In Situ Planarization of Huygens Metasurfaces by Nanoscale Local Oxidation of Silicon

Jonathan Bar-David, Noa Mazurski, and Uriel Levy

Department of Applied Physics, the Benin School of Engineering and Computer Science, the Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Jerusalem, 91904, Israel

Supporting Information

ABSTRACT: Metasurfaces are becoming a flourishing field of research, with diverse applications, such as planar optical components and structural colors. While metallic metasurfaces are typically few tens of nanometers in their thickness, their dielectric counterparts typically span few hundreds of nanometers in thickness variations. This makes the stacking of multilayers a bit challenging. To mitigate this challenge, we have developed a new approach for the realization of dielectric metasurfaces. Our approach is based on the nanoscale local oxidation of silicon (LOCOS), allowing to achieve planar metasurface structures. We have utilized this approach for the design, fabrication and characterization of amorphous silicon based all-dielectric Huygens metasurfaces. These metasurfaces show clear electric and magnetic resonances, which can be structurally tuned. The obtained results are in good agreement with numerical simulations taking into account the unique shape of the nanoantennas. Relying on a robust approach for their realization, and combined with the important feature of in situ planarization, we believe that such planarized metasurfaces will become a viable technology for future applications.

KEYWORDS: Huygens metasurface, dielectric metasurface, LOCOS

Optical metasurfaces are nanopatterned surfaces exhibiting desired optical characteristics depending on the nano patterns and the structures which are defined on the surface.\(^1\)\textsuperscript{−}\textsuperscript{2}\textsuperscript{1} This is in contrast to conventional optical elements that rely on the materials’ bulk properties. One may distinguish between two different types of metasurfaces, being resonant or nonresonant. While the latter relies on concepts such as phase accumulation, effective index and geometrical phase to control light,\(^2\textsuperscript{,}3\textsuperscript{,}5\textsuperscript{−}7\textsuperscript{,}9\textsuperscript{,}10\textsuperscript{,}22\textsuperscript{−}27\) the optical properties of resonant metasurfaces originate at the optical resonant behavior of the individual scattering elements, which are sometimes defined as optical nanoantennas.\(^1\textsuperscript{,}11\textsuperscript{−}13\textsuperscript{,}18\textsuperscript{,}28\textsuperscript{,}29\)

The scattering, transmission, and absorption of electromagnetic waves by small particles is an old topic first considered by Mie,\(^30\textsuperscript{−}32\) who calculated the inner and outer fields for scattering of plane waves by spheres, concluding they are the sum of the basic multipole fields.\(^31\textsuperscript{,}32\) The multipole fields are therefore the electromagnetic eigenmodes of the fields in and around small particles.\(^31\textsuperscript{,}32\) These modes and their resonant frequencies are determined mainly by particle size, geometry, aspect ratio, refractive index, and the index contrast between the particle and surrounding medium. Following the rapid progress in nanofabrication techniques, these observations pioneered by Mie are now of great significance to the photonic research, as nowadays researchers are attempting to harness the optical response of small particles and cavities such as nanoantennas for a large variety of photonic applications. By properly designing nanoantennas, it is now possible to control the amplitude, phase, and polarization of the transmitted and reflected fields and by fabricating arrays of resonant nanoantennas one may fabricate resonant metasurfaces with tailored optical properties for different applications including, for example, color engineering,\(^11\textsuperscript{,}18\textsuperscript{,}19\textsuperscript{,}28\textsuperscript{,}33\textsuperscript{,}34\) nonlinear optics,\(^35\textsuperscript{−}38\) reflectionless surfaces and perfect absorbers,\(^1\textsuperscript{,}6\textsuperscript{,}39\textsuperscript{−}41\) metalenses and other optical elements,\(^10\textsuperscript{,}24\textsuperscript{,}42\textsuperscript{−}44\) to name a few. The common to all these demonstrations is the ability to control the polarization, phase, amplitude and frequency of transmitted and reflected light, as well as the near-field of the metasurface, to design arbitrary optical properties. Many metasurfaces use metals and plasmonic phenomena to achieve such effects.\(^17\textsuperscript{,}18\textsuperscript{,}28\textsuperscript{,}29\textsuperscript{,}45\textsuperscript{−}51\) Yet, metallic metasurfaces suffer significant losses. In contrast, dielectric metasurfaces show only little absorption in most cases and therefore offer high transmission and reflection efficiency reaching the limit of almost no absorption losses and pure control of phase and polarization.\(^1\textsuperscript{,}3\textsuperscript{,}6\textsuperscript{−}9\textsuperscript{,}11\textsuperscript{−}14\textsuperscript{,}39\textsuperscript{,}40\textsuperscript{,}43\textsuperscript{,}52\) On the other hand, while metallic metasurfaces are nearly flat, a typical dielectric metasurface consists of nanoantenna arrays which are situated on the surface of a flat substrate, making the structure

