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## ABSTRACT

In the past decades, the necessity for 3D components became none to be questioned in numerous fields. With these 3D components come new challenges. As an example, the performance of Fabry-Perot based optical filtering devices is dependant on the quality of its sidewalls definition. In this study, we are investigating the mask data preparation method for the patterning of staircase structures thanks to grayscale photolithography. Such structures are used as multiple Fabry-Perot cavities in the context of multispectral imaging. Grayscale photolithography is considered for its offer in 3D micro-fabrication at high throughput. First off, the sidewalls horizontal spread is studied through simulations for different configurations. Metrics are defined and proposed to evaluate the quality of transitions. Secondly, three mask data preparation method are studied : a numerical optimization algorithm as well as an image-to-image deep-learning based workflow are first shown to not meet our application morphological needs. In response, a third method is proposed and is based on local sizings libraries. The recourse to this strategy is shown to have great potential for an improvement of the sidewalls behaviour. However, this methodology taking its first steps, its performance is not pushed to the limit in its current state. As a result, a full mask data preparation flow applied to staircase structures is proposed in the perspectives of this work. With this study we illustrated the importance of the photomask design strategy for the fine tuning of 3D structures sidewalls. We showed the possibility, using a smart mask construction strategy, to produce application-wise enhanced vertical transitions and open the door to further studies toward even steeper sidewalls.

**Keywords:** grayscale lithography, photomask, 3D patterning, optical components, mask data preparation

## 1. INTRODUCTION

For the past decades, the miniaturization of micro and nano-components has been feeding countless studies. The overall goal being to minimize the size of the said components without degrading their performances and, in the end, enhance the performance of the whole device by "cramming more components" within the same surface.[1] Now, what happens of this philosophy for 3D structures such as optical components ? One might say that often, even if the goals and challenges are different, the idea remains the same : for equivalent performances, the smaller the surface covering for an unitary component the better. On another hand, the variety of shapes for 3D components comes with numerous patterning challenges, making them harder to miniaturize. For this study, we are interested in an application for multispectral imaging.

Nowadays, multispectral imaging is a growing field renowned for its interest for many imaging and detection applications.[2,3] The goal is to produce a simultaneous and precise filtering of a high number of different wavelengths to reconstruct with the highest fidelity the spectrum of an incident light. If various multispectral filtering strategies exists, we are here considering the recourse to Fabry-Perot (FP) interferential filters. FP filters are an efficient alternative for multispectral imaging, defining filtered wavelengths depending on the cavities heights, as shown on Fig.1.

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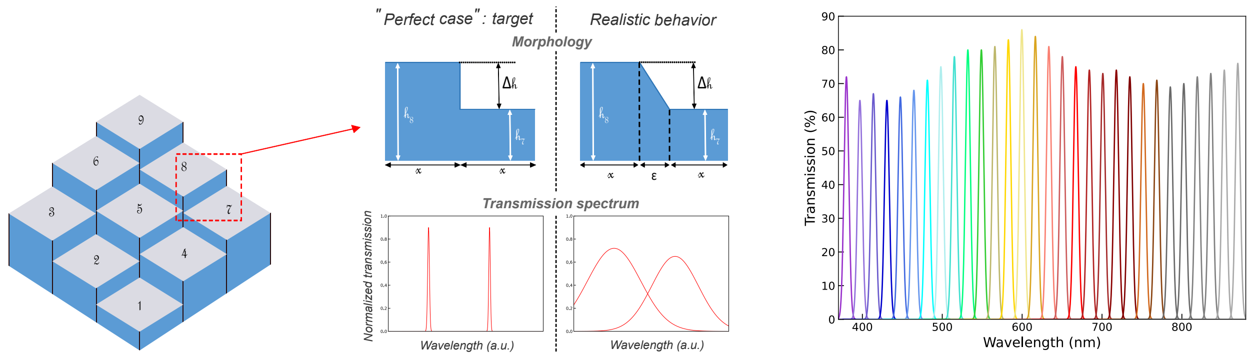



(a) (b)

Figure 1: Patterning challenge of the resort to Fabry-Perot cavities for multispectral imaging. (a) is a representation of the desired 3D structure and shows the challenge on the sidewalls of cavities : a smooth transition from a cavity to its neighbor would result in the deterioration of the performance. (b) is an exemple of the concept of a multispectral filter for 30 filtered wavelengths.

