Design of Si-rich nitride interposer waveguides for efficient light coupling from InP-based QD-emitters to Si$_3$N$_4$ waveguides on a silicon substrate

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Abstract: In this paper, we present a systematic analysis for the design of Si-rich-nitride (SRN) based interposer waveguide layers interfacing InP-based devices and Si$_3$N$_4$ waveguides, towards monolithic co-integration of active and passive elements through a Back-End-Of-Line process. The investigation is performed via extensive 2D-eigenvalue and 3D-FDTD electromagnetic simulations and focuses on three different interposer designs, where performance in terms of coupling loss and back reflections is exchanged for fabrication complexity. In addition, a tolerance analysis is performed for the demonstration of the proposed coupling scheme’s resilience to fabrication misalignments. The calculations use for the refractive index of the SRN interposer, real values extracted from ellipsometry measurements of a novel ultra-Si-rich-nitride material developed and engineered for this purpose. This new material provides tunability in the real part of the refractive index with low-stress crack free samples grown up to 500nm thickness. Test structures with cutbacks featuring waveguides of $500 \times 500\,\text{nm}^2$ cross section formed via e-beam lithography reveal 15dB/cm propagation losses in line with similar amorphous silicon-rich nitride (aSi:N) materials. The proposed coupling concept although assumes an InP active medium, can be applied also with GaAs based lasers and dual facet devices such as Semiconductor Optical Amplifiers (SOAs) and electroabsorption modulators. In addition, all proposed designs are compatible in terms of critical dimensions with low cost 248nm DUV lithography targeting to maximize the low-cost advantage of the Si$_3$N$_4$ platform with very high coupling performance. Our results are expected to pave the way for the generation of a versatile, low cost, high performance monolithic InP-Quantum-Dot (QD)/Si$_3$N$_4$ platform on a common Si substrate.

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1. Introduction

Advances in CMOS technology have led the field of Si photonics to flourish during the last few decades [1]. Nevertheless, one major technical challenge hindering the wider adoption of Si photonics to other applications comes from the incorporation of light sources in the Photonic Integrated Circuits (PICs). Until recently, most silicon photonic circuits have relied on external light sources to couple light in and out of the circuit through novel fiber-PIC I/O interfaces [2]. This approach has the advantage of high yield during assembly and packaging at the expense of higher overall device cost and lower light output power stemming from the fiber-PIC interface losses. The advent of hybrid integration has enabled the next generation of PICs, where the laser source is embedded on the chip through bonding of III-V elements in die [3,4] or wafer level [5]. The light transfer from the laser to the Si waveguide in these PICs is performed either
with adiabatic [6], or end-fire coupling mechanisms [7], with both options providing pros and cons related to coupling loss performance versus alignment accuracy and overall assembly cost. However, the best PIC technology in terms of cost and performance combining active and passive elements is the monolithic co-integration of Quantum Dot (QD) III-V materials on the Si platform. QDs provide the inherent advantages of minimum damage at the active layers from the dislocation propagation formed during the growth of the III-V material at the III-V/Si interface [8], higher temperature insensitivity to output power [9] and higher lasing tolerance to back-reflections [10]. The first trials from this new integration technology have focused almost solely on the integration of QD GaAs lasers [11,12] on Si, with recent results indicating that commercialization is imminent [13]. Additionally, a design strategy for co-integrating monolithically grown GaAs lasers on Si with Si-passive waveguides has recently been presented in [14]. Going to monolithic integration of QD InP, the higher mismatch of the lattice constant relative to GaAs generates additional complexity for the InP/Si buffer, but first results are already reported in [15].

At the same time, the Si₃N₄ technology has gained ground versus traditional Si for fabrication of advanced PICs due to lower cost, lower propagation losses, lower PIC-to-fiber coupling loss [16] and higher temperature insensitivity [17]. The integration of the lasers in this type of PICs is performed through flip chip bonding at the Si₃N₄ waveguide facet and the light is coupled to the passive waveguide with the end-fire mechanism. This solution inspired by the thick (>1μm thick) Si platform mandates sub-micron placement accuracy for the III-V die and provides coupling losses in the order of 1.8 dB [18]. In addition, it is not compatible with dual facet devices e.g. modulator and Semiconductor Optical Amplifiers (SOAs). An approach to overcome all these problems was presented in [19], where a PIC employing a crystalline intermediate Si layer for transferring the light from the InP to the Si₃N₄ low loss waveguide was demonstrated, relying on a rather complex fabrication process involving both die and wafer bonding, without providing any value about coupling loss. In [20] the integration is simpler and the light is propagating from the laser to the Si₃N₄ adiabatically through a hydrogenated aSi waveguide acting as a medium and in this way a fully integrated laser on Si₃N₄ via transfer printing. The coupling losses were 2 dB including propagation to the aSi interposer. Nonetheless, both techniques require multiple taper steps and taper tips widths of 150nm or lower, that render them incompatible with low cost 248nm DUV lithography, while the taper formations also mandate multiple lithography steps, degrading in this way the low fabrication cost advantage coming with the Si₃N₄.

In this work we present the results from the systematic investigation of a low-cost coupling scheme for seamless light transfer between QD InP active elements and the Si₃N₄ passive platform that is relying on a novel SRN material with tunable optical properties in terms of refractive index acting as an intermediate medium. The whole concept is compatible with Back-End-Of-Line monolithic integration process and 248nm DUV lithographic specifications for maximization of low-cost fabrication potentiality. Furthermore, although the analysis assumes an InP active medium, it can be applied also for monolithically grown GaAs based lasers and dual facet devices such as SOAs and electroabsorption modulators, demonstrating the wide applicability of the proposed concept.

