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Formation of antireflection structures for silicon in near-infrared region using AlO_x/TiO_x bilayer and SiN_x single-layer

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ABSTRACT

Antireflection (AR) layers for Si were investigated for applications in optical communication in the wavelength range of 1270–1330 nm. The Essential Macleod software was used to find the optimal thicknesses of the AR coatings with two different structures of AlO_x/TiO_x bilayer and SiN_x single-layer. The simulations revealed reflectances lower than 0.5% for both AlO_x/TiO_x and SiN_x AR structures. Furthermore, atomic layer deposition and plasma-enhanced chemical vapor deposition were used to grow the AlO_x/TiO_x and SiN_x layers, respectively. For the fabricated structures, average reflectances of 0.2% (AlO_x/TiO_x) and 0.3% (SiN_x) were achieved in the wavelength range of 1270–1330 nm. For the AlO_x/TiO_x bilayer, a lower transmittance of ~88% was obtained, compared with that of the SiN_x single-layer of ~99%. An additional air annealing at 300 °C for 2 h led to a crystallization of the amorphous TiO_x into anatase phase, which yielded an improved transmittance of ~99%, comparable with that of the SiN_x single-layer structure. X-ray photoelectron spectroscopy revealed that the oxidation state of Ti in TiO_x influenced the absorption in the near-infrared region.

1. Introduction

Silicon photonics has experienced rapid development with the progress of silicon (Si) technologies. In particular, the development of high-speed optical transceivers has attracted significant interest [1,2]. Copper wiring for data transmission is currently replaced by Si-based optical fibers. Optical signals using light, instead of electrical signals, have been developed for communication. Devices have become smaller and more integrated, and extensive studies have been performed to improve their efficiencies [3–5]. In general, when light from a light source is incident on an optical fiber, approximately 1.2 dB of the light intensity is lost [6]. In order to reduce this loss, an optical coupling lens is used. Owing to the advancement of silicon photonics, Si is mainly used for optical coupling lenses [7]. In Si, approximately 40% of the light intensity is lost owing to reflections at wavelengths of 1310 nm and 1550 nm, which are mainly used in optical communication [8]. One approach to reduce the reflection loss is to introduce an antireflection (AR) coating on the lens surface [1,9]. The AR coating is a thin film that increases the transmittance by reducing the reflection of light at the interface of the medium [10]; it is commonly used in industries where the optical efficiency is required to be increased. It can also be used for solar cells, light-emitting diodes, polarizers, and front plates of displays to improve the device's performance [11,12].

AlO_x, TiO_x, SiO_x, and SiN_x are commonly used as AR coatings for optical coupling lenses [9,10]. All of them have excellent passivation properties and excellent transmittance in the near-infrared (IR) range. Various techniques can be employed to coat these substances on a lens surface, such as the sol-gel process, electron-beam evaporation, plasma-enhanced chemical vapor deposition (PECVD), and atomic layer deposition (ALD). PECVD is advantageous as it can be performed at a lower temperature, compared with the other methods, and in addition, it enables a rapid deposition [13]. ALD provides an excellent step coverage and control of the thickness of the film at the atomic level, which make it suitable for the production of AR coatings whose performance depends on the thickness of the film [14].

In this study, we investigated the possibility of using an AlO_x/TiO_x bilayer and SiN_x single-layer as AR structures for Si, focusing on the wavelengths of 1270–1330 nm. The thicknesses of each layer were optimized by simulations using the Essential Macleod software. Both AR structures were experimentally fabricated using ALD and PECVD, and their performances were compared. Both AR structures lowered the reflectance, close to 0%, at the wavelength band of 1270–1330 nm, which enabled an increase of the transmittance by approximately 40%, compared with bare Si.

