Propagation Loss in Single-Mode Ultrasmall Square Silicon-on-Insulator Optical Waveguides

Frédéric Grillot, *Associate Member, IEEE*, Laurent Vivien, Suzanne Laval, and Eric Cassan

***Abstract*—Silicon-on-insulator (SOI) optical waveguides insure high electromagnetic field confinement but suffer both from sidewall roughness responsible of scattering effects and from leakage toward the silicon substrate. These two mechanisms are the main sources of loss in such optical waveguides. Considering the case of single-mode ultrasmall square SOI waveguides, propagation loss is calculated at telecommunication wavelengths taking into account these two loss contributions. Leakage toward the substrate and scattering effects strongly depend on the waveguide size as well as on the operating wavelength.**

***Index Terms*—Leakage, optical interconnects, optical telecommunications, optical waveguide, propagation loss, roughness, SOI.**

I. Introduction

SILICON-ON-INSULATOR (SOI) wafer is of prime importance for integrated optoelectronic circuits as it offers potentiality for monolithic integration of optical and electronic functions on a single substrate. As silicon is transparent at wavelengths larger than 1.1 μm, including optical communication bands, the silicon film of SOI substrates can be used to fabricate low-loss optical waveguides [1], [2]. Silicon/silicon dioxide (Si/SiO_2) waveguides benefit from a large refractive index difference, inducing high electromagnetic field confinement in the silicon guiding layer that in turn allows to reduce the waveguide size to sub-micrometer values [3]–[6]. Nevertheless, in order to use SOI waveguides for optical communications, both polarization insensitivity and single mode propagation have to be simultaneously fulfilled. It has been shown that these conditions can be achieved using deeply etched rib SOI waveguides with dimensions of the order of 1 μm [7]. At $\lambda = 1550$ nm, compact devices are obtained with square strip waveguides provided a square size smaller than 320 nm is used to insure single-mode condition. Due to the etching process [reactive ion etching (RIE)], those devices generally suffer from sidewall roughness. Such a random phenomenon constitutes the dominant source of propagation loss [8]. The use of an oxidation step or of an anisotropic etching added to an RIE etching process to reduce sidewall roughness has led to demonstrate the feasibility of low-loss SOI submicron waveguides [3]. In order to predict the impact of sidewall roughness on propagation loss, a model based on a planar optical waveguide has been developed [8]. Taking into account two-dimensional (2-D)-confinement, this model has then been extended to the case of 2-D Si/SiO_2 structures [9]. Based on the model described in [8] and [9], a numerical investigation of scattering loss induced by sidewall roughness as a function of the size of SOI square strip waveguides with cross-sections ranging from 500 nm $\times$ 500 nm to 150 nm $\times$ 150 nm has recently been published [10]. It has been demonstrated that scattering loss is not only linked to sidewall roughness but also strongly depends on the waveguide cross-section and decreases when the size is reduced below a given value, due to a lower optical confinement. As a result, scattering loss is strongly correlated to field confinement and the smallest structures can be useful for three-dimensional (3-D) tapers designed for low-loss coupling between polarization-insensitive microwaveguides and single-mode optical fibers [11].

It is well-known that loss in an SOI optical waveguide also comes from leakage toward the substrate. Loss due to leakage toward the substrate has been calculated as a function of the buried oxide thickness (BOX) for SOI rectangular structures with cross-sections ranging from 500 nm $\times$ 220 nm to 300 nm $\times$ 220 nm [4]. A strong loss increase was observed for BOX thickness smaller than 2 μm. Experimentally, an exponential behavior is reported for the total loss as a function of the waveguide width [4]. Other experimental results on SOI strip waveguides with 445 $\times$ 220 nm cross-section have pointed out the influence of the operating wavelength on propagation loss [5].

This paper reports propagation loss calculations taking into account at the same time loss coming from sidewall roughness as well as from leakage toward the substrate for various wavelengths within the standard telecommunications bands. In order to keep polarization insensitivity, these simulations have been done on square strip waveguides. The relative importance of the different contributions mentioned above in the propagation loss evolution is discussed in relation with the device size.

