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1-1-2013

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Heterogeneous lithium niobate photonics on silicon substrates

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Abstract: A platform for the realization of tightly-confined lithium niobate photonic devices and circuits on silicon substrates is reported based on wafer bonding and selective oxidation of refractory metals. The heterogeneous photonic platform is employed to demonstrate high-performance lithium niobate microring optical resonators and Mach-Zehnder optical modulators. A quality factor of $\sim 7.2 \times 10^4$ is measured in the microresonators, and a half-wave voltage-length product of 4 V.cm and an extinction ratio of 20 dB is measured in the modulators.

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OCIS codes: (130.0130) Integrated optics; (230.4000) Microstructure fabrication; (230.5750) Resonators; (130.4110) Modulators.

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1. Introduction

Several unique properties of silicon allow fabrication of ultra-large-scale integrated electronic circuits with extremely high performance. As a result, silicon has been long established as an ideal material for integrated electronics. To date, no material has been able to play a similar unifying role in integrated photonics. Alternatively, hybrid materials and heterogeneous integration solutions are currently being explored, particularly on silicon substrates for compatibility with microelectronics [1]. For instance, several groups are working on technologies to integrate compound semiconductors on silicon photonic chips [1–3]. III-V compound semiconductor waveguides are not very tightly-confined, and hence, silicon itself has been pursued for passive photonics [1]. However, silicon lacks second-order optical nonlinearity for active photonics and, at telecommunication wavelengths, third-order nonlinear silicon devices typically suffer from nonlinear absorptions at the required high optical intensities. Although complicated carrier sweep-out techniques can be employed, they can only partially alleviate the nonlinear absorption problem [1].

Lithium niobate (LiNbO 3) is an ideal material with many interesting properties for integrated photonics. First, it is transparent from the ultraviolet to the infrared range (0.35 to 5.0 µm) of the electromagnetic spectrum [4]. Optical gain can be achieved by doping LiNbO 3 crystals with rare earth elements, such as erbium [5]. A unique advantage is the material’s strong second-order nonlinear optical properties, which are absent in centrosymmetric
semiconductors, like silicon, and amorphous glasses, or are much weaker in noncentrosymmetric crystals like compound semiconductors (it is noted that applying stress can create small birefringence in silicon waveguides but the effect is very weak [6,7]). The second-order nonlinearity of LiNbO3 allows control of the refractive index of the material via the electro-optic (EO) effect. The nonlinearity also allows mixing of optical signals at different wavelengths for parametric amplification, second-harmonic generation, wavelength conversion [8], as well as generation of entangled photon pairs [9]. Even efficient generation of terahertz-frequency signals is reported in the material [10]. Using the piezo-electric properties of LiNbO3, it is possible to make various acousto-optical devices [11]. The most widely used devices based on LiNbO3, meanwhile, are high-speed EO modulators [12]. Extremely high optical modulation performance is possible using the material, since it allows pure phase modulation with virtually no variation in optical absorption. This feature allows vector signal modulation with negligible chirping for advanced telecommunication and other applications [13].

Future applications of LiNbO3 as an integrated optical platform requires a technology that can materialize ultracompact and efficient optical circuits on the material. LiNbO3 optical waveguides are generally very bulky in microphotonic standards and cannot be sharply bent (see Fig. 1). For example, a typical LiNbO3 modulator is 4-5 cm long and tens of micrometers wide [12]. Also, for nonlinear optical applications, due to the low intensity of the pump source in the large cross-sectional optical waveguides, the devices must be a few centimeters long in order to achieve high efficiencies [8,9]. These shortcomings have made LiNbO3 less attractive for integrated photonics, compared to semiconductors.

![Diagram showing effective areas and minimum radii for negligible bending loss at 90° bends for different waveguide technologies.](image)

2. The novel device concept and fabrication method

Conventional LiNbO3 waveguides are typically made by diffusion or proton-exchange methods [14,15]. Here, a novel technology that can realize much more compact LiNbO3 devices on silicon substrates is introduced. It is estimated that the waveguide core size and bending radius of LiNbO3 devices can be reduced by one to two orders of magnitude using this technology, as summarized in Fig. 1.

