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Effects of thin coating on guided mode and sidewall-roughness scattering loss in slot waveguides

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Abstract

Considering utilizing atomic layer deposition (ALD) to depress scattering loss due to sidewall roughness in silicon-on-insulator (SOI) slot waveguides, we discuss the effects of the refractive indexes and the thicknesses of the ALD layers on the modal field, the power confinement factor and the scattering loss of the slot waveguides by numerical simulation. We demonstrate that in applying ALD the decrease of the refractive index contrast on the sidewalls is the main reason for the reduction of the scattering loss, and a single-layer coating with a lower refractive index and a double-layer coating are more effective in depressing the scattering loss. We also show that suitable design of the slot waveguide and the coating scheme is necessary to reconcile both a high confinement factor and a low scattering loss.

Keywords: atomic layer deposition, scattering loss, sidewall roughness, SOI slot waveguide

(Some figures may appear in colour only in the online journal)

1. Introduction

Nowadays, the silicon-on-isolator (SOI) slot waveguide has been an important member in the thriving family of silicon photonics. It manifests unique ability in sensing and nonlinear optics. However, scattering loss in the SOI slot waveguide due to sidewall roughness is a serious problem obstructing its more flourishing applications [1–3]. At present, it is difficult to further reduce the sidewall roughness to a sub-nanometer scale by the lithography process. Therefore, something else needs to be done to depress the sidewall-roughness scattering loss. It is known that the scattering loss can be lessened by increasing the width of the silicon strips or the slot [4, 5], because the electric field intensity of the guided mode at the silicon sidewalls goes down as either of them gets wider. However, enlarging the waveguide size is not conducive to the compactness of an integrated optical chip. In addition, increasing the width of the slot would weaken its confinement on the guided optical power and aggravate substrate radiation [4]. Another way to reduce the scattering loss and increase the power confinement is to fill the slot and clad the waveguide with a low-index material, such as silicon dioxide (SiO_2), SU8 polymer, or aluminum oxide (Al_2O_3) [4–6], whereas in many applications of the slot waveguides, especially in sensing, the slot needs to remain open.

Like depressing the sidewall-roughness scattering loss in SOI strip waveguides [7–9], atomic layer deposition (ALD) has also been proved to be effective for slot waveguides [10]. By ALD, one or several thin dielectric layers, whose refractive indexes are lower than that of silicon, cover the surface of the waveguide to smooth the sidewalls. However, it is still unknown how much the refractive indexes and the thicknesses of the deposited layers are more beneficial. In addition, for the strip waveguide, the coating is completely deposited in the cladding region, which may have very limited influence on the guided mode of the waveguide. As for the slot waveguide, it has two inner sidewalls and two outer ones, and the inner ones are the dominant source of the scattering loss

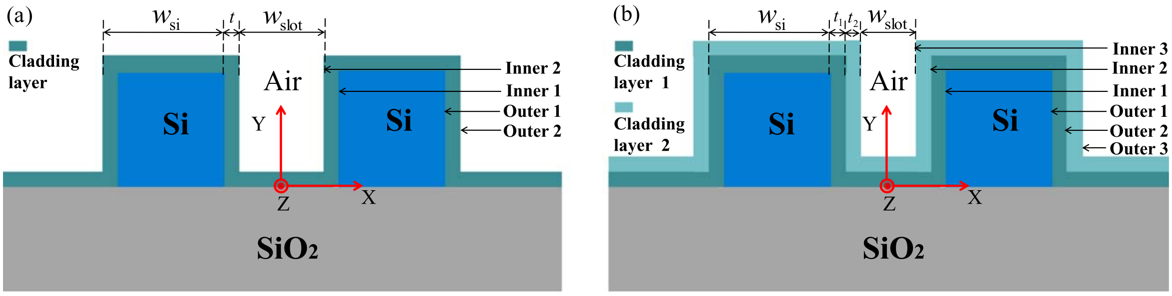

Figure 1. Schematic illustration of the coordinate system and the cross section of the slot waveguides with a single-layer coating (a) and a double-layer coating (b), respectively.