However, the patterning of such a structure also entails challenges : indeed, to perform a precise filtering, the height of the cavities must be precisely controlled and with a low variability, i.e. a high vertical resolution and low surface rugosity are mandatory. Moreover, the patterning of steep transition from one cavity to its neighbor (high spacial frequency) is a challenge to perform the structuration at small scales and with an industrial throughput.

If multiple patterning methods are able to fabricate such structures with high quality, the whole difficulty is to perform the fabrication at a high volume. A promising contestant for this purpose is Grayscale PhotoLithography (GPL). Indeed, GPL reuses classical lithography tools to perform 3D patterning with a high throughput. This method relies on the combinaison of two entities : on one hand, a low contrast photoresist is used, allowing different remaining resist heights post-development for different exposure doses. On another hand, the recourse to non-resolved binary photomasks allows a local control of the light transmission of the mask, without printing the chromium patterns within the resist.[4,5] As discussed in previous studies, since the chromium patterns are not replicated, any geometry can be used as the sub-resolution feature.[6] The recourse to non-resolved binary masks therefore offers a high degree of freedom, but also implies drawbacks, one of them being the lateral resolution. Indeed, due to optical phenomenons, the lateral resolution of the process will be limited by the optical influence radius.

The goal of this study is to investigate and propose a mask data preparation (MDP) method able to enhance the behavior of the sidewalls of GPL-patterned staircase-like structures. In other words, knowing the limitations of our process, we are looking for the mask strategy able to offer the steeper sidewalls possible for stairs structures. This study will be separated in two parts. First, an usecase will be presented and the sidewalls will be evaluated in different configurations. Serving this purpose, dedicated metrics will be proposed. The goal is then to gain a better understanding of the mechanisms at stake, as well as isolating the best configuration. Then, multiple MDP methods will be proposed, used and their performances compared to determine the best candidate. The final objective being to identify and propose the MDP method offering the best performance.

## 2. TRANSITION SPREAD STUDY & METRICS DEFINITION

For simplification purpose, the usecase we will be considering is a simple two heights case presented on Fig.2 : a first chromium density, region A, is circled by a second, region B. When simulating the resist profile obtained via the recourse to such a mask, we obtain a unitary cavity. Simulations were obtained following the methodology presented in.[7]

To begin with this usecase, the impact of the height difference between regions A and B on the transition is studied. Serving this purpose, the density of region A was fixed and we are varying the density of region B. The results for three configurations are visible on Fig.3.