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nonplanar. As a result, special efforts need to be carried out in order to planarize the surface if the stacking of additional layers is needed. Furthermore, the need for etching of the dielectric metasurface structure leads to unavoidable surface roughness and consequently scattering loss. In this work, we demonstrate a novel approach which allows to fabricate smooth and planar dielectric metasurfaces with optical resonances at the telecom regime. By doing so, we address some of the major issues of current metasurface technology and provide a path for even brighter future for metasurfaces.

**FABRICATION**

Our approach relies on the local oxidation of silicon (LOCOS) fabrication technique. LOCOS is a fabrication method originally used for the isolation of adjacent MOS transistors from each other. In short, it is based on the oxidation of silicon in an oxygen reach furnace, with the end result of having silicon dioxide replacing the silicon in desired location across the device. More recently, this approach has been used for the purpose of defining smooth, low-loss optical waveguides on silicon substrate. In this technique, a protective layer is deposited above a silicon (Si) substrate. Next, photo- or electron beam-lithography patterns are transferred to the protective layer by etching. Finally, these patterns are transferred to the silicon substrate by oxidation, rather than by further etch steps. The oxidation process allows for smooth structures to be formed, significantly reducing roughness and consequently undesired scattering of light. The original approach results in a highly nonplanar structure due to the higher volume of the silicon dioxide layer that is formed instead of the silicon. However, Recent publications also show that by partial etching of the Si substrate prior to oxidation, one may

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**Figure 1.** LOCOS fabrication scheme. (A) a-Si, Si$_3$N$_4$ and e-beam resist layers are deposited on a Quartz substrate. (B) ZEP etch mask is defined by electron beam lithography. (C) RIE etch is performed through the Si$_3$N$_4$ and some of the a-Si layer, leaving a thin a-Si layer close to substrate. (D) Silicon oxidation followed by removal of Si$_3$N$_4$ layer. The end result is a quasi-planar metasurface.

**Figure 2.** SEM micrographs of aSi LOCOS nanoantennas. (Left) cylindrical nanoantennas with radius of $\sim$130 nm and gap of $\sim$150 nm. (Right) rectangular nanoantennas with length of $\sim$420 nm, width of $\sim$160 nm, and gaps of $\sim$220 nm. In both antenna types the a-Si thickness is $\sim$270 nm. The a-Si antennas are seen as dark gray areas, and the lighter “frame” around them is the oxide layer.
obtain quasi-planar structures without jeopardizing the smoothness of the obtained structures. An illustration of our fabrication process is shown in Figure 1. Unlike previous demonstrations, in this work, we chose to utilize the LOCOS technique to fabricate quasi-planar nanoantenna arrays in an amorphous silicon (a-Si) layer.

