INVERSE IMAGE PROBLEM OF DESIGNING PHASE SHIFTING MASKS IN OPTICAL LITHOGRAPHY

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ABSTRACT

The continual shrinkage of minimum feature size in integrated circuit (IC) fabrication incurs more and more serious distortion in the optical lithography process, generating circuit patterns deviating from the desired ones. Conventional resolution enhancement techniques (RETs) are facing critical challenges in compensating such increasingly severe distortion. The approach of inverse lithography, which is a branch of mask design methodology to treat the design as an inverse image problem, is adopted in this paper. We apply nonlinear optimization techniques to design masks with minimally distorted output. The output patterns so generated have high contrast and low dose sensitivity. We also propose a dynamic program-based initialization scheme to pre-assign phases to the layout.

Index Terms — Optical lithography, inverse problems, optical proximity correction, resolution enhancement techniques

1. INTRODUCTION

Optical lithography is the process in which we transfer circuit patterns from the mask to the silicon wafer by means of physical optics. However, due to diffraction and other nonlinear phenomena, patterns on the mask cannot be transferred to the wafer perfectly. Rule-based optical proximity correction (OPC) and model-based OPC techniques are the two predominant techniques to improve the resolution by prewarping the mask pattern. Recently, there are researches on inverse lithography, where the design problem is considered as an inverse image problem [1], [2], [3]. In this paper, we applied an inverse method to design phase shifting masks (PSM) by means of nonlinear optimization. We consider the mask pattern as an image so each pixel represents a variable with limited choice of values. We would like to find optimal mask patterns such that the output image on the wafer has minimum error compared to the desired pattern.

Fig. 1. Two processes of a lithography system: projection optics, and photoresist development. [4]

2. PROBLEM FORMULATION

There are two main elements in simulation of the optical lithography process, namely the exposure and resist development. The former is the process where pattern on the mask is transferred to the wafer through optics and the latter is the process where the photoresist profile is derived from the aerial image (See Fig. 1). Let $O(x, y)$ be the object (mask) and $I(x, y)$ be the image (pattern on the wafer). For simplicity we assume that the source is coherent. If the optical transfer function describing the projection optics is given by $H(x, y)$, then the aerial image $A(x, y)$ will be the magnitude square of the convolution between $H(x, y)$ and $O(x, y)$, i.e.

$$A(x, y) = |(H * O)(x, y)|^2.$$ (1)

Consider the simplest case where the aperture is circular in shape. Then the optical transfer function $H(x, y)$ is

$$H(x, y) = \frac{J_1(2\pi r \text{NA}/\lambda)}{2\pi r \text{NA}/\lambda},$$ (2)

where $r = \sqrt{x^2 + y^2}$, $J_1(x)$ is the Bessel function of the first
kind, order 1, $\lambda$ is the wavelength and $NA$ is the numerical aperture.

The second process, resist development, can be approximated by a hard thresholding function. The input output relationship is given by [2]

$$I(x, y) = \frac{1}{1 + e^{-a[A(x, y) - t_c]}},$$

where $a$ is a large constant and $t_c$ determines the transition position.

Our goal is to minimize the error between the output binary pattern $I(x, y)$ and the desired pattern $\hat{I}(x, y)$, with the constraint that a pixel can take values $\{-1, 0, +1\}$ (for alternating phase shifting masks). Therefore, the problem is formulated as

$$\text{minimize} \quad F = \sum_{x, y} \left( I(x, y) - \hat{I}(x, y) \right)^2$$

subject to $O(x, y) \in \{-1, 0, +1\}$.

The constraint in (4) can be relaxed to $-1 \leq O(x, y) \leq 1$ if appropriate regularization terms are added. Poonawala and Milanfar [2] suggested using

$$R = \sum_{x, y} (-4.5O(x, y)^4 + O(x, y)^2 + 3.5),$$

so the minimization problem becomes

$$\text{minimize} \quad F + \gamma R$$

subject to $-1 \leq O(x, y) \leq 1,$

where $\gamma$ is a weighting constant.

\section*{3. ALGORITHM}

Problem (6) is a simple bounded nonlinear optimization problem, where first order derivative is available. Instead of using trigonometric substitution and steepest descent [2] we propose applying active set method and conjugate gradient method to search a local minimum.