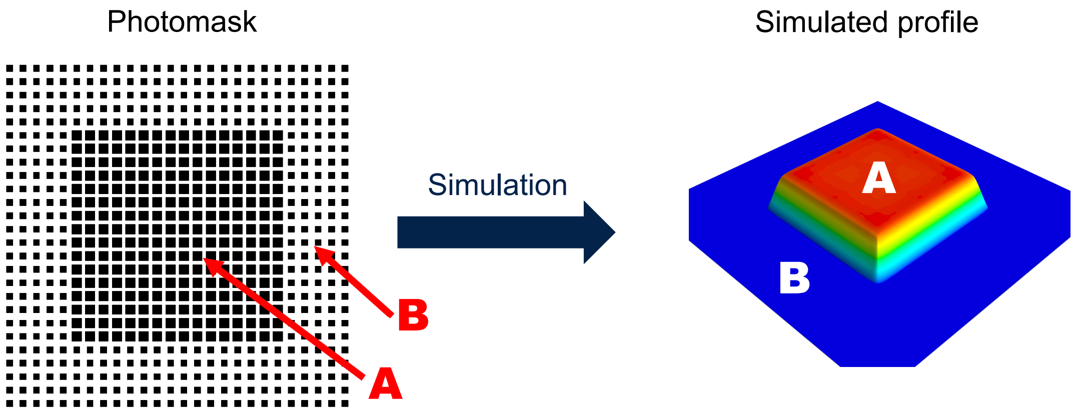



Figure 2: Morphological usecase for this study : representation of the used mask (left) and corresponding simulated profile (right)

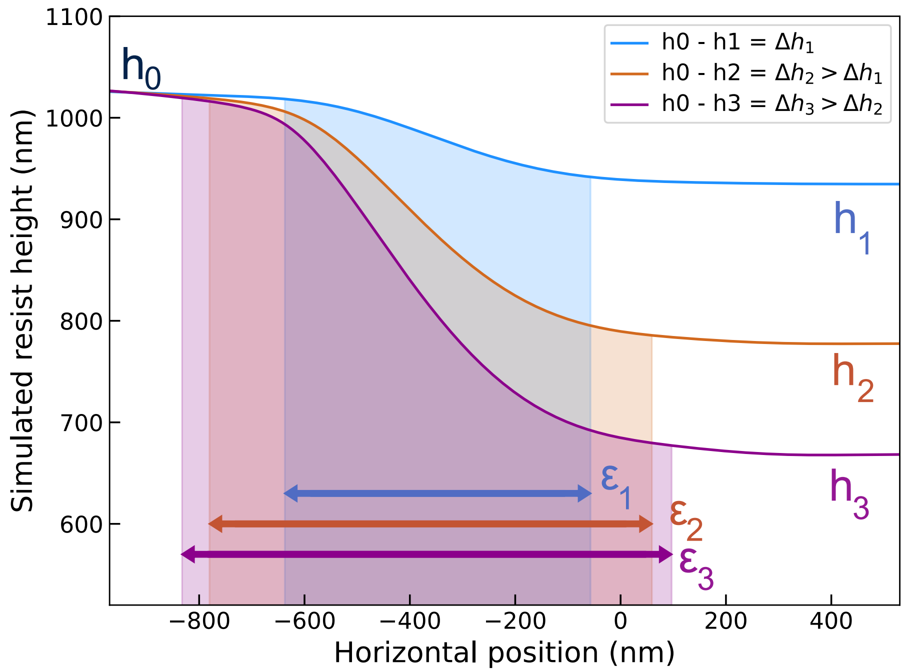
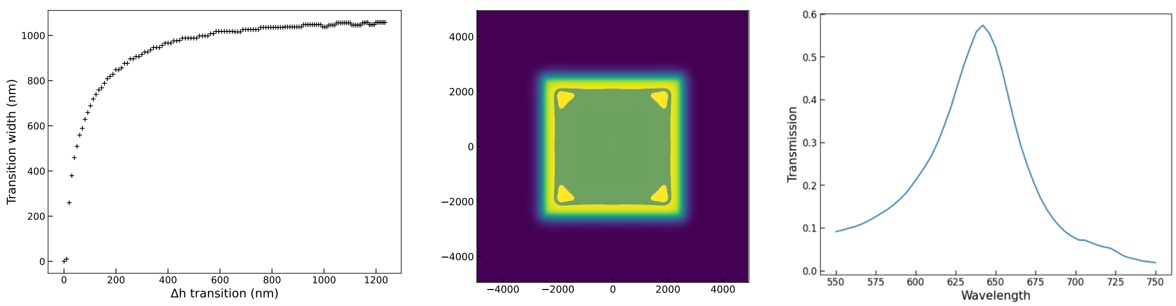



Figure 3: Impact of the vertical amplitude of a transition on its horizontal spread