The fabrication process begins by depositing a 275 nm thick hydrogenated a-Si layer on a quartz substrate by PECVD (Oxford). Atop this layer, we deposited the oxidation-shield layer, a 160 nm thick silicon nitride (Si3N4) by PECVD. Sample was then spin coated with electron beam (e-beam) resist (ZEP 520), and nanoantenna patterns were created by e-beam lithography (Raith eline). Note that ZEP is a positive resist, hence, e-beam patterns are the interantenna gaps. After e-beam lithography, sample was developed and the pattern was transferred to the silicon nitride layer by a reactive ion etch (RIE, Corial), where the ZEP e-beam resist is used as the etch mask. In this step we etched the full height of the silicon nitride layer and exposed the a-Si layer in the bottom of the created trenches. Next, a second etch step was performed, partially etching the a-Si layer, to compensate for oxidation swelling. Finally, the e-beam resist was removed and the sample was oxidized by heating the sample to ~1000 °C in an H2O rich atmosphere. During oxidation, the silicon nitride layer acts as an oxidation shield defining the oxidized regions. Finally, the silicon nitride layer is removed, and the planarized structure of amorphous-silicon nanoantennas, embedded in SiO2, is formed.

A scanning electron microscope (SEM) image showing the top view of some of the fabricated samples is shown in Figure 2. Atomic force microscope (AFM) scans of the fabricated samples are shown in Figure 3. An SEM cross section revealing the detailed subterranean structure of the nanoantennas is shown in Figure 4. These scans clearly show the oxidized ring surrounding each of the Si nanoantennas. The surface height variation is of the order of ±25 nm. The relation between antenna layer thickness and final surface variation was not investigated directly. However, based on current results we assume that the antenna thickness does not have a significant effect on the final flatness, which is governed mostly by the accuracy of the etch and the oxidation steps. We have chosen to fabricate arrays of identical antennas with radii and period varying between arrays in order to better understand and control the fabrication process and the optical properties of the antenna structures.

The cross section shown in Figure 4 further reveals the antenna sidewall geometry which is curved inward. This geometry is an outcome of the oxidation process, the curved structure is a result of oxygen diffusion into the silicon and the in- and outward swelling of the formed silicon dioxide. This unique structure was considered in the numerical simulations, as will be discussed later on.

**NUMERICAL SIMULATIONS**

The optical transmission spectrum of the fabricated structure was simulated by 3D FDTD software (Lumerical FDTD solutions). The transmission of nanoantenna arrays was considered by applying periodic boundary conditions and plane-wave illumination. Due to the resonant nature of these nanoantennas, even a slight change of few nanometers in the simulated antenna geometry, for example, its height, radius, or sidewall profile, results in a noticeable variation in optical performance and shift in the resonance frequency. Figure 5 presents the results of such simulations, calculating the transmitted amplitude for cylindrical nanoantennas with height of 275 nm and varying radii of 60 to 400 nm, for a broad SWIR spectrum with wavelength ranging from 600 to 1600 nm. The gap was kept constant at 200 nm, that is, the period is
increasing with the radius. As may be seen in Figure 5A, the transmission properties of these nanoantennas change with the antenna radius. The change is mostly observable as a wavelength shift and separation of the two distinct transmission minima. These two resonances can also be observed in Figure 5b, which is a line scan of Figure 5a at a constant cylinder radius of 329 nm. Indeed, the two distinct minima, labeled as “electric dipole” (ED) and “magnetic dipole” (MD) resonances are seen, as also reported in, for example, refs 8, 31, 40, and 57. These resonances are actually the two first Mie resonances, which “switch order”, that is, the ED mode is found at a longer wavelength (or lower frequency) than the MD mode, due to the small aspect ratio of the nanoantennas, with a height of 275 nm and a radii of 330 nm. Figure 6 shows the calculated electric and magnetic fields for the two modes indicated in Figure 5B. It may be seen that under illumination with a \( \lambda \)-polarized plane wave, the MD modal field at a wavelength of 1306 nm has the expected strong magnetic field in the \( \hat{y} \) direction and the circular vortex-shaped electric field in the \( \hat{x} \) plane, as depicted in Figure 6 (top row), while the ED modal fields at the wavelength of 1446 nm have a strong electric field at the \( \hat{x} \) direction and a vortex-shaped magnetic field loop at the \( \hat{y} \) plane, as depicted in Figure 6 (bottom row). It may also be noticed that the ED modal fields are actually concentrated close to the nanoantenna boundary due to the asymmetric antenna structure and (relatively) low index contrast between the antenna and the surrounding medium (here, the substrate), which increase the effective volume of the nanoantenna.

