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ABSTRACT
This work proposes and demonstrates the concept of a complementary metal-oxide-semiconductor (CMOS)-compatible electrophotonic monolithic refractive index sensor in which a Si-based light source is directly integrated. The device consists of an embedded light emitter, a waveguide, a sensing area to place an analyte, and a photodetector. The behavior of the system was modeled and simulated using light propagation and semiconductor simulation software. Experimental devices were fabricated using all standard CMOS materials and procedures, and the tests showed changes in detected photocurrent related to the refractive index of the material in the sensing area, demonstrating the potential of the completely Si-based CMOS-compatible electrophotonic systems in the development of fully integrated sensors.

I. INTRODUCTION
Electrophotonics (EPh) introduces the concept of simultaneously controlling and manipulating light and electricity, involving the use of both electrons and photons in a single device according to convenience, as opposed to optoelectronics, in which dedicated photonic and electronic devices are coupled. For instance, in EPh, the insulator of a MIS phototransistor can be, at the same time, the core of a waveguide conducting light in which case the device is not just transducing, not only electronic, nor exclusively photonic but neither a traditional coupling of two devices.

One of the most promising applications of EPh, aside from communications or data managing, is in the sensing field, as it opens the door to monolithically integrate most of the necessary components, including electronics and photonics, as well as sample preparation and waste storage. This would represent a significant step forward in, for instance, the development of lab-on-a-chip (LOC) systems, as it is often regarded as the state of the art in photonic sensing; this is mainly true for advances related to the miniaturization of the light-analyte interaction system and fluidic design and integration, but there are still many challenges to overcome, related to the integration of circuitry and reliable and portable light sources.

However, in order to exploit EPh in a cost-effective manner for this application and any other application, it is imperative to use the existing integrated circuit (IC) fabrication infrastructure for its development. This means that the EPh circuits must ascribe to the strict restrictions imposed by the complementary metal-oxide-semiconductor (CMOS) technology, including fabrication processes and materials, notably Si-based. Strategies to fit into these margins include the use of silicon on insulator (SOI) and silicon nitride-based waveguides (WGs). Nevertheless, the use of these platforms for fully monolithic EPh faces a bottleneck when the light source is addressed, as it is necessary to couple an external light source through fiber optics and gratings, to fabricate hybrid systems butt-coupling the emitting device, or to use heterogeneous integration of III-V semiconductors; none of the former are truly compatible with circuitry integration using
standard CMOS fabrication processes; they all are more expensive, and many present significant light-coupling and packaging challenges.\textsuperscript{18}

Our group recently showed an electroluminescent visible light source directly embedded into a silicon nitride waveguide integrated to a photodetector.\textsuperscript{19} This emitter-waveguide-detector (EWD) system is the first of its kind to the best of our knowledge, as it was fabricated using solely CMOS compatible materials and processes, and no need for external light sources was demonstrated, thanks to a light emitter based on silicon-rich oxide (SRO). The concept introduced in Ref. 19 involves the possibility of distributing light sources across electrophotonic circuits, operating alternatively using photons or electrons as needed, and its characteristics allow it to be easily adapted to create a planar waveguide-based sensor. This cutting edge approach is still to be fully modeled in the frame of its self-contained nature, and the mechanisms taking place in it as well as in its limits must be understood in order to advance toward possible applications.

This work introduces a novel fully monolithic and integrated electrophotonic device based on a EWD scheme with a visible light source fully integrated and obtained using exclusively CMOS-compatible processes and materials. Simulations of the behavior of light in the system based on the characteristics of its conforming elements and their interrelations were performed to understand its operation. A proof of concept system was fabricated and tested, confirming the expected operation from simulation results and demonstrating the possibility of distinguishing materials with different optical characteristics. This work proofs the concept of a photonic sensor using an embedded light source compatible with the integration of processing electronics, demonstrating the possibility of using SRO-based EPh for the full integration of all the main stages of a sensor\textsuperscript{20} including transduction, signal processing, and result interpretation in a single-chip.