We easily notice that the bigger the transition is on the vertical axis, the wider it will spread horizontally. However, we now need to define metrics to efficiently evaluate the quality of a sidewall. Following this objectives, three metrics are proposed :

- The first one, pretty straightforward, is the transition horizontal width, noted $\epsilon$. It is determined simply by a thresholding strategy and provides a visual interpretation of the transition in one direction. The chosen threshold is of 5 nm to be compliant with the previous studies.[6] Indeed, this value is a pertinent reference to observe a shift in the wavelength filtered by a cavity when its height doesn't perfectly meet the target. Typically, an error of 5 nm on a cavity height would produce a 15 nm shift on the filtered wavelength in our configuration (Ag mirrors of 26 nm each, insulator of refractive index 1.653 and thickness 143 nm for a wavelength of 650 nm). The value of this metric for different height difference between region A and B is shown on Fig.4a. As expected, we see an increasing of $\epsilon$ as the vertical transition gets bigger. If this metric already gives precious informations, it has the weakness to be limited to one direction. Therefore, it is not sufficient alone.

- To palliate the weakness of $\epsilon$ being a one dimension metric, we defined a two dimensions metric, called the useful surface, $\Omega$. It corresponds to the part of region A that is close enough to the targeted height. This surface, also determined by thresholding, helps in understanding the impact and particuliar behaviour around the corners. As shown on Fig.4b, the corners response differentiates from the rest of the structure.
- Finally, both previous metrics are geometrical and determined via a thresholding strategy. Because this method is pretty abrupt and weakly represents the real behaviour of a component, the recourse to a physics-based third metric is pertinent. Serving this purpose, the use of optical simulations of the unitary Fabry-Perot cavities is in development. More specifically, the filter transmission and its FWHM (full width at half maximum) are relevant to quantify the quality of the cavity. The example of a transmission spectrum is displayed on Fig.4c.




(a) (b) (c)

Figure 4: Proposed metrics to evaluate the quality of simulated profiles : (a) Transition width for different vertical amplitudes. (b) Top view of a simulated profile. The useful surface is represented in darker green : the spot on corners being excluded for the useful surface highlight their particular behaviour. (c) Example of a simulated transmission filter.

With this metrics, we can efficiently evaluate the quality of a transition between two stairs. It was already shown that an intelligent component design is a first step in minimizing the latter, however, further work on the MDP is also worth considering. Indeed, if it is possible to minimize the vertical amplitude of the transition for multispectral filters, some other applications might require the opposite scheme, i.e. large vertical transitions with steep sidewalls.

In the following, different MDP methods will be proposed and investigated. The performance of each method can be described by the aforementioned metrics and the final objective is to identify and propose the strategy offering the best handling of the transitions between two stairs.

## 3. PHOTOMASK DATA PREPARATION SOLUTIONS

When performing the MDP for GPL, several methods are currently available. Here, three of these methods will be used and compared, with the same objective in mind, represented on Fig.5. The goal can be summed up as follows :

1. When using the basic strategy, each chromium densities will be put next to each other without further considerations, ending in a rectangular density profile.
2. Due to the filtering component of the optical system, the aerial image obtained for this strategy will present rounded edges and a smoother transition.

3. Therefore, the resulting resist profile will display the same behaviour.

4. The idea behind a smarter MDP is to perform an inverse problem resolution, represented by yellow arrows on Fig.5, to obtain the steepest possible profile.

5. To meet this goal, the incident aerial image should be straightened.

6. The goal then becomes finding the density profile offering this straightened aerial image. It is relevant to note that obtaining a perfectly steep resist sidewall using GPL will also be hindered by the intrinsic photoresist response.