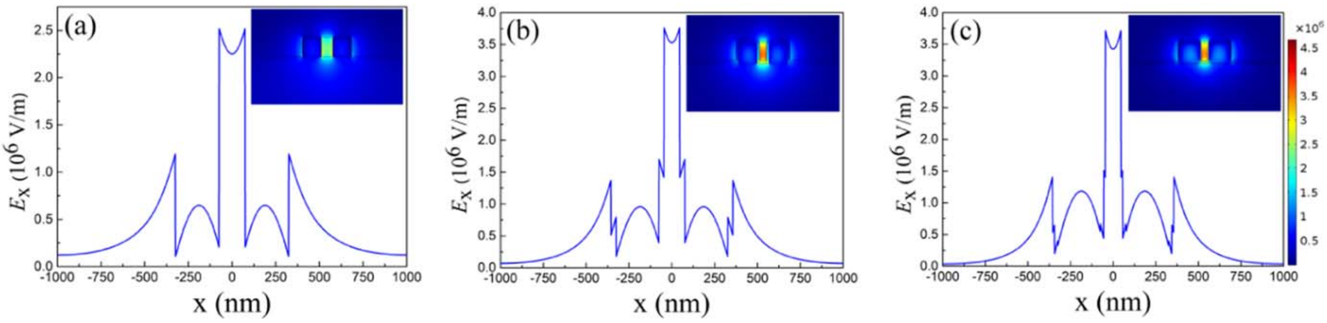

Figure 2. E_x electric field profiles of the fundamental quasi-TE mode along the $y = 110$ nm line in waveguides without coating (a), with an Al_2O_3 single-layer coating of $t = 30$ nm (b), and with a SiC and Al_2O_3 double-layer coating of $t_1 = 20$ nm and $t_2 = 10$ nm (c), respectively. The insets are the distributions of the E_x electric field on the cross sections of the waveguides. The scale bar on the far right is common for all the insets. Before coating, $w_{si} = 250$ nm, $w_{slot} = 150$ nm. The total guided power is 1 mW.

[11–13] and need to be coated. Because the slot is the main region of guiding and confining light, the coating must have a much larger impact on the guided mode and the power confinement for a slot waveguide than for a strip waveguide. Thus, besides considering the reduction of the scattering loss, it is also necessary to demonstrate the influence of the ALD on the modal field of a slot waveguide, especially on its power confinement in the slot, so as to deposit suitable materials with reasonable thicknesses.

In this paper, we demonstrate the effects of the ALD coating on the guided mode and the sidewall-roughness scattering loss in slot waveguides by numerical simulation. Aluminum oxide, titanium dioxide (TiO_2) and silicon carbide (SiC) are considered as representative coating materials with different refractive indexes. Firstly, the effects of the thickness and the refractive index of the coating on the field distribution, the effective refractive index and the power confinement factor of the SOI slot waveguide are calculated. Then, under the premise of an optimal confinement factor, the electric field intensity distributions at the new sidewalls and the interfaces between every two different dielectrics are calculated when different coating materials are employed. Finally, the Payne and Lacey's model [14] is used to estimate the reduction of the relative scattering loss brought by different coating schemes. Some useful guidelines can be derived from work in this paper for the utilization of ALD method in depressing the scattering loss of SOI slot waveguides.

2. Effect of coating on guided mode in slot waveguides

2.1. Change of field distribution and effective refractive index

Figure 1 illustrates the definition of the structural parameters and the coordinate system for the SOI slot waveguides with a single-layer coating and a double-layer coating, respectively. The origin of the *y*-axis is placed on the top of the SiO_2 substrate. In this paper, the slot width of the waveguide is always defined as the width of the air gap and expressed as w_{slot}. The height of the silicon strips is fixed as 220 nm, and their width, w_{Si}, needs to be optimized to obtain as large as possible power confinement in the slot. It is assumed that the thicknesses of the horizontal and the vertical deposited layers are the same and are symbolled as t.

After being coated, the height of the dielectric strips on both sides of the air slot increases, the bottom line of the slot rises, and the slot becomes narrower. Thus, the coating changes the waveguide structure. Although it is thin, the effect of the coating on the modal field distribution and the effective refractive index cannot be neglected because the original slot width is only about 100 nm or less. To illustrate this, guided modes in three waveguides: without coating, with an Al_2O_3 single-layer coating, and with a SiC and Al_2O_3 double-layer coating are solved by the finite element method. The profiles of the dominant electric field component, Ex, of the fundamental quasi-TE mode on the y =100 nm line are shown in figure 2.

