Robustness Analysis of Metasurfaces: Perfect Structures Are Not Always the Best

Hsiang-Chu Wang, Karim Achouri, and Olivier J. F. Martin*

Cite This: ACS Photonics 2022, 9, 2438−2447

ABSTRACT: Optical metasurfaces rely on subwavelength scale nanostructures, which puts significant constraints on nanofabrication accuracies. These constraints are becoming increasingly important, as metasurfaces are maturing toward real applications that require the fabrication of very large area samples. Here, we focus on beam steering gradient metasurfaces and show that perfect nanofabrication does not necessarily equate with best performances: metasurfaces with missing elements can actually be more efficient than intact metasurfaces. Both plasmonic metasurfaces in reflection and dielectric metasurfaces in transmission are investigated. These findings are substantiated by experiments on purposely misfabricated metasurfaces and full-wave calculations. A very efficient quasi-analytical model is also introduced for the design and simulations of metasurfaces; it agrees very well with full-wave calculations. Our findings indicate that the substrate properties play a key role in the robustness of a metasurface and the smoothness of the approximated phase gradient controls the device efficiency.

KEYWORDS: metasurfaces, beam steering, imperfection, plasmonics, dielectric, efficiency

INTRODUCTION

Already at the turn of the 21st century, it was recognized that metallic nanostructures organized on a surface could mold the flow of light by manipulating its phase.1 A few years later, this field of research developed vividly into that of optical metasurfaces: first at microwave and radio frequencies,2−4 later in the infrared,5−11 and finally, in the visible part of the optical spectrum.12−16 This spectral evolution was made possible by tremendous progress in nanofabrication since the dimensions of the structures building the device, the so-called meta-atoms, must be smaller than the operation wavelength to produce a homogeneous response.17,18

Significant efforts have been devoted to the development of precise nanofabrication techniques for metasurfaces.19−21 In most cases, the meta-atoms are defined using electron-beam (E-beam) lithography,22−30 sometimes ultraviolet photolithography is used,31−34 or they are directly carved using focused ion beams.35−37 Meta-atoms are fabricated in either dielectrics16,38,39 or plasmonic metals.40,41 The latter has an especially important interaction with light, due to the excitation of free electron resonances.32 After the exposure step, the meta-atoms are created either by lift-off or by etching.33 Irrespective of the approach, nanofabrication is definitely a rather challenging activity, often with a relatively low yield. Over an entire wafer, it is difficult to fabricate structures that are as perfect as the original design. The size of the meta-atoms can vary with the lithography dose; some nanostructures may be deformed during the lithography by proximity effects associated with neighboring nanostructures.44 The adhesion of some meta-atoms can be poor, such that they disappear during the process; this is especially the case for metal nanostructures on dielectric substrates.45−47 The metal evaporation can produce nanostructures with slanted sides as the photoresist is clogged up during deposition.48

Received: April 13, 2022
Published: June 28, 2022
The aim of this paper is to study the influence of such inaccuracies in nanofabrication on the overall response of metasurfaces, especially the tolerance of nanofabrication that is acceptable without impairing the optical response excessively. Both a quasi-analytical model and full-wave electromagnetic simulations are used to determine the influence of such fabrication missteps. In addition, purposely misfabricated samples are studied experimentally to gain insights into the mechanisms that control the performance of metasurfaces. Although the present study focuses on beam steering gradient plasmonic metasurfaces using gap plasmon meta-atoms,49−51 the findings reported therein can also be applied to other metasurface designs and materials,52−54 since the nanofabrication techniques are very similar.

## RESULTS AND DISCUSSION

The metasurface considered here is based on gold nanostructures of varying dimensions deposited above a gold mirror using a SiO$_2$ spacer (Figure 1). This reflecting substrate provides an additional phase to the scattered light, such that a full $2\pi$ phase range can be engineered for the metasurface response.55 The metasurface is fabricated using E-beam lithography and ion beam etching, as described in the Methods section. In spite of a careful nanofabrication procedure, including dose tests for the electron-beam lithography and optimized etching time, it is almost impossible to avoid imperfections in the fabricated metasurface, especially over the relatively large area (typically tens of $\mu$m$^2$) required to implement a meaningful optical function. Misfabrication leads to defects such as missing elements (Figure 1a,b), displaced elements (Figure 1a,c), or bloated elements (Figure 1d,e). The aim of this paper is to study theoretically and experimentally the influence of such defective elements on the overall metasurface response.