The results of this manuscript complete the previous work presented in [21], [22] and [23], by providing the full analysis of the optimization process through simulations performed for three different interposer waveguide geometry designs exchanging performance for fabrication complexity. The best solution is a three-layer Si-rich nitride (SRN) waveguide stack composed of one layer with n=3.41 sandwiched between two layers of n=3.18 with a 1100 nm total thickness providing 0.9dB coupling losses and back reflection of -52.4dB, when the InP-SRN interface is angled at 15°. In addition, a fabrication tolerance analysis is presented at the QD InP-SRN angled interface for misalignments of 300nm in the y-axis and 200 nm in the z-axis, where the tri-layer SRN exhibits its superiority due to the larger supported modal size. In the worst-case scenario of simultaneous 200 nm misalignment in the z-axis and 300 nm in the y-axis, the
tri-layer SRN achieves a total coupling loss of 1.78 dB and back-reflections lower than -54.4 dB, demonstrating the resilience of the proposed coupling scheme to large errors in the CVD and lithography processes. All simulations use for the refractive index of the SRN interposer the values extracted from ellipsometry measurements of an ultra Si-rich nitride material (SRN) developed and engineered for this purpose. In addition, the paper provides details about this new SRN material that was developed to provide crack free films with thickness up to 500nm. From these samples, cutback structures with waveguides of $500 \times 500\text{nm}^2$ cross section were formed via e-beam lithography revealing 15dB/cm propagation losses in agreement with other works on amorphous Si-rich nitride (aSi:N) waveguides fabricated by PECVD. However, this value can go down to lower than $\sim 10 \text{dB/cm}$ by further optimizing the deposition and especially the etching process [24]. The paper is organized in the following way: Section 2 presents the overall coupling scheme aiming to bridge the InP-based source with the Si$_3$N$_4$ photonics platform considering a BEOL monolithic integration process. Section 3 presents the experimental ellipsometry and profilometry results that demonstrate the feasibility of fabricating SRN waveguides with the desired properties for the proposed light interface. Section 4 describes the detailed design optimization analysis for the interposer SRN waveguiding section by investigating three different cases, i.e. a single-material strip, a single-material rib and the best in terms of performance configuration of the two-material tri-layer rib configuration. Section 4 incorporates also the simulation results when the InP-SRN interface is angled targeting minimization of the back reflections. Therein, a detailed tolerance analysis for the optimum structures of the three cases is presented, validating the supremacy of the tri-layer design.

2. Overall III-V to SiN interface concept and envisaged integration process

Towards monolithically integrating InP-based gain media with a thick-Si$_3$N$_4$ platform in a CMOS compatible and Back-End-Of-Line (BEOL) manner, a suitable SRN material should facilitate light coupling from the semiconductor to the dielectric platform, as a bridging material layer.

Figure 1(a) illustrates a sideview image of the proposed monolithic integrated QD InP laser that shows also the SRN transition waveguide for light coupling to the Si$_3$N$_4$ passive circuitry. The proposed integration platform starts with the 248nm DUV formation of the Si$_3$N$_4$ structures on Si-wafers though Low-Pressure Chemical Vapor Deposition (LPCVD). Then local windows are made on wafer level for the deposition of the QD InP-based layer stack of the active components i.e. lasers and SOAs, followed by etching for facet formation. The gaps in the windows are filled by divinyl siloxane benzocyclobutene (BCB) and then SRN films are deposited with Plasma-Enhanced Chemical Vapor Deposition (PECVD) on the whole surface of the wafer covering the facets of the QD InP elements. The SRN transition waveguides are structured then on the film through 248 nm DUV lithography and etching. All critical parameters in the proposed coupling scheme are defined by the PECVD process and DUV lithography, in contrast to hybrid integration where the coupling efficiency is dictated by the placement accuracy of flip chip bonders that attach the III-V dies to the Si$_3$N$_4$ waveguide.

Figure 1(b) illustrates in a 3D fashion the proposed BEOL interface that can be described in two cascaded discrete coupling stages: i) an end-fire section from the InP-based QD active region of the laser to the interposer SRN waveguide and ii) an evanescent coupling stage from the interposer SRN waveguide to the targeted Si$_3$N$_4$ platform. The design optimization of the overall interface targets two key performance metrics: maximum light transfer to the Si$_3$N$_4$ waveguide and minimum back-reflections to the QD-emitter for uninterrupted operation in high speed Directly Modulated Lasers (DMLs) and external cavity Tunable lasers (ECLs). These two parameters are determined by the cross-sectional geometry and the refractive index of the intermediate SRN waveguide at the two interfacing steps (InP-SRN and SRN-Si$_3$N$_4$) and are thoroughly investigated in this work by 2D and 3D FDTD simulations. The whole configuration
Fig. 1. (a) Sideview image of the envisaged fully monolithically integrated InP-based QD-laser and Si$_3$N$_4$ photonic integrated circuit, (b) 3D geometry model depicting the proposed interfacing scheme. The light is coupled from an InP-based QD emitter to a thick Si$_3$N$_4$ waveguide through an intermediate SRN interposer.

is totally reciprocal and can be employed also for light coupling from Si$_3$N$_4$ to InP-based-QD active elements rendering it ideal for two facet devices, such as SOAs.