**EXPERIMENTAL CHARACTERIZATION**

Following the design and fabrication of the LOCOS based metasurface, we have experimentally characterized its optical response. Transmission measurements were done by illuminating the sample with a white light source (tungsten-halogen lamp) through a microscope condenser lens. The transmitted light is collected by an objective lens (Nikon, 50X, NA 0.45)
and directed into a spectrometer (Horiba, microHR\Ocean Optics, Flame). All measurements are later normalized to the transmission through the system. Figure 7 presents the measured transmission of our fabricated cylindrical nanoantenna arrays. As may be seen, the main features predicted by simulation are clearly seen in our measurements, namely the two resonant modes and their overlap for nanoantennas of radius about 150 nm. To further compare our measured results to the simulated prediction, we present in Figure 8 a comparison of the numerical simulations (left) to the measurements (right) of nanoantennas with gradually increasing radius. This comparison reveals a good agreement between the two. Furthermore, the gradual spectral separation between the electric and magnetic modes can be clearly observed.

In addition to the characterization of cylindrical nanoantennas, we have also fabricated and characterized rectangular nanoantenna arrays (such as depicted in Figure 2). The transmission through such arrays was measured by the same method described above, with light polarized along the nanoantennas’ long axis. Due to the geometry of these nanoantennas, with length of 300–400 nm and width of ∼150 nm, the resonant frequencies of these antennas are closer...
Figure 8. Transmission spectrum of cylindrical nanoantennas with radii of ~90 to ~250 nm. (Left) full wave numerical simulation, (Right) measured results. The shifting of modes toward longer wavelengths and the splitting of the MD and ED modes are clearly seen in both simulation and measured data. The Kerker condition, in which MD and ED resonances overlap is denoted by the red box. Full transmission is not obtained as the wavelength is below the material band gap.

Figure 9. Transmission spectrum of rectangular nanoantennas, with light linearly polarized along the antennas’ long axis: (left) simulation, (right) measurement. Notice the gradual change in resonant frequencies as the antenna length is increased from 300 nm at the bottom row to 400 nm at the top. Spectrum complexity arises primarily from the intrinsic absorption of a-Si for frequencies above the material band gap. The curved sidewall has been approximated by a segment shape with a curvature of about 30 nm inward.
to the visible spectrum (compared to the cylindrical nanoantennas shown previously). As such, the demonstration of LOCOS based nanoantennas allows for an additional degree of freedom in mitigating specific applications toward the visible band, while maintaining dimensions which are not too difficult to fabricate. Figure 9 shows the simulated (left) and the measured (right) transmission of nanoantenna arrays with length varying from 300 to 400 nm. Here, the transmission spectra are more complex due to the intrinsic silicon absorption at these frequencies resulting from interband transition. Nevertheless, we are able to identify the major trends in both simulation and measured data, namely, the general spectral location of the antenna resonances and their gradual shift toward longer wavelengths as the antenna length increases.

**SUMMARY**

We have demonstrated the viability of the LOCOS technique for the fabrication of planar, optically resonant dielectric metasurfaces in a-Si layers. Measurements of our fabricated metasurfaces show good agreement with simulation predictions, indicating that these metasurfaces can operate in the visible and NIR spectral regimes, above and below the Si band gap frequency. We have designed and fabricated metasurfaces based on nanoantennas of different sizes and geometries and by this we have shown the fabrication robustness provided by this approach, as well as its compatibility with current CMOS technologies. Following the results reported here, one may use this technique for the implementation of planar metasurface devices, for example, metalenses, metafilters, metasplitters, metalograms, and more. Finally, the LOCOS technique and the use of PECVD deposited materials on commercially available substrates pave the way for future implementation in optical devices and in few-layer stack structures.

**ASSOCIATED CONTENT**

* Supporting Information
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Figure S1 (PDF).

**AUTHOR INFORMATION**

*Corresponding Author
*E-mail: ulevy@mail.huji.ac.il.

**ORCID**
Jonathan Bar-David: 0000-0002-4464-636X
Uriel Levy: 0000-0002-5918-1876

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**Notes**
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