Influences of silicon nano-crystallized structures on the optical performance of silicon oxynitride rib-type waveguides

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Abstract

Silicon oxynitride (SiON) films were deposited on p-type (100) silicon substrates by plasma enhanced chemical vapor deposition (PECVD), at the temperature of 300 °C, using silane (SiH4), nitrogen (N2), ammonia (NH3) and laughing gas (N2O) as gas precursors. The effects of the processing gas ratio of N2O/(N2 +NH3) on the optical properties, microstructure and chemical bonding evolutions of SiON material, and the influences of silicon nano-crystallized structures on the optical performance of SiON-based rib-type optical waveguides were studied. Microstructure evolutions analysis and optical measurements indicated that the refractive index and the extinction coefficient could be precisely determined by controlling the N2O/(N2 +NH3) ratio and the thermal annealing process. A greater density and dimension of silicon nano-crystallized structures resulted in more optical scattering effect phenomena occurring between the interface of silicon nano-crystallized structure and SiON matrix and more optical propagation loss.

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1. Introduction

In the last few years, following the rapid development of the Internet and multimedia services, the demand for transmission capacity has increased tremendously. This creates a big challenge for the information transmission capacity of the optical fiber network between metropolises and that of the long distance main optical line already set up. Dense wavelength division multiplexing (DWDM) technology is responsible for the original type of transmission capacity variation, and thus enables the capacity of the broadband to increase greatly. Arrayed waveguide grating (AWG) plays a key role in the DWDM system because of its flexibility, low-cost mass production, manufacturing processes similar to VLSI, and ease of integration with other optical electronic ICs.

The optical waveguide can be divided into two main categories in material selection. One is a low index contrast (LIC), such as using silica-based waveguides with a silica cladding [1] and other LIC optical materials [2,3], with low insertion loss performance. However, because of its larger dimension, its application scope is limited. Another is a high index contrast (HIC), such as using silicon waveguides with a silica cladding (silicon-on-insulator, SOI) [4] and other HIC optical materials [5,6]. Silicon oxynitride (SiON), which is considered the candidate material for LIC and HIC optical waveguides, possesses the properties of low residual stress, variations of refractive index controlled by adjusting N2O/(N2 +NH3) ratio, and low absorption phenomena for infrared regions [7].

However, the role of Si nano-crystallized structures in SiON film needs to be further clarified. Therefore, the effects of the processing gas ratio of N2O/(N2 +NH3) on the optical properties and microstructure evolutions of SiON material, and the influences of silicon nano-crystallized structures on the optical performance of SiON-based, rib-type optical waveguides were investigated.

2. Experimental

2.1. Structure simulation

The schematic structure of a rib-type waveguide was adopted by following Pogossian’s single-mode model [8], with indexes...
of 1.50 SiON and 1.45 SiO₂ films as core and top/bottom cladding layers, respectively, as shown in Fig. 1(a). The beam propagation method (BPM), with launch position and optical waveguides length variations for connecting optical fiber and optical waveguides, was studied to achieve reasonable coupling and propagation losses, respectively. Based on the simulation results, the quartz glass masks for AWG devices and straight optical waveguides pattern were designed and manufactured. These straight optical waveguides in the optical mask were used to measure the coupling and propagation losses.

2.2. Fabrication processes

In order to obtain the designed optical properties of SiON film, variations of N₂O/(N₂ + NH₃) ratio, in the range of 0.2~2.0, were adopted to deposit a 3000 nm thickness of SiO₂ and 6000 nm thickness of SiON single layer films on the D263T quartz glass. The ICP-PECVD system was used, with a radio-frequency (RF) of 13.56 MHz at the substrate temperature of 300 °C with the SiH₄ flow rate of 25 sccm, the NH₃ flow rate of 25 sccm, the N₂ flow rate of 75 sccm, the N₂O flow rate in the range of 20~200 sccm, and RF power wattage of 100 W with an operating vacuum pressure of 253 Pa, respectively. The thickness was monitored in-situ by quartz oscillation equipment. The optical transmittances of SiO₂ and SiON single layer films were determined by a Hitachi U-4100 scanning spectrophotometer in the wavelength region of 350~2000 nm. The refractive index and the extinction coefficient were determined by the Swanepoel [9] reported method and obtained a reasonable N₂O/(N₂ + NH₃) ratio to fabricate the designed waveguide. Therefore, we used the obtained N₂O/(N₂ + NH₃) ratio to deposit a 3000 nm thickness of SiO₂ and 6000 nm thickness of SiON films on the six-inch diameter, p-type (100) silicon wafer, respectively. We then proceeded with the optimum photolithography and reactive etching (C₄F₈/O₂) processes, by using the ICP-RIE system with a radio-frequency of 13.56 MHz at the temperature of 300 °C and using the C₄F₈ flow rate of 45 sccm, the O₂ flow rate in the range of 4~8 sccm, RF power wattage of 2500 W with an operating vacuum pressure of 0.67 Pa, respectively, to investigate the effects of etching reactant ratio (C₄F₈/O₂) on the profile and sidewall roughness of SiON optical waveguides. Subsequently, we annealed the determined etched bi-layer films in a thermal furnace with an oxygen atmosphere at the temperature of 1050 °C and operating pressure of 10,133 Pa for 4 h, respectively, to reduce the N–H bonds of SiON film. We deposited a 3000 nm thickness of SiO₂ to serve as the top cladding for the optical waveguides. Finally, we performed cutting, grinding, and polishing processes to finish the rib-type waveguides, and the optical characteristics of optical straight waveguides were measured by the auto optical coupling stage system, as shown in Fig. 1(b).

