameter and the roughness structure, the difference will be discussed. All the correlation measurement is obtaining from the HHCF.

4.1. Method

The resolution decreasing is carried out by averaging the height with their respective height neighbours. The average area is defined by a 3D gaussian. This method allows an isotropic averaging. Thereby, a gaussian is calculated from its own surface, by :

$$\Omega = \frac{FWHM}{2\sqrt{2\ln(2)}} \frac{1}{resolution} \qquad (16)$$

$$Gaussian = \exp\left[-\frac{x^2 + y^2}{2\Omega^2}\right] \qquad (17)$$

With: Ω, the variance | FWHM, full width at half maxima | x and y, position on the surface

The value of FWHM is choosing as an input for the gaussian size. Once calculated, the gaussian is convoluted with the surface. All the pixels inside the gaussian are averaging. For the averaging, all the pixels do not have the same weight due to the gaussian shape. The pixel on the side of the gaussian has the most reduced weight. However, the number of pixels considered is higher on the side than in the middle. It means all the distances (from the first pixel) have the same weight despite the number of pixels. The current resolution is defined by the maximum width at the bottom. This length corresponds to six times the variance, as shown in *Figure 15*. Above this length (diameter) the pixels are uninvolved. Then, the resolution obtains a function from the FWHM.
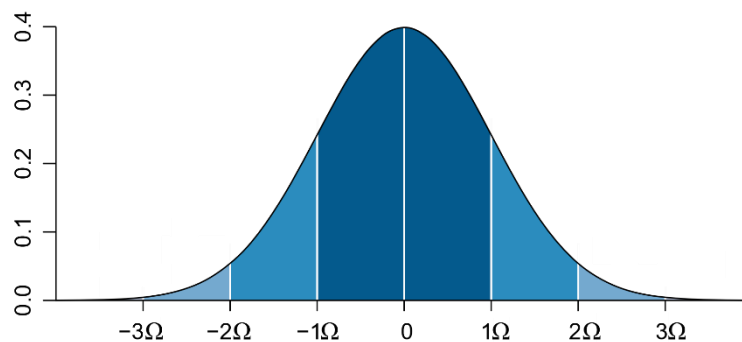

Figure 15 - Scheme of a gaussian divided by the variance (Ω)

4.2. Results and discussion

The resolution decreasing was carried out on the surfaces: Pristine-10, Ultra-smooth, Rough and Ultra-smooth. The initial resolution is 9.8nm and was reduced to 63.7; 127.4nm; 254.8nm; 509.6 and 1273.9nm. The surface cross-sections of Rough are shown in *Figure 16a*. After the

first convolution, the roughness becomes smoother. The jaggedness which belonged to the surface has been loose. However, the roughness height does not change. With a lower resolution, the asperity heights and slope have decreased. The surface becomes more uniform. The lower resolution has changed the roughness structure. Then, the width of asperities has increased, the height decreases, and the jaggedness disappears.