This paper is organized as follows. In Section II, the model developed to calculate scattering loss induced by sidewall roughness is described. Starting from Maxwell's equations, an analytical expression of the scattering loss coefficient is derived. At the same time, the numerical tool used to calculate leakage toward the substrate as well as the effective index is presented. In Section III, the numerical results are presented and discussed. At first, the influence of the operating wavelength both on scattering loss and leakage toward the substrate is investigated. The relative contribution of sidewall roughness and leakage toward the substrate in the propagation loss is then evaluated. Finally, results are summarized in Section IV. This

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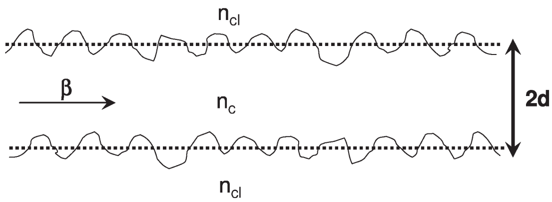

Fig. 1. Geometry of the planar waveguide with rough interfaces. The mean width is $2d$. $\beta = 2\pi n_{\rm eff}/\lambda$ is the propagation constant, with $n_{\rm eff}$ as the effective index and λ as the operating wavelength fixed either at $\lambda = 1550$ nm or at $\lambda = 1310$ nm.

numerical investigation conducted at different wavelengths on single-mode ultrasmall square SOI waveguides allows to understand the propagation loss behavior by taking into account the main contributions.

II. Numerical Model

The geometry of a planar optical waveguide with rough interfaces is represented in Fig. 1. The waveguide width is $2d$ and the propagation wavenumber is $\beta = 2\pi n_{\rm eff}/\lambda$, with $n_{\rm eff}$ as the effective index and λ as the operating wavelength fixed either at $\lambda = 1550$ nm or at $\lambda = 1310$ nm. The silicon core layer ($n_{\rm c} = 3.474$ at $\lambda = 1550$ nm and $n_{\rm c} = 3.505$ at $\lambda = 1310$ nm) is surrounded by a silica cladding ($n_{\rm cl} = 1.444$ at $\lambda = 1550$ nm and $n_{\rm cl} = 1.447$ at $\lambda = 1310$ nm). Sidewall roughness is represented by a random variation of the waveguide width. Such a variation leads to local variations of the effective index, corresponding to the formation of a pseudo-grating along the sidewall. Thus, sidewall roughness acts as a dipole that can be excited by the incident guided light. As a fraction of the dipole cannot be recovered, scattering loss effects take place [12]. Based on [8], the scattering loss coefficient due to surface roughness can be expressed as

$$\alpha_{\rm cm^{-1}} = \varphi^2(d)\left(n_{\rm c}^2 - n_{\rm cl}^2\right)^2 \frac{k_0^3}{4\pi n_{\rm c}} \int_0^{\pi} \tilde{R}(\beta - n_{\rm cl} k_0 \cos\theta)\, d\theta \tag{1}$$

where $\varphi^2(d)$ is a modal function only depending on the waveguide geometrical parameters and $k_0 = 2\pi/\lambda$ is the wavenumber in vacuum. The integral term includes the power spectrum function $\tilde{R}(\Omega)$ ($\Omega = \beta - n_{\rm cl} k_0 \cos\theta$, with θ as the scattering angle relative to the waveguide axis), which takes into account all the spatial frequencies Ω induced by sidewall roughness. Using the Wiener–Khintchine theorem [8] for the calculation of the total radiated power, $\tilde{R}(\Omega)$ can be linked to the autocorrelation function $R(u)$ through a Fourier transform [13]

$$\tilde{R}(\Omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} R(u) \exp(i\Omega u) du. \tag{2}$$

The autocorrelation function $R(u)$ takes into account the local variations of the effective index linked to the evolution of sidewall roughness and corresponds to a measurement of the average correlation between one position along the waveguide with another set at a distance u further along. In the literature, the autocorrelation function is described either by an exponential or by a Gaussian statistic [13]. Experimental investigations have recently shown that an exponential statistic is well suited to characterize sidewall roughness of larger waveguides [14], [15], but no experimental evidence has been yet reported for submicron ones. A sidewall roughness described by an exponential autocorrelation function is assumed in the following such as

$$R(u) = \sigma^2 \exp\left(-\frac{|u|}{L_c}\right) \tag{3}$$

where L_c is the correlation length, and σ is the standard deviation. Using (3), analytical calculations can then be carried out and the scattering loss coefficient in decibel per centimeter can be written as [9]

$$\alpha_{\rm roughness} = 4.34 \frac{\sigma^2}{k_0\sqrt{2}d^4 n_{\rm c}} g f(x) \tag{4}$$

where g and $f(x)$ are complex functions that have already been defined elsewhere [10]. Let us note that $g(V)$ is a function that is determined purely by the waveguide geometry such as