For optimum light coupling in terms of maximization of the achievable coupling efficiency and the minimization of back-reflections to the semiconductor region, the modal field profile of the targeted mode to be excited in the interposer should approach the profile of the mode supported by the gain medium for spatial matching, at the first coupling stage [25]. Identical modal effective indices between the two modes should also minimize the received back-reflections to the semiconductor region. For the second coupling stage, the propagation constant of the mode propagating at the upper SRN layer should be identical to the propagation constant of the targeted TE mode at the final Si$_3$N$_4$ waveguide for phase-matching [25]. Nonetheless, the two conditions that need to be simultaneously met create a trade-off that needs to be dealt with during the design analysis. Optimum spatial matching requires high interposer thicknesses, while optimum phase matching mandates low interposer thicknesses.

The source in the proposed interface scenario is an InP-based QD emitter with a layer stack similar to the one presented in [26] formed by a shallow etched 2µm wide ridge waveguide. BCB acts as the cladding of this QD-emitter. The cross section in the y-z plane of the laser is illustrated in Fig. 2(a). The interfacing design target is to couple light to the final thick Si$_3$N$_4$ waveguide platform. The Si$_3$N$_4$ waveguide platform in this work is relying on the 800nm thick standard platform of Ligentec S.A [27]. In this analysis the width has been set at 800nm, supporting both fundamental TE and TM modes with low propagation losses. However, only the TE Si$_3$N$_4$ mode is of interest due to the TE polarization of the QD-laser mode. Figure 2(c) presents the cross-sectional Si$_3$N$_4$ waveguide geometry with SiO$_2$ over- and under-cladding. On top of the 100 nm SiO$_2$ overclad there is also divinyl siloxane benzocyclobutene (BCB) (n = 1.535 at $\lambda$ = 1550 nm) for compatibility with the III-V monolithic integration. The refractive index values for SiO$_2$ at a wavelength $\lambda$ = 1550 nm has been derived from [28]. For the SRN material, ellipsometry data at 1550 nm have been imported in our numerical simulations. During eigenmode calculations, stretched coordinate PML boundary conditions have been applied at the edges of the computational window to eliminate artefact modes [29]. Figure 2(b) depicts the electric field distribution $|E|$ of the supported fundamental TE mode of the QD-laser. This TE mode spatially extends about 1µm in the z axis and about 4µm in the y axis. The calculated effective refractive index of this mode is $n_{eff}$=3.269. On the other hand, Fig. 2(d) illustrates the supported TE mode of the 800 × 800 nm$^2$ Si$_3$N$_4$ waveguide. The electric field magnitude, $|E|$ extends to a cross-sectional area around 1µm$^2$ with an effective index around $n_{eff}$=1.71.
Fig. 2. (a) Depiction of the InP-based QD-emitter cross-sectional geometry, (b) Electric Field $|E|$ distribution of the fundamental TE-mode supported by the InP-based QD-emitter, (c) Depiction of the $(800 \times 800) \text{ nm}^2 \text{ Si}_3\text{N}_4$ waveguide cross-section, (d) Electric Field $|E|$ distribution of the fundamental TE-mode supported by the Si$_3$N$_4$ waveguide.

As mentioned, since the proposed interface scenario involves two discrete coupling stages, the optimization of the SRN intermediate waveguide will come as a result of accordance with the two conflicting dictations. Therefore, the refractive index of the interposer material should be close to 3.2-3.4, aiming to match the effective index of the TE mode by the InP-based emitter towards minimization of the back reflections. On the other hand, the effective index of the propagating SRN mode should approach the effective index in the Si$_3$N$_4$ waveguide (i.e. $n_{\text{eff}}=1.71$) to satisfy the phase matching condition, approaching the evanescent coupling stage. These two opposing conditions can be met only with a taper structure connecting the two coupling sections. The geometrical characteristics of the transition tapers are presented in the design analysis of the next sections. The gap $g$, i.e. the thickness of the SiO$_2$ overclad, of Fig. 2(c) between the SRN and the Si$_3$N$_4$ layers is fixed at 100 nm in all scenarios considering a minimum value where the quality of the surface roughness can be considered almost ideal. In the next section, we present the fabrication and characterization of a SRN material specifically engineered for the monolithic interposer application.

3. Si-rich Nitride material and waveguide fabrication

The fabricated Si-rich-nitride material that serves the role of the interposer waveguiding layer needs to comply with two fundamental restrictions posed by the utilized coupling schemes. In order to avoid parasitic back-reflections, the refractive index and the thickness of the dielectric material should be large enough, so that the mode in the interposer has a modal profile and an effective index close to those of the mode supported by the QD emitter. The thickness of the material should also be low enough to support a mode with an effective index close to the targeted mode in the Si$_3$N$_4$ PIC, at the end of the intermediate layer section. The temperatures in the whole process should also be lower than 300°C in order to prevent group V element adsorption in the underlying III-V layers. Finally, the material quality should be high enough to prevent intense scattering and absorption phenomena during propagation of the light in this intermediate structure. All these restrictions impose the foundations for the development of the whole fabrication process, that is close to the one presented in [30] for the fabrication of a-Si:H rib waveguides and is described in detail in [22]. One of the key targets in the whole effort was
to maintain low-stresses during material deposition, so that high film thicknesses can be obtained without the occurrence of structural defects.

The process is based on deposition with a PECVD tool (Nextral ND200), using monosilane (SiH₃) and nitrogen (N₂) as precursors, and helium (He) as the dilution gas. The gas chamber temperature and RF power were set to 250°C and 100W respectively, while the variables of the process were the precursor ratio and the chamber pressure. These variables were shown to vary the refractive index and the stress of the developed material respectively. The real and imaginary parts of the refractive index of the grown materials were measured by spectroscopic ellipsometry (HORIBA Jobin-Yvon UVISEL) after SRN deposition on 2-inch Si wafers with a 150-nm-thick cladding layer of PECVD SiO₂, while the material stress was derived from profilometry results (KLA/Tencor P17) before and after the material deposition. This has been deduced from the wafer bowing levels before and after the SRN layer deposition. A 500nm-thick Si-rich-nitride film is the targeted thickness, as derived from the design analysis, enabling ranging effective indices from almost 3 to 1.7.

