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Analytic form for the power spectral density in one, two, and three dimensions

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Abstract. Analytical expressions for the power spectral density (PSD) are often useful in stochastic lithography simulation and the metrology of roughness. Using a common stretched exponential correlation function with three parameters (standard deviation, correlation length, and roughness exponent), the PSD can be computed as the Fourier transform of the autocorrelation function. For the special cases of roughness exponent equal to 0.5 and 1, the PSD can be computed analytically for one, two, and three dimensions. In this paper, the analytical results of these calculations are given. The resulting equations can be used when modeling rough lines, surfaces, or volumes. [DOI: 10.1117/1.3663567]

Subject terms: power spectral density; autocorrelation function; stochastic modeling, line-edge roughness; linewidth roughness.

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1 Introduction

In both stochastic lithography modeling and analysis of roughness metrology data, it is sometimes necessary and often desirable to have an analytical expression for the power spectral density (PSD) that is both grounded in the known physics of stochastic processes and matches experimental evidence for those processes. Many diverse stochastic processes with a single correlation mechanism are known to follow an exponentially decaying autocorrelation function, R:

$$R(r) = \sigma^2 e^{-(r/\xi)^{2\alpha}}, \tag{1}$$

where σ is the standard deviation of the behavior (for example, the rms line-edge roughness), ξ is the correlation length, α is the roughness exponent, and r is the distance (equal to $|x|$ in one dimension, $\sqrt{x^2+y^2}$ in two dimensions, and $\sqrt{x^2+y^2+z^2}$ in three dimensions). This function is often called a stretched exponential or the Kohlrausch–William–Watts function[1] and is frequently encountered in relaxation processes,[2] as well as correlated roughness, where self-affine behavior of the roughness exists on length scales less than the correlation length. It has been used successfully in many studies of line-edge roughness, for example.[3,4]

Since the correlation function of Eq. (1) is frequently encountered in stochastic processes, it makes sense to use this function as the basis for PSD analysis. The power spectral density is simply the Fourier transform of the correlation function (by the Wiener–Khinchin theorem). Unfortunately, analytical solutions to this Fourier transform are possible only for certain values of the roughness coefficient: $\alpha = 0.5$ and $\alpha = 1$. In Secs. 2–4, the analytical forms of the PSD for these two values of α will be derived in one, two, and three dimensions. The PSD for $\alpha = 0.5$ in one and two dimensions has been previously derived,[5] as has the $\alpha = 1$ case in one and two dimensions. Since most experimental line-edge roughness (LER) results show values of the roughness exponent between 0.5 and 1, these represent important limiting cases.

Analytic forms for the PSD are useful in two applications: metrology and simulation. Metrology data for LER and linewidth roughness can be fit by an analytical one-dimensional (1D) PSD, and surface roughness by a two-dimensional (2D) PSD, enabling the extraction of both σ and ξ. When generating random rough lines, surfaces, or volumes for simulation, an analytical form of the PSD can be used to generate random data with the desired autocorrelation response. Thus, it is useful to have as complete a set of analytical PSD functional forms as possible.

2 One-Dimensional Case

Since the autocorrelation function being used here is even, the Fourier transform in one dimension becomes a Fourier cosine transform.

$$G(f) = 2\int_0^\infty g(x)\cos(2\pi f x)\,dx. \tag{2}$$

Applying the Fourier cosine transform to the autocorrelation function of Eq. (1) results in the 1D PSD.

For $\alpha = 0.5$:

$$\mathrm{PSD}(f) = \frac{2\sigma^2\xi}{1+(2\pi f\xi)^2}. \tag{3}$$

For $\alpha = 1$:

$$\mathrm{PSD}(f) = \sqrt{\pi}\sigma^2\xi\, e^{-(\pi f\xi)^2}. \tag{4}$$

3 Two-Dimensional Case

In two dimensions, the radial symmetry of the autocorrelation functions lends itself well to a Fourier transform using polar coordinates. The 2D Fourier transform in Cartesian coordinates is

$$G(f_x, f_y) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} g(x,y)e^{-i2\pi(f_x x+f_y y)}dxdy. \tag{5}$$

Converting both the real space and frequency space coordinates to polar coordinates,

$$x = r\cos\theta,\quad y = r\sin\theta,\quad f_x = f_r\cos\varphi,\quad f_y = f_r\sin\varphi, \tag{6}$$

and

$$G(f_r,\varphi) = \int_0^\infty\int_0^{2\pi} g(r,\theta)e^{-i2\pi f_r r\cos(\theta-\varphi)}r\,dr\,d\theta. \tag{7}$$

For the case of a radially symmetric function, the θ integration can be carried out giving the Hankel transform (also

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called the Fourier–Bessel transform):

$$G(f_r) = 2\pi \int_0^\infty r\, g(r) J_0(2\pi\, f_r r)\, dr, \tag{8}$$

where J_0 is the Bessel function of the first kind, zero order. Applying the Hankel transform of Eq. (8) to the autocorrelation function of Eq. (1) results in the 2D PSD.

For $\alpha = 0.5$:

$$\mathrm{PSD}(f) = \frac{2\pi\sigma^2\xi^2}{[1 + (2\pi\, f\xi)^2]^{3/2}}. \tag{9}$$

For $\alpha = 1$:

$$\mathrm{PSD}(f) = \pi\sigma^2\xi^2\, e^{-(\pi\, f\xi)^2}. \tag{10}$$

4 Three-Dimensional Case

In three dimensions, the 3D Fourier transform can be converted to spherical coordinates. For the special case of a radially symmetric function, the 3D Fourier transform in spherical coordinates becomes

$$G(f_r) = 4\pi \int_0^\infty r^2 g(r) \left[\frac{\sin(2\pi\, f_r r)}{2\pi\, f_r r}\right] dr = \frac{2}{f_r}\int_0^\infty r g(r) \sin(2\pi\, f_r r)\, dr. \tag{11}$$

Applying this spherical 3D Fourier transform to Eq. (1),

For $\alpha = 0.5$:

$$\mathrm{PSD}(f) = \frac{8\pi\sigma^2\xi^3}{[1 + (2\pi\, f\xi)^2]^2}. \tag{12}$$

For $\alpha = 1$:

$$\mathrm{PSD}(f) = \pi^{3/2}\sigma^2\xi^3\, e^{-(\pi\, f\xi)^2}. \tag{13}$$

5 Summary

Letting d be the dimensionality of the problem, the results can be summarized as follows:

For $\alpha = 0.5$:

$$\mathrm{PSD}(f) = \frac{a_d\, \sigma^2\xi^d}{[1 + (2\pi\, f\xi)^2]^{(d+1)/2}}, \tag{14}$$

where $a_1 = 2$, $a_2 = 2\pi$, and $a_3 = 8\pi$.

For $\alpha = 1$:

$$\mathrm{PSD}(f) = \pi^{d/2}\sigma^2\xi^d\, e^{-(\pi f\xi)^2}. \tag{15}$$

These results, especially for the 3D case, should prove useful in many simulation studies.

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