$$g(V) = \frac{U^2V^2}{1+W} \tag{5}$$

with the normalized coefficients

$$U = k_0 d\sqrt{n_{\rm c}^2 - n_{\rm eff}^2} \tag{6}$$

$$V = k_0 d\sqrt{n_{\rm c}^2 - n_{\rm cl}^2} \tag{7}$$

$$W = k_0 d\sqrt{n_{\rm eff}^2 - n_{\rm cl}^2}. \tag{8}$$

The function $f(x)$ is linked to sidewall roughness and describes the integral over the spectral density function. It can be expressed following the relation

$$f(x) = \frac{x\sqrt{1 - x^2 + \sqrt{(1+x^2)^2 + 2x^2\gamma^2}}}{\sqrt{(1+x^2)^2 + 2x^2\gamma^2}} \tag{9}$$

where the normalized expressions of coefficients x, γ, and Δ can be written as

$$x = W\frac{L_{\rm c}}{d} \tag{10}$$

$$\gamma = \frac{n_{\rm cl} V}{n_{\rm c} W\sqrt{\Delta}} \tag{11}$$

$$\Delta = \frac{n_{\rm c}^2 - n_{\rm cl}^2}{2n_{\rm c}^2}. \tag{12}$$

Equation (4) shows that the scattering loss coefficient is linked to the roughness parameters σ and $L_{\rm c}$. However, this equation does not include lateral field confinement. For strip waveguides, scattering mostly comes from etched vertical sidewalls. In order to take into account the 2-D character of the square SOI strip waveguides, the effective index $n_{\rm eff}$ has

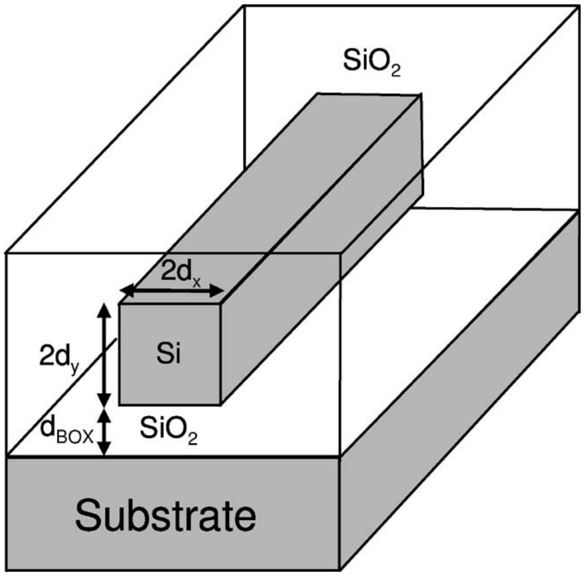

Fig. 2. Cross-section of the SOI strip waveguide under study with $2d_{\rm x} = 2d_{\rm y} = 2d$ ranging from 150 to 500 nm. The buried oxide thickness $d_{\rm BOX}$ is either 3 or 1 μm.

been calculated using the film mode matching (FMM) method, which is well suited to high index contrast structures [16], [17]. It is important to stress that variations of sidewall roughness along the vertical direction are neglected since the height of the waveguide is at most equal to 500 nm. It is also worth noting that such a model does not take into account scattering effects at the top and at the bottom surface of the waveguide. The FMM method is then used to calculate loss induced by light leakage toward the substrate. In the following, scattering loss and leakage toward the substrate are calculated at different wavelengths for square SOI strip waveguides with various widths.

III. Numerical Results

The SOI strip waveguide is schematically drawn in Fig. 2. It is assumed in the calculations that $2d_x = 2d_y = 2d$ ranges from 500 to 150 nm. Only the fundamental guided mode is considered for the largest waveguides and a transverse electric polarization is assumed.

A. Leakage Toward the Substrate

For each value of $2d$, leakage toward the substrate is calculated using the FMM method with a complex mode solver and perfectly matched layers (PML) boundary conditions [16]. Loss due to leakage toward the substrate is plotted as a function of the waveguide width assuming a buried silica thickness $d_{\rm BOX}$ equal either to 3 μm (Fig. 3) or to 1 μm (Fig. 4). In both cases, calculations are also conducted at $\lambda = 1310$ nm (dots) and at $\lambda = 1550$ nm (crosses). These simulations show that loss strongly depends on the operating wavelength and the waveguide size. In Fig. 3, loss rapidly increases as soon as the size of the waveguide is below 230 nm at $\lambda = 1550$ nm (respectively, below 180 nm at $\lambda = 1310$ nm). For instance, when $2d = 200$ nm, loss goes up to 8.5 dB/cm at $\lambda = 1550$ nm, while it remains equal to zero at

