Surface & Coatings Technology 230 (2013) 46–50

Contents lists available at SciVerse ScienceDirect

Surface & Coatings Technology

journal homepage: www.elsevier.com/locate/surfcoat

# Deposition and properties of silicon oxynitride films with low propagation losses by inductively coupled PECVD at 150 °C

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ARTICLE INFO

Available online 13 June 2013

*Keywords:*
Silicon oxynitride
Waveguide
PECVD

ABSTRACT

Silicon oxynitride films were deposited at 150 °C using inductively coupled plasma enhanced chemical vapor deposition, aiming towards low-temperature fabrication of waveguide material with low optical losses in the visible and near-infrared range. The influence of the deposition parameters such as $SiH_4$ fraction, deposition pressure and $Ar/N_2$ ratio on the film properties was experimentally investigated using spectroscopic ellipsometry, X-ray photoelectron spectroscopy and Fourier transform infrared spectroscopy. These findings were consistent with the chemical modeling of gas-phase composition of the plasma thereby leading to better understanding of the deposition process.



## 1. Introduction

In the pursuit of integrated optics [1], the fabrication of high-performance optical waveguides remains a challenge. Low optical losses are required, and in particular in the visible spectrum this is difficult to achieve with commonly applied materials. Process integration considerations lead to the desire for a low fabrication temperature; to make integrated optics on top of integrated circuits, or glass or foil substrates, a fabrication temperature well below 450 °C is needed [2]. Silicon Oxynitride (SiON) with its superb transparency to a wide range of wavelengths and tunable refractive index [3] is very suitable for this purpose. SiON can be deposited below 400 °C by plasma enhanced chemical vapor deposition (PECVD). However such films are hydrogen-rich in the form of Si–H and N–H bonds causing optical losses around 1500 nm [4]. To reduce the hydrogen content in PECVD films, additional process steps are required, typically high temperature anneals or plasma treatment [5–7].

Recently we have reported the fabrication of SiON films with high optical quality deposited at 150 °C using inductively-coupled PECVD. Low propagation losses of 0.5 ± 0.05 dB/cm, 1.6 ± 0.2 dB/cm and 0.6 ± 0.06 dB/cm were measured at 1300 nm, 1550 nm and 1600 nm respectively, very competitive with published results [8]. The findings are consistent with earlier low-temperature deposition experiments of $SiO_2$ in our group [9,10]. In this paper we present a detailed material analysis of the fabricated SiON layers using spectroscopic ellipsometry, X-ray photoelectron spectroscopy and Fourier transform infrared spectroscopy. The film properties are further correlated to chemical modeling results on the gas-phase composition of the plasma at the given process parameters.

## 2. Experiment

The custom-built remote inductively coupled PECVD (ICPECVD) system with a base pressure of $10^{-7}$ mbar was used for the deposition of SiON films using 2% $SiH_4$-in-Ar and $N_2$ also diluted with Ar as the precursor gasses. The purity of the $N_2$ was 99.999% with $O_2 \leq 1$ ppm and $H_2O \leq 3$ ppm as per the provider's specifications. However this $N_2$ line is rather long and also shared by other systems in the cleanroom; this could possibly lead to higher $O_2$ and $H_2O$ levels in the nitrogen-supplying line. The deposition chamber is equipped with an in-situ spectroscopic ellipsometer (Woollam M2000, spectral range 245–1690 nm) and is connected to an automatic load-lock chamber.

The SiON films were characterized using spectroscopic ellipsometry (SE) in ex-situ configuration, X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectroscopy (FTIR). The Tauc-Lorentz model was used for parameterization in SE [11].

As a first step in this study, the plasma power and substrate temperature were varied. Fig. 1a and b depicts the resulting extinction coefficient ($k$) as a function of wavelength. The lowest extinction coefficient was obtained with a plasma power of 300 W at 150 °C; the remainder of this study was carried out using those settings.