Active set method projects all out of bound variables to its closest bound (so that some constraints become active) [5]. In other words, we set

$$O(x, y) = \begin{cases} 1 & \text{if } O(x, y) > 1, \\ -1 & \text{if } O(x, y) < -1. \end{cases}$$

Conjugate gradient method is a first order derivative based method [5]. In general conjugate gradient converges faster than steepest descent which appeared in [2]. We do not apply second order derivative methods (e.g. Newton’s) because the objective function is non-smooth, hence the Hessian is ill conditioned. Moreover, the number of variables is large even if we consider a small circuit pattern. Thus memory becomes an issue if we use Hessian.

\section*{4. INITIALIZATION}

A trivial initial guess for the above algorithm can be the desired pattern itself (i.e. a binary mask without phase component). However, we observe that such initialization may not be the best choice, for the algorithm tends to search a local optimum around the desired pattern. The solution will suffer from poor aerial image slope when two objects are closely located. One intuitive method to resolve this problem is to find an initial mask whose phases are as alternating as possible. In literature this is known as solving the phase conflicts of a layout and there exists plenty of highly specific methods, for example [6]. Since the size of mask that we are considering is small, we propose a simple dynamic program based algorithm to find the initial guess.

We observe that the circuit patterns are often composed of rectangles (for example, Fig. 2(a)). Thus it is intuitive to use vertex locations and edge lengths to present objects. We then apply a distance function (to be discussed below) to measure the “distance” between two objects, hence forming a network (See Fig. 2(c)). Each node represents an object, and path represents a distance. Thus if two objects are close, the path will be short. By finding the shortest sequence of nodes to be passed and assigning phases alternatively, we can get an initial mask with the most alternating phases.

There are various distance functions that can be used and we report three of the reasonable designs below. Let $W$ be the width of overlapping region of two edges, and $G$ be the gap between two objects, as shown in Fig. 2(b). The distance between the $i$-th and $j$-th object can be found using one of the followings, for example:

$$d_1(i, j) = \sum_k G_k/W_k$$

$$d_2(i, j) = \left(\sum_k W_k/G_k\right)^{-1}$$

$$d_3(i, j) = \left(\sum_k \frac{W_k/2}{G_k \sqrt{G_k^2 + (W_k/2)^2}}\right)^{-1}$$

where the index $k$ refers to the $k$-th edge pair under comparison. For example in Fig. 2(b), $k = 2$, as there are two pairs of edges being interacting with each other. It is observed that choice of a particular function is insensitive to the final result.

We use dynamic program to search the shortest route. In each iteration, the algorithm records the cost to reach each
node. Thus at the next iteration, the algorithm picks the path with shortest accumulated cost. Our implementation however needs modification from the standard dynamic program: a node should be removed in the next iteration if a route has passed through it in previous iterations.

The number of nodes in our problem is small, typically less than 10. Therefore, dynamic program is able to solve in seconds. As we mentioned, the solution is in the form of a sequence of nodes. Assigning phases alternatively (i.e. 0, π, 0, π...) we get the desired initial mask (See Fig. 2(d)).

![Fig. 2](image.png)

**Fig. 2.** (a) Mask. (b) Definition of $W$ and $G$. (c) Distance network representing mask shown in (a). (d) Phase initialization result; White = 0, Black = π.

### 5. RESULTS

We demonstrate several test results in this section. The first layout pattern is an XOR gate of size $1700nm \times 1400nm$, and with critical dimension 90nm.

We simulate the source as monochromatic laser with wavelength $\lambda = 193nm$, numerical aperture $NA = 0.85$. As in numerical implementation, we represent the point spread function $H(x, y)$ as an array of size $121 \times 121$, which is adequate to cover 98% energy. For resist development, we set the sigmoid function cut-off threshold as $t_r = 0.3$, and the sharpness of the function $a = 25$. The weighting constant in the algorithm is $\gamma = 0.01$. The initial guess follows from Section 4.

