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Application of atomic layer deposition in nanophotonics
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ABSTRACT
We review our recent results on using Atomic Layer Deposition (ALD) in fabrication of nanophotonic waveguide devices. ALD is a unique thin film deposition method providing atomic level control of film composition and thickness, perfect step coverage, and large-area uniformity. We employ the advantages of ALD in connection with Si-nanophotonics. We present several new structures based on filling silicon slot waveguides or coating the silicon strip waveguides with ALD-grown materials. Also ALD grown TiO\textsubscript{2} strip waveguides are introduced.

Keywords: atomic layer deposition, slot waveguides, strip waveguides, ring resonators

1. INTRODUCTION
During the last decade, silicon photonics has experienced increasing interest for two main reasons: the large-scale manufacturing capacity of the existing silicon microelectronics industry, and the special optical properties of silicon. The high refractive index of silicon enables very efficient light confinement and the small footprints of the silicon photonic devices. The high third-order optical nonlinearity ($\chi^{(3)}$) in silicon, about 200$\times$ higher than in silica, has been enabling the demonstration of the silicon-based all-optical devices with excellent performance.\textsuperscript{1,4} However, silicon has also some challenges such as two-photon absorption. While the high third-order optical nonlinearity enables all-optical functions, it may otherwise be problematic. Therefore, it is necessary to integrate other materials onto silicon photonic chips. In this article, we briefly review our recent advances in the integration of atomic layer deposited thin films with silicon nanophotonic devices.

Atomic layer deposition (ALD) has proven its excellence in the silicon nanophotonics during the last five years. For example, it can be used for reducing the feature sizes of the silicon slot waveguides\textsuperscript{5}, the propagation losses\textsuperscript{6}, the third-order nonlinearity\textsuperscript{7} or the polarization sensitivity of the silicon strip ring resonators\textsuperscript{8}. In ALD, the precursor gases are introduced into the growth chamber sequentially. The different precursors are separated by the purge of an inert gas, typically nitrogen. During the growth pulse, the precursor molecules react with the molecules on the surfaces. After one growth cycle, the fraction of an atomic layer is deposited. In ALD, the growth happens on the surfaces and therefore, the materials are growing conformally. Also the thickness of the film can be controlled accurately due to the nature of the atomic layer deposition. More information about ALD can be found from review articles, for example from Refs. 9 and 10.

A few silicon photonics foundries have been established during the last decades, for example Institute of Microelectronics in Singapore, IMEC in Belgium and Sandia National Labs in the US. Typically, these foundries are using 198 nm or 248 nm deep-UV lithographies which limit the feature sizes to around 100 nm or 160 nm, respectively. However, the optimal slot widths for silicon slot waveguides are below 100 nm and therefore, we proposed the feature size reduction of the silicon slot waveguides by partial filling using ALD materials in 2009\textsuperscript{5}. The filling of the silicon slot test structures using ALD was demonstrated in the same year\textsuperscript{5,11}. The first real silicon slot waveguides partially filled with ALD-TiO\textsubscript{2} were published in 2011 with the reduced propagation losses\textsuperscript{6}. The loss reduction was also observed in the silicon strip waveguides. The ALD-Al\textsubscript{2}O\textsubscript{3} filled silicon slot waveguides were proposed for low-
nonlinearity applications in 2011 and they also showed very low propagation loss, down to ~5 dB/cm\(^7\). In 2012, the ALD-Al\(_2\)O\(_3\) thin films were used to improve the quality factors of the silicon nanobeam cavities (Q-factors higher than 100k)\(^{12}\) and also the multiple slot structure with Al\(_2\)O\(_3\) and TiO\(_2\) films was demonstrated with reasonably low propagation loss\(^{13}\). We also studied theoretically the dispersion engineering of the silicon strip waveguides using the ALD-TiO\(_2\) as a coating material\(^{14}\). In 2013, the polarization sensitivity of the silicon strip ring resonators was dramatically reduced using ALD-TiO\(_2\) coatings\(^8\). The complex merged photonic crystal slot waveguide structure filled with ALD-TiO\(_2\) was also published in 2013\(^{15}\). Finally, ALD grown TiO\(_2\) strip waveguides were demonstrated in 2014 with propagation loss below 2.5 dB/cm\(^{16}\). All of these results prove the excellent quality of ALD deposited thin films in nanophotonic waveguiding applications. In this proceeding, we will give a short overview of these results.