1.1. Experimental details

The Essential Macleod software was used to generate an efficient

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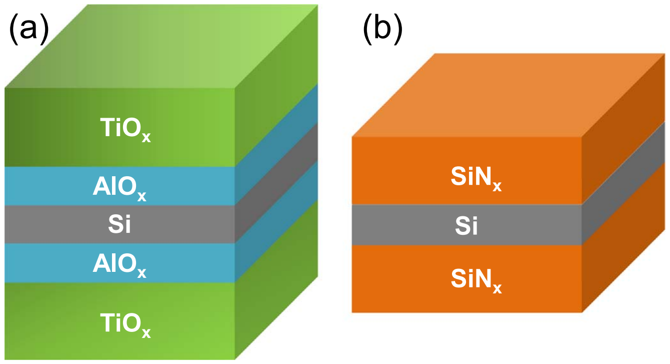

Fig. 1. Structures of the AR-coated Si with an (a) AlO_x/TiO_x bilayer and (b) SiN_x single-layer. The target thicknesses of the two sides of each sample were equal.

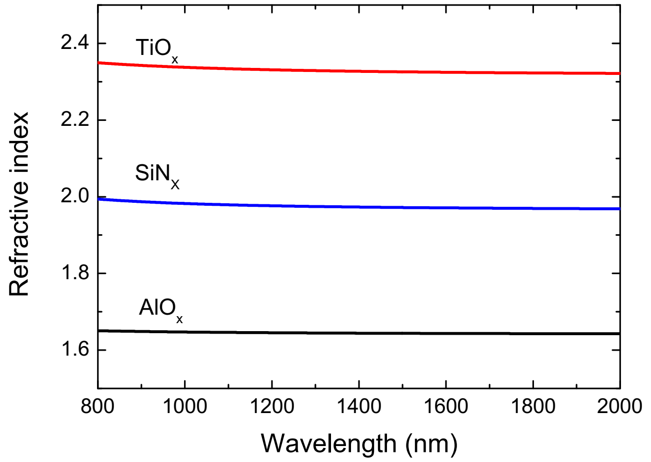

Fig. 2. Refractive indices of the AlO_x, TiO_x, and SiN_x films measured by SE in the wavelength range of 800–2000 nm.

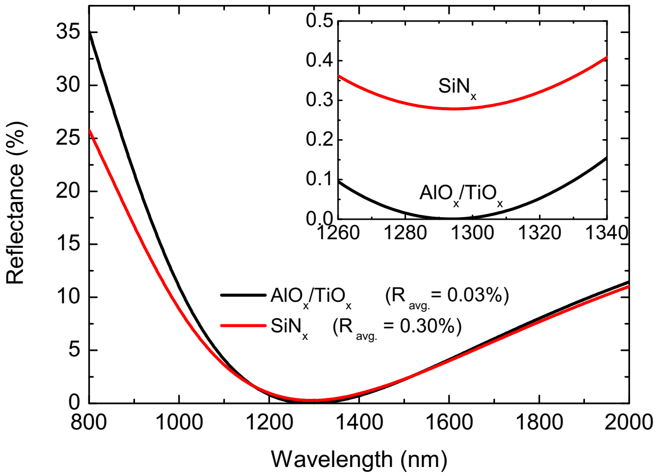

Fig. 3. Simulated reflectance spectra of the AlO_x/TiO_x (black) and SiN_x (red) AR structures; a magnified view of these spectra is shown in the inset. The simulated average reflectances of AlO_x/TiO_x and SiN_x in the wavelength range of 1270–1330 nm were 0.03% and 0.30%, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

thin-film AR structure design, which is a common software package for an efficient design of thin-film optical coatings [15,16]. In this study, an AlO_x/TiO_x bilayer [17] and SiN_x single-layer were considered. AlO_x and TiO_x thin films were deposited using ALD (Atomic classic, CN1, Korea) at 170 °C and 250 °C, respectively. As Al and Ti precursors, trimethylaluminum (TMA, $Al(CH_3)_3$, EGChem, Inc.) and tetrakis(dimethylamino)titanium (TDMATi, $Ti[(CH_3)_2N]_4$, EGChem, Inc.) were used, respectively. Deionized water (H_2O) was used as the oxidant. The sources for TMA and H_2O were set to room temperature, while for TDMATi to 70 °C. The ALD sequences (precursor-pulse–purge–reactant-pulse–-purge) were set to 0.1 s - 10 s - 0.4 s - 25 s for AlO_x and 0.5 s - 15 s - 1 s - 30 s for TiO_x, respectively. SiN_x was deposited by PECVD (VL-LA-PECVD, Uniaxis) at 250 °C using a silane process. Double-side-polished *p*-type (100) Si was used as the substrate. The structure of the sample is shown in Fig. 1. The target thicknesses of the two sides of each sample were equal.