The novel platform on silicon substrates is schematically shown in Fig. 2. The waveguide structure consists of a thin layer of LiNbO3 core region, a silicon dioxide (SiO2) bottom cladding, and a tantalum pentoxide (Ta2O5) rib region loaded on top of the LiNbO3 layer for
Ridge formation. It is noted that, ignoring the birefringence of LiNbO₃, the refractive index of Ta₂O₅ is close to that of LiNbO₃. Hence, a ridge waveguide can be effectively formed, while the difficulties of directly etching LiNbO₃ are avoided. Also, the platform uses submicron layers of LiNbO₃ and Ta₂O₅, which allows creation of high-index contrast optical waveguides with low bending loss on silicon substrates with LiNbO₃ as the active region. It is noteworthy that recently thin layers of LiNbO₃ have been successfully bonded on top of standard SOI photonic devices [16–18]. However, since it is the evanescent tail of the optical mode of silicon waveguides that overlaps the LiNbO₃ cladding layer, the efficiency of the effective EO effect in these devices is low.

To demonstrate the devices schematically shown in Fig. 2, thin films of LiNbO₃ on silicon substrates are needed. Crystal ion slicing has been used for fabrication of thin films of silicon on silicon substrates in the past. That is the silicon-on-insulator (SOI) wafers, which are widely used for silicon photonic devices and circuits [1]. The first author and colleagues have previously demonstrated that a similar technique can be used for fabrication of thin films of LiNbO₃ on LiNbO₃ substrates [19,20]. It was shown that the optical properties of the crystals were preserved in the process and optical waveguides and modulators in submicron thin films of LiNbO₃ are feasible [21].

![Image of waveguide structure](image_url)

**Fig. 2.** (a) Schematics of the demonstrated microring resonators and Mach-Zehnder modulators are shown. The top SiO₂ cladding layer and the ultrathin SiO₂ diffusion barrier shown in (b) are omitted here for simplification. The dimensions are not in scale; (b) Cross-section of the waveguide structure at one arm of the modulator with typical dimensions. The different layers are Si (substrate), SiO₂ (claddings and diffusion barrier regions), LiNbO₃ (core and active region), Ta₂O₅ (loaded rib), Au (metallic contact). Shown also is a simplistic RF electric-field profile in the LiNbO₃ active region; (c) Top-view high-magnification optical microscope image of a fabricated ring-resonator with input and output bent bus waveguides; (d) SEM image of cross-section of a fabricated waveguide.

Since then, significant improvements in bonding techniques allow bonding at room temperature. Thus, fabrication of thin films of LiNbO₃ on silicon substrates is possible, as the difficulties of cracking that exists at elevated temperatures (due to different thermal expansion coefficients between silicon and LiNbO₃) are avoided.

The processing steps proposed and demonstrated here are summarized in Fig. 3. The highly repeatable and reliable process proposed here uses ion implantation and room-temperature wafer bonding to transfer a thin layer of LiNbO₃ to a silicon substrate coated with a thermally-grown SiO₂ buffer (cladding) layer. After the room-temperature initial bonding, a thermal process at 200°C is employed to not only slice the LiNbO₃ wafer at the peak position.
of the implanted ions but also to improve the formed bonding. Chemical-mechanical polishing (CMP) is applied on the films in order to achieve the smooth surfaces needed for high-quality optical waveguides. Figure 3(e) shows an image of a 3” thin film of bonded LiNbO₃ to a 4” silicon wafer with no evidence of cracking or other bonding issues.

Using silicon substrate is not only important for future integration with silicon electronics and photonics, but also significantly simplifies the processing of LiNbO₃ devices. For example, it is well-known that, due to extremely low thermal conductivity of LiNbO₃ and extremely high level of pyroelectric charges, thermal cycling of the material is very difficult. Silicon, on the other hand, is a very versatile material for processing. It can easily go through temperature cycling without any problem. Hence, various processing steps can be performed easily. Also, since the volume of the LiNbO₃ thin film is very small, the formation of pyroelectric charges does not cause sparking.