Figure 3(a) shows the n-k measurements of the fabricated Si-rich nitride material, revealing a refractive index n as high as 3.165 at the wavelength of 1550nm that matches very well the InP value. According to Fig. 3(b) also a 500nm thick deposited material on a 2-inch wafer exhibits low stress with less than 1 µm overall wafer bowing. This is achieved for SiH₄, N₂ and He gas flows of 50 sccm, 40 sccm and 200 sccm, respectively and a chamber pressure of 1400 mTorr. The deposition rate is approximately 60 nm/min. The refractive index of the fabricated material can be varied by modifying the SiH₄/N₂ ratio.

The quality of this novel material was evaluated by the formation of 500nm wide waveguides with the 500nm thick low stress SRN. With more details about the fabrication process given in [22], three waveguides of 0.2, 0.5 and 1 cm were fabricated and the propagation losses were estimated from the cutback measurements to be 15dB/cm, in agreement with other works on aSi:N waveguides fabricated by PECVD. This imposes an additional critical target in the design analysis, specifically the minimization of the taper length due to the high propagation losses. In this case, the high propagation losses have very small effect in the overall interface loss if the length is maintained lower than 200 µm, providing an overall loss of 0.3dB at 200 µm. The high propagation losses however can be drastically reduced by optimizing further the whole process reaching values as low as 6dB/cm in similar dimension waveguides deposited by PECVD [24]. In the next section, an extensive design optimization procedure is presented, leading to three types of configurations, with the optimum one providing close to 1dB coupling losses and less than -50dB back-reflections.
4. Coupling interface design analysis and numerical results

4.1. Strip Si-rich nitride configuration

The strip SRN waveguide configuration is the simplest solution in terms of fabrication that can be utilized as the medium for bridging the InP-based QD laser with the Si$_3$N$_4$ platform. The methodology starts with the identification of the excited targeted fundamental TE mode in the SRN strip waveguide. A 2D-eigenmode analysis reveals the profile of this mode, as well as the rest of the supported modes in the various SRN cross sections. Figure 4(a) illustrates the waveguide geometry under study composed from a strip SRN waveguide covered by a BCB cladding with a refractive index $n=1.535$. The parameters under variation were the waveguide width and thickness. Figure 4(b) presents the power overlap integral values calculated for the modal profiles of the laser and the targeted mode in the SRN waveguide [25].

The integral was calculated for widths ranging from 1$\mu$m to 7$\mu$m and for thicknesses of 300nm, 500nm, 700nm, 900nm and 1100nm. Two refractive indices for the SRN material were investigated, one with $n=3.18$ and one with $n=3.41$, corresponding to the refractive index values of already fabricated SRN low stress and high stress thin films. It is clear that for both materials and all waveguide thicknesses, the power overlap integral values reach a local maximum near a width value of 4$\mu$m. However, the material with $n=3.18$ seems to provide higher overlap integral values than the material with $n=3.41$, therefore for the following calculations only the SRN material with $n=3.18$ was taken into consideration.

In order to identify the optimum waveguide thickness, the evanescent coupling part of the interface was also considered. As mentioned in Section 2, the proposed waveguide thickness needs to solve the contradiction imposed by the obligation to comply with the needs of both coupling steps. This means that the optimum proposed thickness should provide effective indices...
from 3.269, corresponding to the effective index of the mode displayed in Fig. 2(b), to 1.7, close to the effective index of the targeted underlying Si₃N₄ mode, for a variable range of widths. The effective index of the fundamental TE-mode supported by the SRN waveguide for various widths and thicknesses can be seen in Fig. 4(d). The optimum waveguide has a thickness of 500 nm because this waveguide thickness supports a fundamental TE-mode with an effective index ranging from 1.69 to almost 3 for widths ranging from 0.2 µm to 4 µm. The minimum width of 0.2 µm is in line with the limitation of 248nm DUV lithography assumed in our calculations towards mass production at low cost.

Thicker SRN waveguides do not support modes with effective indices lower than 1.7 for minimum 200nm taper width and thinner waveguides cannot achieve effective indices close to 3. Therefore, the optimum geometry defined by the 2D-analysis is a 500nm thick structure that supports a fundamental TE-mode portrayed in Fig. 4(c) with an effective index yielding a real part close to Re(n_eff) = 2.96 when the width is 4 µm for highest spatial matching with the active region of the laser. This is confirmed by the power overlap integral value calculated for this configuration resulting close to 81.4% efficiency or 0.9dB dB coupling loss.

Having the 2D overlap integral analysis as guide, the power coupling efficiency for the first coupling stage has been extracted through 3D-FDTD numerical calculations. The power of back-scattered light that was obtained yielded back-reflections close to -19.79dB and forward propagation coupling efficiency to the targeted mode of Fig. 4(c) of 0.9dB in close agreement with the power overlap analysis. From the 2D-analysis it was observed that the optimum configuration for the selected SRN cross section is multi-mode therefore a small percentage of power from the QD-emitter mode transfers to high-order modes. In addition, as it was mentioned in Section 2, the initially excited mode in the SRN waveguide should be converted to a mode with an effective index close to 1.71. This can be derived through a proper taper design with its operation having a twofold effect, first transform the initially excited SRN mode of Fig. 4(c) to (a) mode with an effective index of 1.71, and secondly, suppress the high-order modes. At the end of the taper, the waveguide will guide a suitable mode to enter the evanescent coupling stage.

