Silicon nanoridge array waveguides for nonlinear and sensing applications

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Abstract: We fabricate and characterize waveguides composed of closely spaced and longitudinally oriented silicon ridges etched into silicon-on-insulator wafers. Through both guided mode and bulk measurements, we demonstrate that the patterning of silicon waveguides on such a deeply subwavelength scale is desirable for nonlinear and sensing applications alike. The proposed waveguide geometry simultaneously exhibits comparable propagation losses to similar schemes proposed in literature, an enhanced effective third-order nonlinear susceptibility, and high sensitivity to perturbations in its environment.

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bottlenecks of conventional CMOS circuits [1–3]. More recently, chip-scale photonic devices
also have been used in such applications as biological and environmental sensing [4,5].
Perhaps the most critical effect which allows silicon waveguides to exhibit improved nonlinear coefficients, response times, and sensitivities is the confinement of electromagnetic fields to a small spatial area [6–9]. In addition to drastically increasing the spatial power density of the supported modes, the reduction of a waveguide’s cross-section also raises its surface-area-to-volume ratio, allowing otherwise negligible phenomena at material interfaces to become strong in comparison to bulk effects [10,11]. As silicon photonics continues to evolve, it is important to design new waveguide topologies capable of exploiting these surface phenomena without consequently compromising other favorable properties.

Slot waveguides show promise as one of the means by which this may be achieved, and
have previously been used to realize high-efficiency electro-optic modulators and wavemixers
[12–14]. Whereas conventional waveguides confine the optical mode to a high-index core, slot waveguides exploit the discontinuities of electric fields across interfaces to trap the mode within the lower-index slot. Sub-wavelength gratings (SWGs), which modify a waveguide’s cross-section along the direction of propagation, are also appealing for various applications due to their high sensitivities to perturbations to the waveguide’s cladding material [15]. A natural integration of these two waveguide configurations, designed with the intent of simultaneously leveraging both of their advantageous properties, would consist of many thin, co-propagating ridges of guiding material, as shown in Fig. 1. Such a waveguide, patterned

over dimensions drastically smaller than the wavelength of light, would preserve the field localization achieved by the slot waveguide while simultaneously allowing the guided mode's effective optical properties to be easily tailored. In this manuscript, we consider the linear and nonlinear characteristics of the so-called nanoridge array (NRA) waveguide and assess its applicability to several photonic applications.

Fig. 1. Illustration showing the size of the proposed waveguide relative to the optical carrier’s approximate free-space wavelength.

2. Basic properties of silicon nanoridge array (NRA) waveguides

In order for an NRA structure to function as a waveguide, it must operate above the cutoff condition for either the fundamental TE- or TM-like mode. However, for applications such as sensing, it is desirable to operate as close to these same cutoff conditions as possible in order to maximize sensitivity. To more explicitly consider this inherent trade-off between confinement and local field enhancement, we consider two cases in which an NRA waveguide is either (1) left unclad, or (2) clad with aluminum oxide. The waveguides in both cases are composed of 500 nm-tall silicon ridges, and differ only in terms of the material used to clad them. We use the finite element method (FEM) software COMSOL to model each case, and the results yielded by this analysis are shown in Fig. 2 [16].

Fig. 2. FEM models showing the x-component of the electric field for the TE-like mode, normalized to 1 W of propagating power, supported by the (a) unclad and (b) aluminum oxide clad NRA waveguide. For both figures, the x- and y-axis are in units of microns.

The TE-like mode of the unclad waveguide, shown in Fig. 2(a), has large electric field discontinuities at each vertical interface, and exhibits local field enhancements within the
lower-indexed material. In addition to interacting strongly with the waveguide's densely integrated silicon-air interfaces, this mode is anticipated to respond strongly to any changes in the refractive index of the space between the ridges. These characteristics are obviously desirable for nonlinear and sensing applications, but they come at the expense of confinement, leading to a larger modal area as well as significant leakage of the mode into the waveguide's substrate. In comparison, the mode supported by the clad waveguide, plotted in Fig. 2(b), shows comparatively less interaction with the cladding material, and this is reflected most clearly by its significantly increased effective index. This may be beneficial, however, because the mode will remain well-confined for smaller waveguide dimensions, whereas the unclad waveguide’s TE-like mode will more quickly reach cutoff. Thus, depending on the intended application of the NRA waveguide, it is critical to determine the proper values of such parameters as the ridge width, the pitch between adjacent ridges, the total number of ridges, the height of the waveguide, and the cladding material.