This was followed by a study on the influence of the deposition pressure set at 0.01 and 0.06 mbar along with two different 2% $SiH_4$-in-Ar flows of 10 and 100 sccm, which amounted to 0.08% and 0.8% of $SiH_4$ (volume) fractions in the reaction chamber, respectively. In addition, the influence of the $Ar/N_2$ flow ratio on the properties of the deposited films was analyzed. The $Ar/N_2$ ratio was varied between 2 and 16 while the total Ar + $N_2$ flow was kept constant at 235 sccm.

The chemical composition of the plasma largely determines the elemental composition of the deposited films and therewith its optical properties. We chemically modeled the deposition process to better

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0257-8972/$ – see front matter 
http://dx.doi.org/10.1016/j.surfcoat.2013.06.010

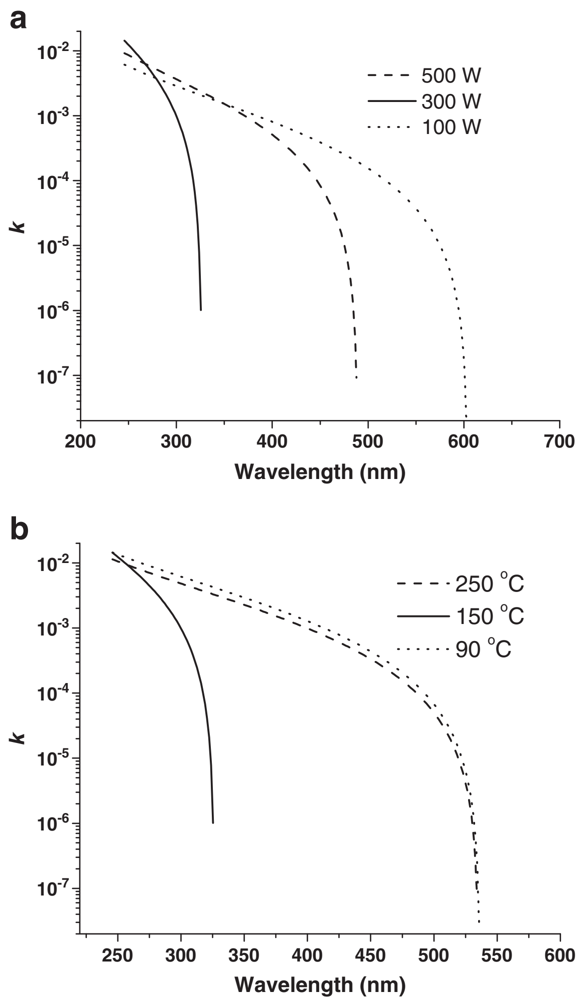


**Fig. 1.** The extinction coefficient $k$ as function of wavelength for different (a) plasma powers and (b) substrate temperatures.