The insets are the distributions of the *Ex* electric field on the cross section of the waveguides. The total power of the mode is always set as 1 mW as calculating the modal fields in this paper.

According to the boundary conditions of electromagnetic fields, at the interface of two dielectrics the electric field intensity along the *x*-axis in dielectric 1, $E_{1,x}$, is n_2^2/n_1^2 times of $E_{2,x}$ in dielectric 2, where n_1 and n_2 represent the refractive indexes of the two dielectrics, respectively. Due to the introduction of the coating, the number of the interfaces of two different dielectrics in the waveguide increases, so the number of the electric field discontinuities increases in the field profiles. The slot waveguide without coating has four vertical sidewalls, while those with one and two coating layers have eight and twelve interfaces, including the new sidewalls, respectively. As can be seen from figure 2, the electric field intensity along the *x*-axis undergoes a discontinuity at each interface, and the amplitude of the discontunity is determined by n_2^2/n_1^2. Because the refractive indexes of the coating layers are between those of the silicon strips and the air, the larger electric field discontinuities on the original sidewalls of the silicon strips are replaced by some smaller ones.

Besides the increase of the number of the electric field discontunities, the coating layers also affect the mode field distribution on the cross section of the waveguide. The insets in figure 2 show that the uncoated waveguide radiates obviously in the substrate and the cladding, and its field confinement in the slot is the weakest among the three waveguides. The field intensity in the silicon stripes of the double coated waveguide is the strongest. However, these changes of the electric field distribution are not deterministic because all the parameters of the original waveguide and the coating play a role. What is deterministic is that the thin coating may impact the mode field distribution significantly, and it is necessary to optimize the parameters of the waveguide and the coating before applying ALD.

Because the refractive index of the coating is between those of silicon and air, if the coating occupies the original region of the silicon strips, the effective refractive index of the waveguide will decrease; otherwise, if the coating is located in the original air region, the effective refractive index will increase. To illustrate the variation of the effective refractive index after ALD, three cases are calculated: (1) the slot width is fixed at 50 nm, and the width of the silicon strips varies with the thickness of the coating but remains $w_{\mathrm{Si}} + 2t = 250$ nm; (2) the width of the silicon strips is fixed at 250 nm, the initial width of the slot is 150 nm, and with the increase of the coating thickness, the slot becomes narrower correspondingly; (3) the widths of the silicon strips and the slot are kept as 250 nm and 100 nm, respectively. The variations of the effective refractive index of the slot waveguide versus the thickness of a Al_2O_3 coating in above cases are shown in figure 3. It can be seen from the figure that the coating has an obvious impact on the effective refractive index. For example, if a 30 nm thick coating is applied, the effective refractive index suffers a change of 0.1659, 0.1433 and 0.085 in the three cases, respectively.

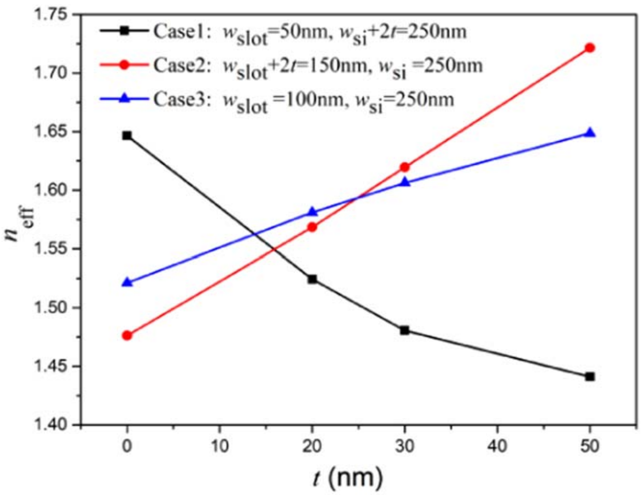

Figure 3. Variation of the effective refractive index with the thickness of the Al_2O_3 coating in three cases.