A second complication faced by the proposed waveguide geometry involves the potential difficulty in exciting its optical modes. Coupling light into an NRA waveguide abruptly from a conventional waveguide is anticipated to be highly inefficient due to the large discrepancy between the two guided modes' electric field profiles. Higher coupling efficiencies are predicted, however, if the conventional waveguide is adiabatically tapered into the NRA configuration as illustrated in Fig. 3(a). To verify this prediction we have modeled both the untapered and tapered cases using the finite-difference time-domain (FDTD) software Lumerical [17]. For the tapered case, a taper length of 10 µm was chosen to reduce the memory requirements of the simulation. The waveguide structure consisted of a 220 nm-tall NRA waveguide clad with 150 nm of aluminum oxide and one micron of silicon dioxide, and a top-down view of the employed model is shown as an inset in Fig. 3(b). The intermediate aluminum oxide layer was included because, when deposited through atomic layer deposition (ALD), it is known to have an exceptionally high degree of conformality.

Our simulations, the results of which are included in Fig. 3(b), clearly indicate that the tapered case couples light into the TE-like mode of the NRA waveguide more efficiently than the abrupt transition, and additionally inhibits reflection back into the counter-propagating mode. This analysis offers some evidence that fabricating and characterizing an NRA waveguide may be feasible, and additionally highlights several of the underlying complexities necessarily entailed by the use of such an atypical waveguide geometry.

![Fig. 3. (a) Schematic showing the simulated structure (not including the top cladding layers of aluminum oxide and silicon dioxide). (b) Normalized transmission (T) and reflection (R) spectra for the tapered and untampered cases (Inset: top-down view of the simulated structure).](image)

### 3. Fabrication

The proposed waveguide design, shown in Fig. 4(a), was fabricated using commercially available SOI wafers with a 220 nm-thick silicon device layer and a 3 µm-thick buried oxide (BOX) layer. The wafers were spin-coated with the negative electron beam resist hydrogen silsesquioxane (HSQ), and the waveguide pattern was written using a Vistec EBPG 5200
Electron Beam Writer. Subsequently, an Oxford Plasmalab 100 Reactive Ion Etcher was used to remove the unwritten portion of the silicon device layer. The gas flow rates during the etching process were 20 sccm for SF₆ and 55 sccm for C₄F₈, and the chamber pressure was maintained at 15 mTorr. These conditions were chosen in order to achieve smooth waveguide sidewalls, and to minimize undercut into the substrate. After etching, the waveguides were clad with a 150 nm-thick layer of thermally deposited Al₂O₃ in a Beneq TFS200 Atomic Layer Deposition at a temperature of 200° C, and finally an additional 2 µm-thick layer of SiO₂ was deposited onto the samples using an Oxford Plasmalab 100 Plasma-Enhanced Chemical Vapor Deposition (PECVD).

The resulting waveguide cross-section, an SEM micrograph of which is shown in Fig. 4(b), exhibited several deviations from the target dimensions. Most prominently, the silicon ridge width was seen to vary with height, reaching a minimum value of approximately 35 ± 5 nm at the ridge’s midpoint. Additionally, air voids with widths of approximately 20 ± 5 nm were observed at regular intervals, likely due to clogging between adjacent ridges during the ALD step. Otherwise, the fabricated waveguides were found to be in good agreement with the proposed geometry, and were predicted to support TE- and TM-like modes as shown in Fig. 4(c) and Fig. 4(d), respectively. It should be noted that, for the TE-like mode, the field is significantly enhanced within the air voids, and this leads to the decreased effective index as compared to the TM-like mode.

Fig. 4. (a) Target dimensions and (b) SEM micrograph image of the NRA waveguide cross-section. (c,d) FEM-generated plot of the dominant field component for the TM- and TE-like modes, respectively.
4. Optical characterization

To measure the propagation loss of the NRA waveguides’ TE-like mode, we fabricated and characterized an NRA ring resonator coupled to an NRA section of a straight waveguide, as shown in Fig. 5(a) and Fig. 5(b). It should be noted that, although not explicitly shown in the SEM micrographs, tapered coupling sections as discussed in section 2 were implemented to couple light into and out of the NRA section of the waveguide. The separation between the bus and ring waveguides was chosen to be 100 nm, and the radius of the ring, which was experimentally characterized, was 40 µm. We coupled light into the bus waveguide using a tunable laser and a lensed tapered fiber, then collected the transmitted power using a metallic output objective and an optical power meter. This measurement setup has been discussed in greater detail in a previous work [18]. The normalized transmission spectrum was found to exhibit sharp dips at each of the ring’s resonant wavelengths, and the shape of these resonances could be fit numerically to the expression [19]:

\[
T = \frac{t^2 - 2t\tau \cos(\theta) + \tau^2}{1 - 2t\tau \cos(\theta) + (\tau)^2}
\]  

