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Sidewall roughness model for optical losses calculation in photonic integrated circuits

E. S. Shamin [1,2]✉, A. A. Sharapov [1,2], I. D. Skuratov [1,2],
S. O. Demidov [1,2], E. S. Gornev [1,2]

[1] Moscow Institute of Physics and Technology, Moscow, Russia;

[2] Molecular Electronics Research Institute, Zelenograd, Russia

✉ yevgeniy.shamin@phystech.edu

Abstract. One of the key performance indicators of photonic circuits is the value of optical propagation losses. Among several factors which impact these losses, the sidewall roughness is considered as the primary focus of this work. The optical signal, propagating along the photonic device, scatters on roughness of its element's surfaces. This decreases the output power, as well as leads to the higher heating and worse transmission characteristics, which in its turn increases the noise ratio and creates undesired phase deviations. Thus, the problem of sidewall roughness simulation (and consequently, losses estimation in microwave photonic circuits caused by it) is relevant at the design stage of the devices. Therefore, a new, highly efficient model of sidewall roughness based on a photolithography simulation and imitational modelling of photoresist exposure is presented. Principles of operation and implementation features of the model are described. Simulation results, obtained using the new roughness model, are demonstrated and an approach on their verification with experimental data is suggested. Additionally, theoretical estimations for the optical losses caused by sidewall roughness in ridge Si waveguides are discussed.

Keywords: sidewall roughness, photolithography modeling, random close packing, photoresist exposure modeling, integral photonics, optical losses

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Материалы конференции
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Модель шероховатости для расчета оптических потерь в фотонных интегральных схемах

Е. С. Шамин [1,2]✉, А. А. Шарапов [1,2], И. Д. Скуратов [1,2],
С. О. Демидов [1,2], Е.С. Горнев [1,2]

1 Московский физико-технический институт, Москва, Россия;

2 Научно-исследовательский институт молекулярной электроники, Зеленоград, Россия

✉ yevgeniy.shamin@phystech.edu

Аннотация. Оптические потери радиофотонных схем является одним из важнейших показателей качества их работы. Среди множества эффектов, влияющих на оптические потери, можно выделить шероховатость боковых стенок оптических элементов

таких схем (далее шероховатость). В данной работе предлагается к рассмотрению высокоэффективная модель появления шероховатости, состоящая из расчета оптической части фотолитографии, а также имитационного моделирования резиста. Описаны принципы функционирования и особенности реализации представленной модели. Продемонстрированы результаты моделирования, полученные с помощью новой модели шероховатости, а также предложен метод их экспериментальной верификации. Приводится теоретическая оценка потерь в волноводной структуре, связанных с шероховатостью.

Ключевые слова: шероховатость, моделирование фотолитографии, случайная плотная упаковка, моделирование проявления фоторезиста, интегральная фотоника, оптические потери

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Introduction

The research activity in the field of integrated photonics is growing steadily. As a result, some aspects of microelectronics technology which were earlier ignored, are becoming more relevant. One of such aspects is a problem of sidewall roughness, which is assumed to be one of the main components contributing to the energy efficiency of photonic integrated circuits [1]. The signal propagating along the photonic device, scatters on roughness of its element's surfaces. This decreases the output power, as well as leads to the higher heating and worse transmission characteristic, which in its turn increases the noise ratio and creates undesired phase deviations. This hinders the use of photonic devices in radiolocation and RF transmission circuits.

Most often, due to the low availability of roughness modeling tools, as well as the high computational complexity of the algorithms used in them, the described problems are identified only at the stage of testing of the final devices. Thus, the problem of estimating losses in photonic circuits caused by sidewall roughness is relevant at the design stage. In this work a highly efficient sidewall roughness model is proposed, which could allow to fill this gap.

Materials and Methods

Roughness simulation, in terms of the model presented, consists of two steps. First step is a modelling of the photolithography which allows to take the effect of photon shot noise on the formation of roughness into account [2]. Second step is an application of the original imitational model of the resist exposure. It is assumed that the etching process used for manufacturing integrated photonic elements is chosen to be highly anisotropic, which results in inheritance of roughness features from the resist to the formed structure.