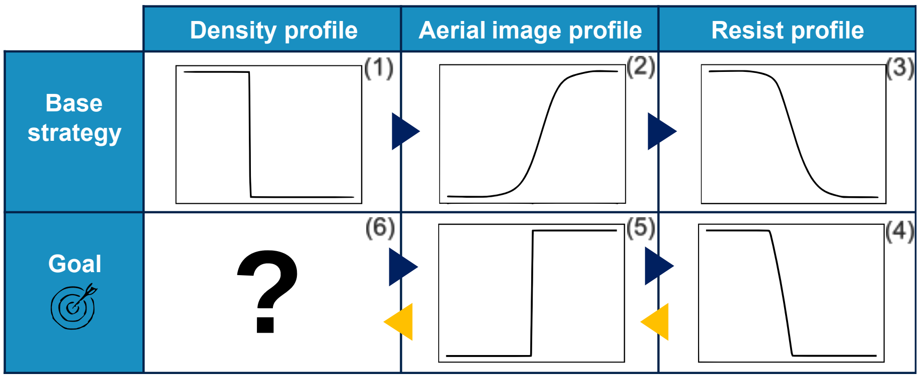



Figure 5: Goal of the MDP : finding the right density profile for a straightening of the aerial image toward steeper resist profiles

In an attempt to answer the problematic of this study, three MDP methods were investigated and will be presented in the following. Each method aimed at a same target, where region A is a stair of height 1174 nm and region B stands at 640 nm height. For every strategy, different strengths and flaws are highlighted. As for the aerial image simulation, we are using the parameters of our illumination : $\lambda = 365$ nm, NA $= 0.57$ and $\sigma = 0.7$.

### 3.1 Rigorous physics-based mask data preparation

Currently, a reference in rigorous MDP applied to grayscale photolithography is the work of Chevalier & al.[7] The principle of the method used here is an iterative, physics-based, mask optimization. A simplified version of this method can be described as follows :

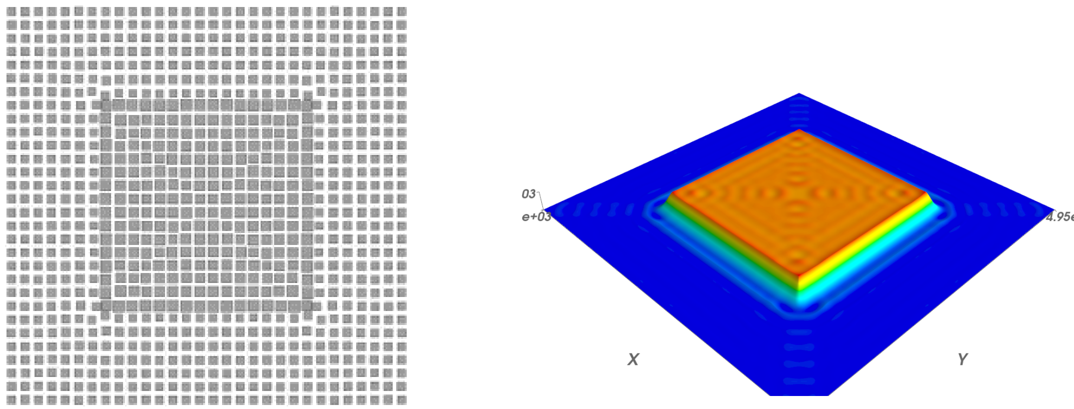
1. A first mask is generated and used for the simulation of a resist profile

2. The obtained resist profile is compared to a target, the difference is then injected into an optimizer that will modify the initial mask (chromium dots position and size), with respect to the Mask Rule Check (MRC).

3. The new mask will be used to produce a new simulation, and the new resist profile will be compared to the target.

4. Step (2-3) will be repeated until the obtained simulated profile is close enough to the target or when the maximum number of iterations has been reached.

This method has been developed and challenged for the realization of microlenses and produces MRC-friendly outputs as shown on Fig.6a. However, Fig.6b shows its limitations regarding our usecase : the produced surface displays important waviness (tens of nanometers), major bumps and holes are present at the border of the transition and the profile seems particularly deteriorated on the diagonals, most likely by the recourse to symmetries.




