Lightwave Circuits in Lithium Niobate through Hybrid Waveguides with Silicon Photonics

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We demonstrate a photonic waveguide technology based on a two-material core, in which light is controllably and repeatedly transferred back and forth between sub-micron thickness crystalline layers of Si and LN bonded to one another, where the former is patterned and the latter is not. In this way, the foundry-based wafer-scale fabrication technology for silicon photonics can be leveraged to form lithium-niobate based integrated optical devices. Using two different guided modes and an adiabatic mode transition between them, we demonstrate a set of building blocks such as waveguides, bends, and couplers which can be used to route light underneath an unpatterned slab of LN, as well as outside the LN-bonded region, thus enabling complex and compact lightwave circuits in LN alongside Si photonics with fabrication ease and low cost.

Lithium Niobate (LN) was once considered the most promising of materials for integrated optics but despite a rich set of properties, the technology of LN integrated optics has not evolved as much as integrated optics in III-V semiconductors and silicon (Si) photonics. Although high performance stand-alone LN devices have been shown and a technique of ion-sliced thin-film LN has been developed, the technology of LN integrated optics has continued to rely on traditional waveguide fabrication techniques based on ion-exchange, diffusion and serial writing, all of which are very different from the modern lithographic techniques and foundry processing available in Si or III-V photonics.

To address this problem, we develop an approach to developing hybrid waveguides in LN based on a two-material core cross-section, consisting of few-hundred nanometer single-crystal thin films of Si and LN bonded face-to-face. We used manufacturer-provided Si-on-insulator and LN-on-insulator wafers which have a SiO₂ cladding layer which is a few microns thick, and a handle material (Si and LN, respectively) for the substrate which is several hundred microns thick. We first pattern all features required for waveguiding in the Si wafer using deep ultraviolet (DUV) lithography (see Methods section). This allows much finer features to be patterned than is possible in LN (especially in comparison to conventional thin film LN waveguides). Since LN is not a CMOS-compatible material and is not processed in CMOS foundries, we developed designs which allow all the waveguiding circuitry to be defined in Si, requiring only a single back-end process step of bonding LN to form the functional chip. DUV lithographic fabrication of Si photonic features is more precise, scalable and manufacturable than the traditional waveguide-fabrication techniques in LN, and the LN layer can be left as an unpatterned slab that is then bonded to the patterned Si. By not patterning, etching or sawing LN, its material properties are kept pristine.

Figure 1 shows images of a bonded chip whose dimensions are that of a typical field size of a stepper projection DUV lithography system (few centimeters squared). Upon bonding, a hybrid waveguide is formed, in which the geometric dimensions of the Si features and LN film dictate how the optical mode is distributed between the Si and LN layers. Techniques have been developed in the past decade for bonding LN of various orientations to Si wafers without incurring thermal stress mismatches. Bonding achieves much higher quality and better optical properties than growth of LN on Si using sol-gel processes or chemical vapor deposition. We directly bonded the LN chip to the Si chip i.e., without any intervening polymeric ‘glue’ layer as used in some approaches, thus permitting the maximum control over the mode distribution.
As will be discussed below, light propagates mainly in the silicon layer in certain sections of the layout, and primarily in the LN layer where desired, and makes transitions between the two layers at several locations while remaining in the transverse-electric (TE) polarized single-mode regime, which is highly desirable for Si photonics. Thus, we can also design devices that are outside the Si-LN bonded region and behave entirely like conventional Si photonics. In this way, the technology for Si photonics can be leveraged to enhance LN integrated optics, and vice versa.

The main advantages of this approach are: (a) the requirements on LN fabrication are reduced to a minimum, i.e., a single bonding step to the manufacturer-supplied wafer after all silicon patterning has been completed (etching LN is possible but is technologically less mature than etching Si, which is available in every foundry process); and (b) both the cross-sectional mode area and the length of components are greatly reduced, compared to traditional LN ion-exchanged or diffused waveguides, allowing complex circuits to be realized in a small area. The tradeoffs are that: (a) the bonding step should be performed at a low temperature since Si and LN have different coefficients of thermal expansion, and (b) the resulting hybrid modes have a higher refractive index dispersion compared to low-index contrast (e.g., doped-glass) integrated optics, and thus, components will be optimized for a desired vacuum wavelength range, e.g., the telecommunications band around 1550 nm.

**Hybrid Modes and Mode-Transition Tapers**

The dimensions of the Si features and LN film determine what fraction of the optical mode resides in Si and in LN. Two distinct waveguide cross-sections, labeled ‘A’ and ‘B’, are selected, as shown in Fig. 2a, and used in the microchip layout. These cross-sections vary only in the width of the Si structures, which allows for convenient fabrication in a single step of lithography. The numerical values of the widths and heights chosen here are suitable for wavelengths between 1530 nm and 1565 nm (i.e., the telecommunications C-band).