2.2. Effect of coating on power confinement factor

The power confinement factor of a slot waveguide is defined as the fraction of the guided power localized in the slot. Supposing the slot width before coating is 150 nm, the power confinement factor is calculated at different widths of the silicon strips and different coating thicknesses of three coating materials. The contours of the power confinement factor shown in figure 4 are obtained. As can be seen from figure 4, the higher the refractive index of the coating has, the greater the maximum confinement factor is, and the narrower the silicon strips to obtain this maximum confinement factor is. The total width ($w_{\mathrm{slot}} + 2w_{\mathrm{Si}} + 4t$) of the waveguide with the optimal confinement factor also decreases with the increase of the refractive index of the coating. The specific data are as follows: With a Al_2O_3 coating of a refractive index of 1.64, the maximum confinement factor is 13.9%, the width of the silicon strips is 250 nm, the thickness of the coating is 15 nm, and the total width of the waveguide is 680 nm; With a TiO_2 coating of a refractive index of 2.27, the corresponding data are 16.9%, 210 nm, 30 nm and 630 nm, respectively; With a SiC coating of a refractive index of 3.1, the data are 18.8%, 170 nm, 30 nm, and 550 nm, respectively. Because the confinement factor is the most important parameter of a slot waveguide, similar calculation as above should be carried out when considering applying ALD to slot waveguides, and appropriate parameters of the original waveguide and the coating should be adopted.

3. Effect of coating on modal electric field intensities at interfaces and scattering loss

3.1. Model of estimating scattering loss due to interface roughness

The Payne and Lacey's model is widely used in estimating scattering loss due to sidewall roughness in planar waveguides [14]. According to this model, the expression of the

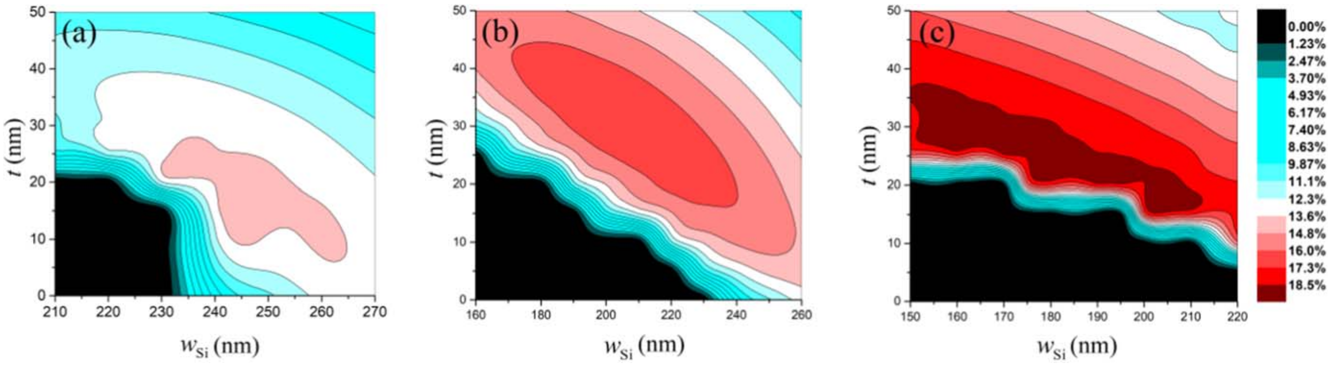

Figure 4. The effect of the coating thickness and the width of the silicon strips on the confinement factor. Before being coated the width of the slot is 150 nm. The coating materials are Al_2O_3 (a), TiO_2 (b) and SiC (c), respectively.

scattering loss coefficient of a planar waveguide with two uncorrelated sidewalls is

$$\alpha = \frac{\sqrt{2}\,k_0^3}{4n_1}A\varphi_{\mathrm{sw}}^2(n_1^2 - n_2^2)^2\sigma^2 L_c, \tag{1}$$

where the factor A is

$$A = \sqrt{\frac{\{4\beta^2L_c^2 + [1 - L_c^2(\beta^2 - n_2^2k_0^2)]^2\}^{1/2} + 1 - L_c^2(\beta^2 - n_2^2k_0^2)}{4\beta^2L_c^2 + [1 - L_c^2(\beta^2 - n_2^2k_0^2)]^2}}. \tag{2}$$