II. RESULTS AND DISCUSSION

A. System and principle of operation

A conceptual representation of the monolithic emitter-waveguide-detector scheme in which the sensor is based is presented in Fig. 1. The main novelty of the proposed system is the direct embedding of the light source while maintaining its full compatibility to materials and techniques used for standard electronics, enabling its fabrication in well-established IC foundries and the future direct integration with driving and processing electronics. The scheme is based on a planar EWD with a dual layer SRO-silicon nitride light emitting capacitor (LEC), which is seamlessly integrated in a planar silicon nitride waveguide conducting the light to an integrated photodiode. The planar WG is cladded with SiO\textsubscript{2} on top and bottom. A section of the top cladding is exposed to allow the contact with a substance to be analyzed. The characteristics of the light emitter spectrum and of the WG transmission make this EWD a very good candidate for evanescent field-based optical detection. The photodiode detecting the light is electrically accessed by an upper Al pad (anode terminal) and the bottom of the substrate (cathode terminal). The light emitter is electrically pumped using two Al pads fabricated on the top of the substrate, one directly over the gate of the LEC and the other connected to its bottom through a heavily doped region. Section III C describes the fabrication process in detail.

When the light emitter is stimulated, the light produced is directly injected into the WG, and much of the evanescent field propagates through the cladding. In order to have a sensor, the cladding is interrupted at some point to define the sensing region of the device by a trench able to accommodate an analyte in the upper part. The interaction of the analyte with the propagating light will modify the way it is transmitted, and different analytes can result in different light intensities being detected by the photodiode.

In the end, the system delivers a value of photocurrent in the photodiode, which depends on the medium in the sensing area. Its general behavior will be dictated by three main interrelated phenomena and its characteristics: the light emission and injection into the waveguide (spectrum), the transmission of light through the waveguide and its interaction with the analyte (field configuration and transmittance), and the conversion of arriving light into detectable electrical current by the photodiode (responsivity).

Modeling and controlling all phenomena taking place in the system is a complicated task, and its monolithic nature makes it nearly impossible to characterize its main elements individually to later relate their behaviors. Then, the system must be analyzed as a whole considering the several parameters, phenomena, and models taking place simultaneously and their close interrelation.

B. Light propagation and interaction with analyte

To model and simulate the behavior of light through the system, it must be addressed that the LEC presents a continuous emission spectrum, while the simulations of light insertion are generally limited to a single wavelength $\lambda$. The normalized light emission spectrum of the fabricated LEC according to studies on the active material, which can be considered the input light, is presented in Fig. 2. More detailed studies on the emission characteristics and mechanisms can be found in Refs. 21 and 22.

In order to approximate how the injected light propagates through the system considering the continuous spectrum,
simulations were performed for wavelengths from 400 nm to 800 nm with a step of 5 nm. This covers both the range of the LEC emission\(^2\) and the range in which it can be transmitted through the waveguide.\(^3,24\) The simulation software can handle the transmission characteristics of the WG material, but an input power of the light must be declared by the user. To account for the different intensities in which light with a specific wavelength is emitted, the spectrum was normalized to its maximum value and the input power for each wavelength was multiplied by the correction factor corresponding to the crosses in Fig. 2. This allows adjusting the relative contribution for the total transmitted power accordingly with the specific system transmittance for each wavelength.