(1)

where \( \theta \) was the phase accumulated by the mode in one round trip, in turn defined as:

\[
\theta = \frac{4\pi^2 n_{\text{eff}} r}{\lambda}
\]  

(2)

In the previous two expressions, \( t \) is the self-coupling coefficient of the bus waveguide, \( \tau \) is the attenuation coefficient of the ring, \( r \) is the ring radius, \( n_{\text{eff}} \) is the effective index of the mode supported by the ring, and \( \lambda \) is the optical wavelength. The loss coefficient may be calculated at a given resonance as [19]:

\[
\alpha [\text{dB/\mu m}] = \frac{-20\log_{10}(\tau)}{L[\mu m]}
\]  

(3)

where \( L \) was the length of the ring. The transmission spectrum of the ring resonator, shown alongside the wavelength dependent quality factor (Q) in Fig. 5(c), displayed resonances with an approximate free spectral range of 5 nm. Our experimental data was used in combination with Eq. (1) and Eq. (3) to calculate both the effective index and loss coefficient of the TE-like mode at a wavelength of 1552 nm, and the two values yielded were, respectively, 1.501 ± 0.001 and 0.0217 ± 0.0013 dB/µm. The loss measured here is comparable in magnitude to the values exhibited by subwavelength gratings [15], and is most likely due both to the NRA waveguide’s high surface-area-to-volume ratio and to interface charge-induced free-carrier effects [20]. It is important to note that this value may be significantly reduced in future iterations by approximately 70% through the application of a post-etch RCA clean to reduce sidewall roughness and/or the modification of the deposition recipe to reduce the magnitude of interface fixed charges [20–22]. Additionally, the number and spatial density of ridges and slots may be reduced according to the desired application, further lowering the loss as necessary.
Fig. 5. (a,b) SEM micrographs showing the NRA ring resonator coupled to a bus waveguide, and (c) the transmission spectrum measured at the output of the bus waveguide, additionally showing the Q-factor of each resonance.

5. Applications

5.1 Nonlinear optics

Materials patterned on a deeply subwavelength scale often exhibit enhancements to the second- and third-order nonlinear susceptibility tensor [23–26], and this effect is believed to be due primarily to (1) the highly localized electric field profiles supported by such structures, and (2) the high spatial density of optical nonlinearities along each material interface. These two effects combine to produce an effective third-order nonlinear susceptibility in the patterned material. To determine whether such enhancements were present for our fabricated waveguides, we carried out surface third-harmonic generation from large (1 mm by 1 mm) silicon surfaces which were patterned similarly to our NRA waveguides, using a multiphoton microscope as shown in Fig. 6(a). The measurements were taken using a linearly polarized fs-pulsed laser operating at a wavelength of 1560 nm with a repetition rate of 8 MHz [27]. Figure 6(b) shows the multiphoton spectra for the patterned and unpatterned sections of the sample, for an input beam with its polarization perpendicular (TE) to the silicon ridges, and this data clearly illustrates that the third-harmonic signal, observed as a sharp peak at 520 nm, increased drastically due to the patterning of the surface. The strongest signal was reached for a ridge width of 70 nm and a trench width of 70 nm, and the factor of enhancement observed for these dimensions, in comparison to the unpatterned silicon surface, was approximately equal to 500. Additionally, the effective third-order nonlinear susceptibility of the patterned area is anticipated to be highly anisotropic. Whereas one electric field polarization (TM) is oriented parallel to the silicon-air interfaces and is consequently continuous across them, the orthogonal polarization (TE) is oriented perpendicular to them and will instead be highly discontinuous, exhibiting higher field values in the lower-indexed material. In order to confirm this hypothesis, we measured the reflection third-harmonic signal as a function of the angle of polarization of the input beam for the sample with ridge and trench widths of 70 nm. The results shown in Fig. 6(c) confirm that the measured third-harmonic signal reaches its maximum for two angles separated by 180 degrees, corresponding to the TE polarization,
while exhibiting minima at the orthogonal TM polarization. Figure 6(d) shows the spatially resolved optical images of the third-harmonic signal for the TE and TM polarizations. Because the power contained in the third-harmonic signal was highly dependent on the exact geometry of the patterning, further work may be done to optimize the combined response of the cascaded silicon surfaces and the electric field enhancement. Nonetheless, these initial results suggest that NRA waveguides may be highly beneficial to processes which rely on third-order wavemixing.