Equation (1) indicates that the scattering loss due to sidewall roughness is proportional to φ_{sw}, $(n_1^2 - n_2^2)^2/n_1$ and σ^2L_c. Here, we define $n_r = (n_1^2 - n_2^2)^2/n_1$, and refer to it as the contrast parameter of the refractive indexes. Thus, the scattering loss due to sidewall roughness can be depressed in three ways: depressing the field intensity, decreasing the refractive index contrast and abate the roughness at the sidewalls. Obviously, a deposited layer fills the grooves on the sidewalls of the silicon strips, so the roughness of the coating will be lower than that of the original etched sidewalls, and the thicker the coating is, the smoother the new sidewalls are. The refractive index of the coating should be between those of silicon and air. Increasing the refractive index of the coating will lower n_r on the coating-silicon interfaces but increasing that on the new air-coating sidewalls. Specifically, at the coating-silicon interfaces, $n_1 = 3.48$, i.e. the refractive index of the silicon strips, and n_2 is the refractive index of the coating, which can be any value within 1-3.48; at the air-coating sidewalls, $n_2 = 1$, i.e. the refractive index of air, and n_1 is the refractive index of the coating. Variations of n_r with the refractive index of the coating at the coating-silicon interfaces and the air-coating sidewalls are illustrated in figure 5. It can be seen that the refractive index of the coating may change n_r within 0-35.47 for both of the interfaces, but its effects are reversed. Therefore, it is necessary to compromise the refractive index of the single coating layer, or to deposit two coating layers and let the refractive index of the inner layer near the silicon strips be larger than that of the outer one near the air.

In (1) and (2), φ_{sw} is the electric field intensity of the guided mode at the waveguide sidewalls, n_1 and n_2 are the refractive indexes of the waveguide's core and cladding, respectively, k_0 is the free-space wavenumber, β is the modal propagation constant, and σ and L_c are the standard deviation and the correlation length of the sidewall roughness, respectively. Combined with the effective refractive index method, this model can also be used to estimate the scattering loss of three-dimensional strip waveguides [15, 16]. In this paper, we apply this model to each interface of a slot waveguide and take their sum as the total scattering loss to evaluate the effect of the coating on depressing the scattering loss of the slot waveguide. Because the coefficient A given by equation (2) is little affected by waveguide parameters [16], we ignore its influence on the variation of the scattering loss and calculate the scattering losses of the waveguides at every interface by the rest part in equation (1), and called the results as relative scattering losses. The higher and the lower refractive indexes of the two sides of each interface are chosen as n_1 and n_2, respectively. As mentioned above, the electric field intensities on the two sides of the interface are discontinuous, and the ratio of them is n_2^2/n_1^2. We consider only the larger one on the side with a lower refractive index and employ it as φ_{sw} in equation (1). Since the Payne and Lacey's model was derived for solid-core planar waveguides, accurate scattering loss cannot be obtained directly by it for strip and slot waveguides. However, it is reasonable for us to utilize it to estimate the relative scattering loss of the coated slot waveguides, because the influence of the refractive index contrast, the electric field intensity and the roughness at the sidewalls on scattering loss is similar for different kinds of waveguides [12], [13], [16].

In addition, it should be noted that the original silicon surfaces do not disappear, and its roughness does not decrease after ALD. What happens there are only the decrease of the refractive index contrast and the possible change of the modal field intensity, which will be discussed later. More importantly, the number of the interfaces increases significantly after the introduction of the coating, which is unfavorable to

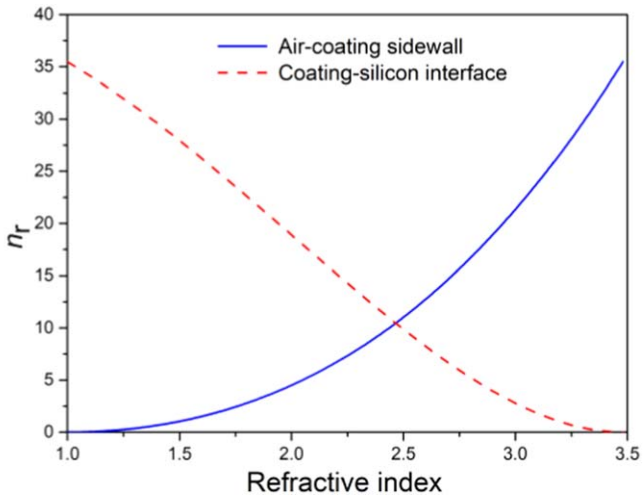

Figure 5. The effects of the refractive index of the coating on the contrast parameter of the refractive indexes at the air-coating sidewalls (the solid line) and the coating-silicon interfaces (the dotted line).

the reduction of the scattering loss. Therefore, in order to determine whether the total scattering loss can be effectively depressed by ALD, we need to compare the scattering losses before and after ALD.