For each surface and resolutions, the roughness parameters have been plotted in *Figure b-d*.
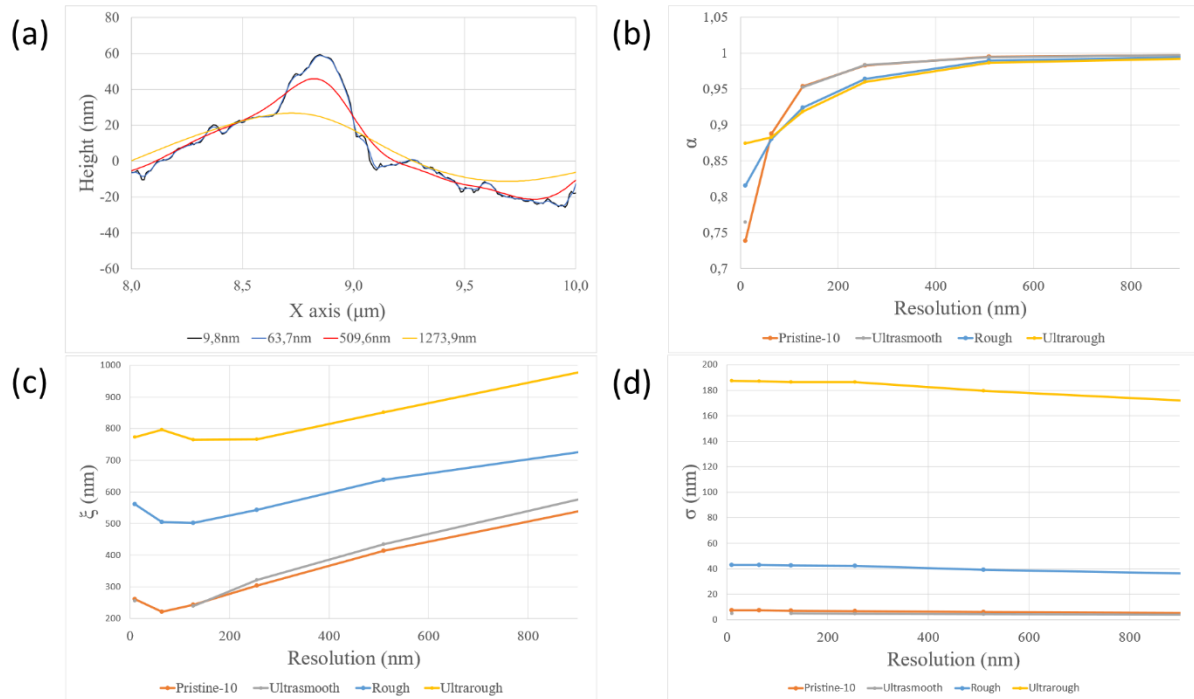

Figure 16 - Influence of the resolution on (a) the Rough surface cross-section, (b) the Hurst exponent, (c) Correlation length, (d) Root-mean-square of heights

In *Figure 16c*, the correlation according to the resolution is plotted. The evolution is composed of 2 parts. For high resolution, the slope presents either a valley or a hill. This phenomenon is due to the Hurst exponent determination. This variation is still low regarding the second part. The second part starts after a threshold where the correlation length increase. This threshold operates for resolutions under the initial correlation length. As seen with the window size in the previous part (3.), when the resolution is above $\xi/10$, the fractal structure is badly detected. The correlation lengths calculated above the threshold resolution could be like the gaussian structure (due to the convolution). The same threshold is observed with σ, in *Figure 16b*. Firstly, the value is constant. Above the threshold, the root-mean-square decrease. The decreasing means that higher heights involve the average. Moreover, before the threshold, the Hurst exponent is influenced by the resolution. In *Figure 16c*, regardless of the initials α value, the parameter is above 0.95 at the threshold value. Above they trend to 1 which is le limit.

Then, when the gaussian size is lower than the correlation length. Only the Hurst parameter is influenced by the resolution decreasing. By extension, slightly the correlation length due to the calculation method of HHCF. Then, only the fractal structure is influenced. When the resolution reaches the threshold, the correlation length increase and the root-mean-square of heights

decrease. These trends correspond to the differences seen with the surface cross-section in *Figure 16a*.

Moreover, the Hurst exponent is highly influenced by the high resolutions. The Hurst exponent is bond to the fractal dimension (Df, by Df = 2 – α), representing how the line (surface) fills a plan. The total structure needs to be characterized in a way to determine the real Df, so α.
The value of α is relevant only for the comparison of one resolution. Only a part of the fractal roughness is measured.
In the goal to obtain an α characteristic to the surface, the atomic structure should be detected. It is the underneath structure from the fractal one. However, the lower resolution on the AFM is 10nm (tip size). Therefore, this measurement is completed by the other measurements performing on smaller scales, as the Transmission Electron Microscopy [16].