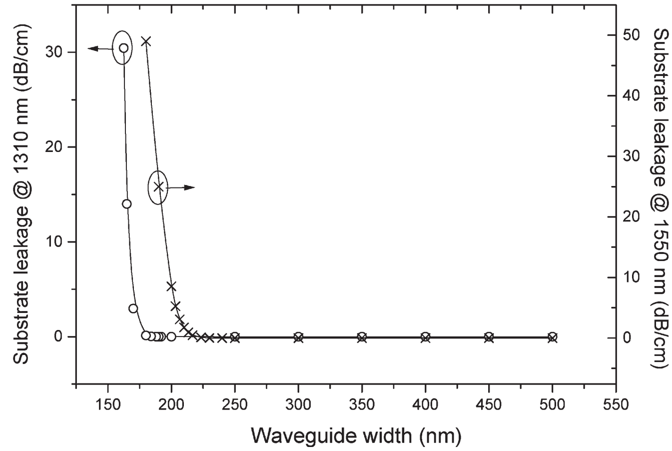

Fig. 3. Calculated loss due to leakage toward the substrate versus the waveguide size at $\lambda = 1310$ nm and at $\lambda = 1550$ nm. The buried silica thickness is fixed to 3 μm.

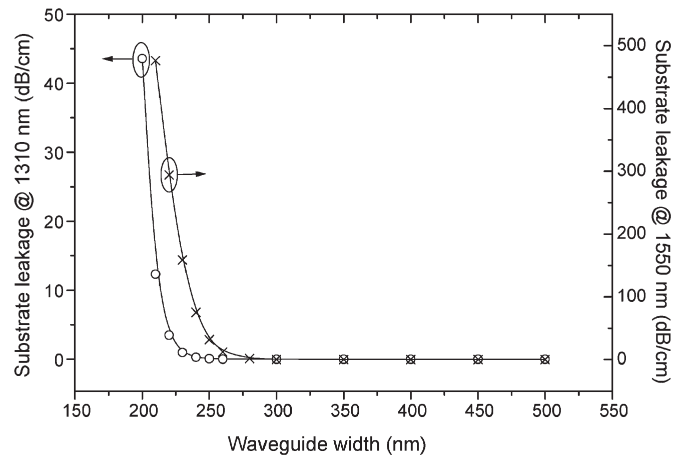

Fig. 4. Calculated loss due to leakage toward the substrate versus the waveguide size at $\lambda = 1310$ nm and at $\lambda = 1550$ nm. The buried silica thickness is fixed to 1 μm.

$\lambda = 1310$ nm. When the buried silica thickness is decreased to 1 μm, calculated loss is much more important at $\lambda = 1550$ nm, for which it reaches 30 dB/cm assuming a waveguide width such as $2d = 250$ nm. To conclude, the influence of the operating wavelength is attributed to mode confinement, which is better at $\lambda = 1310$ nm. As a result, loss due to leakage toward the substrate is smaller. However, above all, calculations show that such a loss is drastically enhanced when a BOX thickness smaller than 2 μm is used.

B. Scattering Loss Calculations

For each value of $2d$, scattering loss is calculated for the fundamental mode from (4). Results are plotted in Fig. 5, where the variation of the calculated scattering loss is reported versus the waveguide size $2d$, assuming a correlation length $L_{\rm c}$ of 50 nm and a standard deviation σ equal to 2 nm. The roughness parameters (σ, $L_{\rm c}$) have been chosen according to recent measurements obtained on similar structures, if an oxidation or an anisotropic etching step is added to the RIE process [3]. Calculations have been done for wavelengths equal either to $\lambda = 1550$ nm [case (a)] or to $\lambda = 1310$ nm [case (b)].