Based on the photolithography modelling data (Fig. 1, *a*), a region of "Unreliable illumination" is calculated [3] (Fig. 1, *b*). In this region there might be statistical deviations in energy, transferred to resist which may lead to local under- or over-exposures. Thus, it is assumed that sidewall roughness will be localized inside the "Unreliable illumination" region. Formally this region could be defined as by equation (1) on the aerial image plane (distribution of intensity over the resist, obtained as a result of modeling the optical part of photolithography). Here $I_{imaging}$ is defined as an average intensity over which photoresist becomes exposed and σ_I is defined by (2). $E(I)$ denotes an expected value of intensity, which could be substituted with intensity, obtained from CAD simulations. This reflects the statistical nature of roughness modeling.

$$\begin{bmatrix} I + 3\sigma_I(I) \geq I_{imaging}, & I \leq I_{imaging} \\ I - 3\sigma_I(I) \leq I_{imaging}, & I > I_{imaging} \end{bmatrix} \quad (1)$$

$$\sigma_I(I) = \sqrt{\frac{E(I)}{TA\frac{\lambda}{hc}}} \quad (2)$$

where I is intensity, T is exposure time, A is an elementary area unit on the XY simulation plane and λ is a photolithography wavelength.

The contribution of photoresist effects to sidewall roughness is taken into account by applying an imitational model of the resist exposure. In terms of this model, the macromolecules of the photoresist material are represented as tightly packed spheres or as referred further – grains. The resist grains mass (and, accordingly, size) variations are taken into account by specifying the grains radii distribution. If resist grain is partially or completely located within "Unreliable illumination" region, its exposure occurs only with some probability, which contributes to the roughness of the final structure.

After processing the initial data and obtaining the "Unreliable illumination" region, a smooth buffer region is built around it on a distance of two maximum radii from given grain radii distribution (Fig. 1, *b*). This ensures that every placed grain would give noticeable impact to final roughness modeling result as well as there would be minimal number of grains to be processed. Over the smooth buffer region, a grid data structure and a grid-based buffer are built with cell size of four maximum radii from given radii distribution (Fig. 1, *c*). The former one allows to address paced grain's location by their number and numbers of placed grains by the number of grid cell. This allows the close packing algorithm to compute in linear time with respect to the number of balls to be processed. The latter one allows to efficiently calculate if placed grain is inside valid region and thus is used as a shape to be filled. The close packing algorithm, used in this work is a highly optimized for photoresist modeling 2D realization of 3D version of algorithm, presented at [4]. The result of the application of this algorithm could be seen at Fig. 1, *c*.

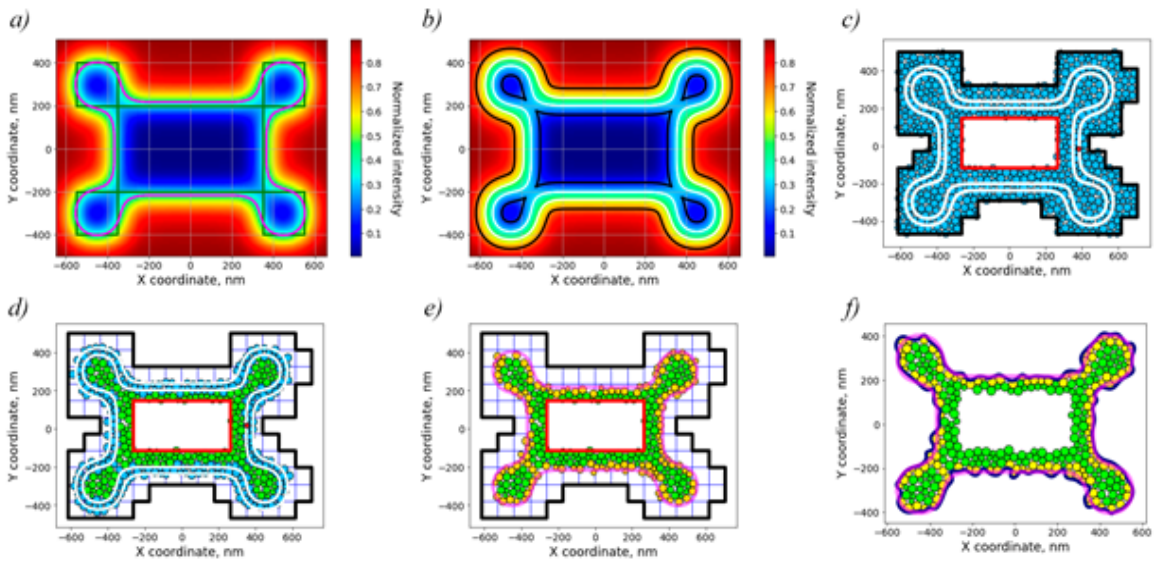

Fig. 1. Initial data for unreliable exposure model: aerial image and exposed resist contour (marked as purple). Initial topology polygons are presented with green lines (*a*); Buffer region (marked as black) is built around "Unreliable illumination" region (marked as white) (*b*); Result of the close packing algorithm application on a grid-based region (marked as black), built around buffer region, shown on Fig. 1, *b*)(*c*); Grains labeling: blue ones (in contrast to green ones) are exposed by chance (*d*); Exposed grains (marked as yellow). Initial resist contour (marked as transparent purple) is presented for comparison (*e*); Result of the patching and smoothing algorithms application. Initial resist contour (marked as transparent purple) is presented for comparison (*f*)