Spectroscopic ellipsometry (SE, V-VASE Ellipsometer, J. A. Woollam Co.) was used to determine the refractive index (*n*) and extinction coefficient (*k*) of each film. The Cauchy equation was used for the analytical model. A single-wave ellipsometer (LSE-USB, Gaertner, 632.8-nm wavelength) was also used to measure the thickness and refractive index of the AlO_x, TiO_x, and SiN_x thin films. An UV-Vis-near-IR spectrophotometer (Cary 500, Agilent) with a wavelength range of 800–2000 nm was used to measure the reflectance and transmittance of the Si wafers with and without AR coatings. An atomic force microscope (AFM, XE100, PSIA) was used to scan the surface morphologies of the Si wafers with and without AR coatings. Chemical states of the grown films were analyzed using X-ray photoelectron spectroscopy (XPS, K-Alpha + , Thermo Fisher Scientific). The XPS spectra of the TiO_x films were obtained after an Ar^+-ion beam etching for 20 s in order to remove surface contaminations. X-ray diffraction (XRD, X'Pert Pro MPD, PANalytical) was used to investigate the crystallinity of the TiO_x film.

2. Results and discussion

The refractive index of each material was measured using SE. Fig. 2 shows that the refractive indices of the AlO_x, TiO_x, and SiN_x single-layers are 1.64–1.65, 2.32–2.35, and 1.97–1.99 in the wavelength range of 800–2000 nm. Considering that the refractive index of Si is 3.5–3.8, these materials are suitable for AR structures for a silicon lens in the near-IR region. The simulated extinction coefficients of these materials were 0 in this wavelength range.

The reflectance was simulated using the Essential Macleod software, as shown in Fig. 3. The simulations were performed using the simplex parameter function of the program. We designed the AR structure by setting the reflectance target at 0% in the wavelength range of 1270–1330 nm to obtain the minimum reflectance. Both AlO_x/TiO_x and SiN_x AR structures exhibited an average reflectance close to 0% in the wavelength range of 1270–1330 nm, as shown in the inset of Fig. 3. The average reflectance of the AlO_x/TiO_x AR structure decreased to 0.03%, while that of the SiN_x AR structure decreased to 0.30% in the wavelength range of 1270–1330 nm. The optimized thicknesses of the AlO_x/TiO_x and SiN_x AR structures were 98.4 nm for AlO_x, 47.3 nm for TiO_x, and 164.3 nm for SiN_x. Based on the simulations, bilayer and single-layer AR structures were fabricated using ALD and PECVD.

Fig. 4 shows the measured reflectance and transmittance of the fabricated AR structures on both sides of Si substrates, designed according to the above simulation results. As light with a small wavelength of 1100 nm (or smaller) has a sufficiently larger energy than the band gap of Si, the light reflected from the backside is absorbed in Si; however, light with a larger wavelength is not absorbed in Si, hence it is emitted to the surface again, thus increasing the reflectance. In order to mitigate the backside reflection, we fabricated the above AR structure on both sides of the Si substrate, as depicted in Fig. 1. The measured thicknesses of the AlO_x, TiO_x, and SiN_x films were 98, 41, and 167 nm, respectively. The dashed curves in Fig. 4 represent the measured values for bare Si, while the solid curves represent the measured values of the AlO_x/TiO_x (black) and SiN_x (red) AR structures. Fig. 4(a) shows that the reflectances of bare Si are approximately 33% and 47% at wavelengths of 800 nm and 1100 nm, respectively. The reflectance of the fabricated