(a) (b)

Figure 6: Outputs of the physics-based optimization (a) is the generated photomask. (b) is the corresponding simulated resist profile.

If suppressing the symmetries might partly ameliorate the results, it goes against another major difficulty: the runtime of this method, even if depending on many parameters and improvable, is not optimized and therefore is massive due to the optimization of every chromium features and the recourse to physical simulations.

Ultimately, both the morphological results and the required runtime are positioning themselves against the recourse to this method for our usecase. To try to palliate these drawbacks, the resort to AI-based MDP has been investigated.

### 3.2 AI-based mask data preparation

When considering complex problems and aiming at shorter runtimes, a natural contestant is artificial intelligence (AI). An AI-based MDP strategy is in development by Moreau & al.[8] The goal is to resort to a deep-learning workflow to design non-intuitive binary photomasks for given GPL resist targets. Once a model is trained, the numerical cost to generate the photomask for a 3D target is negligible regarding the physics-based optimization.

However, as mentioned earlier this method is still in its early phase of development and needs improvements on multiple levels. Firstly, the generated masks are not compliant with MRC limitations as displayed on Fig.7a.

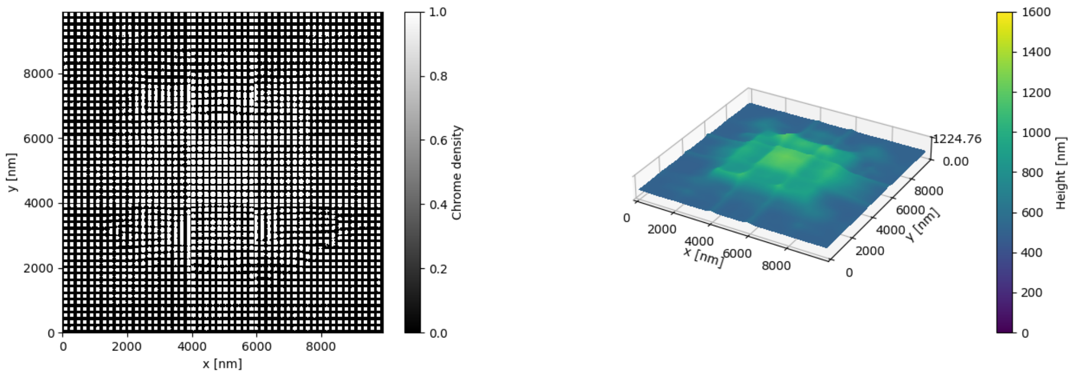
Moreover, the current performance of this strategy does not meet our needs, as visible on Fig.7b. This can be partly explained by two facts :

- First, flat surfaces is a particuliar geometry on which the current model has not been extensively trained, resulting in difficulties to handle it.
- Then, for large objects a stitching of multiple masks is necessary. This transformation is yet also at early stages of development and therefore lacks maturity.

In the end, both of the advanced MDP methods we investigated aren't suited for our usecase in their current state. The development of a new strategy consequently becomes justified. In an attempt to attain the goal presented on Fig.5, a strategy based on the sizing of the chromium features defining the sidewalls has been studied.

### 3.3 Sizings-based mask data preparation

As previously presented, the horizontal spread of the transition between two stairs mainly originates from the transformation of the illuminated mask to the aerial image in which high spatial frequencies are lost. To prevent this, the idea of a sizing of the chromium features defining the transition is introduced, inspired from previous




(a) (b)

Figure 7: Outputs of the AI-based method. (a) is the generated photomask. (b) is the corresponding simulated resist profile.

studies.[9] This straightforward method presents the advantages of necessiting no long runtime and is adapted to produce manufacturable masks.