The propagation of light in the waveguide of the system in Fig. 1 was simulated for each sampled wavelength. Figure 3 shows a longitudinal section where the materials, boundaries, and ports are defined. The length of the device was scaled down. The thicknesses of the core and cladding were declared according to the actual physical dimensions of the device. Three additional regions were included: silicon substrate at the bottom of the lower cladding, air at the top of the upper cladding, and the sensing area, which is obtained after removing the SiO\(_2\) at the upper cladding in order to modify the propagation characteristics, defining this region as a material with the refractive index of air and water. Optical modes were determined from modal simulations. Symmetric and asymmetric waveguides were analyzed. Before the fabrication of the sensing region, the waveguide can be considered symmetric, since the core of Si\(_3\)N\(_4\) is surrounded by a SiO\(_2\) cladding; an asymmetric waveguide is created when the upper cladding in the sensing region is removed. The supported modes are modified when the upper cladding is varied. Hence, the propagation characteristics depend on the interaction of some analyte with the light in the sensing region. Modes supported by the waveguide were determined by the analysis of the effective refractive index, \(N_{\text{eff}}\), which should be in the range of \(n_{\text{cladding}} \leq N_{\text{eff}} \leq n_{\text{core}}\).\(^25\) An optical mode is highly confined when \(N_{\text{eff}}\) is close to the upper limit, \(n_{\text{core}}\), and becomes leaky as it approaches to the lower limit, \(n_{\text{cladding}}\). The results of modal simulations by COMSOL Multiphysics revealed that the planar structure supports \(E_0\) and \(TM_0\) modes, as shown in Fig. 4. High order modes (\(m = 1\)) are not supported by the waveguide, since \(N_{\text{eff}}\) is lower than the refractive index of SiO\(_2\). The symmetric waveguide is able to transmit all the spectrum from the emitter. However, when the upper cladding is removed, the resulting guided-wave behavior strongly depends on the wavelength, analyte, and mode (TE or TM). From Fig. 4, it is observed that, as expected, \(N_{\text{eff}}\) reduces as the refractive index of the analyte decreases. Additionally, TE modes are better confined than TM modes, and shorter wavelengths are supported even for TE modes in asymmetric waveguides. Modes that are not supported after the interaction with the analyte are scattered out of the waveguide, as shown in Fig. 5.
The images in Fig. 5 present examples of the intensity of the field as it propagates through the waveguide for $\lambda = 500 \text{ nm}$ and different analytes in the reservoir.

It can be observed how the part of the field that reaches the detector is rapidly transmitted to the silicon in the diode within the first two micrometers. This allows the detection of the arriving optical power and the generation of a photocurrent. Figure 2 presents the results for integrated power arriving to the photodiode as extracted from simulations for each wavelength. Intuition may suggest that the higher the contrast between the core and analyte, better light confinement in it and hence larger intensities in the light arriving to the detector, but the results from simulations presented in Fig. 2 indicate otherwise. Figure 5 illustrates why, as it can be observed, the contrast between the cladding and analyte increases dispersion, causing higher losses and the consequential lower field intensities after the interaction. This was confirmed experimentally as will be discussed later. The simulations of both TE and TM modes showed that the latter presents no significant contribution to the light arriving to the detector.

Transmittance values relating the input and output power for each wavelength are presented in Fig. 6. Transmittance exhibits a complex behavior when propagating modes interact with the integrated silicon photodetector and the cavity formed in the sensing region. Nevertheless, a tendency is clearly observed for all the wavelengths, as higher the refractive index of the analyte the higher the transmittance. However, there are some wavelengths particularly sensitive for some refractive index. This could be of potential use for systems incorporating wavelength selective photodetectors, such as differential spectral response photodiodes.

C. Light detection

The intensity of the detectable light (i.e., the light arriving to the photodetector) for each wavelength can be estimated using the transmittance data presented in Fig. 6 and the known emission spectrum shown in Fig. 2. Figure 2 also presents an approximation of the light intensities arriving at the photodiode region according to the characteristics of the injected light for the different analytes studied.

As expected from the transmittance results, there is a significant diminution of light intensity after interaction with the analyte in all the cases. In addition, there are also noticeable distinct results among the different analytes. The possibility of successfully transducing such differences from light power to photocurrent will be related to the responsivity of the photodiode. Due to the heavily integrated and monolithic nature of the system, an experimental characterization of the responsivity is very challenging, and while experiments are being performed for further studies, for the purposes of this work, such parameters can be estimated by simulating the fabrication process of the system using the Athena module of Silvaco TCAD and then simulating the electro-optical response of the diode using the Atlas module of Silvaco TCAD. This was carried out as described in Sec. III B.