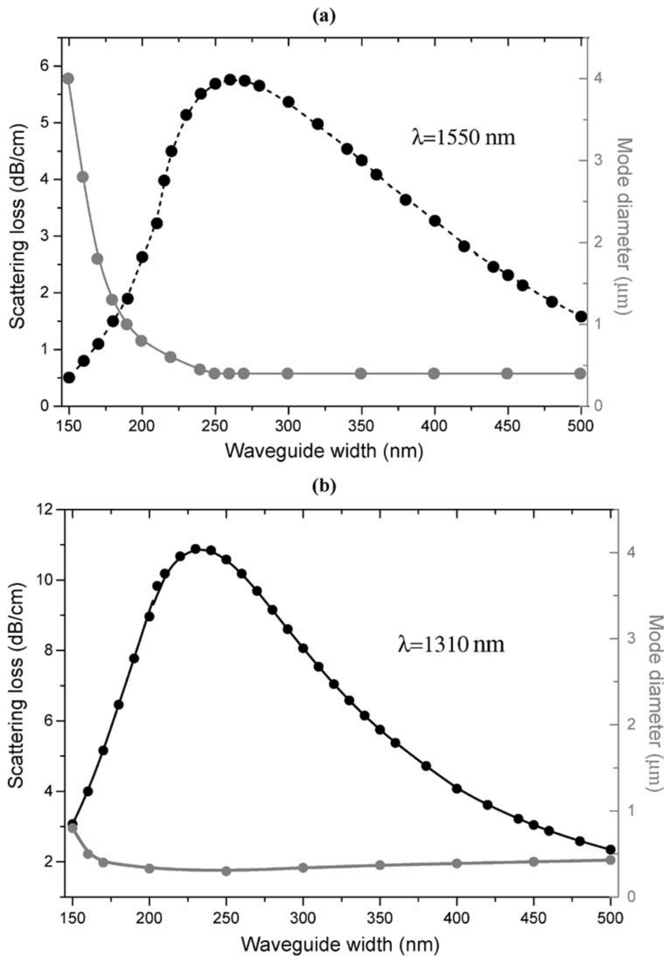

Fig. 5. Calculated scattering loss versus waveguide width (150 nm $< 2d <$ 500 nm) for roughness parameters equal to ($\sigma = 2$ nm, $L_c = 50$ nm) at $\lambda = 1310$ nm and at $\lambda = 1550$ nm (black curves). Calculated mode diameter at $1/e^2$ versus waveguide width and at $\lambda = 1310$ nm and at $\lambda = 1550$ nm (gray curves).

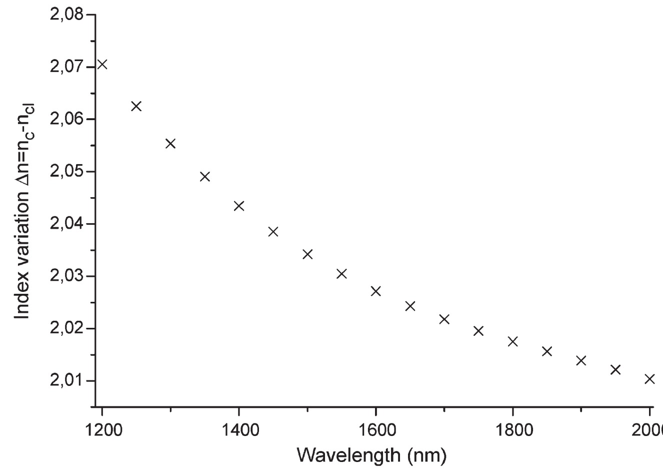

Fig. 6. Calculated index difference between silicon core and oxide cladding $\Delta n = n_c - n_{cl}$ versus the operating wavelength.

The mode diameter is also plotted versus the waveguide width for both cases. Two regions can be clearly distinguished. When the waveguide width decreases from $2d = 500$ nm to the value corresponding to the maximum loss ($2d = 260$ nm at $\lambda = 1550$ nm and $2d = 230$ nm at $\lambda = 1310$ nm), the sensitivity to sidewall roughness is strengthened since the mode confinement increases. Scattering loss is enhanced from 1.6 to 5.7 dB/cm at $\lambda = 1550$ nm and from 2.3 to 10.9 dB/cm at $\lambda = 1310$ nm. As no coupling with higher order modes is taken into account, scattering loss is underestimated in the calculations. On the other hand, when the waveguide width decreases from the values corresponding to the maximum loss to $2d = 150$ nm, loss decreases for both wavelengths. As it has been already shown [10], the effective index decreases and becomes very close to the refractive index of the silicon oxide cladding. This effect is accompanied by a significant deconfinement of the optical mode, which is favorable to loss reduction. If the mode diameter is defined at $1/e^2$ (although the field profile is exponential on each side of the waveguide core), mode deconfinement can be quantified and the mode diameter is plotted in Fig. 5. As an example, for $2d = 150$ nm, the predicted mode diameter at $1/e^2$ is 4 μm at $\lambda = 1550$ nm (0.8 μm at $\lambda = 1310$ nm) and the calculated scattering loss does not exceed 0.5 dB/cm at $\lambda = 1550$ nm (3 dB/cm at $\lambda = 1310$ nm). According to [10], such results show that scattering loss depends on the waveguide size. Scattering loss induced by sidewall roughness is enhanced as the wavelength decreases. Part of this enhancement is attributed to the variation of the silicon index with the wavelength. In Fig. 6, the refractive index difference between silicon and silica $\Delta n = n_c - n_{cl}$ is reported versus wavelength. The index difference goes up as the wavelength decreases, leading to a higher confinement and larger scattering loss. The other part mostly comes from the factor $k_0^3/4\pi$ located in (1) and strongly depending on the wavelength. As it is multiplied by 1.7 when the operating wavelength decreases from $\lambda = 1550$ nm to $\lambda = 1310$, $k_0^3/4\pi$ takes part to enhance scattered light from the waveguide. These simulations allow to predict scattering effects as a function of waveguide size and point out the main variations with the operating wavelength.