The application of this strategy is presented on Fig.8 : sizings are applied on the chromium features at both sides of the transition between two stairs. On the side of the bigger density (the higher stair), the chromium features will be magnified. On the other side, defining the ”lower” stair, they are shrinked. For the rest of the study, the non-resolved features employed will be chromium dots for more similarity with the physics based method for comparison purpose. However, as discussed in previous studies,[6] the resort to non-resolved lines could be made, providing similar results.

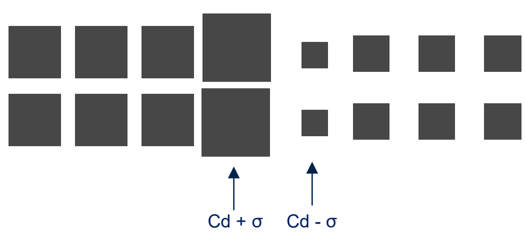
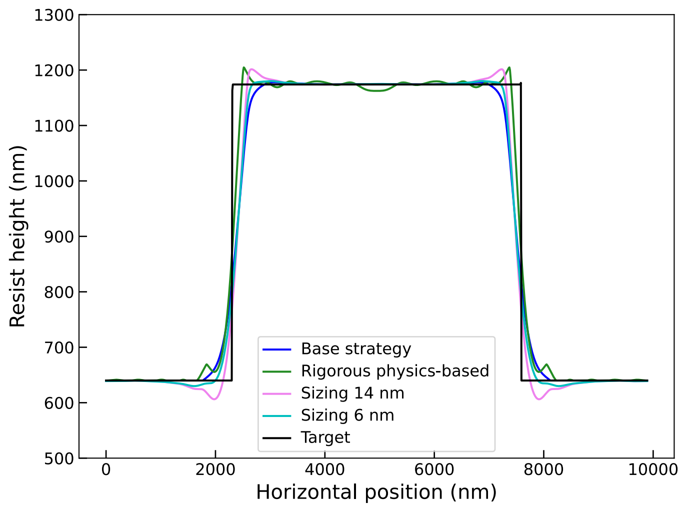



Figure 8: Sizing strategy on the chromium features bordering the transition. $\sigma$ is the sizing value applied.

The results for the different strategies are shown on Fig.9, as well as the geometrical metrics values for each case. Numerous observations are possible :

- First, for the base strategy (for which A and B are next to each other with no further considerations), we see a transition width estimated at almost 1 µm as well as a lost of almost 40% of the useful surface.
- For the physics-based method, the waviness at the surface of the profile prevents the calculation of the transition width, as for the useful surface, 45% is lost. This confirms that this alternative is not performant for our usecase in its current state.
- The results for the three sizings presented are rich in informations. For small sizings (i.e. 2 nm), we notice a slight improvement both on the transition width and the useful surface. A large sizing (i.e. 14 nm) in another hand is producing bumps at the top of stairs and trenches at the foot, from which both metrics are suffering. For a medium sizing (i.e. 6 nm), the transition width is much reduced, by more than a third of its original size, which is really promising. However, at the same time, the useful surface is adopting an opposed behaviour and decreases. With further investigations, this result was explained by

the transformation of the corners of the stair : when adding a medium sizing on the chromium features, the transition is reducing on the sides of the stairs. On the corners however, bumps and holes are appearing similarly as what is observed for large sizings.




| | ε (nm) | Ω (%) |
|---|---|---|
| Target | 0 | 100 |
| Base strategy | 979 | 62,3 |
| Rigorous physics-based | NA | 55,0 |
| Sizing 2 nm | 870 | 64,3 |
| Sizing 6 nm | 613 | 57,5 |
| Sizing 14 nm | 1917 | 45,2 |

Figure 9: Cutlines of the simulated profiles obtained for different mask data preparation strategies. The values of $\epsilon$ (transition width) and $\Omega$ (useful surface) for each strategy are provided in the table. The profile for the sizing strategy with a value of 2 nm is not displayed for more visibility as it almost blends with the base strategy.