3.2. Effect of single-layer coating on modal field at interfaces and scattering loss

For three-dimensional waveguides, the distribution of the electric field of the guided mode along each interface is not uniform. For the SOI slot waveguides shown in figure 1, because the materials of the substrate and the cladding are different, the distribution of the electric field is not symmetric with respect to the central point of the interface. Hence, the field intensities at the interfaces at the $y = 110$ nm line shown in figure 2 cannot be utilized to represent the electric field intensity on each interface. Therefore, we calculate the E_x field distribution of the fundamental quasi-TE mode on the cross section of the waveguide like what is shown in the insets of figure 2 and extract the electric field intensity distribution along the interfaces. Since the waveguide is symmetrical with respect to the y-axis, we need only obtain the field on the interfaces beside one of the silicon strips. For the single-layer coating, there are four interfaces to be considered, and for the double-layer coating, there are six.

Since the power confinement in the slot is very important for slot waveguides, we choose to compare the scattering loss of the waveguides having an optimal confinement factor. For the reference uncoated waveguide, we set its slot width as 100 nm. When $w_{si} = 250$ nm, the confinement factor of the waveguide is maximum (16.0%). The electric field intensity profiles along the two sidewalls of one of the silicon strips are shown by the black solid and the black dotted lines in figure 6, respectively. As can be seen from figure 6, the electric field intensity along the inner sidewall of the silicon strip is much higher than that along the outer one. This illustrates the necessity of coating the inner sidewalls of the slot waveguides. Because the refractive index of the SiO_2 substrate is higher than that of the air cladding, the electric field intensity on the lower part of a sidewall is larger than that on the upper part. At the four vertexes of the silicon strip, the electric field intensity has a rapid increase due to the right-angle turnings there.

For waveguides with a single-layer coating of the three materials, optimal structural parameters for a maximum confinement factor given in section 2.2 are chosen. When the input power is 1 mW, the field intensity profiles at the interfaces are shown in figure 6. It can be seen from figure 6 that the sidewall adjacent to the air slot (Inner 2) still has the largest electric field intensity, which is comparable to that on the inner sidewall of the uncoated waveguide. The electric field intensities on other interfaces resemble that on the outer sidewall of the uncoated waveguide.

Using equation (1), we estimate the reduction of the relative scattering loss in slot waveguides with a single-layer coating relative to that of the uncoated one. In calculation, utilizing the electric field profiles along the interfaces shown in figure 6, we obtained the average electric field intensity at each interface and set it as φ_{sw} in equation (1). Suppose the sidewalls of the original etched silicon strips have a roughness of $\sigma = 5$ nm and a correlation length of $L_c = 15$ nm [10]. Considering that the thicker the coating layer, the smoother its surface is, and the correlation length is inversely proportional to the roughness, and referring to [8], [15] and [16], we infer the roughness and the correlation lengths for the coating layers as provided in table 1. The obtained relative loss coefficients are normalized to that of the uncoated waveguide and listed in the table. Also given in the table are the proportions of the loss at each interface.

Table 1 shows that the coating can depress the scattering loss dramatically. Especially for the Al_2O_3 coating, although its thickness is only half of that of the SiC and the TiO_2 coatings, its effect is the most remarkable: the loss can be reduced to 15% of that of the uncoated waveguide. Actually, according to the data in table 1, for the single-layer Al_2O_3 coating, the value of $\sigma^2 L_c$ on the air-coating sidewalls is 332 nm^3. It is not much smaller than that of the original air-silicon sidewalls, 375 nm^3. In addition, as mentioned above, the electric field intensity on Inner 2 is very close to that on the inner sidewalls of the uncoated waveguide. Therefore, the small loss proportion of Inner 2 must be attributed to the decrease of the contrast of the refractive indexes. Indeed, n_r on the uncoated inner sidewalls is 35.47, while on the air-Al_2O_3 sidewalls it is only 1.74. As for Inner 1, although n_r is still pretty large (25.5), the electric field intensity there gets smaller (less than half of those on Inner 2 and the uncoated inner sidewalls). This also contributes to the decrease of the scattering loss, but the contribution is much smaller than that from Inner 2.

