Surface & Coatings Technology 332 (2017) 262–266

Contents lists available at ScienceDirect

Surface & Coatings Technology

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

Simulation and deposition of near-IR anti-reflection layers for silicon substrates

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ARTICLE INFO

Keywords:
Atomic layer deposition
Anti-reflection
Silicon lens
Reflectivity
Humidity test

ABSTRACT

Anti-reflection (AR) layers for Si were investigated for potential application in optical communications in the wavelength range of 1270–1330 nm. The optical simulation module of the Essential Macleod program was used to find the optimal thickness of single-layer and double-layer structures using Al_2O_3 and TiO_2. Al_2O_3 was found to be a better AR single-layer because of a lower reflectance. Less than 1% reflectance was simulated using double-layer structures for both stack sequences Si/TiO_2/Al_2O_3 and Si/Al_2O_3/TiO_2. For experimental work, atomic layer deposition (ALD) of Al_2O_3 and TiO_2 was employed to fabricate two different stacks. Reflectance measurements were conducted and 1.9% and 1.7% maximum reflectance was recorded in the wavelength range 1270–1330 nm. This reflectance establishes the possibility that the two stacks can be used as effective AR layers for Si lenses designed for optical communications. Resistance against humidity was tested for the two structures and only the Si/Al_2O_3/TiO_2 structure was impermeable. Analyses using Fourier transform infrared spectroscopy and atomic force microscopy revealed that ALD-Al_2O_3 is easily hydroxylated while ALD-TiO_2 acts as a good humidity barrier.

1. Introduction

An expansion of the optical network is necessitated by the rapidly increasing demand for high capacity mobile services. Because of this need, transmission rates of 100 Gbps through high-speed optical networking are rapidly applied on optical modules of data centers [1–4]. Increased efforts have been concentrated on silicon photonics and on combining optical communications for condensing more information within a limited bandwidth by minimizing the number of optical devices and reducing optical loss [5–10]. The role of a coupling lens is to combine optical devices and optical fiber so that it increases the coupling efficiency [11–14].

In the recent years, the wavelength used in optical communications has been distributed on a broad range from 780 to 1770 nm. Wavelengths ranging from 1270 to 1330 nm characterized by the lowest losses are utilized to send and receive data [15]. A conventional lens consists of fused silica or glass with a low refractive index of approximately 1.4–1.5. In contrast, silicon has attracted attention as a material for optical coupling lenses because of ease of manufacturing and a high refractive index of approximately 3.5 within the near-IR range [5–8]. Optical lenses with a high refractive index are an attractive option because photonic devices can be miniaturized.

Research in anti-reflection (AR) coatings that can drive the reduction of surface reflectance of optical coupling lenses is crucial to achieving high coupling efficiency. AR coatings enhance light transmittance instead of reflection on the interface between the two materials using destructive interference. The effect of AR coatings on Si has been extensively studied for photovoltaic applications, but the wavelength of interest was mainly in the visible light range of 400–800 nm [11,12,16–22].

AR coating for optical coupling lenses usually consists of TiO_2, SiO_2, Al_2O_3, or Si_3N_4. There are several methods for making AR structures including a sol-gel process, electron beam evaporation, plasma enhanced chemical vapor deposition (PECVD) and atomic layer deposition (ALD). Among them, ALD offers the advantage of easy thickness control at the atomic scale [23]. It also forms thin films of high purity [24,25]. In order to reduce the reflection from the surface of the optical lens, precise control of AR coating thickness is one of the most important factors. In addition, deposited films with high purity and a smooth surface are ideal in realizing optimized AR coatings.

In this study, we first simulated the effects of Al_2O_3 and TiO_2 AR coatings on the reflectance of Si substrates concentrating on the 1270–1330 nm wavelength range, which is common in optical communications. Single-layer and double-layer structures were compared to find the optimal thickness of each layer. Deposition of Al_2O_3 and TiO_2 on Si substrates was performed with ALD and reflectance was

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http://dx.doi.org/10.1016/j.surfcoat.2017.06.094
Received 19 April 2017; Received in revised form 25 June 2017; Accepted 27 June 2017

measured to compare simulated and measured data. Reflectance values of 1.9% and 1.7% were obtained from double-layer AR coatings on Si. The respective layers deposited were 50 nm TiO_2/170 nm Al_2O_3 and 90 nm Al_2O_3/50 nm TiO_2. Resistance against high humidity was also investigated and it was found that the ALD-Al_2O_3 film exhibits poor water permeability. A 50 nm-thick TiO_2 layer on the surface was found to have high resistance against moisture.