Attaining the discussed thin films of LiNbO₃ is critical for vertical optical confinement in submicron waveguides. For lateral confinement in the waveguides, an etching technique may be employed. However, etching LiNbO₃ is very hard and it might be impossible to achieve the ultralow surface roughness required for low-loss waveguides. Ion beam milling [21–23], and wet etching [24] are some of the techniques pursued for achieving LiNbO₃ ridge waveguides. The latter technique has been more successful in achieving reasonably low-loss waveguides [24]. However, non-vertical sidewalls, low etch rates and undercutting are common issues of wet etching recipes. As a result, the waveguide widths are typically several microns and hence tightly-confined submicron waveguides cannot be achieved. Also, accurate control of small feature sizes, like the submicron gaps required for coupling in and out of microring resonators, is hardly possible by wet etching.

We have recently developed a novel method for fabrication of nanophotonic devices in Ta₂O₅ using selective oxidation of the refractory metal (SORM), tantalum (Ta) [25]. We have shown that this method eliminates the surface roughness and also allows fabrication of Ta₂O₅ waveguides and couplers with submicron gaps easily [25]. As mentioned, Ta₂O₅ has a refractive index roughly matched to that of LiNbO₃ and hence it can be used as a rib-loaded layer in combination with a LiNbO₃ slab layer to form a composite ridge waveguide (see Fig. 2).

In the demonstrated fabrication process, first, an ultrathin (30 nm) layer of SiO₂ is deposited on LiNbO₃-on-Si wafers as a diffusion barrier to prevent out-diffusion of oxygen from LiNbO₃ in the Ta oxidation step (COMSOL™ simulations confirm that the existence of this ultrathin SiO₂ layer does not disturb the optical mode of the waveguides). Then, Ta is deposited on LiNbO₃ thin films that are prepared by the explained crystal ion slicing method. A plasma-enhanced chemical vapor deposition (PECVD) SiO₂ mask is then patterned on tantalum by lithographic techniques for selective oxidation of Ta at 520°C. After oxidation, a composite rib-loaded waveguide is formed consisting of Ta₂O₅ ridge layer and LiNbO₃ slab layer. The mask layer is subsequently removed, the remaining non-oxidized tantalum layer is dry-etched by a chlorine-based recipe, and the device is covered with SiO₂ or other materials for passivation. In the next step, the top cladding layer is etched and metal electrodes are deposited or electroplated to form a device structure using standard fabrication techniques. Oxidation of Ta to form Ta₂O₅ could cause stress, which is disadvantageous for processing. However, since the waveguide width are very narrow, the oxidation step does not create wafer bending as might be anticipated. Figure 2(d) shows a scanning electron microscopy (SEM) image of a fabricated optical modulator.
3. Design of prototype devices

Having established the fabrication process described in the previous section, optical waveguides, Mach-Zehnder modulators and microring resonators were designed. A refractive index value of 2.1 to 2.2 for Ta$_2$O$_5$ layers were measured in the 1550 nm range by ellipsometry techniques. It is noted that the dispersion properties of Ta$_2$O$_5$ is dependent on the preparation method, as reviewed elsewhere [26]. For future applications, such as nonlinear optical effect that require phase-matching, the material dispersion of Ta$_2$O$_5$ versus LiNbO$_3$ must be carefully accounted for in the waveguide design. Nonetheless, for the present demonstration, as long as the indices of the two materials at 1,550 nm are within ± 0.1 of each other the waveguides can be properly designed according to our COMSOL simulations.

In order to achieve small bending radii using this geometry for telecommunication wavelengths, slab layers of ~400 nm thickness with rib height of ~200-400 nm are required (see Fig. 2(b)). Figure 4(a) shows the calculated optical mode for a 200-nm-tall, 1-µm-wide Ta$_2$O$_5$ rib on a 400-nm LiNbO$_3$ slab layer with 4-µm gap between the electrodes shown in white. Calculation results using COMSOL™ show negligible bending loss for devices with bending radius of approximately 100 µm for this structure. Bending radius of 50 µm is also possible using a 300-nm LiNbO$_3$ slab height. Further reduction of bending radius is possible at the expense of lower confinement of the optical mode and less power overlap with the LiNbO$_3$ slab region. As can be seen in Fig. 4(a), the optical mode is confined to an area of approximately less than 1 µm by 2 µm. This is smaller, by at least an order of magnitude, compared to diffusion-based devices. Hence, it is expected that highly efficient nonlinear optical devices become practical using our proposed approach.