C. Propagation Loss Calculations

Taking into account both sidewall roughness and leakage toward the substrate, the propagation loss coefficient α is now calculated in decibel per centimeter following the relation

$$\alpha = \alpha_{\text{roughness}} + \alpha_{\text{substrate}} \tag{13}$$

where $\alpha_{\text{roughness}}$ is the contribution due to sidewall roughness while $\alpha_{\text{substrate}}$ corresponds to that related to leakage toward the substrate. Propagation loss is plotted in Fig. 7 as a function of the waveguide size both at $\lambda = 1310$ nm and at $\lambda = 1550$ nm for a BOX thickness of 3 μm. On one hand, simulations show that for waveguides such as $2d > 200$ nm, the roughness has an influence much more important than leakage toward the substrate itself. The maximum encountered in Fig. 5 can be easily recognized in both situations. On the other hand, when $2d < 200$ nm, the contribution of leakage toward the substrate is predominant. Those numerical results are qualitatively in good agreement with those published in [5]. In [18], a propagation loss equal to 6 dB/cm has been measured at $\lambda = 1550$ nm on 300 $\times$ 300 nm SOI strip waveguides. These experimental results also match very well our theoretical investigations

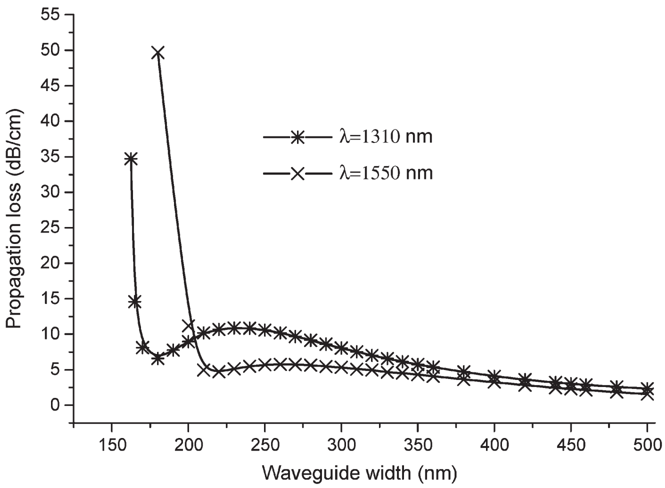

Fig. 7. Calculated propagation loss versus the waveguide width at $\lambda = 1310$ nm and at $\lambda = 1550$ nm.

since in Fig. 7, a propagation loss coefficient close to 5.5 dB/cm is predicted considering a similar structure. In conclusion, these results are of prime importance since they constitute the first theoretical quantification of the duality phenomenon existing between sidewall roughness and leakage toward the substrate.

IV. Conclusion

A numerical study has been performed to evaluate propagation loss in square SOI strip waveguides arising from both sidewall roughness and leakage toward the substrate. The dependence of scattering loss on the waveguide size is related to the mode diameter. It has been shown that scattering loss is very sensitive to the operating wavelength. A stronger resistance to sidewall roughness has been predicted as long as the wavelength increases. Loss due to leakage toward the substrate increases more rapidly at shorter wavelengths. Propagation loss has then been derived by taking into account the two previous contributions. Thus, sidewall roughness appears more detrimental for larger waveguides whereas leakage toward the substrate becomes predominant for smaller ones. These results allow to clearly distinguish the contribution between scattering and leakage toward the substrate in the propagation loss of guided mode in ultrasmall SOI waveguides.

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