The xy-plane (top-view) of the simulated tapered structure in 3D-FDTD numerical calculations can be seen in Fig. 5(a). Figure 5(b) illustrates the |E| field distribution on a xy-plane located at the middle of the SRN waveguide. The source is located at the cross-section of the QD-emitter and is the mode depicted in Fig. 2(b). Therefore, the |E| field includes both phenomena, that of end-fire coupling and that of the adiabatic transition. Intensive simulations revealed that a linear taper with a length of 150µm fulfills the adiabaticity criterion, exhibiting a coupling loss of only 0.037dB during the transformation from the mode of Plane A (Fig. 4(c)) to the targeted excitation mode of Plane B (Fig. 5(d)). The excited mode at the taper tip of Plane B is portrayed in Fig. 5(d) and has an effective index close to 1.69, i.e. close to the targeted mode in Si₃N₄ thereby complying with the phase-matching condition of the evanescent coupling step. The smooth conversion of the initially excited mode from Plane A to Plane B as well as the suppression of the high-order modes can be seen in the electric field distribution |E| of Fig. 5(b), as derived by the FDTD numerical calculation. At the end, before light enters the directionally coupling step, the optical mode is deconfined, being closer at the edges of the SRN waveguide cross-section as depicted in Fig. 5(d).

As in the end-fire case, the directional coupling stage was initially studied with a 2D-eigenmode analysis at the yz- cross sectional plane of Fig. 6(a) with the 210 × 500 nm² SRN layer lying over the targeted 800 × 800 nm² Si₃N₄ strip waveguide. A small SiO₂ gap with thickness g=100nm separates the two waveguides. The 2D- analysis revealed TE-polarized supermodes of quasi-even and quasi-odd symmetry, supported by the hybrid structure. Figure 6(b) depicts the E_y-component of the symmetric mode while Fig. 6(c) depicts the same component for the anti-symmetric supported mode. The beating of the two, a quasi-even and a quasi-odd symmetry supermodes leads to directional coupling of light to the Si₃N₄ waveguide. Theoretically the full
amount of the initially inserted energy will pass to the Si$_3$N$_4$ at the coupling length $L_c$, given by the relation [25].

$$L_c = \frac{\pi}{\beta_s - \beta_a}$$  (1)

By inserting the effective indices of the two supermodes displayed in Fig. 6(b) and Fig. 6(c) in Eq. (1), a coupling length of 6.6µm was calculated. This was also verified by a strict 3D-FDTD simulation of the directional coupling step. The side-view of the simulated geometry is depicted in Fig. 6(d). The SRN taper tip mode of Fig. 5(d) was set as the excitation in the simulation. Stretched coordinate PML boundary conditions were once again utilized to absorb incoming waves at the edges of the computational window. The calculated $|E|$ field distribution depicted in Fig. 6(e) indicates a seamless transition from the SRN to the Si$_3$N$_4$ waveguide with a coupling loss of only 0.13dB for the targeted TE-mode of the final Si$_3$N$_4$ waveguide at 1550nm. Finally, taking into account all coupling and conversion steps of the proposed interface, a coupling loss of 1.06dB is achieved for the overall configuration of the strip SRN strip intermediate waveguide.

4.2. Rib Si-rich nitride configuration

In this section a single material ($n=3.18$) rib SRN waveguide geometry is investigated as a means to reduce the high back reflection value of -19.79dB exhibited by the simple strip SRN configuration. Initially, two total rib waveguide thicknesses of 900nm and 1100nm were taken into consideration in 2D-eigenmode calculations. A slab thickness $h$ with a value of 300nm, 500nm, and 700nm for a total thickness of H=900nm and a slab thickness $h$ with a value of 300nm, 500nm, 700nm, and 900nm for a total thickness of H=1100nm were initially studied. Figure 7(a) depicts cross-sectional yz-plane of the simulated geometry, that was inserted in eigenmode calculations. The power overlap integral value was calculated for all these waveguide thicknesses with waveguide widths ranging from 1µm to 7µm with the results illustrated in Fig. 7(b) and Fig. 7(c). For both thicknesses the power overlap integral values reach an optimum point near a 4µm rib width. In terms of slab thickness even though values above 500nm yielded higher power overlap integral values, they are discarded from thereon, since they cannot support directional coupling to the final 800 × 800 nm$^2$ Si$_3$N$_4$ waveguide with minimum 200nm wide taper tips. More specifically, it was observed that for increasing SRN slab thicknesses the effective index value of the supported TE mode at the double taper tip is increased, thus leading to phase
Fig. 6. (a) Depiction of the hybrid cross-sectional geometry at the yz-plane of the directional coupling step, (b) Real part of the $E_y$-component of the quasi-even TE-supermode supported by the hybrid geometry, (c) Real part of the $E_y$-component of the quasi-odd TE-supermode supported by the hybrid geometry, (d) xz-representation of the simulated geometry for the directional coupling step, (e) Electric field distribution $|E|$ at the xz-plane derived by a 3D-FDTD calculation, at the middle ($y=0$) of the computational window.