Conclusion

In summary, we have characterized the surface topography of SiN samples with various roughness. For all of them, the PSD and HHCF allowed us to qualify the roughness characteristics from the nano to the macro-scale. By the calculation of the root-mean-square height, the correlation length and the Hurst parameter; the two methods appeared to show a similar analysis quality but also their own drawback. The differences reside in their response to the surface anisotropy. For the PSD, it solely influences the curve shape. That property induces easier overlapping of the curves. However, the value is still different. Thus, the overlapping should consider many PSD to overcome surface anisotropy. On the opposite, the HHCF amplitude is strongly influenced by the statistical drift of σ. The curves are too different to obtain an overlapping. The discrepancy of these curves profile points out of the sensitivity of the HHCF outcomes on the measurement window size.

Secondly, as the fractal structure characterizes the lateral variation of the topography, the resolution has a strong influence on the roughness parameter. In this manner, when the resolution is close enough to the initial correlation length, ξ increases. This change corresponds to the convolution of the tip (from AFM) or the gaussian. Accordingly, the Hurst parameter trends to 1 and is highly influenced by the high-resolution variation. The comparison of two α values from surfaces with different resolutions lacks relevance. To find the true value of α, the information entailed within the structure underneath must be taken into account. All the fractal information will be considered.

My work at ARCNL represents a great experience. All the friction phenomena about the nano-scaled surface are still under debate. Hence, many subject mixing physics and/or chemistry was carried out using such analysis. During this internship, I have developed my English skills and the knowledge to understand and characterize nano-scaled topography. Through this work, we provide tools and interpretations that shall help future scientists to understand and compare surface topographies for a large range of length scales.