In summary, the effect of the Al_2O_3 coating on depressing the scattering loss stems from following two factors: (1) the position of the largest electric field intensity is moved from the inner silicon sidewall to the inner air-coating sidewall (Inner 2), which has a much small n_r and a slightly smaller $\sigma^2 L_c$; (2) both the electric field intensity and the n_r get

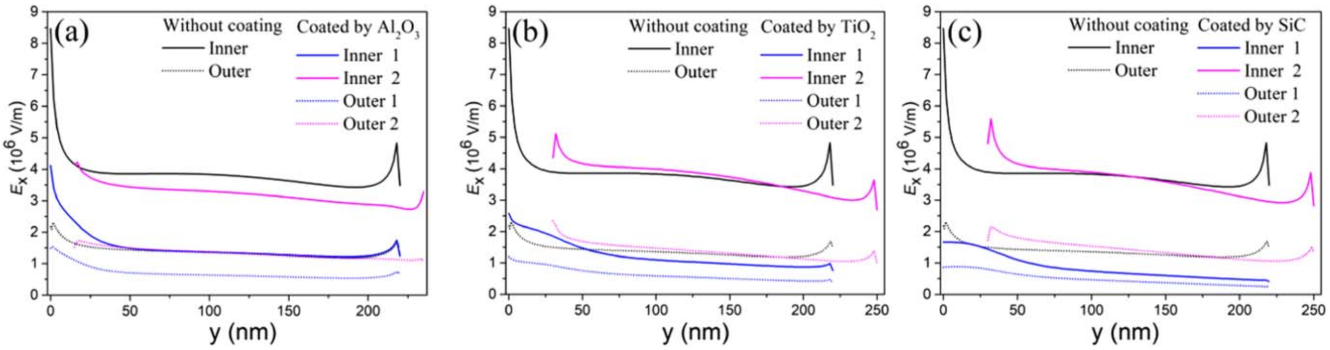

Figure 6. E_x field profiles of the fundamental quasi-TE mode along the sidewalls of slot waveguides without coating and with single-layer Al_2O_3 (a), TiO_2 (b) and SiC (c) coatings, respectively.

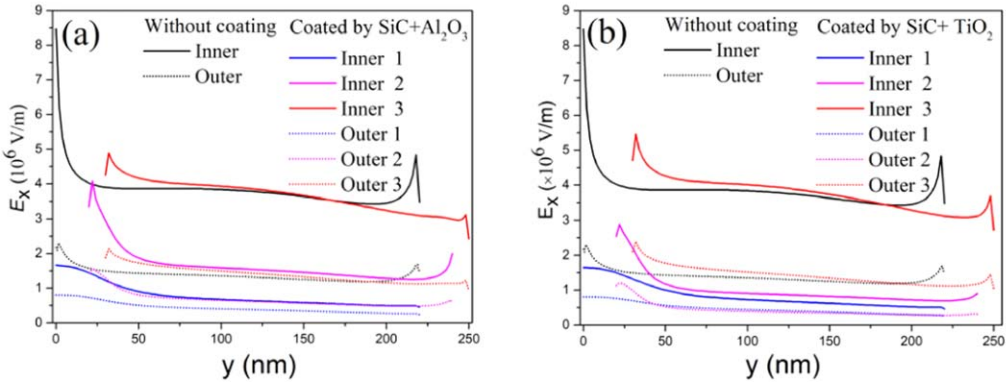

Figure 7. E_x field profiles of the fundamental quasi-TE mode along the sidewalls of slot waveguides without coating and with a double-layer coating. (a) Coated by SiC and Al_2O_3 layers; (b) Coated by SiC and TiO_2 layers.

Table 1. Normalized relative scattering loss coefficients of slot waveguides with a single-layer coating and loss proportion of each interface.

Single-layer coating					Proportion of scattering loss at each interface (%)			
Material	t (nm)	σ (nm)	L_c (nm)	Normalized total relative scattering loss	Inner 1	Inner 2	Outer 1	Outer 2
None	0	5	15	1	88.67		11.33	
Al_2O_3	15	4.3	18	0.15	65.14	17.76	14.05	3.05
TiO_2	30	4.1	20	0.22	16.09	72.30	4.10	9.51
SiC	30	4.1	20	0.54	0.39	86.41	0.13	13.06

smaller on the inner silicon interface (Inner 1) comparing to the uncoated situation. These are the same for the effect of the TiO_2 and the SiC coating layers. With the increase of the refractive index of the coating material, the effect of the first factor decreases, while that of the second increases, because n_r increases on Inner 2 and decreases on Inner 1. Clearly, the influence of n_r is the dominant and larger than those of the electric field intensity and the roughness. Therefore, a coating with a lower refractive index is more efficient in reducing the scattering loss. However, it is worth mentioning that as discussed in section 2.2, the available maximum confinement factor of the waveguide with a lower-refractive-index coating is the smaller, and its waveguide width is larger.