Due to the 500nm slab thickness, the same directional coupling step exploited in the strip cross section analysis and depicted in Fig. 6(e) can also be employed through a double taper structure for efficient coupling to the Si$_3$N$_4$ waveguide. The initially excited TE mode of Fig. 7(d)

Fig. 7. (a) yz-plane of the simulated single material SRN rib waveguide, (b) Power overlap integral values for SRN single material rib waveguide and for total thickness $H=1100$nm, (c) Power overlap integral values for SRN single material rib waveguide, for total thickness $H=900$nm, (d) Fundamental TE-modal profile $|E|$ supported by the single material SRN rib waveguide
is converted through the taper in the intermediate waveguide to the mode of Fig. 5(d), that in turn is employed as the excitation in the following evanescent coupling step. The design of the conversion taper was performed utilizing consecutive numerical 3D-FDTD calculations. A minimum tip width condition of 200nm was imposed again to the designed structures for compliance with limitations from 248nm DUV photolithography processes.

A 3D-representation of the SRN based rib waveguide transition utilizing a double taper can be seen in Fig. 8(a) and the xy-plane of the simulated geometry for the optimization of the double taper structure is displayed in Fig. 8(b). The double taper is formed by separately etching the slab and the rib of the waveguide. PML boundary conditions were once again employed at the edges of the computational window. In the analysis the upper and lower taper tip widths were fixed at \( w_1 = 200 \text{nm} \) and \( w_2 = 210 \text{nm} \), respectively. The initial dimensions of the rib waveguide before double tapering had been \( w_1\text{(initial)} = 4 \mu\text{m} \) and \( w_2\text{(initial)} = 20 \mu\text{m} \). The slab is initially extended out of the PML boundaries. The corresponding results from the 3D-FDTD simulations are illustrated in Fig. 8(c) where there is a minimization of coupling loss at 0.5dB or close to 89% coupling efficiency for a 100\( \mu\text{m} \) taper length. In addition, from the numerical calculation, the coupling loss for the end-fire at the III-V to SRN interface is calculated at 0.36dB in agreement with the correspondent power overlap integral value. The level of back-reflections is near -30dB for a 0° facet angle. Figure 8(d) depicts the smooth butt-coupling and transition of the light in the double taper structure, after the initial excitation of the mode that was used as the source. Along with the fundamental TE-mode, higher order TE-modes are initially excited in the taper, but are later suppressed, as in the strip waveguide case. Again, at the end the mode mostly resides at the edges of the SRN waveguide.

![Fig. 8](image-url)

**Fig. 8.** (a) 3D-depiction of the double taper formed at the SRN rib waveguide based interface, (b) xy-representation of the simulated single material SRN rib waveguide based transition layer, (c) Coupling efficiency (%) for increasing double taper length – The upper taper terminates at the same spot as the lower taper, (d) \( |E| \) field distribution propagated along the xy-plane of the double taper structure after excitation from the InP-based QD-emitter. The xy-plane resides at the middle z-axis of the lower taper.

### 4.3. Tri-layer waveguide configuration

For further performance optimization a tri-layer rib waveguide was investigated, leveraging the versatility of our engineered SRN material. Instead of a single material with a thickness of 900nm and \( n = 3.18 \), this improved geometry consists of a material with \( n = 3.41 \) sandwiched by two layers.
with n=3.18, as shown in Fig. 9(a). The total waveguide thickness was set to 1100nm targeting supported modes with effective index as close as possible to the ones emitted by the QD laser for minimization of the back reflection. Also, the thicker waveguide enables better tolerances in vertical misalignment during the deposition of the SRN stack at the laser facet. The slab thickness is set to 500nm, corresponding to a SRN waveguide thickness suitable for the directional coupling configuration of Fig. 6(d). Figure 9(c) presents the power integral overlap values from scanning the rib width w and middle material thickness t, while Fig. 9(b) illustrates the corresponding effective index for each cross section. What should be noted is that by increasing the middle material thickness t, a trade off appears. While the achievable effective indices increase, the coupling efficiency indicated by the power overlap integral calculations slightly deteriorates. This is attributed to the larger modal confinement in the middle layer from the higher refractive index. Figure 9(d) reveals that the overlap integrals reach a local maximum near w=4µm rib width. Also, from Fig. 9(b) it is deduced that for a total thickness of H=1100nm and t=400nm, the effective index of the fundamental-TE mode supported by the tri-layer waveguide is 3.2675, matching very well the laser mode. For this cross section, the power overlap integral calculation yields a transition efficiency value of 91.8% or 0.37dB loss. For the optimum geometry, the modal |E| field profile of the fundamental-TE-mode presented in Fig. 9(d) has a spatial distribution very similar to that of the mode of the InP-based QD-emitter shown in Fig. 2(b).

As already mentioned, the selection of 500 nm total slab thickness allows the employment of the directional coupling step shown in Fig. 6(d) and (e) coming directly from the strip SRN waveguide. A suitable double taper structure adiabatically transforms the initially excited mode shown in Fig. 9(d) to the desired mode of Fig. 5(d), with the corresponding top-view depicted in Fig. 10(a). The InP-based QD-laser mode was the excitation in cascaded 3D-FDTD calculations that were carried out to determine the double taper shape and geometry. PML boundary conditions were utilized at the edges of the computational window, similarly to the previous configurations. The upper taper has a length of 200um ending to a tip width of w1=100nm that adiabatically couples light to the targeted cross-section of Fig. 5(c). The lower taper features a tip width of w2=210nm and length of 200um. The upper taper geometrical characteristics were selected aiming at optimum coupling performance. The higher thickness of the upper taper requires an

Fig. 9. (a) Depiction of the simulated tri-layer SRN waveguide at the yz-plane, (b) Effective index of the fundamental TE-mode supported by the tri-layer interposer for varying width w and middle material thickness t, (c) Power overlap integral values for varying width w and middle material thickness t of the tri-layer waveguide, (d) |E| field distribution of the fundamental TE-mode supported by the optimum tri-layer SRN waveguide.
upper taper width as low as 100nm in order to be adiabatic. However, the selection of an upper taper with a 200nm width instead, for the same length, would only cause a deterioration of 0.1dB to the overall device performance, based on 3D-FDTD calculations.