The metasurface unit cell is illustrated in Figure 2: $h = 30$-nm-thick Au nanostructures (meta-atoms) with a width $w = 140$ nm and different lengths $L$ are deposited atop a gold mirror (thickness $150$ nm, such that the mirror can be considered as semi-infinite) with a $t = 40$ nm SiO$_2$ spacer (Figure 2a). The system builds unit cells with dimensions $P_x = 180$ nm and $P_y = 430$ nm in x- and y-directions, respectively.

Changing the nanostructure length $L$ controls the phase of the reflected light for illumination with y-polarized light, as shown in Figure 2b for the operation wavelength $\lambda = 980$ nm. These data were obtained using full-wave simulations, as described in the Methods section. Varying the nanostructure length $L$ between 0 and 400 nm changes the phase of the reflected light over a $2\pi$ range while maintaining the amplitude of the reflection coefficient relatively constant around unity, except for $L = 150$ nm, where the excitation of a localized resonance increases absorption and reduces reflectance. To analyze missing meta-atoms, we replace the missing element with a bare substrate, i.e., with its corresponding amplitude (0.99) and phase ($10^\circ$) of the reflection coefficient, computed at the same height as the other elements.

The deflection angle $\theta$ for a beam steering device under normal incidence illumination is defined as $\theta = \sin^{-1}(\lambda/L)$, where $\lambda$ is the working wavelength and $L$ is the superlattice period, which is $L = nP_x$, where $n$ represents the number of discretized elements used for the metasurface, which is eight in this work. Two different designs can achieve the same beam steering functionality: an eight-level design, which maximizes the phase discretization levels and has a smoother phase gradient (Figure 2c), or a four-level design, with a coarser phase discretization (Figure 2d). Both designs have been reported in the literature. According to our simulations, the phase of the reflected light over a $2\pi$ range while maintaining the amplitude of the reflection coefficient relatively constant around unity, except for $L = 150$ nm, where the excitation of a localized resonance increases absorption and reduces reflectance. To analyze missing meta-atoms, we replace the missing element with a bare substrate, i.e., with its corresponding amplitude (0.99) and phase ($10^\circ$) of the reflection coefficient, computed at the same height as the other elements.

A simple quasi-analytical model is derived in the Methods section to compute the momentum provided by the metasurface upon reflection. Based on Fourier transforms, this model is extremely efficient for computing the metasurface response and can be used to evaluate its performance. In short, the superlattice period is replaced by a collection of discrete points, each representing one meta-atom by its reflection amplitude and phase, as illustrated at the bottom of Figure 2c,d. These amplitude and phase values were obtained from full-wave simulations, as described in the Methods section. With this approach, it is also very simple to compute the response of a metasurface with one or several missing meta-atoms, which are then replaced by the amplitude and phase of the substrate reflection.

Let us first use this model to study in Figure 3 the performance of eight-level metasurfaces with different missing elements. We label the intact structure as Sample #0 and a metasurface where the meta-atom m is missing as Sample #m. For a perfect eight-level device, the efficiency is 0.66, meaning that 66% of the incoming energy is redirected into the diffraction order at an angle $\theta$ (see Sample #0 in Figure 3a). The remaining energy is absorbed in and scattered by the device. When one element is missing, light is still redirected into the direction $\theta$, but part of the energy is also specularly reflected and absorbed, making the device less efficient (see for example Sample #5 in Figure 3a), which has only an efficiency of 37%. Surprisingly, each meta-atom does not have the same influence on the performance, as summarized in Figure 3c: counterintuitively, it is not when the largest elements #7 and #8 are removed that the efficiency deteriorates most but rather missing elements around #5 appear especially detrimental to the metasurface performance. On the other hand, when the first meta-atom is missing (Sample #1), the performance is the same as the complete structure (Sample #0), because both the substrate and the first meta-atom ($L = 20$ nm) produce the...
same amplitude and phase for the reflected field (see Figure 2b).