The losses due to material absorption in the case of passive WG are typically negligible, and silicon nitride single strip WGs with increased width have proven to present even lower losses. Furthermore, studies on WG fabricated using the same technology and operating in the same wavelength ranges show losses between 0.51 dB cm$^{-1}$ and 2.25 dB cm$^{-1}$, which in the case of the 1 mm long experimental fabricated device means a worst-case scenario of less than 5% losses in the WG. This means that the transmittance results obtained by the simulations for a reduced geometry can be directly extended to the longer fabricated devices in the case of $\text{SiO}_2$ as an
analyte (or no sensing area), since the losses related to the length of the WG are negligible. With this information and the known responsivity of the photodiode, the radiant power of emitters in fabricated devices was estimated. According to photocurrent values at a photodiode reverse bias of \( V_{pn} = -15 \) V and a LEC voltage of \( V_{LEC} = 15 \) V, the power produced by the emitters and inserted in the WG is in the order of nanowatts.

Considering the responsivity of the photodiode as well as the spectral characteristics of the light arriving to the diode in Fig. 2, the photocurrent produced by each simulated wavelength can be estimated. Figure 7 presents these values for a sampling step of 50 nm of the spectrum assuming a total optical power injected of 1 nW. Then, the total current of the photodiode when the emitter produces an optical power of 1 nW can be calculated by integrating these curves. To adjust the normalized values to an emitter power closer to reality, fabricated systems were characterized and the values from simulations were scaled using the results obtained with air in the sensing area (\( n = 1 \)). The results for the expected photocurrent as extracted from simulations and experimental results (discussed in Sec. II D) are presented in Table I.

The estimations indicate that, even for the broad emission spectrum, it is possible to detect photocurrent variations for the studied refractive indices.

### TABLE I. Total photocurrent produced in the photodiode.

| Analyte   | Photocurrent \( \times 10^{-11} \) (A) |
|-----------|-----------------------------------------|
| Air (\( n = 1 \)) | \(-3.61\) | \(-3.61 \pm 0.07\) |
| H\(_2\)O (\( n = 1.33 \)) | \(-8.54\) | \(-5.54 \pm 0.28\) |
| SiO\(_2\) (\( n = 1.47 \)) | \(-12.12\) | \(-13.9 \pm 3.42\) |

\(^*\)The match between simulations and experiments was assumed ideal for \( n = 1 \).

### D. Experimental proof of concept

As presented in Fig. 5, changes in the field intensity arriving to the photodetector with different materials in the sensing region are to be expected, according to simulations.

In order to verify this, experiments were performed with fabricated systems. The photocurrent detected by the integrated photodiode for a constant LEC bias was monitored when placing 3 \( \mu \)l of deionized water in the sensing area, when no liquid was placed (air), and in systems with no cladding interruption (SiO\(_2\)). The same chip was used for the air and water measurements. Cleaning and drying of the system were performed prior to each droplet measurement. A micrograph of one tested chip with a drop of liquid in the sensing region of one structure is presented in Fig. 8.

Figure 9 shows the values of photogenerated current (dark current subtracted) for the three different cases when applying a voltage of \( V_{LEC} = 15 \) V to the emitter and a reverse bias of \( V_{pn} = -15 \) V to the photodiode for 5 s. Reversibility of the system can be concluded from the observable low deviation from the average values of photocurrent for air presented in Fig. 9 and Table I (the error bars are shorter than the size of the symbols and hence not visible in Fig. 9), as the same device was used in all 5 interspersed air–water tests. This means that except for the first measurement, the results for air correspond to a device that was already used to test water and then dried, with the photocurrent returning to the initial air value within the error margins every time.

From the experimental measurements, it is confirmed that as the refractive index of the material in the sensing area is increased, the photogenerated current also increases. Moreover, the cladding layer behaves as expected increasing the light confinement by around one order of magnitude.

The discrepancies between the simulations and the experimental results presented in Table I clearly indicate room for improvement of the complex modeling of the systems. This can be attributed to a variety of reasons, including experimental such as the need for precise temperature control for low index variations and of design such as the lack of optimization of both WG and photodiode for the most sensible wavelengths. However, the observed trends proof the concept and the viability of a detector under the proposed scheme, and the system showed clear capabilities to differentiate analytes.
with a refractive index difference in the order of tenths, showing potential for more sensitive detection in further iterations. In this regard, the Si-wafer platform not only would allow for electronic integration but wafer-level assembled watertight microfluidics can also be included using one of the already available techniques, like those using polymers such as SU-8 or polydimethylsiloxane (PDMS), which are applicable for the proposed technology.

