

# Efficient source mask optimization with Zernike polynomial function-based source representation

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**Abstract:** This paper introduces a Zernike polynomial function-based source representation method for the aerial image calculation of optical lithography. It is shown that this representation enables computation reduction for both mask optimization and source optimization.

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## 1. Introduction

As the critical dimension (CD) in the semiconductor industry has come to the sub-22nm region, the process factor  $k_1$  becomes very low, and the continuation of ArF optical lithography depends heavily on resolution enhancement techniques (RETs), especially computational lithography such as source mask optimization (SMO) [1,2]. In this technique, source representation methods are fundamental for both aerial image simulation and inverse optimization [3]. There is a trade-off between the traditional methods, which utilize a few parameters to represent the sources, and the recent pixel-based methods. While the traditional methods take advantage of fewer number of variables, the solution spaces of their optimization are also limited, and the natural optical imaging theory cannot be revealed in the optimization, leading to non-linear problems [4]. The recent pixel based representation methods can bring larger solution spaces with more pixel variables, but suffer from huge optimization problems with a large number of variables, and total variation regularization may be required to limit the source complexity [5].

This paper addresses this problem by introducing a Zernike polynomial function-based source representation method, where the sources are represented as a series of source coefficients [6]. Based on this representation, we derive a linear relationship between the Transmission Cross Coefficient (TCC) in optical imaging systems and the coefficients, so that the aerial image simulation for mask optimization can be accelerated. We also derive a linear relationship between the aerial images and the coefficients, and then the source optimization can be formulated as a convex problem. Both of these two linear relationships can reduce the computation, and the number of variables can be greatly reduced at the same time, making this algorithm quite suitable for SMO.

## 2. Theory

The imaging process of optical lithography is often modelled as a partially coherent imaging system, where the aerial images can be expressed as in Abbe's formulation or in Hopkins' formulation

$$I(x, y) = \iint_{-\infty}^{\infty} J(f, g) |FT[O(f', g')H(f' + f, g' + g)]|^2 df dg, \quad (1)$$

$$= \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} T(f_1, g_1; f_2, g_2) O(f_1, g_1) O^\dagger(f_2, g_2) e^{-i2\pi[(f_1 - f_2)x + (g_1 - g_2)y]} df_1 dg_1 df_2 dg_2. \quad (2)$$

Here,  $J$  is the illumination source,  $O$  is the Fourier Transform (FT) of the mask pattern,  $H$  is the projection pupil,  $\dagger$  is the complex conjugate, and  $T$  is the TCC defined as

$$T(f_1, g_1; f_2, g_2) = \iint_{-\infty}^{\infty} J(f, g) H(f + f_1, g + g_1) H^\dagger(f + f_2, g + g_2) df dg. \quad (3)$$

Since the sources of partially coherent imaging systems are limited to a circular investigation with a unit radius after normalization, we can introduce a novel method to represent the sources, which is a combination of a series of Zernike polynomial functions:

$$J(f, g) = \sum_{l,m} \psi_m^l Z_m^l(f, g) = Z\Psi, \quad (4)$$

where  $Z_m^l$  are the Zernike polynomial functions with an order  $m$  and rank  $l$ ,  $\psi_m^l$  is the source coefficient,  $Z$  is the stacked Zernike polynomial functions, and  $\Psi = [\psi_0^0, \psi_{-1}^1, \psi_0^1, \dots]^t$ . Substituting this source representation in Eq. 1 and Eq. 3, we get

$$I(x, y) = \iint_{-\infty}^{\infty} \sum_{l,m} \psi_m^l Z_m^l(f, g) |FT[O(f', g') H(f' + f, g' + g)]|^2 df dg, \quad (5)$$

$$T(f_1, g_1; f_2, g_2) = \iint_{-\infty}^{\infty} \sum_{l,m} \psi_m^l Z_m^l(f, g) H(f + f_1, g + g_1) H^\dagger(f + f_2, g + g_2) df dg, \quad (6)$$

Since both the aerial image and the TCC are linearly related to the source, we can separate the source coefficients  $\psi_m^l$  from the above equations. What then remains is only involved with the Zernike polynomial functions, mask patterns and pupils. Denoting  $I_m^l$  as the aerial images formed from the Zernike polynomial functions with the mask patterns and the pupils,  $T_m^l$  as the corresponding TCC, we can calculate the aerial image as  $I = \sum_{l,m} \psi_m^l I_m^l$ , and TCC as  $T_m^l = \sum_{l,m} \psi_m^l T_m^l$ . If we vectorize the matrices, and stack the vectors, we can get the following matrix representation:

$$I = \hat{I}\Psi, \quad (7)$$

$$T = \hat{T}\Psi, \quad (8)$$

where  $\hat{I} = [I_0^0, I_{-1}^1, I_0^1, \dots]^t$ ,  $\hat{T} = [T_0^0, T_{-1}^1, T_0^1, \dots]^t$ .  $I, T$  are vectorized versions of  $I$  and  $T$ , respectively. Thus, we get an efficient way to calculate the TCC and the aerial images when the source changes.