The final step before exposure simulation is grains labeling (Fig. 1, *d*) – algorithm defines, which grains from close packed ones fall into "Unreliable illumination" region and which ones are definitely exposed. Consequently, unreliable grains are processed using the criterion, described further in this work. Remaining (exposed) grains could be seen at Fig. 1, *e*. Finally – patching algorithm is applied between each neighboring grain which returns their convex hull – this and an additional spline interpolation algorithm allows for overall smoothness of the final result (Fig 1, *f*).

To simulate the exposure process – an exposure probability function is calculated for each of the unreliable grains, which could be expressed as (3). Each unreliable grain is split into 3 parts – reliable one, which is located in the definitely exposed region, unreliable one – according to the name, and underexposed one, as shown in Fig 2, *a*. Those correspond to values Ain, Aur, and Aout in (3) – which represent the fractions of overall grain area. Important to note that sum of this values equals to one.

$$P(Exposure) = A_{in} + A_{ur} \cdot P(I) + 0 \cdot A_{out} \tag{3}$$

where $P(I)$ is derived from Poisson cumulative distribution function and Ain, Aur and Aout are fractions of grain area, defined by Fig. 2, *a*.

For photoresist that becomes exposed over low intensity values, $P(I)$ in (3) has the meaning of probability that less than the threshold number of photons (proportional to Iimaging) strikes the grain in average over its area. This probability is calculated using the Poisson cumulative distribution function (Fig. 2, *b*), which is built for each grain by the average number of photons over all yellow points shown in Fig. 2, *a*. Respectively, for photoresist that becomes exposed over high intensity values, $P(I)$ should be calculated as $1 - P(I)$ for low intensity resist.

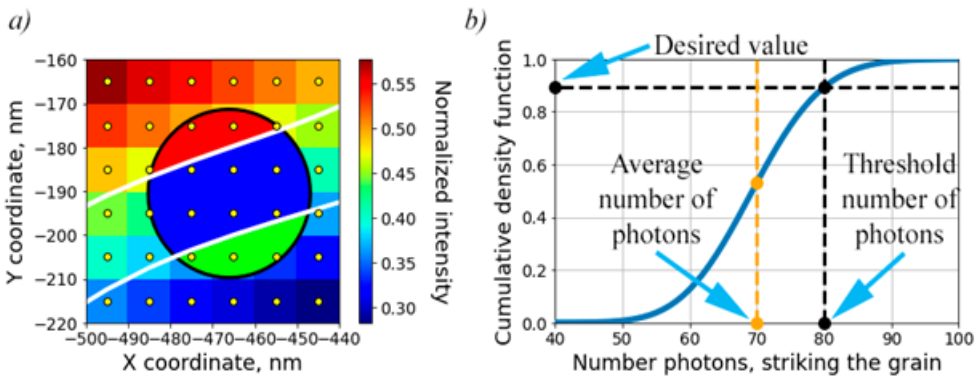

Fig. 2. Location of intensity points (yellow) that are averaged for each grain for probability calculation. Additionally, 3 split parts, calculated for each grain are shown – each corresponding to one of three fractions of area, used in (3): red part corresponds to A_{out} fraction of grain area, blue part corresponds to A_{ur} fraction and green part corresponds to A_{in} fraction (*a*); Probability calculation that less than threshold number of photons will strike the grain on average (*y* axis value, corresponding to horizontal black dotted line). Calculation is performed with the use of Poisson cumulative distribution function (*b*)

Results and Discussion

As could be seen on Fig. 3, *a* – resulting distribution of grain sizes (grains are shown on Fig. 1, *c*) is closely matched with initial one. It is also worth noting that overall running time of all applied algorithms is close to linear in respect to number of grains needed to be processed (as shown in Fig. 3, *b*). Results of high-precision modeling are shown on Fig. 3, *c*. Initial number of resist grains was about 3.5k. Full computation time needed to achieve the result presented was about 13s.

