Grounds and problem statement for software complex for photolithography optimization for minimization of losses in optical structures of photonic integrated circuits

A A Sharapov\textsuperscript{1,2,3}, E S Shamin\textsuperscript{1,2}, I D Skuratov\textsuperscript{1,2} and E S Gornev\textsuperscript{1}

\textsuperscript{1} JSC Molecular Electronics Research Institute, 12/1 Academician Valiev Street, Zelenograd, Moscow, 124460, Russia
\textsuperscript{2} Moscow Institute of Physics and Technology, 9 Institutskiy per., Dolgoprudny, Moscow Region, 141701, Russia
\textsuperscript{3} E-mail: andrey.sharapov@phystech.edu

Abstract. The losses in optical components are the key obstacle in development of photonic integrated circuits (PIC). This makes the developers to include additional signal gain elements into the optical scheme. One of the major and optimizable factors of signal loss is the sidewall roughness of the optical components. After analysis of factors causing the line-edge roughness (LER), we developed the basic model of the roughness emerging process during forming of photolithography nanostructures. We proposed an approach to optimize the photolithography process in order to minimize the optical losses in fabricated optical structures. The software complex on the basis of this approach is currently under development.

1. Introduction

The continuous development in integrated circuits manufacturing is associated with technology node scaling [1]. However, the edge roughness of nanostructures cannot be decreased with the same factor [2]. Hence, the roughness-to-size ratio is growing for single elements, which makes devices on their basis unstable in terms of electrotechnical performance. Such issues are particularly relevant for structures having dimensions about the size limit of used technology.

For example, figure 1 shows the I-V curves modeled for a single FinFET having certain values of LER. Due to shortness of transverse dimensions in comparison to the roughness amplitude, the gate width is obviously subject to effects linked with the edge roughness emergence. The modeling of this structure was performed in Synopsys TCAD, and the existence of structure unevenness was simulated by applying the built-in method of edge transformation by noise function. This function is given by an inverse Fourier transform of autocorrelation function with predefined values of standard deviation $\sigma$ and correlation length $\Lambda$:

$$f_{\text{autocorrelation}} = \sigma^2 \sqrt{\pi} \Lambda e^{-x^2/\Lambda^2}.$$ (1)
Figure 1. Scheme of FinFET and current–voltage curves modeled for fin with different line edge roughness values. Geometrical parameters of the fin structure – 8 × 40 × 100 nm; gate length – 30 nm; correlation length – 5 nm.

Not only electrotechnical performance of silicon microelectronic devices is affected by edge roughness, but this phenomenon is also an issue for silicon photonics. Despite the fact that this realm of science and technology develops rather quickly, sidewall roughness in optical waveguides which gives the main impact into the propagation losses in photonic circuit elements, continues to be a serious concern.

Due to light scattering at short-period roughness of waveguides, the loses may reach several decibels per millimeter, while total area of optical integrated circuits may span up to several square centimeters. Losses calculation method for waveguides with account for the sidewall roughness is described in [3]. These losses for fin waveguides which are one of the most common structures in silicon photonics, are given by the following expression [4]:

$$\alpha(TE,TM) = \frac{4,34 \sigma^2}{\sqrt{2d^4\beta_{TE,TM}}} g(V) \cdot f_e(x,\gamma),$$

where

$$g(V) = \frac{n_2V^2}{1+p^2} \quad f_e(x,\gamma) = \left( \frac{((1+x^2)^2+2x^2\gamma^2)^{1/2}+1-x^2}{[1+(x^2)^2+2x^2\gamma^2]^{1/2}} \right)^{1/2}.$$

These functions in turn are defined by the set of standard parameters:

$$x = p(L_c/d), \quad \gamma = \frac{n_2V}{n_1\sqrt{\Delta}}, \quad \Delta = \frac{n_1^2-n_2^2}{2n_1^2},$$

$$h = d\sqrt{n_1^2k_0^2-\beta^2}, \quad V = k_0d\sqrt{n_1^2-n_2^2} \quad p = d\sqrt{\beta^2-n_2^2k_0^2}.$$

Here $k_0$ is the wavenumber in air, $\beta$ is the effective propagation constant of certain mode, $d$ is the half-width of the waveguide, $L_c$ is the roughness correlation length, and $\sigma$ is its standard deviation.