Another advantage of the highly-confined optical waveguides is that it is possible to place the metallic electrodes in much closer proximity of the waveguides without introducing metallic optical absorption. This leads to a lower voltage to attain the same radio-frequency (RF) electric field for EO modulation. Calculations show that the gap between the electrodes can be as small as 4 µm in this structure without significant absorption of light by the electrodes. This is smaller by a factor of 5 compared to conventional LiNbO$_3$ devices. As can be seen in Fig. 4(a), there is negligible optical power close to the metallic electrodes with 4 µm gap in between. The crystalline orientation of the LiNbO$_3$ layer can be chosen to be Y- or X-cut, since in either case, electrodes can be conveniently placed laterally and an electric field along the Z-axis can be applied to the nonlinear material for EO modulation. In this work, Y-cut LiNbO$_3$ was chosen. Figure 4(b) shows the calculated RF field for the modulator by applying 1 V of bias to the electrodes. Also, the electrodes are in direct contact with the LiNbO$_3$ thin film layer. This design eliminates the problem of weak electric field previously...
reported in the LiNbO$_3$ region in Z-cut thin-film devices [21] due to very large dielectric constant difference that exists between SiO$_2$ and LiNbO$_3$. As can be seen in Fig. 4(b), the resulting electric field is approximately $2 \times 10^5$ V/m, which is close to the value of $2.5 \times 10^5$ V/m, that is, when uniform electric field with a gap of 4 µm is assumed. The estimated half-wave voltage, $V_{\pi}$, of this design is 1.5 V.cm, which is about 10 times lower than commercially available devices.

![Diagram](image)

**Fig. 4.** (a) Calculated optical mode profile with 400-nm-thick lithium niobate and 200-nm-tall, 1-µm-wide tantalum pentoxide ridge waveguide; (b) Calculated RF mode profile with 4 µm gap between electrodes. High confinement allows short gaps between electrodes without introducing absorption loss.

### 4. Performance of demonstrated prototype devices

As a first demonstration of a photonic device using this technology, microring resonators were considered. Microring resonators have a wide range of photonic applications and are also ideal for accurate measurement of waveguide propagation losses. Resonators with high quality factor, $Q$, have been demonstrated in silicon and other materials, such as polymers and glass [27–30]. It is possible to achieve ultracompact EO modulators using microring resonators, as demonstrated first on polymers [30]. Using thin films of LiNbO$_3$ bonded to LiNbO$_3$ substrates by an adhesive polymer, and by employing ion milling for etching the waveguides, and very low $Q$ microring resonators have been demonstrated in the past [23]. Here, much higher $Q$ values and relatively low-loss waveguides are reported on the proposed platform, as follows.

Microresonators with two coupled waveguides were fabricated as shown in Fig. 2(a) and 2(c) in our proposed platform. Several devices with different diameters and coupling gaps were designed and fabricated. Curved input-output waveguides (buses) were used to study the impact of bending and the microresonator on the optical transmission as a function of wavelength. The coupling and bending losses were calculated and designed using finite element modeling tools. Figure 2(c) shows an image of a fabricated photonic circuit with a ring radius of 150 µm. The devices were characterized using a tunable semiconductor laser. Light was coupled into the chips by a lensed fiber and coupled out via an objective lens into a low-speed photodetector. Standard micromanipulator stages were used for manual alignment. Figure 5(a) presents the measured transverse-electric (TE) mode transmission spectrum of a fabricated microresonator, with 150 µm radius, in the vicinity of the 1550-nm telecommunication wavelength range. The bending loss for this radius is negligible as was discussed in designs of Section 3. The estimated unloaded $Q$ obtained by curve fitting [30] is $7.2 \times 10^4$ and the unloaded finesse is 50. The extracted propagation loss is 5 dB/cm. The loaded $Q$ of the device presented in Fig. 5(a) is $4.5 \times 10^4$, which is over an order of magnitude higher than previous results [23]. The somewhat high value of loss could be due to material
absorption or scattering of light in the Ta₂O₅ ridge region, as we have seen in Ta₂O₅ waveguides on silicon too [25]. One possible explanation is that during deposition of the Ta layer, there is a high percentage impurities in Ta and hence the loss is attributed to this impurity in the rib layer. Another possible explanation is that Ta₂O₅ is prone to polycrystalline forms with α- and β-phases, whose grain boundaries can lead to scattering loss. Further investigation of these and other possible causes is underway.