If we do not perform any correction to the layout pattern and use it as the mask, the aerial image is seriously blurred (Fig. 3(a)). Some objects even merge together. On the other hand, if we apply the algorithm and use the optimal phase shifting mask, then the image fidelity is significantly improved (Fig. 3(b)).

![Fig. 3](image.png)

**Fig. 3.** Comparison of using original layout as mask and using optimally designed phase shifting mask.

The second testing layout is a two-rectangle pattern (Fig. 4(a)). The size of the layout is $1000nm \times 1000nm$, and the critical dimension is 50nm. Since the critical dimension of this pattern is much smaller than the previous case, we observe that if we use the layout directly, the two rectangles merge together (Fig. 4(b)). But, using optimal phase shifting mask, the two objects are separated, as seen in Fig. 4(c).

![Fig. 4](image.png)

**Fig. 4.** (a) Desired pattern. (b) Aerial image of using layout as mask. (c) Aerial image of using optimal PSM.

### 6. ROBUSTNESS ANALYSIS

We can further investigate the robustness of our algorithm using the second example. We make a cross section cut at the middle row, and plot the intensity curves, as shown in Fig. 5.

#### 6.1. Contrast

We can numerically evaluate the contrast, as [7]

$$V = \frac{I_{\text{max}} - I_{\text{min}}}{I_{\text{max}} + I_{\text{min}}} \times 100\%.$$  \hspace{1cm} (10)

It is the measure of the difference between the largest and the smallest intensity value. High contrast is always desired because it implies sharper edges. In Fig. 5, the contrast of the aerial image using original layout as mask is

$$V_0 = \frac{0.7413 - 0.6566}{0.7413 + 0.6566} \times 100\% = 6.06\%,$$
where the values are taken at Distance = 490nm, which is the falling edge of the first rectangle. Without performing any OPC, the aerial images of the two rectangles merge because of the wide point spread function \( H(x, y) \) (large \( \lambda \)). Therefore, as we see in Fig. 5, the contrast is very low.

On the other hand, the contrast of the aerial image using optimal PSM is

\[
V_{PSM} = \frac{2 - 0}{2 + 0} \times 100\% = 100\%.
\]

Since we use PSM, the alternating phases cause the intensity to drop to zero at the trough. This is the reason why contrast can be 100%. Moreover, even if we are not using alternating PSM, the contrast will still be high [3], because when the algorithm searches a mask that gives good fidelity, contrast is enhanced at the same time.

Therefore, the contrast is improved significantly after using the OPC scheme stipulated by our algorithm.

6.2. Dose Sensitivity

Another measure that we can compare is the dose sensitivity, which is usually quantified as the normalized image log slope [7]:

\[
\text{NILS} = \left| \frac{\partial I_{\text{threshold}}}{\partial x} \right|_{\text{threshold}},
\]

where \( I_{\text{threshold}} \) is the threshold intensity (i.e. \( t_r \)), CD is the critical dimension. NILS measures the tolerance of the aerial image when facing fluctuation in dose concentration. Therefore, a higher value is preferred.

In this example, if we use the original layout as the mask, NILS can be found as

\[
\text{NILS} = \left| \frac{50 \times 10^{-9}}{0.3} \times \frac{0.681 - 0.668}{10 \times 10^{-9}} \right| = 0.2167,
\]

where we have set \( t_r = 0.3 \), CD = 50nm, and use forward difference with \( \Delta x = 10\text{nm/pixel} \).

On the other hand, if we use the optimal PSM, the NILS calculated is

\[
\text{NILS} = \left| \frac{50 \times 10^{-9}}{0.3} \times \frac{0.5475 - 0.2581}{10 \times 10^{-9}} \right| = 0.4823.
\]

It is clear that the algorithm also improves the tolerance to dose fluctuation significantly.

7. CONCLUSION

We demonstrated a nonlinear optimization method to inversely synthesize phase shifting masks in optical lithography. We used conjugate gradient and active set method as the core algorithms to solve the problem, with initialization found using simple dynamic program. Results showed that the aerial images generated by our optimal phase shifting masks outperform those generated by using the original layout as the mask: both in contrast and tolerance to dose variation. Further investigation will be focused on regularizing the complexity of the mask.

8. REFERENCES