2. Theoretical description of edge roughness for waveguides formed by photolithography

All the phenomena causing the edge roughness of nanostructures during nanofabrication process, can be divided into the following groups by physical principles [5]:
1. Photonic shot noise is the lithographic phenomenon which takes place during aerial image formation.
2. Effects caused by chemical properties of resist and peculiarities of chemical reactions modifying the resist and affecting the resist imaging.
3. Effects associated with diffusion properties of photoresist.
4. Effects caused by plasma etching (also referred to as dry etching).

We suggest to implement the optimization algorithm which allows to find technology process parameters, which provide minimal losses in fabricated PIC due to decreasing of edge roughness magnitude.

2.1. Brief description of optical effects in photolithography
Photolithography process modeling is one of the key stages in microelectronic devices fabrication. It can be divided into modeling of aerial image and resist modeling.

As known from optics, description of light propagation principles through holes in the screen, are determined by three parameters, which are holes diameters, distance from the screen to observation plane, and wavelength of used light source. The three regimes of optics can be well demonstrated for the case of a screen with a single hole and monochromatic normal incident light beam. These cases are called geometrical optics, Fresnel diffraction, and Fraunhofer diffraction [6].

Practically important cases for photolithography are the diffraction optics regimes. Moreover, due to continual development in microelectronics, critical dimensions of the structures are decreasing, and the impact of diffraction effects becomes more and more significant. These effects lead to fuzzy boundaries, corner rounding, line-end shortening, and as for most critical, illumination of undesired area on the wafer [7].

Common view of intensity distribution cutline is presented on figure 2. This distribution apparently has smooth tails that exceed the bounds of initial topology elements. Further theoretical description in this work is essentially the impact analysis of these distribution tails on the structure unevenness.

Figure 2. Common view of aerial image cutline at the position of red line. Geometrical parameters of the dark-field topology elements with 140 nm pitch: 100 nm × 1 μm for short lines, 100 nm × 2 μm for middle line. Intensity is normalized by the full illumination intensity.
2.2. Impact of photonic shot noise into edge roughness

First phenomenon causing the edge roughness, is photonic noise [8]. Let us consider the light source, which emits photons at the rate $F$ per unit time and unit area. Let us also consider the binary random phenomenon of photon emission during the time segment $\Delta t$, that is short enough so no more than one photon can be emitted during it, i.e. $\Delta t \ll 1/F$. The probability of photon emission during $\Delta t$ is $F \Delta t$.

Let us now find the probability that exactly $n$ photons will be emitted during time interval $T$, which is $N$ time periods each equal to $\Delta t$:

$$P(n) = C_N^n (F\Delta t)^n (1 - F\Delta t)^{N-n}. \tag{5}$$

We can use the Poisson limit theorem for binomial distribution in (5) if $N \to \infty$ and $N F \Delta t = TF = \text{const}$, which is a practical case for photolithography:

$$\lim_{N \to \infty} C_N^n (F\Delta t)^n (1 - F\Delta t)^{N-n} = \frac{(TF)^n}{n!} e^{-TF} \tag{6}$$

From Poisson distribution properties one can estimate expected value of photon amount, emitted during time interval $T$:

$$E(n) = \sum_{n=0}^{\infty} n \frac{(TF)^n}{n!} e^{-TF} = e^{-TF} \sum_{n=1}^{\infty} \frac{(TF)^n}{(n-1)!} = TF e^{-TF} \sum_{m=0}^{\infty} \frac{(TF)^m}{(m)!} = TF, \tag{7}$$

and the variance of photon amount is

$$\sigma_n^2 = E\left(\left(n - E(n)\right)^2\right) = E(n^2) - \left(E(n)\right)^2 = TF. \tag{8}$$