5.2 Mode-split sensing

As mentioned, NRA waveguides exhibit large spatial discontinuities in their index of refraction. This makes them ideal candidates for sensing applications, particularly if they can be exploited in a resonant configuration. Currently, one of the most common techniques in on-chip nanoparticle detection is to measure the change in the resonant wavelength of a resonator induced by the presence of a nanoparticle. Although effective, this method is limited in terms of the magnitude of the spectral shift it can attain, and is additionally highly susceptible to unintended perturbations to the ring. But perhaps even more importantly, the spectral shifts of such resonators depend strongly on both the nanoparticle's size and location, and decoupling these two variables from one another is not always possible [28,29].

Recently, a self-referencing detection mechanism based instead on the splitting of degenerate modes, achieved using a high-Q silica microtoroid resonator, has been demonstrated to overcome the limitations of conventional chip-scale sensors [30]. This new
mechanism relies not on a single mode, but on the degenerate clockwise- and counterclockwise-traveling modes of a perfectly symmetrical ring resonator. Upon the introduction of an impurity, the degeneracy of the two modes is lifted, leading to a split in their resonant frequencies. The strength of this splitting is again strongly dependent on both the size and location of the particle, but in this case both variables may readily be extracted from the resonator's transmission spectrum. Additionally, the two non-degenerate resonances encounter the same noise, and this makes the measurement of their frequency difference more robust than the analogous measurement of traditional sensors.

Here, we evaluate unclad NRA whispering gallery mode (WGM) ring resonators as possible devices for sensing based on self-referential mode-splitting. Because of their topology, trenched structures allow nanoparticles to interact with the core of the optical mode, rather than the evanescent tail. This leads to a stronger perturbation of the structure's resonances, which in turn yields a more appreciable eigenfrequency splitting and a higher overall sensitivity. To demonstrate this effect, two-dimensional models of a 40 µm-radius ring resonator were constructed in COMSOL and used to simulate the eigenmodes supported at 1.55 µm, assuming (1) an ideal unclad NRA waveguide consisting of eleven 50 nm-wide ridges separated by 50 nm, and (2) a traditional ring resonator of comparable size. A dielectric particle with a diameter of 30 nm and a permittivity of 25 was incorporated into the model to induce the splitting of the resonances' eigenfrequencies, as shown in Fig. 7(a-d). To achieve the strongest possible response, the particle was initially assumed to be in the central slot of the NRA waveguide. We observed that the split in resonances, Δf, for the case of the NRA ring was approximately 7.0 GHz, while the corresponding value in the traditional ring resonator was approximately 8.2 MHz. Figure 7(e) illustrates how, even as the particle was moved to slots farther away from the NRA waveguide's center, the splitting of the eigenfrequencies remained orders of magnitude larger than that of the conventional ring. Although unclad waveguides can be used in the detection of airborne analytes, many practical applications involve the detection of analytes immersed in a liquid medium like water [31]. Because of water’s higher index of refraction (∼1.31 at λ = 1.55 µm), the field enhancement in the slots is reduced by approximately 40%, reducing the absolute value of Δf for both the NRA and conventional geometries. It is also worth noting that while a 2-D simulation of an unclad waveguide structure leads to exaggerated values of Δf, a more detailed 3-D simulation is expected to yield a similar trend and consequent enhancement of the NRA device sensitivity. An additional concern is that, in waveguides patterned on such small scales, it can be difficult to introduce particles into regions of interest with a high degree of success and accuracy [31]. However, the number and dimensions of slots can be tailored according to the intended application without drastically compromising the degree of field enhancement, and this may improve the ease with which analytes penetrate into the waveguide's core. We emphasize that the geometry considered here represents the most ambitious slot and ridge widths attainable with the fabrication tools at our disposal.
7. Conclusion

To summarize, we have modeled, fabricated, and characterized a new waveguide topology consisting of closely spaced silicon ridges clad with aluminum oxide in combination with silicon dioxide. The waveguide was found to support a TE-like mode which exhibited a competitively low propagation loss coefficient [15], and was additionally shown to offer unique advantages in terms of both nonlinear optics and sensing applications. As integrated silicon photonics continues to evolve, the NRA waveguide may be leveraged to improve the efficiencies of a wide range of linear and nonlinear optical device components including but not limited to modulators and switches, wave mixers, wavelength- and polarization-sensitive filters, and on-chip spectrometers.

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