The total tri-layer double intermediate taper has a total length of 200µm and achieves a coupling efficiency of 94.2%, or equivalently, induces losses near 0.26dB. A smooth excitation of the targeted TE mode before the directional coupling step is seen at the end of the taper at plane B in Fig. 10(b). The end fire transition loss at the InP-SRN interface according to the 3D-FDTD calculations is 0.37dB loss (91.8% coupling efficiency), identical to the power overlap integral value. In total by summing the losses from the end-fire coupling, taper transition and directional coupling (0.13dB) of Fig. 6(d) and 6(e), the proposed tri-layer based interface yields an overall coupling efficiency of 0.77dB, while back reflections are as low as -34.95dB for a 0° facet angle at a wavelength λ=1550nm. So, overall the tri-layer SRN waveguide achieves the optimum results compared to the other structures, evidently being a suitable configuration for coupling of light between QD-emitters and thick Si₃N₄ waveguides in monolithic integration scenarios. However, this enhanced performance is coming at the expense of additional fabrication complexity for the deposition of three materials with suitable thicknesses for the formation of the final waveguide geometry.

4.4. Investigation of angled facets for the minimization of back-reflections

In the analysis presented so far, the SRN based interface schemes have yielded coupling loss values even at the sub-dB range for the tri-layer interposer. However, the back-reflections were higher than -40dB. In the co-integration of the laser sources in Si photonics PICs, back reflection requirements are highly relaxed by utilizing QDs in the active region. The QDs with recent experimental studies of QD-DMLs on Si have exhibited penalty-free transmission at 10 GHz external modulation even with -7.4dB parasitic optical feedback [31]. However, in order to ensure seamless light transfer under any III-V material an angle was induced to the InP-Si₃N₄ interface for further minimization of the back reflections. Figure 11(a) depicts the top-view depiction of the modified simulated interface, repeated for all three configurations. The facet angle was set to 0°, 2°, 8°, 10° and 15°, as dictated by fabrication capabilities, and the corresponding results for back reflections and coupling efficiency are presented in Fig. 11(b), and (c), respectively. Back-reflections were calculated behind the plane of the source that was used as the excitation. The monitor for the calculation of the coupling efficiency is at plane B, i.e. the end of the modal transformation region. The 3D-FDTD calculations reveal for the strip SRN waveguide reduced back reflection levels close to -49.7dB at 8°. This comes at the expense of reduced coupling efficiency, where coupling loss are increased by 0.09 dB at 8°, as the asymmetry in the end-fire interface leads to the generation of high-order modes in the SRN waveguide structure. This part of light is eventually guided to the cladding and fades away after a few tens of um. In the same
Fig. 11. (a) xy-plane representation of the angled-facet based interface for the SRN strip configuration, (b) Calculated back-reflections (dB) for increasing angle values for all three SRN-based geometries, (c) Calculated coupling efficiency (%) for increasing angle values for all three SRN-based geometries.

graph it is shown that the rib cross section is the most insensitive to the facet angle, based on the studied angles. The back reflections are reduced to -34.81 dB at 8° and the coupling losses drop by 0.097 dB at the same angle. On the other hand, for the tri-layer structure the introduction of the angled facet improves the overall performance of light transition, where at an angle of 15°, record low coupling losses of 0.6 dB (equivalent coupling efficiency of 87.02%) and back reflections of -52.6 dB are achieved. The small increase of the device performance at 15° is attributed to a more gradual effective index matching between the supported modes in the SRN waveguide and the III-V source after the perturbation of the angle. This leads to slightly higher coupling efficiency at the end-fire stage and lower back-reflections. However even with the small angle of 2° the performance is very good with only 0.632 dB losses and -50 dB back reflections. Again, the enhanced performance of the tri-layer waveguide is coming with the drawback of the increased fabrication complexity.

4.5. Tolerance analysis of monolithic interfaces

In the three coupling interfacing schemes presented in the previous sections, the alignment of the SRN waveguide was considered ideal in terms of matching the center points of the QD laser active region and the SRN waveguide. In this section the resilience of the proposed coupling scheme is demonstrated through a fabrication tolerance analysis performed with 3D-FDTD simulations. In the setup of Fig. 11(a) for the optimum angle of the three SRN cross sections i.e. 15° for the strip, 8° for the rib and 15° for the tri-layer rib, the SRN waveguide central point was misplaced by up to 300 nm in the y-axis (horizontal) and 200 nm in the z-axis (vertical). Figure 12(a) shows the corresponding results in the y-axis, where it is revealed that the performance degradation from optimum value is approximately 0.15 dB (or 3.4%) for all three SRN geometries. This is something that was expected due to the large horizontal dimensions of both the emitted mode from the laser and the initial width of the SRN waveguides, before tapering. Figure 12(b) presents the results from the misalignment in the z-axis and demonstrates the superiority of the tri-layer SRN rib cross section relative to the single layer strip and rib approaches by supporting larger mode in the z-plane. The coupling efficiency drops for the tri-layer SRN waveguide by only 1 dB (20%) for 200 nm misalignment, while for the other two, the corresponding values are 1.74 dB and 1.25 dB, respectively and provide total loss of 1.62 dB (68.9%), 3 dB (50.1%) and 2.24 dB (59.7%). At the same time, the back-reflections for 300 nm y-axis misalignment are
Fig. 12. Coupling efficiency (%) from Plane A to Plane B of the optimum Strip (black), Rib (red) and Tri-Layer (blue) interfacing configurations for varying misalignment in the (a) y-axis, (b) z-axis, (c) Coupling efficiency (%) of the SRN-to-Si$_3$N$_4$ directional coupler for varying misalignment in the y-axis.