Cross-section A consists of 650 nm wide and 150 nm tall Si features, bonded to LN. The lowest-order mode of the waveguide is quasi-TE-polarized and is similar to the quasi-TE0 mode in conventional silicon photonics (see Fig. 2a). Wider waveguides are close to becoming multi-modal, which is undesirable. A waveguide using cross-section A can transition from an SiO2-clad silicon photonic section to the bonded Si-LN region, as shown in Fig. 1c, with less than −0.3 dB loss calculated by numerical simulation (Lumerical software package). We have not experimentally confirmed the mode-transition loss at this time. As shown by Fig. 2b, waveguides using cross-section A can support compact bends with radii of 3–5 μm without incurring bending losses higher than that of a standard rib waveguide (650 nm × 220 nm surrounded by SiO2, labeled ‘Si/SiO2’ in Fig. 2b) with a radius of 0.5–1 μm.
Cross-section B consists of 320 nm wide Si features at the same height as cross-section A. With an air upper cladding, this waveguide is unable to support a waveguide mode by itself, and thus requires the bonded LN layer to support a well-defined mode at C-band wavelengths. Cross-section B cannot be used for compact low-loss bends (see Fig. 2b). Instead, it is used when we want the light to interact with the crystal properties of LN; otherwise, cross-section A is used to route light on the hybrid chip. Therefore, it is desirable to maximize the fraction of light in LN for the mode in cross-section B. The confinement factor is defined as follows:

\[ \Gamma = \frac{\int \int_{\text{LN}} (E \times H^* \cdot \hat{y}) \, dA}{\int \int (E \times H^*) \, dA} \]

where \( \hat{y} \) is the direction of light propagation and the range of integration in the integral in the numerator is restricted to the LN region. In waveguides using cross-section A, \( \Gamma_{\text{LN}} \approx 32\% \) whereas in waveguides using cross-section B, \( \Gamma_{\text{LN}} \approx 87\% \). The transition between the two cross-sections is discussed below.

A modified version of cross-section A, in which SiO\(_2\) replaces LN as the upper cladding, is used outside the LN bonded region to demonstrate all-Si components made on the same platform and at the same device level. Another cross-section with a reduced Si width of 180 nm is used for couplers at the edge of the Si chip, as is commonly used in Si photonics\(^{27}\), and can also be fabricated in the same step.

All these waveguide shapes are simple rectangles without relying on slots, tilted sidewalls or other difficult-to-fabricate shapes. There is no patterning in the LN layer which eliminates many of the challenges faced in the past\(^{13}\). Conceptually, the waveguide structure is similar to that of the strip-loaded waveguide film studied in the 1970s\(^{28}\), but scaled to the deep sub-micron regime. The modal area of cross-section A (0.22 \(\mu\)m\(^2\)) is, in fact, smaller, and that of cross-section B (1.25 \(\mu\)m\(^2\)) is only slightly larger, than those of the smallest-area waveguides reported in LN, fabricated by the ion-milling technique\(^{29}\).

As shown in Fig. 1d, large rectangular areas were defined in the Si device layer at distances of about 30 \(\mu\)m from the waveguide edge. These “bonding pads” between the Si and LN chips are far from the waveguide core and serve no optical purpose, but instead provide a large surface area for bonding. They are precisely at the same height as the Si rib features, since they are formed in the same lithographic step. They are similar to “dummy fill” features inserted to assist in chemical-mechanical polishing, but without a fragmented pattern. The etched
trenches between the Si ribs and the bonding pads not only provide optical confinement but may assist in bonding by defining convenient outgassing channels, and for local stress relaxation.