2. ATOMIC LAYER DEPOSITION ON SILICON SLOT STRUCTURES

2.1. ALD filling of slot test structures

First, we fabricated grooves into standard silicon wafers to carry out initial studies on how ALD materials grow on silicon slot waveguide like patterns. The fabricated grooves are shown in Fig. 1a. In Fig 1b, the test structure has been coated by ALD-TiO\(_2\). A narrow air slot is retained in the widest two grooves, while the narrower grooves are perfectly filled without any clear interface in the middle. This structure demonstrated how conformally the ALD film has grown. Similar grooves covered first with ALD-Al\(_2\)O\(_3\) and then with ALD-TiO\(_2\) are presented in Fig. 1c. We also studied the slot filling with an ALD nanolaminate. In Fig. 1d., 5 x (10 nm x Al\(_2\)O\(_3\) + 10 nm x TiO\(_2\)) nanolaminate has been deposited on silicon slot test structure. Different layers are clearly visible in cross-sectional SEM image. The nanolaminates can be used to optimize optical properties of ALD grown thin films. We have demonstrated TiO\(_2/\)Al\(_2\)O\(_3\) and ZnO/Al\(_2\)O\(_3\) nanolaminates with enhanced third-order optical nonlinearities\(^{17,18}\). Also the propagation losses were reduced in TiO\(_2/\)Al\(_2\)O\(_3\) nanolaminates compared to crystalline TiO\(_2\). All of these structures shown in Fig. 1. demonstrate that ALD is an excellent method for filling silicon slots in a controllable way.

![Fig. 1. a) Uncoated slot test structure, b) same structure coated with ALD-TiO\(_2\) layer, c) similar structure coated first with ALD-Al\(_2\)O\(_3\) and then with ALD-TiO\(_2\) layer, and d) slot structure coated with TiO\(_2/\)Al\(_2\)O\(_3\) nanolaminate fabricated by ALD\(^{15}\).](image-url)
2.2. Feature size reduction

Due to diffraction limit, the silicon slot waveguides with optimal slot width cannot be fabricated using the deep-UV lithography. Therefore, an additional high-index coating on top of the silicon slot structure is crucial. Fig. 2a shows a schematic of a feature size reduced silicon slot waveguide. The cross-sectional SEM images of the silicon slot waveguide fabricated by 248 nm deep-UV lithography and coated with a 45 nm thick ALD-TiO2 layer is in Fig. 2b.

![Schematic of the feature size reduced silicon slot waveguide](image)

Fig. 2. a) Schematic of the feature size reduced silicon slot waveguide and b) the silicon slot waveguide covered with a 45 nm thick ALD-TiO2 layer.

The slot mode appears to the structure shown in Fig. 2a when the thickness of the ALD-TiO2 layer is 40 nm or higher.

2.3. Multiple slot waveguide

A schematic of the dual-filled silicon slot waveguide structure is presented in Fig. 3a and the cross-sectional SEM images of the fabricated structure in Fig. 3b. In Fig. 3b we can see that the 50 nm thick ALD-Al2O3 covers silicon slot structure perfectly. Even the voids below the silicon rails are completely filled.

![Schematic of the dual-filled silicon slot waveguide](image)

Fig. 3. a) Schematic of the dual-filled silicon slot waveguide and b) the cross-sectional SEM images of the dual-filled silicon slot waveguide.