The special role of element #5 is also observed for a four-level device, as indicated in Figure 3c. Those devices have somewhat lower performance than the eight-level devices, with an efficiency of only 56% for the perfect metasurface due to the coarser phase gradient. However, the decrease in performance caused by element #5 missing is similar for eight- and four-level devices. On the other hand, the scattering direction \( \theta \) is maintained for both devices, even when a meta-atom is missing.

Figure 3c also provides the efficiency for the defective devices computed with full-wave simulations (see the Methods section). The agreement between those simulations and the model is very good and we also recover with full-wave simulations the strong influence of element #5. The small differences between the full-wave simulations and the model stem from the fact that the latter does not include the near-field interactions between neighboring elements. The efficiency computed with full-wave simulations for the four-level device is quite surprising: sample #8, with a missing element, has a higher efficiency (56%) than the perfect one (52%), and only sample #5 drops noticeably in performance (31%) (see the purple diamonds in Figure 3c). To gain insights into the underlying mechanisms, Figure 3b shows the amplitude of the total electric field for Samples #1 (left part) and #5 (right part). Surprisingly, it is very difficult to distinguish in the electric field distribution any difference between both devices.

To investigate this further, we have fabricated samples for both eight-level (Figure 4a) and four-level devices (Figure 4b). Purposely misfabricated samples with missing specific elements were realized, as described in the Methods section and in the Supporting Information (Figure S1). The left parts of Figure 4a,b illustrate the large area samples that were produced; this was also the case for the misfabricated metasurfaces, of which only excerpts are shown in the right parts. Complete misfabricated metasurfaces are shown in the Supporting Information, Figure S2 for eight-level devices and in the Supporting Information, Figure S3 for four-level devices. The optical response of these different metasurfaces was measured using an optical microscope as detailed in the Methods section and in the Supporting Information, Figure S4. Figure 4c shows the measured intensity profiles for both devices (purple lines for the four-level devices and green lines for the eight-level devices). For each device, the efficiency is computed as the power integrated over the entire deflected beam with its center at the angle \( \theta \approx 43^\circ \), divided by the measured power reflected by a mirror that replaces the sample. The corresponding values

![Figure 2](https://pubs.acs.org/doi/10.1021/acsphto22000563)

Figure 2. (a) Schematic of the metallic meta-atom and (b) corresponding amplitude and phase of the reflection coefficient as a function of the length \( L \) of the gold nanorod at \( \lambda = 980 \text{ nm} \). Two common configurations to achieve beam steering with a phase gradient metasurface covering a full \( 2\pi \) range for the phase modulation with an (c) eight-level unit cell with meta-atoms of lengths \( L = 20, 120, 135, 143, 150, 160, 175, \) and 345 nm and a (d) four-level unit cell with meta-atoms of lengths \( L = 20, 135, 150, \) and 175 nm (each element being repeated). The discrete elements used for the corresponding simplified model are shown beneath panels (c, d).
are reported in Figure 4d, where the error bars correspond to a series of measurements with different measurement areas, as described in the Methods section and in the Supporting Information, Figure S4. According to the experimental results, for the eight-level device (green squares), as expected, Sample #1 has almost the same performance as the perfect sample (sample #0). Surprisingly, Samples #2 and #3 have higher performance than the perfect one, while the others follow a similar trend as the semianalytical model and the full-wave simulations with Sample #5 exhibiting the lowest performance. For the four-level devices (purple squares in Figure 4d), as expected from the calculations, sample #8 has an outstanding performance, while Samples #3 and #4 perform also better than the perfect one (Sample #0). In addition to Sample #5, Sample #7 also has the lowest efficiency.