Along the direction of light propagation, adiabatic tapered transitions were defined in the Si layer (see Fig. 3a) as a linear change in the Si rib width over a distance of 150 μm. The quasi-TE-polarized mode TE₀ has the highest effective refractive index in cross-section A (and is used extensively in conventional Si photonic waveguides, which are wider than they are tall). In cross-section B, it is actually the quasi-TM-polarized mode TM₀ which has the higher refractive index. This is due to both the anisotropic properties of LN (LN has a lower material index along the z-axis) and the low index lateral air cladding on either side of the Si. However, the taper-induced coupling between these modes is zero to first order because the electric field of the former is a symmetric mode, and that of the latter is an anti-symmetric mode. Thus, we are able to draw the waveguide down to a narrow width that pushes a very large fraction of the light into LN while maintaining its state of polarization all the way from the feeder waveguides. For the Si rib widths used in this design, the higher-order quasi-TE polarized mode labeled TE₁ in Fig. 3b) is not guided; however, by using wider Si rib widths, tapers can couple between this anti-symmetric mode and the TM₀ mode, which may be useful for polarization rotators etc. Thus, compared to other hybrid Si-LN structures, our design achieves the highest TE-polarized (lowest-order) mode-fraction in LN while also providing a pathway for integration to Si photonics by first coupling light into cross-section A (which is similar to a traditional Si photonics cross-section), and then transitioning into cross-section B adiabatically. Attempting to couple from an external input to the quasi-TE mode in cross-section B would render the device very susceptible to roughness and bending losses, because it is not the fundamental mode. Widening the Si waveguide effectively pulls the light back into Si again, and, because it remains in the TE-polarization, allows for the benefits that have been realized by Si-only waveguides, such as tight bends and compact directional couplers, among others.

Another important consideration is that the propagation loss of a hybrid mode can increase significantly due to lack of transverse confinement, if the LN thickness falls within a range of values, depending upon the Si rib dimensions, at which one of the vectorial field components becomes slab-like (in the LN region). This effect, studied and measured in standard rib waveguides, has recently been highlighted for quasi-TE modes in x-cut LN proton exchanged channel waveguides. Similarly, in our configuration, it originates from the TE ↔ TM mode coupling at the Si strip boundaries. Quasi-TE mode leakage then occurs when the modal effective index becomes smaller than that of the TM slab mode in LN, i.e., when the minor TM-polarized field is no longer a bound mode and propagates in the LN planar waveguide. Due to the LN birefringence, this condition cannot be met for the quasi-TM modes which is therefore immune to leakage. This is shown in Fig. 3c: for LN thicknesses...
between 850 nm and 1750 nm (not used in our present design), the propagation loss would be significantly higher than at other thicknesses. A similar behavior is observed when the width of the Si region is reduced and the LN thickness is fixed, as in Fig. 3d.

**Waveguides, Directional Couplers and Photonic Circuits**

Photonic circuits can be assembled from the basic building blocks of waveguides and directional couplers. Hybrid waveguides of lengths between 1.8 cm and 4.6 cm were fabricated with the majority of the length consisting of waveguides using cross-section B. Cross-section A was used at the semi-circular bends, in order to fit the longer waveguides into a compact footprint using “paperclip” structures. The longest waveguide involves 10 transitions between cross-sections A and B. Since the edge facets were roughly diced and not polished, the fiber-to-chip insertion loss was high (about 9.5 dB without index-matching liquid) and non-uniform. As shown in Fig. 4, by measuring transmission versus length across several chips, we were able to build up an ensemble of measurements from which a propagation loss of $\pm 0.32 \, \text{dB/cm}$ was extracted at 1550 nm wavelength with only minor changes across the wavelength range 1530 nm to 1570 nm. At this time, we are unable to separate the bending loss from the straight waveguide propagation loss, but the former is expected to be very small based on the large bending radius of 25 $\mu m$. Numerical simulations reported in Fig. 2b suggest that the bending loss should drop to less than 0.001 dB per $90^\circ$ bend for bending radius greater than 3 $\mu m$ using cross-section A.

By way of comparison, the propagation loss of the same Si waveguides with 3 $\mu m$ SiO$_2$ top-cladding (rather than LN) was measured to be $3.1 \pm 2.1 \, \text{dB/cm}$, indicating that bonding and incorporation of LN as the top cladding did not significantly worsen the propagation characteristics. In fact, the propagation loss is similar to that measured in rib Si photonic waveguides$^{30}$ despite the thinner Si layer in our structures.

The loss values in these hybrid Si-LN waveguides using cross-section B are significantly lower than other reported values, e.g., 16 dB/cm in etched thin-film LN waveguides$^{31}$ and 6–10 dB/cm in thin-film LN waveguides (600 nm thickness, not too different from the 750 nm thickness used here) with oxidized titanium stripe$^{35}$. Although the loss is still an order-of-magnitude higher than that of traditional in-diffused waveguides which have a much larger mode area, our circuits are also more than an order-of-magnitude more compact. Furthermore, we expect that with improved Si waveguide fabrication (e.g., roughness reduction), and filling of the air pockets on the lateral sides of the Si rib with a low-optical-loss gap-fill dielectric material, the overall propagation loss will decrease.