Let us switch to dimensional units to associate these estimations with physical quantities. The key quantity is light intensity, which expresses the amount of energy transferred by $n$ photons per unit time $T$ to unit area $A$:

$$I = \frac{n \ h c}{TA \ \lambda} \tag{9}$$

Then at each spatial segment intensity expected value can be calculated as follows:

$$E(I) = \frac{E(n) \ h c}{TA \ \lambda} = \frac{F \ h c}{A \ \lambda}. \tag{10}$$

The same substitution can be used to obtain intensity standard deviation:

$$\sigma_I = \frac{1}{TA \ \lambda} \sigma_n = \frac{E(I)}{\sqrt{TF}} = \frac{E(I)}{\sqrt{E(n)}} \tag{11}$$

As a result, we get the relation between intensity standard deviation and its expected value for each spatial segment:

$$\sigma_I = \frac{\sqrt{E(I)}}{\sqrt{TA \ \lambda \ h c}} \tag{12}$$

Equation (12) allows to calculate an area in which photonic shot noise could affect the edge.
roughness. Expected value of intensity in (12) could be substituted for modeled values of intensity, unit area $A$ could be substituted for a pixel area of the modeled intensity and time period $T$ could be substituted for exposure time. Then we could build the map of intensity standard deviations over the intensity distribution. When modeling intensity distribution (also referred to as aerial image) and subsequent resist imaging using empirical models based on the data from fabrication results, one can estimate the average imaging intensity $I_{\text{imaging}}$, which characterizes the boundaries of the areas where resist becomes exposed (blue line at figure 3). This value is closely related to the simplest of resist models, the so-called constant threshold resist models. The average imaging intensity value applied as a threshold on the intensity distribution plot, gives an isoline, which is surely not the same as the imaging contour due to performed averaging, though it is a simple and robust estimation. Using three-sigma rule at each point of the aerial image, we can define the area of unreliable illumination as follows:

$$
\begin{align*}
I + 3\sigma_I(I) &> I_{\text{imaging}} \quad \text{if } I < I_{\text{imaging}} \\
I - 3\sigma_I(I) &< I_{\text{imaging}} \quad \text{otherwise.}
\end{align*}
$$

(13)

We will have a closer look at this area in the next section.

Figure 3. Schematic explanation of area of unreliable illumination definition (between green contours) for a dark-field topology element. Blue isoline corresponds to the average imaging intensity.

A common practice for microelectronic manufacturers is to calculate normalized aerial image distribution. This is appropriate for the use of empirical resist models and significantly simplifies the calculations. To get the dimensional quantities of intensity, one shall use the factor of light source power for the certain photolithography setup.

2.3. Impact of photoresist imaging effects into edge and sidewall roughness
Resist imaging process is enabled by illumination of resist molecules. For a positive resist, incident light breaks the molecular bonds in illuminated areas on the resist layer surface, and solubility of resist in these areas increases. For a negative resist, on the contrary, the solubility of illuminated areas decreases. Significant part of modern photoresists are so-called chemically amplified resists, which represent a mixture of a polymer and a photo-sensitive compound called photoacid generator. The latter substance decomposes upon exposure and releases acid, which dopes polymer during post-exposure baking and is being released into resist again, i.e. behaves as a catalyst. In the doped areas, polymer becomes soluble, and reacted products are removed in etching.
In all mentioned types of photoresist, it is the chemical reaction that plays the key role in imaging. This reaction is characterized by a certain activation energy.

In order that the resist in different areas of surface had similar properties in relation to incident illumination, its composition shall have as narrow distribution of molecular weights. If confined to consideration of resist as absolutely uniform substance having fixed threshold of chemical reaction activation, the ratio of this activation energy to the unit area is essentially the resist threshold exposure dose $D_{\text{threshold}}$.