III. MATERIALS AND METHODS

A. Optical simulations

The optical behavior of the system was simulated using COMSOL Multiphysics. The Wave Optics module was used to perform the simulations by the electromagnetic wave frequency domain (ewfd) physics interface. Some assumptions were considered to enable optical simulations due to finite computational resources because the device shown in Fig. 1 is a three dimensional (3D) structure with the width and length in the millimeter scale and the height in micrometer scale, which would require an unmanageable large number of mesh elements. The mesh size was set to 5 elements per wavelength. The refractive index and extinction coefficient for Si, SiO₂, and c-Si were determined from the data widely available in the literature and web resources. The Sellmeier model was used for data fitting; the properties obtained in the range of 400 nm–800 nm were used for simulations. Modal and propagation simulations were analyzed. Optical modes that are supported in the waveguide were obtained by simulations in a two dimensional (2D) section, transverse to the propagation direction. Transmittance was obtained from 2D simulations by the propagation of the optical modes through a longitudinal section of a waveguide of 0.1 mm of length. The optical waveguide was modeled as a two-port element, at the input port is coupled the light generated by the emitter, which was normalized to 1 nW according to estimations based on previous studies to discrete emitters. Then, the light propagates through the waveguide and interacts with the analyte at the sensing region, which acts as an evanescent field transducer. Finally, at the output port is obtained the transmittance; these results are used in the electro-optical simulations to determine the photogenerated current in the detector.

B. Electro-optical simulations

In order to estimate the responsivity of the photodetector, the fabrication process of the photodiode was simulated using Silvaco TCAD. All the fabrication processes of the complete system, including thermal annealing for the active materials, were included in the simulations. Using ATHENA-Silvaco, all the process steps described in Sec. III C were simulated to obtain a bidimensional p-n structure with a junction depth of approximately 2.95 μm. The electric response in dark condition and under illumination was simulated for the resulting structure using ATLAS-Silvaco. Results were obtained for applied reverse voltage (Vin) values from 0 V to −20 V. Regarding the incidence of light, Ray Tracing (RT) mode was used, as it is useful for devices with planar geometries. The model considers an uniform light beam, ignoring second order effects, such as diffraction or interference. The incidence of the beam was declared normal to the substrate surface, with wavelength values varied from 500 nm to 800 nm using sampling steps of 50 nm. The simulations were split into two parts: first, the real component of the refractive index was used to calculate the optical intensity in each point on the defined structure; second, the imaginary component was used to obtain the carrier concentration in each point of the structure under illumination conditions. The photogeneration rate G was calculated using the following equation:

\[ G = \frac{P \lambda}{h c} \gamma e^{-\alpha \gamma}, \]

where \( P \) is an intensity factor including all accumulative effects of reflections, transmissions, and losses after the ray absorption; \( \eta_0 \) is the internal quantum efficiency; \( \gamma \) is the distance to the light source; \( h \) is Planck’s constant; \( \lambda \) is the wavelength of the incident light; \( c \) is the speed of light; and \( \alpha \) is the absorption coefficient.

Once G has been obtained, the total current values were calculated under specific bias and illumination conditions, which in turn delivered the ratio of optical power to photocurrent to obtain the responsivity of photodiodes.