![Graph](image1)

**Fig. 5.** (a) Transmission spectrum of a microresonator with 300 µm diameter for the TE mode around 1550 nm wavelength. The resonance linewidth is 2.7 GHz; (b) Applied sawtooth electrical signal and the measured modulation response of a 6-mm-long Mach-Zehnder modulator. The measured $V_\pi$ is 6.8 V.

To demonstrate improvement in the functionality of a widely used active device using this technology, Mach-Zehnder modulators consisting of two $Y$-junctions and two straight 6-mm-long arms were designed and fabricated on $Y$-cut thin films. Push-pull electrodes were utilized, as shown in Fig. 2(a). The gold (Au) electrodes were deposited and patterned by standard lithographic techniques to achieve the final structure shown in the SEM image of Fig. 2(d). The devices were characterized by applying a sawtooth modulation voltage around 1 kHz using the same setup as discussed above. It was confirmed that no current flows through the electrodes, as expected from the dielectric nature of SiO₂ and LiNbO₃. Figure 5(b) shows the applied low-frequency electrical signal and the measured optical modulation signal for a device with 7 µm gap between the electrodes.

As can be seen in Fig. 5(b), the $V_\pi$ of the device is 6.8 V. Since the electrodes are 6 mm long, the measured half-wave voltage-length product, $V_\pi L$, is equal to ~4 V.cm. This record value of $V_\pi L$ for LiNbO₃ is lower, by at least a factor of 3, than the best optimized diffusion-based modulators [31]. The simulated value of $V_\pi L$ (using the EO coefficient, $r_{33}$, of LiNbO₃ single crystals) is ~4.1 V.cm for this device (this is higher than the aforementioned value of 1.5 V.cm because of larger gap between the electrodes and slightly thicker Ta₂O₅ layer used in the fabricated devices compared to the simulations of Section 3). The agreement between experimental and simulated value of $V_\pi L$ indicates that the extracted value of $r_{33}$ is approximately 31 pm/V, which is very close that of LiNbO₃ single crystals. This means that the crystalline quality of the LiNbO₃ layers is not degraded after annealing the ion implanted thin films.

When the transmission in Fig. 5(b) is plotted in logarithmic scale, an extinction ratio (ER) of approximately 20 dB is measured in the modulator. This high ER value, possible through the EO effect, is a clear advantage over silicon optical modulators, based on free-carrier plasma effect, which typically suffer from low ER in the modulation response [32]. Also, a fit to the results of Fig. 5(b) confirms that the response is sinusoidal, as expected in a Mach-
Zehnder-type device. The fit error is less than 3% with respect to the applied sawtooth voltage.

As was discussed in Section 3, with more optimized design, smaller electrode gaps and higher fabrication tolerances, it is predicted that $V_{\pi}L$ as low as 1.5 V.cm is feasible, which will be approximately 10 times lower than the state of the art. By combining this reduction in $V_{\pi}L$ of the device with folded-waveguide schemes, which can become possible for the first time in LiNbO$_3$, it will be then practical to reduce the footprint of LiNbO$_3$ Mach-Zehnder optical modulators by two orders of magnitude to less than 0.5 mm $\times$ 0.5 mm and achieve a $V_{\pi}$ of $\sim$1 V.

The high-speed modulation properties of the device using non-RF-terminated electrodes were also measured using a network analyzer. The devices are certainly functional up to several GHz according to the measured $S_{21}$ parameter of the modulated signal. However, full characterization of the modulation properties and extraction of the modulation bandwidth requires careful design and fabrication of devices with travelling-wave electrodes and RF termination, which is beyond the scope of this work.

5. Conclusions

In conclusion, the present work demonstrates a novel integrated photonic platform based on thin films of LiNbO$_3$ on silicon substrates fabricated by room-temperature bonding and SORM methods. The platform allows significantly improved performance for various photonic devices based on LiNbO$_3$. Here, improvements for a typical passive optical device (microring resonators) and a typical active device (optical modulators) are reported. It is expected that high-performance nonlinear devices for second-harmonic generation, parametric amplification, and entangled photon generation can be attained on the platform in the future.

Acknowledgment

The work is being supported by the U.S. Office of Naval Research (ONR) Young Investigator Program (YIP) under the Grant Number 11296285.