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Annexes

Annexe 1. HHCF script

```matlab
%-------------------Important variable----------------------
%For r distance part
Size = 90E-6;          % the picture size in meter
%-------------------Advanced option------------------------
%For document choice
delated_part = 2;    %2 = rid second half of hhcf values | 4 = rid the last quart
%For sigma determination
multiplicator = 10;


%%
%---------------------Document choice------------------------

% Variables :
% file (string) : Name of the file choose
% matrix (matrix) : matrix of the heights
% dimension (vector) : dimension of the mactrix
% Length (float) : size of croped HHCF

file = uigetfile('*.txt');                       % Ask to the user to choose his file (.txt)
matrix = readtable(file);                         % Aparts the different values
matrix = table2array(matrix);                    % Convert to output type
dimension = size(matrix);                        % Matrix size determination
Length = dimension(1)-(dimension(1)/delated_part);  % Length of croped HHCF

%%
% Variables :
% R_distance (vector) : values of R (horizontale values)
% HHCF (vector) : HHCF values of the surface (Ordinate values)
% alpha (float) : value of alpha (Hurst exponent)
% sigma (float) : value of sigma (Root mean square of roughness amplitude)
% xi (float) : value of xi (Correlation length)
% FitCurve (vector) : values of the fitting curve

R_distance = R_func(Size,dimension, Length); % R distances calculation

HHCF = HHCF_func(matrix, dimension(1), Length);  % HHCF calculation

[alpha,sigma,xi] = parameter(R_distance,HHCF,multiplicator,Length); % fitting parameters calculation

FitCurve = 2*sigma^(2)*(1-exp(-(R_distance.^(2*alpha)/xi.^(2*alpha)))); % fitting curve calculation
```

```matlab
%%
%------------------------ PLotting Curves ------------------------
% Variables
% h (diagram) : plotting diagram
% txt (string) : Text displaying the hhcf parameters
% dim (vector) : size of the display box

%------- Ploting part -------
%figure( 'Name', file );
h = loglog(R_distance, FitCurve, R_distance, HHCF );
loglog(R_distance, FitCurve, 'LineWidth', 1.5, 'Color', [1 0 0]);
hold on;
loglog(R_distance, HHCF,'LineWidth', 1.5, 'Color', [0 0 1]);
hold on;
legend('Fitting curve', 'HHCF');
% Disp coeff on diagram
txt = ['Alpha: ' num2str(alpha) ' | ', 'Sigma: ' num2str(sigma) ' nm | ', 'Xi: ' num2str(xi) ' nm'];
dim = [0.2 0.5 0.3 0.3];
annotation('textbox',dim,'String',txt,'FitBoxToText','on');
% Label axes and title
%title(file)
xlabel( 'Horizontal distance (nm)', 'Interpreter', 'none' );
ylabel( 'Heigh-Height Correlation Function (nm²)', 'Interpreter', 'none' );
grid on

function hhcf = HHCF_func(matrix,dimension,Length)
    % Variables:
    % r (inter) : number of pixel between the two height
    % xp (inter) : number of the column of the pixel (X axis)
    % yp (inter) : number of the line of the pixel (Y axis)
    % y (vector) : HHCF (line)
    % hhcf (vector) : HHCF (column)
    % sum (value) : sum of all the difference for one distance r
    % persentage (value) : indicate the process advancing

    % Setting
    r = 1;                      %Start from the smaller distance
    xp = 1;                     %Start from the first value of the row
    yp = 1;                     %Start from the first row
    sum = 0;                    %Initialisation
    y = zeros(1, Length);           %Initialisation of the hhcf length
```

```matlab
    % ----HHCF calculation loop----
    % for each r -> calculation of height difference along the row for each row until half of the image size
    while r < Length
        while yp <= dimension            % row loop
            while xp <= dimension-r          % column loop
                a = ((matrix(yp, xp + r) - matrix(yp, xp))^(2))*10^(18);    % HHCF Calculation
                sum = sum + a;                         % sum all the values
                xp = xp + 1;                           % column incrementation
            end
            xp = 1;                               % reset the column indice
            yp = yp + 1;                          % new row
        end

        y(r) = sum /(dimension*(dimension-r));       % average of the sum
        sum = 0;                          % reset of the sum for the next r
        yp = 1;                           % reset the row indice
        r = r + 1;                        % new distance (next point on hhcf curve)
        persentage = round(r/Length*100);        % calculation of the advancement
        disp(['HHCF process : ', num2str(persentage), '%']);    % display the percentage
    end

    % ---- End HHCF calculation loop ----
    % from line to column
    hhcf = y';
end

function xscale = R_func(Size,dimension, Length)
    % Variables :
    % Res (float) : picture resolution value
    % Size (float) : the picture size in meter
    % x (vector) : distances (line)
    % xscale (vector) : distances (column)
    % dimension (vector) : dimension of the mactrix
    % Length (float) : size of croped HHCF

    %Calcul the size of one pixel, the resolution
    Res = Size/dimension(1);
    %Calculation of the R distances
    x = (1:Length);
    x=x*(Res*10^9);
    %From line to column
    xscale = x';
end
```

```matlab
function [ALPHA,SIGMA,XI] = parameter(xscale,HHCF,multiplicator,Length)
%   Variables :
%   i (integer) : counter
%   xfit (vector) : R distance data belonging to the slope
%   yfit (vector) : HHCF values belonging to the slope
%   ft (function) : fittng function
%   fitresult  : fitting parameters
%   gof : error data
%   rsquare (float) : fitting error
%   persentage (value) : indicate the process advancing
%   coeffs (vector) : fitting parameters values
%   alpha (float) : value of alpha parameter
%   high_limit (value) : plateau edge
%   A_coeffs (vector) : fitting parameters values
%   alpha (vector) : values of alpha parameter
%   Mean (float) : mean value of the plateau
%   sigma (vector) : values of sigma
%   xi (vector) : values of xi
%   ALPHA (float) : final value of alpha
%   SIGMA (float) : final value of sigma
%   XI (float) : final value of xi


    %Setting
    low_limit = 6;                   % start from the third point on the curve
    alpha = zeros(1,20);
    sigma = zeros(1,20);
    xi = zeros(1,20);
    rsquare = zeros(1,20);

    while low_limit <= 20
        xfit = log10(xscale(1:low_limit));          % select the x scale for alpha fit (R)
        yfit = log10(HHCF(1:low_limit));            % select the y scale for alpha fit (HHCF)

        % Set up fit type and options.
            % a : log10 of the coefficient with no meaning | b : Alpha
            % coefficent | x = log10(r)
        ft = fittype( 'a+b*x', 'independent', 'x', 'dependent', 'y' );
        opts = fitoptions( 'Method', 'NonlinearLeastSquares' );
        opts.Display = 'Off';
        opts.StartPoint = [1 1];

        % Fit model to data.
        [fitresult,gof] = fit( xfit, yfit, ft, opts );
        rsquare(low_limit) = gof.rsquare;       % pick up the rsquare error
        coeffs_alpha = coeffvalues(fitresult);  % pick up the function coefficient, alpha
        A_coeff = 10^(coeffs_alpha(1));
        alpha(low_limit) = coeffs_alpha(2)/2;
        % ---- Sigma determination -----
        high_limit = low_limit*multiplicator;
        % Do the average of all HHCF values in the range [k length(HHCF)]
        Mean = mean(HHCF(high_limit:Length));
        sigma(low_limit) = sqrt(Mean/2);                % calculation of sigma from the mean

        % ---- Xi determination -----
        % Calculate the xi
        xi(low_limit) = (Mean/ A_coeff)^(1/(2*alpha(low_limit)));

    persentage = round((low_limit-2)/18*100);       % calculation of the advancement
    disp(['Fitting process : ', num2str(persentage), '%']); % display the percentage
    low_limit = low_limit + 1;  % incrementation
    end

    Error_min = max(rsquare);           % Find maximum of all the rsquare calculated
    Index = find(rsquare==Error_min);   % Find the maximum value index
    ALPHA = alpha(Index);               % Final alpha value at the index
    SIGMA = sigma(Index);               % Final sigma value at the index
    XI = xi(Index);                     % Final xi value at the index
end
```