Next, we elucidate why the fifth element has such a significant influence on the metasurface performance: when it is missing and replaced by a highly reflective substrate, the device efficiency decreases most. After investigating different parameters, we came to the conclusion that this behavior is related to the phase provided by the substrate upon reflection. In Figure 5a, we take the same configuration of an eight-level device as in Figure 2c, but this time we keep the reflection amplitude of each meta-atom as unity while keeping the phase gradient very smooth. Since in a four-level metasurface, both meta-atoms #3 and #4 produce the same phase, one could think that having either of them missing would deteriorate the performance of the eight-level device more than their four-level counterparts. Even for the ideal case used in the simplified model, where each element reflects a phase equal to 1, the performance is only 83% due to the coarser phase gradient (it reaches 97% for the eight-level devices, Figure 5). The surprising fact that a metasurface with missing elements can perform as well or even better than a complete metasurface is easily understood by the fact that it approximates the phase gradient better. For example, if we consider the phase substrate \( \phi_{\text{sub}} = 0 \) and remove the meta-atom #4, which provides the best performance in the Supporting Information, Figure S5a, the corresponding phase distribution, shown in the Supporting Information, Figure S5b, is very smooth. Since in a four-level metasurface, both meta-atoms #3 and #4 produce the same phase, one could think that having either of them missing would deteriorate the performance in a similar fashion. Supporting Information, Figure S5c indicates that this is not the case and, from the previous discussion, we have learned that the origin is the worse phase discretization when #3 is replaced by the substrate. Note that one could make good use of these observations to optimize device performances.

Let us now resort to full-wave simulations to study other imperfections such as displaced or bloated nanostructures. In Figure 6, the performance of the eight-level device is not significantly affected by the displacement of a single
nanostructure in $x$, $y$, or $xy$-directions. Maximum possible
displacements are $\delta x = 35$ nm and $\delta y = 30$ nm (for larger $\delta y$, the largest meta-atom would overflow the unit cell). Since the spacing along $x$-direction between two adjacent nanorods is only 40 nm in the original design, a $\delta x = 35$ nm displacement for one nanostructure leaves only 5 nm between neighboring nanostructures. Surprisingly, those displacements barely influence the overall device performance. This observation holds for displacements along both directions, as well as in the diagonal. Overall, the exact nanostructure alignment is not required for the device performance; it does not influence the steering angle $\theta$ either.

We also study in Figure 7 the influence of the meta-atoms size on the metasurface performance for an eight-level device. Structures that are larger or smaller than the original design are usually the result of an over- or under-exposed lithographic process and all structures will be affected in a similar way. Hence, we consider here that all of the eight structures that build the metasurface superlattice are modified in a similar amount in either $x$, $y$, or $xy$-directions. Both a positive (enlarged nanostructures) and a negative (shrunk nanostructures) variation $\Delta$ is considered. We observe in Figure 7 that size variations in $x$-direction do not influence much the device performance, since the light of interest is polarized in the $y$-direction. On the other hand, over- or under-sized nanostructures in the $y$-direction deteriorate the device performance since a change in the nanostructure length $L$ modifies the amplitude and phase of the reflected light (Figure 2b). This effect is however quite marginal for variations between $\Delta y = -10$ nm and $\Delta y = 5$ nm, leading to a maximal efficiency reduction of only 5%. For larger variations, the performance begins to be affected significantly, for example, for $\Delta y = 20$ nm, the efficiency drops to half that of the perfect one, although the steering angle $\theta$ is not affected by all of these changes.

Let us now briefly investigate another type of device: dielectric metasurfaces that operate in transmission. The meta-atoms are TiO$_2$ cylinders with a fixed height $H = 600$ nm and varying diameters $D$ (Figure 8a). Changing $D$ tunes the phase shift of the transmitted light over $2\pi$ while keeping the transmission amplitude constant (Figure 8b). Similar to the metallic metasurface, we investigate both eight-level and four-level devices (Figure 8c,d) and study with full-wave calculations the response of imperfect metasurfaces with a missing element $m$. The efficiency as a function of the sample number is summarized in Figure 8e. For the eight-level dielectric devices, sample #8 has about the same performance (79%) as sample #0 (the complete device). For sample #2, the efficiency drops to only 63%. Surprisingly, sample #8 for the