With this efficient way to calculate the TCC and the aerial images, the amount of computation in source mask optimization can be largely reduced. For mask optimization, the Sum Of Coherent Systems (SOCS) theory can be introduced for aerial image simulations [7], replacing the traditional methods based on Abbe's theory that are often used in SMO. The number of Fourier Transforms can be greatly reduced since only a small number of kernels are needed, while the traditional methods require a Fourier Transform for each pixel source. Thus, though the inverse mask optimization is still a non-linear problem, the amount of computation can be reduced because of the faster aerial image simulation algorithm. This problem can be solved through gradient-based methods as described in our previous work [5].

In terms of source optimization, it is possible to formulate the problem as a convex problem based on the linear relationship indicated in Eq. 7. The cost function for source optimization can be defined for the aerial images as

$$\mathcal{F}_s\{I(x, y), I_t(x, y)\} = \sum_{x,y} |I(x, y) - I_t(x, y)|_2^2, \quad (9)$$

$$= \sum |\hat{I}\Psi - I_t|_2^2, \quad (10)$$

where  $I_t$  is the target pattern, and  $I_t$  is its vector form. Regarding the constraints, total variation regulation of the sources is not required to constrain their complexity because the Zernike polynomials are naturally smooth functions. We only have to constrain the values of the source pixels to be larger than 0 and less than a normalized value such as 1. Therefore, the source optimization can be formulated as

$$\text{minimize } \mathcal{F}_s\{I(x, y), I_t(x, y)\},$$

$$\text{subject to } 0 \leq Z\Psi \leq 1$$

As the cost function take a quadratic form for the source coefficients, and the constraint is linear, it is a convex problem that can be solved through convex optimization tools such as CVX.

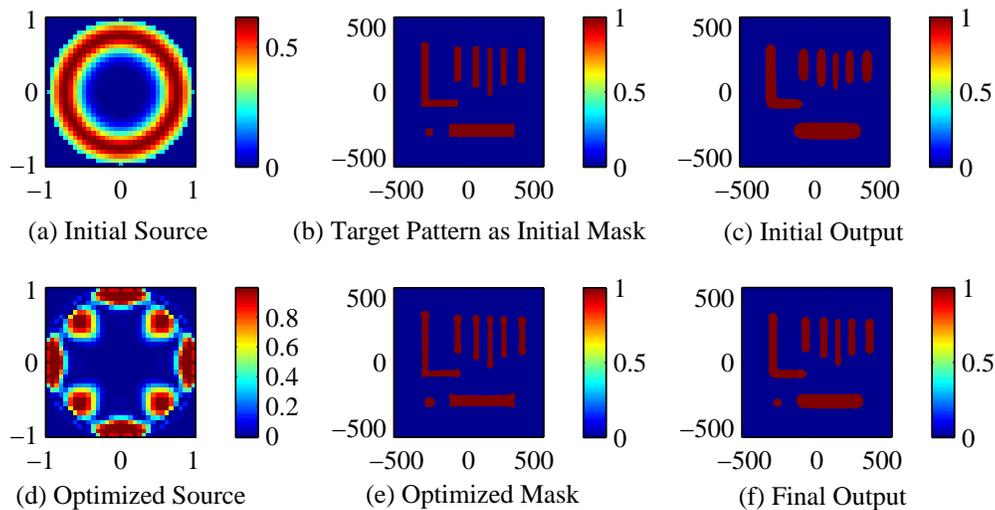


Fig. 1. Simulation Results of SMO with Zernike polynomial-based source representation. The frequency coordinate is  $[-1, 1]$ , and the spatial one is  $[-572, 572]$  nm.

### 3. Results and Conclusions

In the simulations, the wavelength of the illumination source was set as 193 nm, and the numerical aperture was set as 1.35, which were quite normal for the current immersion lithographic tools. The mask patterns were represented as pixel-based images, where each pixel represented 4.57 nm, and 251 pixels were used in each axis of the mask. We selected 42 Zernike polynomial functions that are symmetric to both axes for the source representation. We also used a sigmoid function to model the threshold process during the optimization as in [5].

As shown in Fig. 1, the target mask pattern contains some bars, with the smallest width of about 37 nm (8 pixels), and also a contact with a CD of 55 nm (12 pixels). Simulation results demonstrated the pattern fidelity can be greatly improved (Pattern errors decreases from 1197 to 716) after several sequential optimizations are performed for both the sources and the mask patterns. The number of iterations is less than 25 in each of the source optimization. It should also be noted that no initial value of the source is required for its optimization, since it can be globally optimized through CVX.

Overall, this paper has presented a novel source mask optimization algorithm by introducing a Zernike polynomial function-based source representation method. Simulation results have demonstrated the feasibility and suitability of this algorithm.

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