Sidewall roughness inflict and therefore highly correlated with optical losses. In agreement with Yap-form Payne-Lacey model [5], losses caused by sidewall roughness scattering in ridge optical waveguide can be expressed as (4):

$$\alpha_{PL}(TE/TM) = \frac{4.34\sigma^2}{\sqrt{2}d^4\beta_{TE/TM}} g(V) \cdot f_e(x,\gamma) \quad (4)$$

where σ is root-mean-square roughness, d is ridge waveguide half width, $\beta_{TE/TM}$ is a propagation constant. $g(V)$ and $f_e(x, \gamma)$ are functions described in [5].

By measuring these losses one can calculate device sidewall roughness and, consequently, verify new roughness model. On this basis, we propose a verification methodology that could be divided to three steps:

- Fabrication of test waveguide structures;
- Evaluation of numerical roughness characteristics by using a scanning electron microscope [6];
- Measurement of the transmission characteristic of the devices obtained.

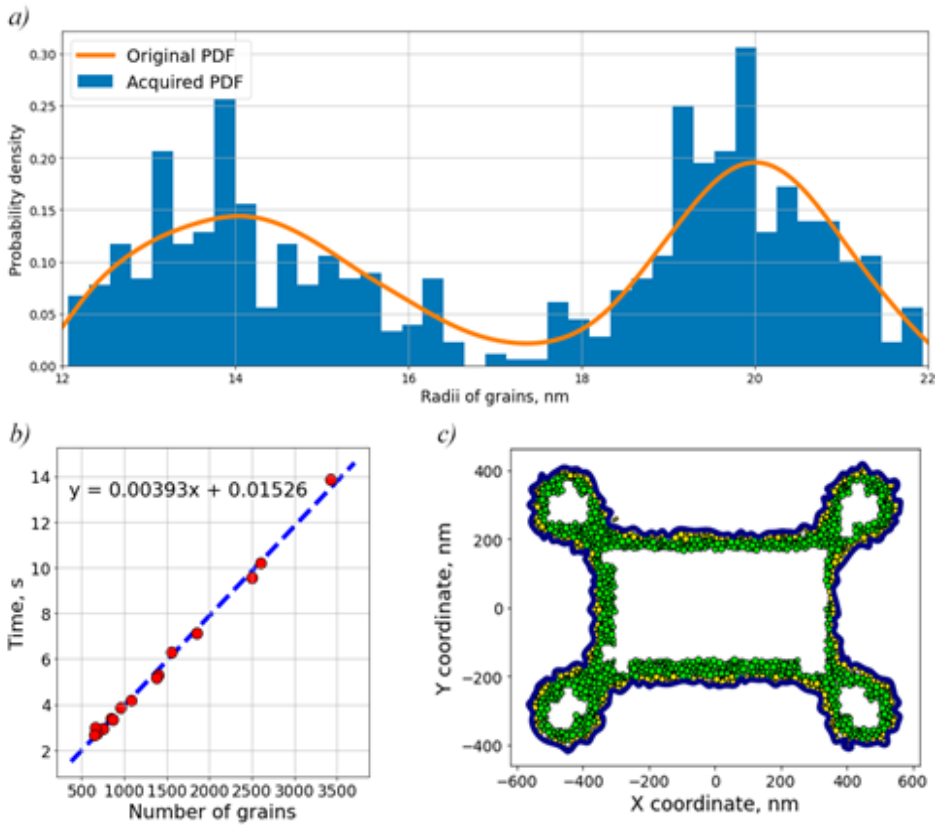

Fig. 3. Acquired probability density function (shown with histogram) and original probability density function (shown as orange curve) of grain's radii distribution (*a*); Time vs resulting number of grains processed by all applied algorithms (*b*); Results of high-precision modeling. Initial number of grains was about 3.5k. Running time was about 13s (*c*)

Conclusion

In this work simulation results, obtained using the new, highly efficient sidewall roughness model, were demonstrated. Principles of operation and implementation features of the model were described. An approach on their verification with experimental data was suggested. Additionally, theoretical estimations for the optical losses caused by sidewall roughness in Si waveguide are discussed.

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THE AUTHORS

SHAMIN Evgeniy S.
yevgeniy.shamin@phystech.edu
ORCID: 0000-0002-0470-350X

SHARAPOV Andrey A.
andrey.sharapov@phystech.edu
ORCID: 0000-0001-9945-3875

SKURATOV Ilya D.
ilya.skuratov@phystech.edu
ORCID: 0000-0002-4045-2883

DEMIDOV Stanislav O.
demidov.so@phystech.edu
ORCID: 0000-0003-0115-8822

GORNEV Evgeniy S.
egornev@niime.ru
ORCID: 0000-0003-1706-4142

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