Figure 4. Experimental results for eight-level and four-level devices. Fabricated samples (a) for the eight-level devices and (b) for the four-level devices. The images on the left show part of the perfect Sample #0 (scale bars: 1 $\mu$m), while the images on the right show excerpts taken out of the misfabricated samples (the complete misfabricated samples are shown in the Supporting Information, Figures S2 and S3). (c) Intensity profiles were measured in the Fourier plane (green for the eight-level devices and purple for the four-level devices). (d) Measured efficiency for each device at the deflection angle $\theta \approx 43^\circ$ (see the text for details).
four-level dielectric device has the highest performance (83%), which is 18% higher than the perfect sample #0 (65%).

It is very surprising that some imperfect metasurfaces, both dielectric and metallic, can outperform perfect devices. To shed some light on this phenomenon, we use full-wave electromagnetic simulations in the Supporting Information, Figure S6 to compute the field distribution for perfect and imperfect dielectric devices. Four-level metasurfaces are chosen because sample #8 outperforms the ideal structure most for those devices. By comparing the different phase distributions, we observe that sample #8 exhibits a smoother phase gradient, compared to sample #0. On the other hand, sample #5, which has the worst efficiency, produces a very rough phase distribution (Supporting Information, Figure S6b). Consequently, although sample #8 is imperfect, its steady-state electric field distribution has a better fitting with the designed phase gradient and gives rise to a higher efficiency.

**CONCLUSIONS**

In summary, we have analyzed theoretically and experimentally the robustness of phase gradient metasurfaces to fabrication inaccuracies, considering both metallic devices in reflection and dielectric devices in transmission. To this end, a simple semianalytical model has been developed, which provides the response of a metasurface at almost no numerical costs and is in very good agreement with full-wave numerical simulations. This simple model could be used to design more complex metasurfaces, such as meta-holograms, for example.

Missing meta-atoms are the defects that deteriorate most of the device efficiency, reducing it typically by 20%. In that context, and quite surprisingly, it is not the meta-atom size that matters most, but rather its associated phase, with respect to the phase provided by the substrate. Elements that have the largest phase difference with the substrate (e.g., in the order of 180°) are the most sensitive ones. Consequently, by modifying...
and for both types of devices; we notice that the steering angle is not influenced by such defects $\theta$.

Measurements on misfabricated metallic metasurfaces, both eight-level and four-level, fully support these findings, which indicate that one can design a metasurface with less stringent considerations than anticipated. This work paves the way for revisiting the design of metasurfaces afresh, beyond the constraints of a periodic perfect lattice, possibly with the help of a deep learning approach. $^{56}$

**METHODS**

**Nanofabrication.** Supporting Information, Figure S1 shows the process flow for nanofabrication. A Silicon wafer (100/P/SS/01-100, Center of MicroNanoTechnology at EPFL) was first baked on a hot plate (fabricant) for 5 min at a temperature of 180 °C to dehydrate it (humidity appears detrimental to nanofabrication$^{57,58}$). Then, 1 nm Ti as the adhesion layer followed by 150 nm Au as the mirror, 1 nm Ti and 40 nm SiO2 as the dielectric space, 1 nm Ti, 30 nm gold as the meta-atoms, and finally, 20 nm Cr as the sacrificial layer were deposited using an evaporator (Leybold Optics LAB600H). A negative tone electron-beam photoresist hydrogen silsesquioxane (HSQ, XR-1541-006 DuPont) was then spun-coated on top at 6000 rpm. After electron-beam exposure (Vistec EBPG5000 system, 100 keV and 100 pA) and development (Tetramethylammonium Hydroxide 25%, Honeywell), ion beam etching (Veeco Nexus IBE350, 300 V and 500 mA collimated Ar ion beam) is used to reveal the meta-atoms while maintaining the SiO$_2$ substrate. The sample is finished by etching the sacrificial Cr layer (TechniEtch Cr01, Microchemicals GmbH) to remove the remaining HSQ and cleaned in isopropanol alcohol and deionized water.