This dual-filled silicon slot waveguide forms a multiple slot structure for TE-polarization. The simulated mode field is shown in Fig. 4. The measured propagation loss of the dual-filled slot waveguides was as low as 8 dB/cm for TE-polarization and 4 dB/cm for TM-polarization. These reasonably low losses prove that the Al2O3/TiO2 interface must be smooth.
3. LOSS REDUCTION WITH A THIN ALD-TiO$_2$ COATING

The propagation loss was measured from the silicon slot waveguides fabricated by 193 nm deep-UV lithography without any coating and with 20 nm, 30 nm and 50 nm thick ALD-TiO$_2$ coatings. The lowest loss values of silicon slot waveguides with different coatings are presented in Table 1. The lowest loss for uncoated slot waveguides was ~65 dB/cm proposing that the waveguide mode was not well guided. The propagation loss was reduced down to 7 dB/cm for the silicon slot waveguides with a 50 nm thick TiO$_2$ coating. The loss values decrease when the thickness of the coating layer increases. There are two explanations for that: first the effective indices of the modes increase when the high-index material (amorphous TiO$_2$) is deposited on top of the slot structure and second one is that the edge roughness of the silicon rails is decreased due to the conformally grown TiO$_2$ film.

<table>
<thead>
<tr>
<th>Silicon slot waveguides</th>
<th>Lowest loss value (dB/cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uncoated</td>
<td>~65</td>
</tr>
<tr>
<td>20 nm TiO$_2$ coating</td>
<td>~14</td>
</tr>
<tr>
<td>30 nm TiO$_2$ coating</td>
<td>~11</td>
</tr>
<tr>
<td>50 nm TiO$_2$ coating</td>
<td>~7</td>
</tr>
</tbody>
</table>

Fig. 5. shows schematically how the edge roughness decreases when the thickness of the ALD-TiO$_2$ increases. In reality, the roughness of the edge of the silicon rails does not decrease, but the refractive index difference at this interface decreases dramatically.

4. STRIP TO SLOT WAVEGUIDE COUPLER AND ALD-Al$_2$O$_3$ FILLED SLOT WAVEGUIDES

Schematic of the strip to slot waveguide coupler we designed is presented in Fig. 6a. Insets in the input and output sides show the mode fields of the TE-polarized light in the strip and slot waveguides, respectively. The SEM image of the 1 µm long strip to slot waveguide coupler is in Fig. 6b.
The measured losses per coupler as a function of the coupler length are plotted in Fig. 7. These couplers were coated with 166 nm thick ALD-Al₂O₃ films. The propagation loss in ALD-Al₂O₃ filled slot waveguides was very low. The lowest value was ~4 dB/cm. These ALD-Al₂O₃ were proposed to be suitable for the applications requiring low nonlinearities.

5. REDUCTION OF POLARIZATION SENSITIVITY IN SILICON STRIP RING RESONATORS

The ring resonators had a radius of 50 µm and a waveguide width of 460 nm. The whole chip area was first covered with 2 µm of PECVD SiO₂, and then the ring resonator parts were completely exposed to ambient by a highly selective SiO₂ etching (shown in Fig. 8). Such a design enables the deposition on the ring parts, leaving the rest of the waveguide parts intact. The ring resonators were covered with different thicknesses of ALD-TiO₂ film.

In Ref. 8, we demonstrated the potential to control the free spectral range (FSR) of the two orthogonal polarizations by tuning the TiO₂ overlayer thickness. Fig. 9. shows how the wavelength dependence of the FSR is drastically modified by increasing the TiO₂ overlayer thickness. The effect is particularly intense for the TM polarised mode since its profile experiences a strong influence from the change in surrounding material. The dispersion properties of the deposited TiO₂ govern the wavelength dependence of $n_{eff}$ and promote the corresponding FSR shift. Thus, when the TiO₂ thickness is 100 nm (Fig. 9c), both the absolute values and the slopes of the FSRs for TE and TM fundamental modes start to coincide remarkably. Finally, as the thickness achieves 150 nm (Fig. 9d), the peak-to-peak spacings of the two polarizations exhibit a good alignment with each other across the broad bandwidth.
In order to illustrate the peak-to-peak spacing for the TE and the TM input polarizations, the transmission spectra of the ring resonator with a 150 nm thick TiO₂ overlayer is presented in Fig. 10. As can be seen from that figure, the dips in the spectra are very near each other for both polarizations and the FSRs are staying same over this spectral range.

