Improved the Surface Roughness of Silicon Nanophotonic Devices by Thermal Oxidation Method

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Abstract- The transmission loss of the silicon-on-insulator (SOI) waveguide and the coupling loss of the SOI grating are determined to a large extent by the surface roughness. In order to obtain smaller loss, thermal oxidation is a good choice to reduce the surface roughness of the SOI waveguide and grating. Before the thermal oxidation, the root mean square of the surface roughness is over 11 nm. After the thermal oxidation, the SEM figure shows that the bottom of the grating is as smooth as quartz surface, while the AFM shows that the root mean square of the surface is less than 5 nm.

Key words- thermal oxidation, SOI, silicon waveguide, surface roughness

I. INTRODUCTION

Silicon is an inexpensive and mature semiconductor material. Silicon waveguide is a basic component of silicon-based optoelectronics. SOI has met the needs of microelectronics technology development. Furthermore, it also has many advantages in the field of optoelectronic devices. Since silicon has a very low absorption loss in the infrared band. In the SOI waveguide, the refractive index difference between silicon and silica is nearly 2. The large index difference makes the optical field of the waveguide restricted more compactly, which will greatly reduce the propagation loss of the waveguide [1].

Fabrication of silicon gratings on an SOI wafer can be achieved by RIE (reactive ion etching) or ICP (inductively coupled plasma etching). The high-energy ion attacking will lead serious roughness of the etched surface of the silicon grating grooves and the silicon waveguide [2]. The transmission loss of the waveguide and the coupling loss of the grating are determined to a large extent by the surface roughness of silicon waveguide and grating [3]. In order to obtain smaller loss, using thermal oxidation to reduce surface roughness of the silicon grating is a good method [4].
II. PHYSICAL AND CHEMICAL MECHANISMS

The thermal oxidation method is categorized as dry oxygen oxidation and wet oxygen oxidation. Pure oxygen is used in the dry oxygen oxidation as the oxidizing ambient. During the dry oxidation, the silicon reacts with the ambient oxygen, forming a layer of silicon dioxide on its surface. In the wet oxidation, hydrogen gas and oxygen gas are introduced into a torch chamber where they react to form water molecules, which are then pumped into the reactor where they diffuse toward the wafers. The water molecules react with the silicon to generate the oxide. Since the reaction materials are a mixture of oxygen and water vapor, the oxidation rate of the wet oxygen oxidation is much faster than the dry oxygen oxidation.

The chemical equation of the dry oxygen oxidation is shown as following:

\[ \text{Si} + \text{O}_2 = \text{SiO}_2 \]  

(1)

Besides the chemical equation (1), there is another chemical equation for the wet oxygen oxidation which is:

\[ \text{Si} + 2\text{H}_2\text{O} = \text{SiO}_2 + 2\text{H}_2 \]  

(2)

The oxidizing ambient gas may also contain several percents of hydrochloric acid (HCl). The hydrochloric acid removes metal ions that may be contained in the oxide. The thermal oxide layer reacted with silicon consumed from the substrate and oxygen supplied from the ambient. Thus, it grows both down into the wafer and up out of it. For every unit thickness of consumed silicon, 2.27 unit thickness of the oxide will be engendered.

According to the commonly used Deal-Grove model, the time \( t \) required to grow an oxide thickness \( X_o \), at a constant temperature, on a bare silicon surface, is:

\[ t = \frac{X_o^2}{B} + \frac{X_o}{B/A} \]  

(3)

where the constants A and B is determined by the characteristics of the reaction and the oxide layer, respectively. If a wafer that already contains oxide is placed in an oxidizing ambient, equation (3) must be modified by subtracting a corrective term \( \tau \) at the right side of the equation, the time which would be required to grow the pre-existing oxide under current condition [5].

Solving the quadratic equation and obtaining \( X_o \) as below:

\[ X_o(t) = A/2 \cdot \sqrt{1 + \frac{4B}{A^2}(t + \tau) - 1} \]  

(4)

Fig. 1 shows the kinetics of silicon thermal oxidation. In thermal oxidation of silicon, oxygen travels through the silica layer by diffusion. Oxygen reacts with silicon and then silica is formed around the silicon-silica interface. Silicon at the interface is consumed when oxidation takes place. As the oxide layer grows, the Si-SiO\(_2\) interface moves into the silicon substrate. As a result, the Si-SiO\(_2\) interface will always be below the original Si wafer surface. The SiO\(_2\) surface, on the other hand, is always above the original Si surface. SiO\(_2\) formation therefore proceeds in two directions relative to the original wafer surface. The shorter the diffusion distance
is, the easier the diffusion is. When the oxidation time is short, the thickness of the silica increased linearly with the oxidation time. When the oxide grows thicker, there is a parabolic relationship between the thickness of the silica and the oxidation time.

![Fig. 1. The kinetics of silicon thermal oxidation](image)

The compactness of the oxide formed by the dry oxygen oxidation is much better than that of the oxide formed by the wet oxygen oxidation, and the damage to the silicon by the dry oxygen oxidation is smaller than that by the wet oxygen oxidation. Furthermore, the thickness of silica is easier to control by the dry oxygen oxidation. Therefore the dry oxygen oxidation is chosen for the further experiment of the thermal oxidation method.