Ultimately, no method has been shown to propose satisfying result. The performances for each investigated solutions are presented on Tab.1. Nevertheless, the test with sizings showed the potential for smart mask considerations to alterate and enhance the profiles. Following this proof of concept, multiple strategies might be studied and/or combined :

- First, we opted for sizings to straighten the aerial image. We could also think of other/complementary solutions such as : changing the position of the chromium features around the border or inserting holes in the features to lower the density for the small stair.
- If the previous strategies as well as the sizings are very straightforward, they are not optimized. For a sturdier implementation into the MDP, there are several optimization options. A modelisation of the transformations impact on the transition is a first alternative. Similarly, the recourse to libraries might be conceivable. In both case, a massive simulation work must be carried out beforehand.
- Finally, a more mature methodology would aim toward an automatized combination of multiple strategies. As an example, for our usecase, a simplified flow could take this path : (1) The initial size of each chromium features is determined by the base strategy. (2) The sizing-based method or equivalent is applied only to the chromium features bordering the transition. The right transformation being determined via the recourse to either models or libraries. (3) The chromium features defining the corners are optimized thanks to a physics-based rigorous optimizer. Limiting the optimization to the features defining the corners would result in a viable runtime and no deterioration of the rest of the profile.

## 4. CONCLUSIONS AND PERSPECTIVES

The current growth of interest for variety, performance and miniaturization of 3D micro-structures is highly demanding in patterning strategies able to produce the desired morphologies. An exemple of these challenges is the obtention of steep sidewalls within 3D structures.

Table 1: Summary of every mask data preparation strategies performance for the staircase morphology with steep sidewalls

| | Morphological performance | Runtime | Maskshop friendly | Potential |
|---|---|---|---|---|
| Base strategy | - | ++ | ++ | - |
| Physics-based optimizer | - - | - - | ++ | + |
| AI-based method | - - | ++ | - - | ++ |
| Sizings | + | ++ | ++ | ++ |

In this study, we used the fabrication of Fabry-Perot cavities for multispectral imaging as a vehicle, highlighting the need for steep sidewalls. However, this problematic might be applied to various other applications. The patterning method investigated is grayscale photolithography. More precisely, the aim is to determine a mask design strategy offering the desired behaviour. With this goal in mind, different configurations were first investigated and used to :

- Characterize a structural behaviour and determine a best-case configurations
- Define metrics dedicated to the quality of a sidewall and an overall structure

Using the defined metrics, a single usecase has been used to evaluate the performance of different MDP strategies, compared to a basic strategy with no considerations for the sidewalls behaviour. On a first hand, two existing advanced methodologies were confronted to our usecase : a rigorous physics-based optimization and an AI-based flow. The physics-based strategy inability to produce a satisfying result both in morphology and runtime is shown. As for the AI-based strategy, if the runtime is satisfying, the morphological performance is currently far from the goal. As a response, a sizings-based strategy is proposed and shown to have potential for an improvement on the metrics used. This method consists of a sizing of the chromium features bordering the transition with the aim to straighten the aerial image. However, if it has a clear potential, it is not a mature alternative and needs further studies. Furthermore, in the future, the recourse to a physics-based metric such as optical transmission would be pertinent and is currently in development.

While the MDP propositions investigated in this work are not fully-satisfying our needs, they are numerous perspectives for the following of the studies. Firstly, the creation of an automated flow mixing the strengths and flaws of various MPD strategies has great potential to answer the application specifications. In such a process, the sizings-based strategy or equivalent might be used to handle the transition at the sides of stairs. The value of the sizings could be chosen thanks to the resort to previously established libraries. The handling of the corners, being a harder task, could be managed by an adapted physics-based optimizer. On another hand, further development of the AI model is also promising. Providing the results of every strategy as a part of the training dataset is also worth considering. Finally, the more natural way of reducing the transition horizontal size between two stairs patterned using GPL would be to use a smaller illumination wavelength. This would also require an adapted low contrast photoresist and lithographic process.

## ACKNOWLEDGMENTS

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