Optimization of Masks for High Aspect Ratio UV-Lithographic Patterning

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ABSTRACT

In this paper we present an optimization method for mask layouts used in high aspect ratio UV-lithographic patterning. Different levels of microstructures and substrate cause diffraction effects during the exposure which lead to a distortion of the original mask pattern. A simulation tool for the estimation of diffraction effects during the exposure of complex three-dimensional structures was developed and coupled to an evolutionary optimization algorithm. The simulation tool itself enables a designer to calculate intensity profiles on the resist surface and to estimate the impact of diffraction effects on the resulting resist pattern. Together with the newly implemented optimization method an automatic generation of compensation elements could be achieved.

The simulation method and the used algorithm is described in detail. Finally, an example is used to show how the tool can be used for the optimization of mask structures by generating compensation structures.

Keywords: proximity correction, electro-depositable photo resist, mask design tool, evolutionary algorithms

1 INTRODUCTION

Single crystal silicon still plays a prominent role in MEMS technology. However, there is increasing interest in metallic and polymer micro structures with high aspect ratios which find application, for example, in magnetic micro systems and microfluidic devices. For such purposes thick-film photo resists like SU-8 or AZ9260 enable the fabrication of high aspect ratio 3D structures (see figure 1) [1,2].

Figure 1: Aspect ratio of AZ9260 and Epon SU-8

Figure 2: Uniform coating of arbitrary geometries using electro-depositable photo resists

Such high aspect ratios lead to increasing difficulties in lithographic pattern transfer, as traditionally used photo resists are unable to build a uniform layer by spin-coating and even spray-coating fails on certain geometries. Electro-depositable (ED) photo resists have been successfully used to coat arbitrary geometries. Uniform layers could be produced and structured, particularly on vertical sidewalls of high structures (see figure 2) [3]. Nevertheless, having reached a uniform resist layer is only one precondition for a true to dimension pattern transfer. The main difficulty now exists in the different levels of the microstructures and substrate which results in a proximity distance, where diffraction effects distort the original mask structure (see figure 3). These effects mainly depend on the used exposure dose, the structure geometries and the proximity distance.

Figure 3: Schematic illustration of proximity effects at 3D microstructures
Optical Proximity Correction (OPC) is a widely known technique for compensating such diffraction effects in subwavelength lithographic patterning [4, 5]. Such rule based methods are only suitable for compensating effects generated by a fixed proximity distance. Furthermore, there are simulation tools available for exposure processes in semiconductor industries [6]. However, such tools work only in the near field within a proximity distance of up to some microns. The level differences in the presented application can be 150 microns and more.

To estimate diffraction effects for the presented case, where arbitrary mask geometries and several different proximity distances, caused by the topology of the underlying structures, determine the patterning result, a special simulation tool has been developed [7].

This simulation tool is now coupled to an evolutionary optimization algorithm in order to derive a suitable mask structure for a given design problem. The idea of using genetic algorithms (GA) for calculating lithographic masks for wet-chemical etching of silicon was described in detail in earlier papers [8, 9, 10].

This paper reports on how this approach was adapted for the high aspect ratio UV-lithography process to alter the geometrical parameters of the mask structures. Figure 4 gives an overview of the algorithm. Inside the main iteration loop an individual, represented by a mask layout, is manipulated in the manner of a DNA string evolving over generations. The simulation tool is used to assess the quality of each layout. Each layout is simulated and the result is compared by an exclusive-or of the resulting intensity plot with a reference bitmap. Depending on the resulting score a layout is either removed from the optimization process or selected for the next generation. Recombination of the selected individuals on the one hand and mutation on the other hand are used to derive new layouts.

In the following section the simulation method will be described in detail. Afterwards the optimization algorithm is described and an example is used to illustrate the functionality of the approach.

### 2 SIMULATION METHOD

The intensity profile on the resist surface is calculated by an adapted Fresnel diffraction analysis. Together with the resist sensitivity on a certain wavelength, it can be used to calculate the absorbed dose using equation 1, whereas $D$ is the deposited dose, $I$ the intensity and $t$ the exposure time.

$$D = I \cdot t$$  \hspace{1cm} (1)

The algorithm used is based on the numerical solution of the Fresnel-Sine $S(w)$ and Fresnel-Cosine $C(w)$ integrals [11]. The energy ($E_p$) for a given point $P$ on the screen, i.e. the resist surface, can be calculated by equation 2, where $A$ is the amplitude of the incoming wave and $w$ states the distance of the point from the edge of the aperture. The intensity ($I$) is then calculated by the square of the absolute value of $E_p$ (eq. 3).

$$E_p = A \cdot [C(w) + iS(w)]$$ \hspace{1cm} (2)

$$I = |E_p|^2$$ \hspace{1cm} (3)

The shape of the aperture, i.e. the masking layer, can be defined as an arbitrary polygon including curves as possible shapes. To reduce the calculation effort a simplification is used: the simulation calculates the intensity function for straight edges only. The intensity for a given point ($I_p$) can then be calculated by equation 4. $I_0$ is the intensity of the incoming wave just in front of the aperture.

$$I_p = \frac{I_0}{2} \left[(0.5 - C(w))^2 + (0.5 - S(w))^2\right]$$ \hspace{1cm} (4)

To generate straight edges from arbitrary polygons the calculation algorithm in a first step subdivides the mask geometry into an even grid of squares. In a second step the number of edges is reduced by merging as many of the single squares as possible to larger rectangular regions. For each edge of such a rectangle the Fresnel integrals are numerically solved and the calculated energies are superimposed to form the resulting intensity plot as depicted in figure 5. If more than one wavelength is dominant during the exposure, the intensities for every relevant wavelength are calculated and superimposed to form the resulting intensity profile.