The SOI wafer, on which the silicon waveguide and silicon grating is etched, is placed into a high-temperature furnace. The furnace is then vacuumized, heated to 1000 degrees Celsius and exposed in oxygen flow. The thickness of the oxide can be controlled by the oxidation time. It is important that all the materials put in the high-temperature furnace can withstand high temperature and will not import other impurities. The new impurities will increase transmission loss and coupling loss. After the high temperature process, a thin oxide layer will be generated over the SOI grating surface, which can be removed by immersed in the hydrofluoric acid buffer. A smooth grating surface is realized.

**III. RESULTS AND DISCUSSION**

The silicon structures were etched by RIE first. The wafer is etched for 8 min in an air environment of 80% CHF₃, 3% O₂ and 20% SF₆ with an electrical power of 30 W. Then the thermal oxidation of the SOI devices is achieved by putting the wafer in the high-temperature furnace for one hour with 200 cc/min O₂ current under one thousand degrees.

The surface conditions of silicon grating before and after the thermal oxidation are observed by AFM (atomic force microscopy) firstly. The AFM testing results are shown in Fig. 2 and Fig. 3. Fig. 2 (a) is the AFM scanning result before the thermal oxidation and the right picture of Fig. 2 (a) is the sectional drawing of the back line in the left picture. Those sharp deep rags near the left sides of the grating bars are caused by measurement error of AFM. They are caused by the width of the scanning needle.
Before the thermal oxidation, the sidewalls are nearly perpendicular, and the needle scans from left to the right. When the right side of the needle reaches the left sidewall of the bars, the needle has to rise steeply to the top of the grating surface. A small gap is missed for the tip of the needle, and the tip touches nothing. In this case, the AFM considers it is a very deep gap as default. On the right sidewall, the needle scans from the top to the bottom and the needle has no encumbrance in its way. In this case, the top side and the bottom side are concatenated with a line. Fig. 2 (b) shows the AFM scanning result after the thermal oxidation and the red line and the green line in the right picture of Fig. 2 (b) are the sectional drawings of the red line and the green line in the left picture respectively. After the thermal oxidation, the sidewalls are less steep and thus the deep gaps caused by the measurement error of AFM are disappeared. Comparing the two figures, it can be seen that the roughness of the etched grooves of the grating has been greatly improved by the thermal oxidation method. Fig. 3 is the three dimension diagram of the grating after the thermal oxidation drawn by AFM, which shows that the bottom of the grating grooves is smooth and the roughness caused by the etching is removed by the thermal oxidation.

Fig. 2. (a) The surface conditions before the thermal oxidation by AFM. The right picture is the sectional drawing of the back line in the left picture. (b) The surface conditions after the thermal oxidation by AFM. The red line and the green line in the right picture are the sectional drawings of the red line and the green line in the left picture respectively.
Fig. 3. 3D AFM diagram of the grating after the thermal oxidation.

The AFM data shows that before the thermal oxidation, the bottom of the etched grooves of the grating is very rough with many obvious protuberances and the root mean square of the surface roughness is over 11 nm. After the thermal oxidation, the peak protrusions have been eliminated mostly and the roughness of the bottom of the grating grooves has been approximately removed, while the root mean square of the surface is less than 5 nm.

The surface conditions of SOI grating before and after the thermal oxidation are also observed by SEM (scanning electron microscope). Fig 4 (a) is the SEM picture of a curved waveguide before the thermal oxidation. The etched surface is seriously rough according to the picture and there are many significant protuberances. Fig. 4 (b) is the SEM picture of the grating after the thermal oxidation. The roughness of the etched grooves of the grating is greatly improved and the notable protuberances are removed by the thermal oxidation, and the bottom of the grating is as smooth as quartz surface. Even the two objects are different, they are on the same wafer before and after the thermal oxidation, thus the results are comparable. The SEM results shows that the surface roughness have been greatly improved by the thermal oxidation method.

The oxide growth rate is affected by time, pressure and temperature. More specifically, oxide growth is accelerated by increasing oxidation time, pressure or temperature. When the thickness of oxide layer is small, the improvement of surface roughness is not obvious. Increasing oxidation time and oxygen flow can produce thicker oxide layer and make better improvement of the surface roughness, because the oxidation rate is the same at the beginning. With the oxidation time passing much longer, the oxidation rate of the vertex and the sidewall becomes smaller. Long-time thermal oxidation can reduce the surface roughness more significantly, but it also leads to more silicon consumption and thus narrower grating grooves. Proper dry etching and thermal oxidation parameters can lead to good surface-roughness improvement, which will reduce the scattering loss of the waveguide and guarantee the coupling efficiency of the grating.
Fig 4. (a) Top view of the surface condition of a curved waveguide before the thermal oxidation by SEM. (b) Top view of the surface condition of the grating after the thermal oxidation by SEM.

**IV. CONCLUSION**

In this paper, the thermal oxidation method is used to improve the surface roughness of the etched grating grooves. Experimental results are shown by AFM and SEM. Before the thermal oxidation, the bottom of the etched grooves of the grating is very rough with many obvious protuberances. The root mean square of the surface roughness is over 11 nm. After the thermal oxidation, the peak protrusions have been eliminated mostly; the roughness of the bottom of the grating grooves has been approximately removed, and the SEM figure shows that the bottom of the grating is as smooth as quartz surface, while the AFM show that the root mean square of the surface is less than 5 nm. The surface condition of silicon grating is greatly improved. The thermal oxidation parameters can be properly chosen for good improvement of surface roughness of the grating.
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