Surface roughness of the films was measured below the 5000 nm × 5000 nm size by using an atomic force microscope (AFM, Solver Scanning-probe-Microscope SPM-P7LS). Cross-sectional transmission electron microscopy (XTEM) samples were prepared by cutting, mechanical grinding, chemical mechanical polishing, and ion-milling (Gatan Duo-mill) to an electron transparency. High-resolution transmission electron microscopy (HRTEM) was used to observe the cross-sectional microstructure of the SiON core layer, with a JEOL JEM-4000EX type electron microscope operated at a voltage of 400 kV. The density and dimension of silicon nano-crystallized structures in the amorphous SiON optical films were quantitatively calculated with at least 5 TEM images. Optical waveguides profile analysis of the core layer was performed by scanning electron microscopy (SEM, JSM-6400).

3. Results and discussion

3.1. Simulation results

Optical waveguides, with the width of 5000 nm, the height of 6000 nm, the slab height of 4000 nm, and the length of 20 mm, revealed reasonable spectral performance by 3-dimension (3D) simulation, as indicated in Table 1. The waveguide of the smaller dimension, rib-type waveguide design, with an index of
films could achieve the designed refractive index and extinction coefficient by controlling the \( \text{N}_2\text{O}/(\text{N}_2+\text{NH}_3) \) ratio at the value of 1.0 and performing a thermal annealing process.

3.2.2. Microstructure analysis

It was found that the SiON films possessed a similar amorphous XRD pattern to that of the glass substrate. AFM analysis indicated that the average roughness of the SiON films increased as the \( \text{N}_2\text{O}/(\text{N}_2+\text{NH}_3) \) ratio increased, and found that the average roughness values were 0.578 nm, 6.836 nm, and 7.478 nm at the \( \text{N}_2\text{O}/(\text{N}_2+\text{NH}_3) \) ratios of 0.2, 1.0 and 1.8, respectively. Increasing the \( \text{N}_2\text{O}/(\text{N}_2+\text{NH}_3) \) ratio, that is, a higher \( \text{N}_2\text{O} \) flow rate, would form a higher density of

### Table 1

<table>
<thead>
<tr>
<th>Items</th>
<th>Large size waveguide</th>
<th>Small size waveguide</th>
</tr>
</thead>
<tbody>
<tr>
<td>Center wavelength</td>
<td>1552.25 nm</td>
<td>1552.25 nm</td>
</tr>
<tr>
<td>Output channels</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>Optical waveguides structure</td>
<td>Rib</td>
<td>Rib</td>
</tr>
<tr>
<td>Optical waveguides height</td>
<td>6000 nm</td>
<td>5000 nm</td>
</tr>
<tr>
<td>Optical waveguides width</td>
<td>5000 nm</td>
<td>3000 nm</td>
</tr>
<tr>
<td>Slab height</td>
<td>4000 nm</td>
<td>2500 nm</td>
</tr>
<tr>
<td>AWG Device dimension</td>
<td>11 cm × 3 cm</td>
<td>4 cm × 1.4 cm</td>
</tr>
<tr>
<td>Arrayed optical waveguides numbers</td>
<td>46</td>
<td>36</td>
</tr>
<tr>
<td>Center optical waveguides loss (3D)</td>
<td>−0.5 dB</td>
<td>−2.35 dB</td>
</tr>
<tr>
<td>Uniformity of loss (3D)</td>
<td>−3.6 dB</td>
<td>−1.9 dB</td>
</tr>
<tr>
<td>Center optical waveguides loss (EIM)</td>
<td>−0.05 dB</td>
<td>−0.15 dB</td>
</tr>
<tr>
<td>Uniformity of loss (EIM)</td>
<td>−2.9 dB</td>
<td>−1.5 dB</td>
</tr>
<tr>
<td>Device crosstalk</td>
<td>−20 dB</td>
<td>−15 dB</td>
</tr>
<tr>
<td>Device side-lobe</td>
<td>−35 dB</td>
<td>−40 dB</td>
</tr>
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</table>

Fig. 2. (a) The refractive index and the extinction coefficient, (b) the deposition rate of SiON film are dependent on the \( \text{N}_2\text{O}/(\text{N}_2+\text{NH}_3) \) ratio.
oxygen free radical atoms than the lower N\textsubscript{2}O flow rate, resulting in a larger deposition rate and roughness of SiON film.