To get relation with photolithography parameters, the dose can be expressed in terms of quantities introduced in the previous section:

$$ D = \frac{n \ h c}{A \ \lambda} = TI $$

Hence, having certain exposure time $T$, resist illumination area matches the area, surrounded by contour, corresponding to fixed intensity value $D_{\text{threshold}}/T$. Due to the absence of lateral shifts of such contour, the line edge roughness, which is defined as standard deviation of line points from the average edge position, equals zero.

In fact, edge roughness of fabricated structures is defined by random deviations of illumination intensity in the area of unreliable illumination. For each molecule in this area, the condition to start chemical reaction $I > D_{\text{threshold}}/T$ is satisfied with certain probability. This means, that for a large number of molecules there are such ones, that are not modified, despite the fact that they are formally in the area of illumination. In case of chemically amplified resists, acid diffusion during post-exposure baking “smooths” the resist properties, and the interface between different states of photoresist becomes more even. The width of the formed structure, however, is still uneven.

Let us now consider the impact of discrete polymer-based resist structure on edge roughness. To a basic approximation, the polymer macromolecule can be represented as freely-jointed chain of monomers. This allows not to account for the peculiarities of single atom interaction while describing spatial polymer configuration. In addition to structure discreetness of the substance, one shall also take into account the fact that there is a certain variation in mass and radius of constituent molecules. Taking all this into consideration, and assuming that all the molecules within the area of unreliable illumination, form the interface and thus define the edge roughness, one can make a schematic illustration of these phenomena (see figure 4).

**Figure 4.** Schematic demonstration of impact of intensity dispersion, non-zero width of molecular size distribution, and resist discreetness, to edge roughness forming. Geometric size of molecules is increased by several decades for the sake of visibility.

Estimation of roughness characteristics for given topology and materials, including correlation length and power spectral density analysis, is performed using stochastic modeling. Input parameters for this
technique are molecular mass distribution of photoresist, and resist illumination dose distribution.

Due to requirements of high etch selectivity, and in order to prevent the negative effect on the width evenness of fabricated elements, the most common is plasma etching, which forms a sidewall with roughness inherited from the top edge of the structure downwards in the material (see figure 5). Hence, it is acceptable to assume that roughness of the structure as well as its linear qualitative characteristics, stay unchanged.

![Sidewall morphology of fin structure pictured by atomic force microscopy](image)

**Figure 5.** Sidewall morphology of fin structure pictured by atomic force microscopy [9]. Edge roughness is inherited along the etching direction.

3. **Optimization algorithm**

Now having information on sidewall roughness of structures for certain fabrication process, one can estimate the qualitative parameters of width unevenness for waveguides, and also optical losses using equations (2) – (4). In order to decrease the resulting losses, one shall adjust certain parameters of technology process using the optimization algorithm presented on figure 6.

![Scheme of suggested optimization algorithm](image)

**Figure 6.** Scheme of suggested optimization algorithm for photolithography adjustment to minimize losses of fabricated optical elements.
Verification of suggested algorithm shall be conducted both comparing the relative optical losses in PIC before and after technology adjustment, and also by assessment of roughness for fabricated structures. The set of test structures to conduct such measurements is under development.

Sidewall roughness in silicon microelectronics is usually measured using scanning electron microscopy (SEM) [10], and the most stable on-wafer technique to estimate LER value is by calculation of the standard deviation of edge points position sampled from the SEM image [11]. Optoelectronic structures are currently also fabricated on silicon wafers, which gives a reason to use mentioned roughness analysis methods in photonic integrated circuits manufacturing.

4. Conclusion
In this work we considered how do certain processes of microelectronic technology influence the amplitude of edge roughness of fabricated structures. We suggested the algorithm of photolithography optimization to minimize the optical losses in structure of photonic integrated circuits. The implementation and verification of the algorithm suggested in this work is the subject of further research.

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