Directional couplers were defined by lithography in the Si layer, but act on the hybrid mode using cross-section A, with a gap of 0.4 $\mu m$ between the waveguide edges. The typical length was only 150 $\mu m$, compared to a typical length of about 5 mm for directional couplers with diffused or ion-exchanged waveguides. Because the mode in cross-section A resides primarily in Si, there was no measurable crosstalk at milliwatt power levels, unlike the traditional waveguide LN devices which are susceptible to photorefractive artifacts$^{36,37}$. However, long-term (>1 day) tests have not yet been performed since the chips are not fully packaged and we rely on manually-adjusted fiber coupling to the silicon waveguides.

Optical circuits can be designed if two fundamental parameters are known: the optical (modal, i.e., “effective”) refractive index of a waveguide, which determines the rate of accumulation of optical phase with distance, and the directional coupling coefficient of two adjacent waveguides. Both these parameters are functions of the optical wavelength. To measure these parameters and compare with numerical calculations, we designed an interferometric test structure (see Fig. 5) which can also perform several functionalities useful in integrated optics such as spectral filtering, interleaving or multiplexing/de-multiplexing for wavelength-division multiplexing (WDM). Such a device does not use microring or standing-wave (e.g., Fabry-Perot) resonators, in which the intensity enhancement (due to the infinite impulse response nature of the transfer function) may cause photorefractive

![Figure 4. Waveguide characterization.](image-url)
artifacts in LN. The circuit consists of several building blocks where the optical pathway is indicated by the red arrows and consists of four transitions, two directional couplers and twenty 90-degree bends, incurring a cumulative insertion loss of about -15 dB. (The circuit does not need to be so complicated to realize only a Mach-Zehnder interferometer, but showcases some of the capabilities of the platform.)

Discussion
To experimentally show the large difference in the effective modal refractive index between the A and B cross-sections, we measured two distinct MZIs in which the path imbalance of one arm with respect to the other was formed using waveguides of cross-section A and B, of length $L_A$ and $L_B$, respectively. In each case, the free-spectral range (FSR) of the MZI was approximately 10 nm near the central wavelength of 1550 nm. The Supplementary Information shows the 'Cross' (in 1 to out2 or in2 to out1) and 'Thru' (in 1 to out1 or in2 to out2) transmissions measured at the two output ports for each input port (a total of four combinations for each MZI structure) while the laser wavelength was varied between 1520 nm and 1620 nm, and describes the data fitting procedure.

Figure 5b shows the wavelength variation of the effective refractive index of the A and B waveguides. The two branches (cross-section A and cross-section B) are sufficiently far apart that the results confirm a clear distinction between the A (Si-like) and B (LN-like) guided modes. The group velocity dispersion (GVD) coefficients of the two modes at $\lambda = 1550$ nm are as follows: $D_A \approx -3100$ ps/nm-km for cross-section A, and $D_B \approx -4300$ ps/nm-km for cross-section B, which are of the same order-of-magnitude as that of a typical silicon photonic waveguide whose modal effective area is similar to that of cross-section A, $D_A \approx -1500$ ps/nm-km.

Figure 5c shows the wavelength variation of the coupling coefficient of a directional coupler which was formed using waveguides of cross-section A, with a gap of 0.4 $\mu$m between the waveguide edges. As may be expected, the change in the magnitude of the coupling coefficient over the wavelength range of 1520 nm–1620 nm is similar to the behavior seen in all-Si waveguides.

On the same chip, outside the LN-bonded region, waveguides and devices may be designed as usual in Si photonics, i.e., with SiO$_2$ cladding. Because of the high refractive index of Si, light is tightly confined for waveguides of cross-section 'A' whether LN or SiO$_2$ is used as the upper cladding. We designed and measured a Mach-Zehnder interferometer outside of the LN-bonded region, using waveguide with cross-section 'A' and with...
SiO₂ replacing LN as the upper cladding (and with SiO₂ side- and lower-claddings in our fabrication process), as reported in Fig. 6. Although our test chip shown in Fig. 1 was designed for LN covering nearly all of the Si surface, it is equally possible to design “mixed” chips with smaller-sized LN pieces, which combine traditional Si photonic components with hybrid LN-Si photonic components on a monolithic platform.

We have restricted this fabrication process for reasons of cost and complexity to exclude dopants and electrodes as part of the Si chip, which could be used for electro-optic effects. Simulations show that gold electrodes can be positioned directly on the LN thin-film layer (surface opposite to the bonded interface to Si) at a lateral distance of only 0.4 μm from the Si edge for cross-section A and 4 μm from the Si edge for cross-section B, for an estimated additional propagation loss of 0.1 dB/cm. Alternatively, electrodes can be fabricated on the LN layer after substrate removal, following the traditional approach.