**Quasi-Analytical Model.** A simple quasi-analytical model is implemented to calculate the momentum provided by the metasurface. For a normal incident plane wave propagating in $-z$-direction, the phase gradient metasurface provides a momentum horizontally in $+x$-direction and the reflected light is redirected into the angle $\theta$ as described by the generalized Snell's law.$^{59}$ The simplified one-dimension model considers each unit cell as a point light source with its own amplitude and phase: $E(x) = E(x)e^{i\phi}$. This information after the Fourier transform can be converted into the momentum $k_x$ parallel to the surface. Once the unit cells' periodicity and the superlattice period are determined, we apply Fourier transforms to convert the complex amplitude from direct space into spatial frequencies

$$\tilde{E}(k_x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} E(x)e^{-ik_xx}\,dx \quad (1.1)$$

where $\tilde{E}(k_x)$ is the Fourier transform of the electric field $E(x)$ and $\exp(-ik_xx)$ the phase term associated with the metasurface. The efficiency in the Fourier plane is normalized to the maximum intensity for a perfect mirror, such that the performance of the device can be quantized. A Matlab code implementing this simple model is available in the open dataset (Section 1) associated with this article.

**Full-Wave Simulations.** The full-wave simulations are performed with COMSOL version 5.6. Periodic boundary conditions are applied in $x$- and $y$-directions at the edges of the superlattice. The system is illuminated at normal incidence with a plane wave polarized in the $y$-direction ($\lambda = 980$ nm). The following references are used for the refractive index of gold,$^{60}$ silicon,$^{61}$ titanium dioxide,$^{62}$ and silicon dioxide.$^{63}$

---

**Figure 8.** Another example of beam steering devices made of dielectric meta-atoms in transmission. (a) Schematic of the dielectric meta-atom: a TiO$_2$ cylinder (varying diameter $D$ and fixed height $H = 600$ nm) supported by a glass substrate with the periodicity $P = 250$ nm. (b) Corresponding amplitude and phase shift in transmission as a function of $D$ at $\lambda = 632$ nm. (c) Eight-level unit cell with dielectric meta-atoms of diameters $D = 100, 130, 150, 165, 180, 195, 210$, and 225 nm and (d) four-level unit cell with meta-atoms of diameters $D = 100, 150, 180$, and 210 nm (each element being repeated once). The discrete elements used for the full-wave simulations are shown in the insets of panels (c, d). (e) Metasurface performance as a function of the sample number for eight-level and four-level metasurfaces computed using full-wave simulations.
Perfect match layers are applied on both ends. The energy in the different diffraction orders can be obtained directly from COMSOL or extracted from the electric and magnetic fields above the surface at 2 and 2.5 μm using the post-processing provided in the open dataset (Section 2) associated with this article.

**Optical Characterization.** Supporting Information, Figure S4a shows the optical setup used for the optical characterization of the different metasurfaces fabricated. The measurements are conducted with an inverted microscope (Olympus IX-73) and a 50x objective with NA = 0.9, which can collect the light up to 64°. The light source (LP980-SF15, Thorlabs) is a laser diode coupled into an optical fiber. To generate a linearly polarized plane wave, a collimator and a subsequent linear polarizer are placed at the end of the fiber. A lens with focal distance f = 200 mm is used to convert light reflected from the sample into the Fourier plane, thus providing angular information. As indicated in the main text, the light diverted by the metasurface is normalized to that reflected by a silver mirror to determine the metasurface efficiency. On the contrary, the beam steering metasurface is capable of deflecting the incoming light toward an angle, as shown in the Supporting Information, Figure 4b. The efficiency is defined as the total power of the deflected beam divided by the total power of the light reflected by the silver mirror. A Matlab code is provided in the open dataset (Section 3) associated with this article to post-process the experimental data.

**REFERENCES**


(64) Wang, H.-C.; Achouri, K.; Martin, O. J. F. Data set for the manuscript 'Robustness Analysis of Metasurfaces: Perfect Structures are not always the Best' (2.0) [Data set]. https://zenodo.org/record/6606461#YphfYhByUk (accessed Jun 02, 2022).