### 3 OPTIMIZATION OF MASKS

The optimization algorithm was implemented to the software module OMAGA (Optimization of MAasks using Genetic Algorithms), which is forming one part of the TCAD environment for MEMS developed at the TU Braunschweig within the collaborative Research Center (Sonder-
forschungsbereich 516) titled, ‘Design and Fabrication of Active Microsystems’.

Evolutionary algorithms are very well suited to be used in this context, since a large amount of parameters have to be optimized and the optimization problem has to search a multi-dimensional, non-linear design space.

3.1 Assessment of Individuals

The crucial point of any optimization algorithm is the assessment of the quality of a given solution. In this case the grade of a lithographic pattern has to be evaluated. This is done by performing an intensity profile simulation with a defined set of parameters as described in section 2.

3.2 Configuration of the Genetic Algorithm

Each chromosome is formed as a two-dimensional bitmap mask. Based on 2D bitmap descriptions of the mask layouts, OMAGA offers high flexibility and is capable of treating nearly any mask geometry. According to the discrete structure of the underlying simulation the solution is gained at a certain problem resolution. To speed up the optimization a low start resolution can be chosen and the model can be refined after a certain number of generations or after reaching a predefined quality of the mask.

A configurable amount of individuals is used to form the initial population (see fig. 5), which can be regarded as the genetic pool. Such a population represents one generation in the optimization process, whilst the designer specifies the actual number of generations.

Having configured an initial population, further parameters have to be defined to determine the algorithms behavior[10]. The new individuals of the next generation are formed by a recombination of the best genotypes of the parent generation. As recombination method a uniform block crossover was chosen. Stochastically chosen rectangular regions determine the crossover points. Additionally mutation is used to enrich the genetic pool with new information.

Finally the assessment method must be configured. An XOR-comparison is used to determine the score of a certain individual. A 2D Bitmap acts as reference structure and can be configured with an editor.

3.3 Optimization Cycle

For each generation every individual has to be evaluated, which is done by comparison of the intended geometry with the resulting geometry after simulation. The quality of the result is highly dependent on the evaluation criteria. Therefore a weighting system is introduced giving the designer the opportunity to define regions of the mask layout of greater or lesser importance to the resulting structure by specifying appropriate weighting factors.

Depending on the assessment of the current generation particular individuals can be removed from the population (death) or recombined and then mutated for building the next generation. Attention must be paid to the eventuality, that the genetic information of the single individuals of one generation becomes too similar. In this case the optimization process would run the risk of remaining in a local optimum, which might not produce a result of sufficient quality. Is a determined percentage of similarity to the intended structure not yet reached, the optimization tool will use mutation for generating new genetic information, thus generating new individuals and causing the process to search a different area of the available design space. If the desired quality of the results is not reached within the specified number of generations the optimization process stops and a new run or a change in parameters becomes necessary. However, it has to be kept in mind that it might not be possible to generate the intended structure and that therefore a satisfactory solution cannot be found. Depending on the number of individuals and generations, the size of the masks and the specified resolution for the etch simulation the optimization procedure requires a substantial amount of processing time.

4 EXAMPLE

Figure 6 shows an example of a calculated intensity plot in comparison to a fabricated microcoil. Four windings of the upper copper conductor were simulated. The distance between the windings is 40 µm and the width of the copper layer is set to 60 µm. The calculation was done at a single wavelength of 365 nm.

Figure 5: Intensity plot in comparison to an SEM of a fabricated microcoil. The thin grey line marks the position of the 100 µm deep step. The white line is the boundary of the resulting resist structure.

Regions were the calculated intensity is larger than 60 % of the incoming intensity are painted as white areas. This proofed to be very close to the limiting dose where the resist still reacts and will be completely developed. The thin grey line marks the position of the 100 µm deep step as shown in the SEM. The white line qualitatively states the boundary of the resulting resist structure. In comparison to the technological result the simulation shows a high degree of matching: a sharp image on top of the ferromagnetic core and a distorted outline in the lower regions of the microstructure.

To generate compensation structures for the layout depicted above, the optimization algorithm was set up and
started. An initial set of four masks and a grid size of 4 \( \mu m \) were used. Figure 6 shows some of the first 350 iteration steps as an example on how the final structure evolves from simple start geometry over generations into a complex set of compensation structures compensating the diffraction effects. The dotted line of the diagram shows the maximum score reached for the best individual. The black curve states the mean score over all individuals in a generation. The continuous variation of the mean score is an evidence for mutations occurring during the optimization process. Whenever the individuals become too similar, i.e. the mean score gets too close to the maximum score, mutation occurs and the mean score decreases.

![Optimization Project Helix](image)

**Figure 6:** The first 350 iteration cycles show how the mask structure evolves from a simple start geometry to a complex set of compensation structures.

5 SUMMARY AND PERSPECTIVE

A robust optimization tool for lithographic masks was presented. The algorithm, which was formerly used to derive mask structures for wet-chemical etching of silicon, was enhanced to be capable of handling a new simulation method as evaluation criteria for deriving high aspect ratio UV-lithographic masks. An example was used to illustrate the usefulness of the presented approach.

Future work will focus on strategies to speed up convergence by using rule based assumptions for creating initial populations.

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REFERENCES