Conclusion
These results show that, even though LN is not a CMOS-compatible material, foundry-fabrication technologies can play a very useful role in a new generation of LN integrated optics. While LN has always been a desirable material for its nonlinear and electro-optic properties, it has not been possible in the past to make compact and complex waveguide circuits as is possible nowadays in Si photonics using precise and highly-repeatable DUV lithography. We have shown a suite of hybrid building blocks from which optical circuits can be assembled alongside traditional Si photonics components. While improved wafer-scale bonding techniques are being developed by industry for commercial applications, here we have shown chip-scale direct bonding of chips that are a few centimeters squared (the size of a typical field size of a DUV stepper lithography system), with enough bond strength to permit dicing and simple packaging for test and measurement. A similar approach may also be applied to design and investigate optical circuits using other thin-film materials in place of LN, leveraging the advanced foundry fabrication capabilities of Si photonics as a waveguiding template for the hybrid modes without needing to pattern the thin-films.

Methods
Fabrication. The silicon features were patterned using DUV lithography on silicon-on-insulator wafers with a substrate oxide thickness of 3 μm at Sandia National Laboratories. A blanket etch was used for height reduction of the device layer from 250 nm to 150 nm followed by patterning to define waveguides and bonding pads simultaneously (i.e., at the same height). The thin-film LN on insulator wafers were procured from a commercial source (NanoLN Jinan Jingzheng Electronics Co. Ltd.), with a nominal top LN thickness of 750 nm, silicon oxide buffer of thickness 2 μm and LN handle of thickness 0.5 mm, diced into chips of size 2.1 cm × 1.7 cm. The materials properties of such thin-films have been documented elsewhere.

Bonding. There are several techniques that could be used for bonding Si to LN, most of which rely on managing the temperature budget of the process, in view of the different thermal coefficients of expansion of the two crystalline materials. In this work, we used a room-temperature bonding process without any intermediate layers, i.e., direct bonding, which relies on van der Waals or hydrogen bonding. The cleaning process was as follows: 1) a solvent clean of the Si and LN chips in an ultrasonic bath; 2) a buffered oxide etch of the Si chip only for 4 seconds; 3) a piranha acid (2:1, H₂SO₄:H₂O₂) clean of the Si and LN chips for 5 minutes, followed by a two-stage water bath (10 sec. in first bath, 1 min. in second bath); 4) N₂ blow dry both chips; 5) plasma surface
activation (PSA) of both chips with O₂ gas for 45 sec. at 200 W and 200 mT in a Technics PEIIB; 6) water bath for both chips immediately after the PSA, for at least 1 min.; 7) N₂ blow dry both chips. After drying, the chips were aligned manually such that the z-axis of the (x-cut) LN was perpendicular to the long axis (y) of the optical waveguides. Since our direct bonding technique does not rely on high pressure, bonding was initiated at room temperature by gently pressing and sliding outwards from the center using plastic tweezers or the backside of a clean room swab. After bonding, approximately 825 nm of SiO₂ was sputtered at room temperature (Denton 635, 400 W, 5 mT; growth rate approximately 275 nanometers of SiO₂ per hour).

We performed a bond strength analysis using an Imada force gauge and test stand to measure tensile “pull-apart” force.44 The average bond strength measured over a few test bulk Si-LN chips was 0.31 MPa for chips cleaned using an ultrasonic cleaner, and 0.37 MPa for chips cleaned using a megasonic cleaner. While the bond strengths are not as high as commercially-bonded wafers, these results eliminate the possibility of the sputtered oxide being an ad-hoc “glue” holding the wafers together. These bond strengths were sufficient for handling and testing the chips, which have remained bonded for more than four months without any special storage techniques. However, additional processing to achieve stronger bonds will be required for commercial applications, which may involve proprietary recipes.

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Author Contributions
P.O.W. designed the photomask, did the bonding, and performed the measurements. M.S. assisted in the measurements and performed the data fitting. Both P.O.W. and M.S. performed numerical simulations. C.T.D., A.L.L., A.T.P. and A.L.S. performed the silicon foundry fabrication at the Microsystems and Engineering Sciences Applications (MESA) facility, Sandia National Laboratory. V.S. contributed information, insights and techniques regarding thin-film LN. S.M. developed the hybrid Si-LN integration concept and supervised the project. All authors read and contributed to the manuscript.

Additional Information
Supplementary information accompanies this paper at http://www.nature.com/srep

Competing financial interests: V. Stenger is an employee of SRICO Inc., a small business that manufactures and sells thin-film lithium niobate components. Other authors report no competing financial interests.

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