**Fig. 10.** Transmission spectra of the ring resonator with the 150 nm thick TiO₂ overlayer.

### 6. MERGED PHOTONIC CRYSTAL SLOT WAVEGUIDES

The concept of a merged nanoscale photonic crystal slot waveguide that acts as a bandpass filter in the near infrared region of the spectrum was demonstrated in Ref. 15. The device is based on the integration of a photonic crystal cavity...
in a slot waveguide on a SOI substrate. The device was coated by amorphous ALD-TiO₂, which allows to reduce two-
photon absorption losses and creates the possibility to combine nonlinear guided-wave optics resulting from the strong
field confinement in the slot region with slow light effects in the photonic crystal cavity. The simulated electric field and
the SEM images of the fabricated structure before ALD coating are presented in Fig. 11.

![Simulated electric field in the merged photonic crystal slot waveguide](image)

Fig. 11. a) Simulated electric field in the merged photonic crystal slot waveguide, b), d) and e) SEM images of the fabricated structure
before ALD-TiO₂ coating and c) SEM image of the strip to slot waveguide coupler.¹⁵

The simulated and measured transmission spectra of the merged photonic crystal slot waveguide are shown in Fig. 12.
The experimental spectra in Fig. 12b confirms that the merged photonic crystal slot waveguide with the cavity works as a
bandpass filter at the wavelength around 1350 nm.

![Transmission spectrum of the merged photonic crystal slot waveguide](image)

Fig. 12. Transmission spectrum of the merged photonic crystal slot waveguide. a) Simulated by 3D-FDTD, and b) measured for a 10
periods photonics crystal on each side with the cavity. All spectra were filtered using a Fourier transform band pass filter.¹⁵
7. ALD-TiO$_2$ STRIP WAVEGUIDES

TiO$_2$ strip waveguides were fabricated on oxidized silicon wafer using ALD and reactive ion etching. The SEM images of the fabricated TiO$_2$ waveguides are shown in Fig. 3a and b. The width of the waveguides was 1 µm and the height was 450 nm. TiO$_2$ was grown at low temperature (at 120 °C) and therefore the film is in an amorphous phase. The width of the coupling region was 3 µm and then the waveguide was tapered down to 1 µm. The propagation loss was estimated to be 5 dB/cm just after the etching process. The propagation loss was reduced down to 2.4 dB/cm by growing an additional 30 nm thick TiO$_2$ layer on top of it. The reason for the loss reduction is the reduced edge roughness as we discussed earlier in chapter 3.

Fig. 13. SEM images of a) the coupling facet of the TiO$_2$ waveguide and b) the whole waveguide structure. c) Transmitted power as a function of the waveguide length with different coating conditions.

8. CONCLUSIONS

Atomic layer deposition has been shown to work well with the silicon waveguide structures. ALD materials can fully fill the silicon slot waveguides without any air gap or rough interface in the middle. This allows introducing different materials with desired optical properties into the silicon photonic structures. For example, the silicon slot waveguides filled with Al$_2$O$_3$ have low nonlinearities compared to silicon strip waveguides, and we demonstrated ALD-Al$_2$O$_3$ filled Si slot waveguides with reasonably low propagation loss. Atomic layer deposition has also been used to reduce the feature size of the silicon slot waveguide and to reduce propagation loss in silicon strip and slot waveguides. ALD-TiO$_2$ can be used for dispersion engineering of the silicon waveguides due to the dispersion properties of ALD-TiO$_2$ and highly accurate thickness control. Recently, also the ALD-TiO$_2$ strip waveguides were demonstrated to exhibit low loss at the wavelength of 1.55 µm and in the future, they will be used for visible wavelengths too. We believe that the atomic layer deposition will be a highly used method in the nanophotonic applications in the future.
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6. REFERENCES