Table 1 also illustrates that with the coating, the scattering losses on the outer interfaces (Outer 1 and Outer 2) also decrease significantly and still take a small proportion in the total loss.

3.3. Effect of double-layer coating on modal field at interfaces and scattering loss

As depositing two layers, the refractive index of the inner layer should be higher than that of the outer one. We use a SiC layer with a thickness of 20 nm inside and 10 nm thick TiO_2 and Al_2O_3 layers outside, respectively. High confinement factors of 18.1% and 16.4% can be achieved by the two coating schemes, respectively. The electric field intensity profiles at the interfaces are shown in figure 7. Similar as the calculation results shown in figure 6 for the single-layer coating, the coating layers move the largest electric field

Table 2. Normalized relative scattering loss coefficients of slot waveguides with double-layer coating and loss proportion of each Interface.

Coating materials	Normalized total relative scattering loss	Proportion of scattering loss at each interface (%)					
		Inner 1	Inner 2	Inner 3	Outer 1	Outer 2	Outer3
None	1	88.67			11.33		
SiC+Al_2O_3	0.11	1.58	54.32	30.37	0.48	8.86	4.38
SiC+TiO_2	0.20	1.05	4.70	81.42	0.33	0.84	11.66

distribution from the inner silicon sidewall of the uncoated waveguide to the inner air-coating sidewall (Inner 3), and the electric field intensities on other interfaces are much smaller and comparable to each other.

Supposing $\sigma = 4.3$ nm and $L_c = 18$ nm for Inner 2, and σ=4.1 nm and L_c= 20 nm for Inner 3, using equation (1), the total relative scattering losses of the slot waveguides of the two coating schemes are estimated and the results are provided in table 2. Also, the scattering losses are normalized to that of the uncoated slot waveguide. As shown in table 2, the normalized relative scattering losses of the waveguides with a SiC + Al_2O_3 coating and a SiC + TiO_2 coating are 0.11 and 0.19, respectively. Comparing these data with the calculation results in table 1, it can be seen that although the number of the interfaces is further increased, the scattering loss goes down further. The reason for this is that the contrast parameters of the refractive indexes at some of the interfaces decrease more significantly than in the single-layer coating situation. The SiC + Al_2O_3 coating scheme cuts down more scattering loss than the SiC + TiO_2 one mainly because on Inner 3, where the electric field intensity is the largest, the refractive-index difference between the Al_2O_3 layer and air is smaller than that between the TiO_2 layer and air.

4. Conclusions

In conclusion, we have shown that although the number of the waveguide interfaces increases with the introduction of the coating, and the roughness of the original silicon surfaces remains unchanged, the total scattering loss can still be significantly reduced. By the coating, the position of the largest electric field intensity distribution is moved from the inner silicon sidewalls to the inner air-coating sidewalls, which has a lower refractive index contrast, and on the inner silicon surfaces, both the electric field intensity and the refractive index contrast get smaller. In both of these two aspects, the reduction of the refractive index contrast plays a role. Since the contrast parameter of the refractive indexes can be changed from 35.47 of an air-silicon sidewall to 1.74 of an air-Al_2O_3 sidewall, it has the most efficient effect to the depression of the scattering loss. By a thin coating, the decrease of $\sigma^2 L_c$ is very limited, so the reduction of the roughness does not contribute a lot.

Concerning the suppression of the scattering loss, coating with a low-refractive-index material is a better choice, and a multi-layer coating is better than a single-layer coating. However, the single-layer high-refractive-index coating and the double-layer coating are more favorable to the power confinement in the slot. In addition, both the parameters of the original waveguide and the coating determine the confinement factor. Therefore, it is necessary to optimize the waveguide structure and the coating scheme before applying ALD in order to ensure a remarkable depression of the scattering loss and a high confinement factor simultaneously.

Acknowledgments

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