Caractérisation de la topographie de surfaces à travers différentes échelles

La topographie nanométrique de surface a été caractérisée. La variation de hauteur considérée comporte une structure fractale sur les faibles faible distance. Sous la longueur de corrélation (ξ), deux hauteurs sont corrélées. Pour ces distances (et fréquences), la rugosité est dépendant de l'exposant de Hurst (α). Lorsque les deux hauteurs sont séparées d'une distance supérieure à celle de corrélation, elles n'appartiennent pas à la même structure. Elles n'ont plus d'influence l'une sur l'autre. La moyenne quadratique des hauteurs (σ) est ainsi calculée. La rugosité de surface est définie par l'élargissement latéral et horizontal (ξ et σ) moyenne des aspérités, et aussi leur évolution à travers l'échelle (α). La densité spectrale de puissance (PSD) et la fonction de corrélation entre hauteurs (HHCF) nous permettent de décrire et de quantifier la topographie à l'aide des trois paramètres. Le HHCF considère la variation de hauteur relative par rapport à la distance horizontale, tandis que le PSD considère la variation de hauteur absolue. Les mesures de corrélation ont été réalisées sur les surfaces artificielles et SiN. Avec une optimisation (sur σ) de la fonction de fitting du PSD^{2D}, les deux méthodes ont les mêmes interprétations de la surface. Cependant, le fonctionnement de l'AFM influence les résultats. Alors que le HHCF est influencé uniquement par la distribution statistique des hauteurs, le PSD dépend en plus d'une variation de référence. Le second point est que la modification de résolution montre la limite de mesure pour α.

Characterization of topography across the scales

The nanometric surface topography has been characterized. The height variation considered has a fractal structure over short distances. Under the correlation length (ξ), two heights are correlated. For these distances (and frequencies), the roughness is dependent on the Hurst exponent (α). When the two heights are separated by a greater distance than the correlation, they do not belong to the same structure. They do not influence each other. The root-mean-square of heights (σ) is thus calculated. The surface roughness is defined by the average lateral and horizontal widening (ξ and σ) of the asperities, and their evolution across the scale (α). Power spectral density (PSD) and height correlation function (HHCF) allow us to describe and quantify topography using the three parameters. The HHCF considers the relative height variation with respect to the horizontal distance. While the PSD considers the absolute height variation. The correlation measurements have been performed on artificial surfaces and SiN.

With an optimization (on σ) of the fitting function of the PSD^{2D}, the two methods show the same analysis. However, the AFM operation influences the results. While the HHCF is influenced only by the statistical distribution of heights, the PSD additionally depends on a reference variation. The second point is that the changes in resolution show the limit of the measure of α.