TEM analysis was used to observe the localized microstructure. The cross-sectional features of HRTEM analysis for the SiON films, with N\textsubscript{2}O/(N\textsubscript{2} + NH\textsubscript{3}) ratios of 0.2, and 1.0, respectively, were shown in Fig. 3(a)–(b). TEM examination clearly revealed no evident void formation observed in these unthermal annealing treated specimens. It was also revealed that on the films there existed few silicon nano-crystallized structures with various dimensions and densities as shown in Table 2. The silicon nano-crystallized structure amounts increased as the N\textsubscript{2}O/(N\textsubscript{2} + NH\textsubscript{3}) ratio decreased, and this resulted in a higher extinction coefficient.

The substrate holder of the PECVD system is self-biased at the voltage of −200 V by the RF power supply. Si nano-crystallized structures might be nucleated and grown in the vicinity of the defects which are formed by plasma positive ions bombarded the substrate. Moreover, the presence of nitrogen could increase the precipitation density of Si nano-crystallized structures in SiON thin films as in the study of Ebara and Machida [10]. Under the PECVD process, the Si nano-crystallized structures were embedded randomly in the amorphous SiON films by random bombardment of plasma positive ions.

<table>
<thead>
<tr>
<th>N\textsubscript{2}O/(N\textsubscript{2} + NH\textsubscript{3}) ratio</th>
<th>Dimensions (nm)</th>
<th>Densities (× 10\textsuperscript{13}#/cm\textsuperscript{3})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>10–50</td>
<td>−20</td>
</tr>
<tr>
<td>1.0</td>
<td>10–30</td>
<td>−3</td>
</tr>
<tr>
<td>1.8</td>
<td>&lt;10</td>
<td>−1</td>
</tr>
</tbody>
</table>

Fig. 3. Transmission electron microscope (TEM) cross-sectional features of the SiON films under the N\textsubscript{2}O/(N\textsubscript{2} + NH\textsubscript{3}) ratios of (a) 0.2 and (b) 1.0.

Fig. 4. Optimum cross-sectional etching profile of rib-type SiO\textsubscript{2}/SiON films under the C\textsubscript{4}F\textsubscript{8}/O\textsubscript{2} ratio of 45 sccm/6 sccm.

The substrate holder of the PECVD system is self-biased at the voltage of −200 V by the RF power supply. Si nano-crystallized structures might be nucleated and grown in the vicinity of the defects which are formed by plasma positive ions bombarded the substrate. Moreover, the presence of nitrogen could increase the precipitation density of Si nano-crystallized structures in SiON thin films as in the study of Ebara and Machida [10]. Under the PECVD process, the Si nano-crystallized structures were embedded randomly in the amorphous SiON films by random bombardment of plasma positive ions.

Fig. 5. The coupling loss was about −2.3 dB, and the propagation losses were −0.57 dB/cm, −0.34 dB/cm, and −0.15 dB/cm for the N\textsubscript{2}O/(N\textsubscript{2} + NH\textsubscript{3}) ratios of 0.2, 1.0, and 1.8, respectively.
3.2.3. Etching processes and optical characteristics of waveguides

The topography of rib-type SiO₂/SiON films was influenced by the etching reactant C₄F₈/O₂ ratio of 45 sccm/4 sccm, 45 sccm/6 sccm, and 45 sccm/8 sccm, respectively, and indicated that the optimum vertical etching profile existed at the ratio of 45 sccm/6 sccm, as shown in Fig. 4. It is well-known that the C/F ratio will effectively influence the etching profile for the competition of polymerization and etching processes, and providing sufficient oxygen atoms would evidently reduce the polymerization phenomena [11].

The coupling loss was about −2.23 dB, and the propagation losses were −0.57 dB/cm, −0.34 dB/cm, and −0.15 dB/cm for the N₂O/(N₂ + NH₃) ratios of 0.2, 1.0, and 1.8, respectively, as shown in Fig. 5. It was found that the more density and dimension of silicon nano-crystallized structures in the amorphous optical films resulted in more propagation loss, and this might be contributed mainly to a more scattering effect phenomenon which occurred between the interface of silicon nano-crystallized structure and SiON matrix.

4. Conclusion

The refractive index and the extinction coefficient of a SiON film could be precisely determined by controlling the N₂O/(N₂ + NH₃) ratio. The silicon nano-crystallized structure amounts would be increased as the N₂O/(N₂ + NH₃) ratio decreased, and the more density and dimension of silicon nano-crystallized structures in the amorphous optical films would result in a larger extinction coefficient and more propagation loss. We must consider their unavoidably negative influences on the rib-type waveguide usage in the future.

Acknowledgements

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