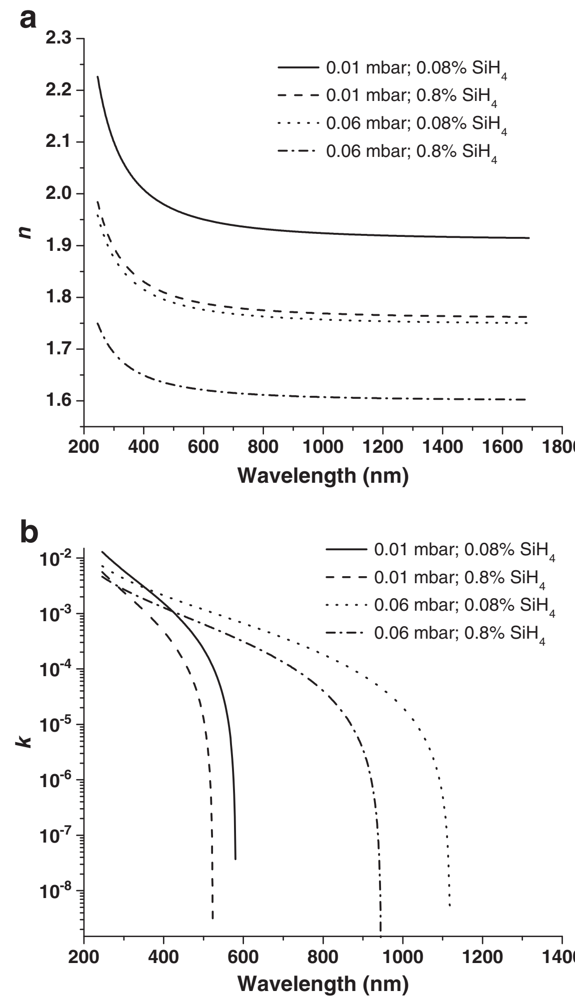


**Fig. 2.** (a) The refractive index $n$ and (b) extinction coefficient $k$ as function of wavelength for two different deposition pressures and $SiH_4$ fractions. The plasma power is 300 W, the $Ar/N_2$ ratio is 4, and the substrate temperature is 150 °C.

understand the influence of the deposition parameters such as pressure and $SiH_4$ fraction on the plasma composition and on the film properties. The $Ar-SiH_4-N_2-O_2$ plasma is modeled with 173 reactions and using this model we compute the concentrations of important chemically-reactive species such as $SiH_x$ ($x = 0$–3), H, N, O, O($^1$D), and synthesized $H_2O$. For a detailed description of the chemical modeling approach we refer to [12].

## 3. Results and discussion

For SiON to be suitable as a waveguide material it should first of all be uniform, homogeneous and flat, which can be readily achieved using CVD deposition. Further it should have the right composition, material density and chemical bonding. For this class of materials it is known that excess silicon leads to high absorption mainly at visible wavelengths. In the infrared spectral range, Si–H and N–H bonds lead to absorption due to bond vibrations around 1500 nm [4].

In the following subsections, we analyze SiON films deposited under varying $SiH_4$ fraction, deposition pressure, and $Ar/N_2$ ratio. We deduce the composition of these films from the SE, XPS and FTIR measurements and relate this to the gas phase composition as calculated with our chemical model.

### 3.1. Influence of $SiH_4$ fraction

Fig. 2 shows how increasing the $SiH_4$ fraction from 0.08% to 0.8% leads to a decrease in the refractive index ($n$) and shift of $k$ towards lower wavelengths. XPS analysis show that this increase in the $SiH_4$ fraction unexpectedly leads to an increase in the film's oxygen concentration from 5% to 26% at 0.01 mbar and 26% to 50% at 0.06 mbar. For reference, the atomic concentration of N, Si and O versus the film thickness for SiON film with 5% (average value) oxygen is shown in Fig. 3.

For SiON films the refractive index can vary between 1.48 ($SiO_2$) and 2.02 ($Si_3N_4$) depending on the composition of the material. Increase in the oxygen content can therefore result in decrease of refractive index as indicated in Fig. 2a. FTIR results shown in Fig. 4 point to the growing prominence of Si–O–Si (stretching) and Si–O–Si (bending) absorption peaks at around 1090 $cm^{-1}$ and 800 $cm^{-1}$, respectively, in addition to shifting Si–N peak (from 850 $cm^{-1}$ to 940 $cm^{-1}$) and decrease in its intensity for films deposited at higher $SiH_4$ fractions. This is caused by an increase of the oxygen content in the films corroborating the XPS results.

Both the increase of the $SiH_4$ fraction and the total gas pressure lead to a higher partial pressure of $SiH_4$. The relation between the partial pressure and oxygen concentration in the films is however not obvious. This relation can be further clarified using the results obtained from chemical modeling. Here we look at the relative concentration of N with respect to $H_2O$, O and O($^1$D), four major factors that can heavily influence the N to O ratio in the deposited films, by deriving the ratios of $N/H_2O$, N/O and N/O($^1$D) for each individual set of deposition parameters. Fig. 5a and b shows the change in these ratios during the change in the $SiH_4$ fraction for two deposition pressures of 0.01 and 0.06 mbar. It can be observed that there is a dramatic decrease in the