lower than -54 dB, -34 dB and -52 dB for the strip, rib, and tri-layer cross sections, respectively. The corresponding values for 200 nm z-axis misalignment are -55 dB, -34.9 dB and -56.9 dB. Finally, for the combination of 300 nm in the y-axis and 200 nm in the z-axis i.e. the worst-case alignment scenario, the total coupling loss is only 1.78 dB and the back-reflections are lower than -54.4 dB for the tri-layer SRN, revealing the high fabrication tolerances of this proposed coupling scheme and fully justifies the required extra fabrication complexity.

Figure 12(c) illustrates the performance degradation analysis in the SRN-to-Si$_3$N$_4$ evanescent coupler and confirms the high tolerances expected from the directional coupling scheme. For 300 nm y-axis misalignment the coupled power drops only by 0.5 dB with the total coupled power calculated at 0.62 dB (86.4%). In terms of z-axis misalignment, the thickness error from the CVD process is typical ±1.5% across a 4" wafer from the targeted value and thus is considered negligible for all three critical parameters i.e. Si$_3$N$_4$ thickness, SiO$_2$ gap, and SRN thickness that determine the coupling efficiency at the SRN-to-Si$_3$N$_4$ interface.

Table 1 summarizes the calculated performance of all three proposed coupling schemes with other InP-to-Si$_3$N$_4$ experimentally demonstrated coupling interfaces. Our work is the only one compatible with monolithic integration and 248 nm DUV lithography for lowest possible PIC fabrication cost in large scale. For the tri-layer SRN the total coupling loss, including the

| Reference | Integration Process | Coupling Losses (dB) (InP-to-SRN + SRN-to-Si$_3$N$_4$ Propagation Losses) | Back Reflections (dB) | Minimum Feature Size (nm) |
|-----------|---------------------|---------------------------------------------------------------|----------------------|--------------------------|
| [18]      | Hybrid              | <1.8                                                           | -                    | -                        |
| [19]      | Heterogeneous       | _                                                             | _                    | 150nm                    |
| [20]      | Heterogeneous       | <2                                                            | _                    | 120nm                    |
| [32]      | Heterogeneous       | 0.66 + 0.32                                                   | -36dB                | 120nm                    |
| [33]      | Heterogeneous       | 0.2                                                           | _                    | 100nm                    |
| This work - Strip | Monolithic              | 1.26 + 0.13 + 0.3 (Sim.)                                      | -54.4 (Sim.)         | 210nm                    |
| This work - Rib    | Monolithic              | 0.98 + 0.13 + 0.3 (Sim.)                                      | -34.81 (Sim.)        | 200nm                    |
| This work – Tri-Layer | Monolithic              | 0.6 + 0.13 + 0.3 (Sim.)                                      | -52.6 (Sim.)         | 200nm                    |
propagation losses in the SRN intermediate waveguide, is 1.03 dB with the potential to go to sub-dB by further improvement in the SRN etching process. Further coupling performance improvement could be obtained from higher resolution lithography for the formation of narrower tip in the SRN.

5. Summary

This work presents a systematic analysis for the design of SRN interposers, suitable for seamless light transfer from QD-InP-based gain sections to Si$_3$N$_4$ waveguides in a BEOL process targetingPICs with advanced functionality. Based on an extended set of simulations results, three types of interposer waveguide configurations have been designed that exchange performance for fabrication complexity. The simplest one relies on 500nm thick SRN strip waveguide with 1.06 dB couple loss and -19.79 dB back-reflections, while the rib one with the same overall thickness manages to improve the coupling loss to 0.86dB and lowering the back reflections to -30dB. The tri-layer sandwich material provides finally 0.77dB overall coupling loss and back reflections as low as -34.95dB. All these results are for $0^\circ$ angle at the QD InP-SRN interface and by introducing a $15^\circ$ angle, the tri layer stack manages to lower the back reflections and coupling loss to -52.4dB and 0.6dB, respectively. The tri-layer also exhibits the higher fabrication tolerance by imposing only 1.78 dB total loss and -54.4 dB back reflection for the worst case scenario of simultaneous 300 nm in the y-axis and 200 nm in the z-axis misalignment between the center points of the InP QD laser and the SRN waveguide. The proposed concept although assumes an InP active medium can be easily transferred also to monolithically grown GaAs based lasers and also to dual facet devices such as SOAs and electroabsorption modulators. In addition, the critical dimensions of all geometries in the three proposed designs are larger than 200nm that render them compatible with 248nm DUV lithography targeting to maximize the low-cost potentiality of the Si$_3$N$_4$ platform. The accuracy of the simulations is enhanced by taking into account for the refractive index of the SRN interposer the values extracted from ellipsometry measurements of an ultra-Si-rich-nitride material (SRN) developed and engineered for this purpose. This new material provides tunability in the real part of the refractive index, while crack free samples were grown up to 500 nm in thickness. Test structures with cutback waveguides of $500 \times 500 \text{nm}^2$ cross section formed via e-beam lithography featured 15dB/cm propagation losses in line with similar SRN materials. The proposed work is expected to pave the way for the next generation of a versatile, low cost, high performance monolithic InP-QD/Si$_3$N$_4$ platform on a common Si substrate.

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