C. Fabrication of devices

The fabrication process of the EWD started with the etching of 1.5 μm deep trenches in the wafer in zones corresponding to the bottom cladding of the waveguides. Then, local oxidation of silicon (LOCOS) was used to fill the volume of the trenches with SiO₂, and a process consisting of successive deposition-fluidification-etching of orthosilicates was used to planarize the surface of the wafers. Each oxide-filled trench will be the bottom cladding of a WG. After this, p++ wells were created by implanting boron in the zones where the surface contact to the light emitting capacitor and the p-n junction forming the photodiode were needed, i.e., at opposite ends of the WG. Then, we used LPCVD to deposit a Si₃N₄ layer of 30 nm thickness and a lithography and wet etching process to define the areas corresponding to the lower half of a waveguide. The following steps: PECVD deposition, lithography, and wet etching were used to fabricate SiO₂ films with 60 nm thickness in the LEC areas (input of the WG). Afterwards, there was deposited and defined another LPCVD Si₃N₄ film with 30 nm thickness to obtain the upper layer of the LEC as well as the upper half of the nitride waveguide. The zone corresponding to the SiO₂-Si₃N₄ bilayered LEC was then implanted with Si ions using doses and energies tuned to
have a silicon excess in the middle of the SiO₂ film. Next, wafers were annealed for 240 min at 1100 °C to activate the boron in the LEC bottom contact and photodiode wells and to nucleate Si atoms implanted in the SiO₂ to obtain SRO. Detailed fabrication and results of structural and luminescence characterization to the SRO-Si₃N₄ films are detailed in Ref. 22. No silicon excess was obtained in the nitride. After the main EWD components were obtained, a SiO₂ film with a thickness of 1.5 μm was deposited on top of the wafer. Finally, lithography and wet etching were used to completely and selectively remove the SiO₂ from the zones corresponding to the metallic pads and to the points of contact between the WG and analyte.

D. Light-emitting material optical characterization

During the fabrication of the devices, pilot wafers were introduced in all the fabrication steps up to the deposition of the active materials (SRO-nitride bilayer). These samples were also submitted to any subsequent thermal treatment, but no materials were deposited on top of them. This provided samples with the exact same luminescent materials for optical characterization. The emission spectrum of the active materials was obtained using an Ocean Optics QE65000 spectrometer connected to an optical fiber with its input placed normal to the surface of the sample when pumping the active material with UV light at 325 nm from a 30 mW He-Cd laser. Cutoff filters were placed in order to avoid noise from wavelengths below 400 nm. Detailed studies on the emission characteristics, luminescence mechanisms, and PL-EL correlation can be found in Refs. 37, 21, and 22.

E. Device characterization

The electrical characterization of the EWD was performed using a dual channel Keithley 2636B source-meter. Tungsten microprobes were placed in the corresponding pads to stimulate the emitter (see Fig. 1). The response of the photodiode was characterized contacting a probe to the anode pad and the wafer holder to the other terminal of the channel. Channel A of the source-meter was connected to the emitter terminals to apply the power for its operation and channel B to the photodiode to polarize it in reverse bias while registering its current values. The source-meter was controlled using a custom made software to synchronize all the registered values of both channels. The measurements were conducted in controlled illumination conditions. At least 5 measurements were performed for each analyte, and the liquid and air measurements were performed alternately (one after the other) to the same device to corroborate reversibility of the system and approximate as much as possible the measurement conditions for water and air cases. The fluid in the sensing area was placed using a microscope and micropipettes with submicroliter precision.

IV. CONCLUSION

The concept of a CMOS-compatible electrophotonic microsystem for sensing was demonstrated. The behavior of the monolithic device consisting of a Si-based light source directly embedded into a Si₃N₄ waveguide, a sensing area to place an analyte, and an autoaligned photodetector was simulated, and experiments on fabricated chips carried out. The experimental and simulation results were compared. A clear match between the trends on both was observed, showing in all cases an increase in photocurrent delivered by the photodetector with an increment in the refractive index of the material in the sensing region. Modeling indicated that this was caused mainly by higher light dispersion in the system, and the difference between cladding and analyte refractive indices increases. Despite the match of the simulation and experimental trends, the capabilities of the system in its current state for detecting refractive index differences is in the order of tenths, requiring optimization of the geometries and photodetectors in the system. In this case, all the spectrum of the emitter was used, but wavelength filtering or selection by photodetectors may improve sensitivity. On the other hand, simulations showed that the sensor working principle is related to dispersion, which indicates potential for the detection of dispersive or opaque analytes. The theoretical results and the experimental proof of concept indicate that a sensor using this general system can be developed if the geometries are optimized for specific applications and microfluidics are included when necessary.

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