2. Experimental

The Essential Macleod software, a powerful tool for optical analysis of thin films, was used to simulate the single-layer and double-layer Al_2O_3 and TiO_2 AR structures. The refractive indices for Si, Al_2O_3, and TiO_2 were set to 3.88, 1.66, and 2.47, respectively, at 632.8 nm. Atomic layer deposition (Atomic classic, CN1, Korea) was used to deposit TiO_2 and Al_2O_3 AR coatings on (100) *p*-type silicon substrates. Titanium(IV) isopropoxide (TTIP, EGChem, Inc.) and trimethlyaluminum (TMA, Al $(CH_3)_3$, EGChem, Inc.) were used as the Ti and Al precursors, and deionized water (H_2O) was used as the oxygen source. The deposition temperature was all set to be 250 °C. The pulse sequence (precursor pulse-purge-reactant pulse-purge time) was optimally arranged to be 0.05 s–10 s–0.2 s–20 s and 0.15 s–10 s–0.2 s–20 s for Al_2O_3 and TiO_2 growth, respectively. The deposited Al_2O_3 and TiO_2 were amorphous and crystalline (rutile) phases, respectively.

Ellipsometer (LSE-USB, Gaertner) was used to measure the thickness and refractive index of Al_2O_3 and TiO_2 thin films. The UV–visible spectrophotometer (Cary 500, Agilent) with a wavelength range from 800 to 2000 nm was used to measure the reflectance of silicon wafers with and without AR coatings. The optical module has to be maintained at constant humidity when used outdoors [26] so we conducted resistance tests for humidity. Si wafers with AR coatings were boiled at 80 °C for 10 h in deionized water. The reflectance before and after boiling was compared. Fourier transform infrared spectrometry (FTIR, Spectrum 400, PerkinElmer) was used to investigate the structural change after the humidity test. Surface morphologies of the fabricated AR coatings on Si wafers were scanned using the atomic force microscope (AFM, XE100, PSIA).

3. Results and discussion

3.1. Simulation with single- and double-layer structures

AR structures with TiO_2 and Al_2O_3 single-layers on Si were simulated and Fig. 1(a) shows the maximum reflectance of each AR layer as a function of film thickness. In this graph, the maximum reflectance is defined as the highest reflectance value recorded among wavelengths ranging from 1270 to 1330 nm from simulation results with thickness intervals of 20 nm. At 0 nm of each film, which represents a bare Si substrate without AR coating, the maximum reflectance was 31.0%. As the thickness of either TiO_2 or Al_2O_3 increases, maximum reflectance shows a gradual drop and the lowest reflectance values are 6.38% and 1.94% for 130 nm of TiO_2 and 190 nm of Al_2O_3, respectively. Simulated total reflectance for wavelengths in the range of 800 to 2000 nm is also shown in Fig. 1(b). The simulated reflectance of a bare Si wafer is included for comparison. Based on this simulation, we can confirm that compared to TiO_2, Al_2O_3 is a better AR coating for Si substrates in the IR range. However, the reflectance value of 1.9% is not as low as required for higher coupling efficiency in Si lenses. Therefore, we investigated double-layer AR structures to verify if the reflectance can decrease further.

Two different models were designed based on Si/TiO_2/Al_2O_3 and Si/Al_2O_3/TiO_2 layered structures. Fig. 2(a) shows the maximum reflectance of Si/TiO_2/Al_2O_3 AR structures with increasing TiO_2 thickness. In this graph, data for three different thicknesses of Al_2O_3 (100, 130, and 170 nm) are illustrated. For 100 nm-thick Al_2O_3, the minimum reflectance is 1.68% when the thickness of TiO_2 is set to 100 nm. A maximum reflectance of less than 1% is observed for a 90 nm TiO_2 layer with 130 nm of Al_2O_3 (the actual value is 0.40%). A similar value is observed for a 50 nm TiO_2 layer with 170 nm Al_2O_3 (the actual value is 0.73%). The results for the structure Si/Al_2O_3/TiO_2 with inverted layers are also illustrated in Fig. 2(b). Low maximum reflectance values of 0.25% and 0.28% were simulated when TiO_2/Al_2O_3 thicknesses were 40 nm/105 nm and 50 nm/90 nm, respectively. The simulation demonstrates that both double-layer structures can effectively function as good AR layers. Based on the simulation, two sets of AR structures were selected for experimental validation by considering their respective maximum reflectance and TiO_2 thickness. These were the Si/50 nm-TiO_2/170 nm-Al_2O_3 and the Si/90 nm-Al_2O_3/50 nm-TiO_2 structures. The 50 nm TiO_2 thickness was fixed for both models because the growth rate of TiO_2 ALD is slower than that of Al_2O_3 and both experiments can be performed with the reliable ALD process.

3.2. ALD fabrication of double-layer AR structure

Fig. 3(a) shows the simulated (dotted line) and measured reflectance (solid lines) of Si/50 nm-TiO_2/170 nm-Al_2O_3 AR structures. It is noted that the overall shape of the experimentally obtained reflectance curves replicate the trend of the simulation, suggesting that the thickness of both TiO_2 and Al_2O_3 layers are near the target values. In this regard, ALD is a powerful tool that validates the simulation results experimentally. The exception is the reflectance from 1130 to 1600 nm which is somewhat higher than the simulation result. Maximum reflectance at 1270–1330 nm was 2.9% while the simulated value is 0.73%. A wavelength of 1130 nm corresponds to the photon energy of 1.1 eV and it is consistent with the bandgap energy of Si. Longer wavelength than the bandgap energy is not well absorbed by Si

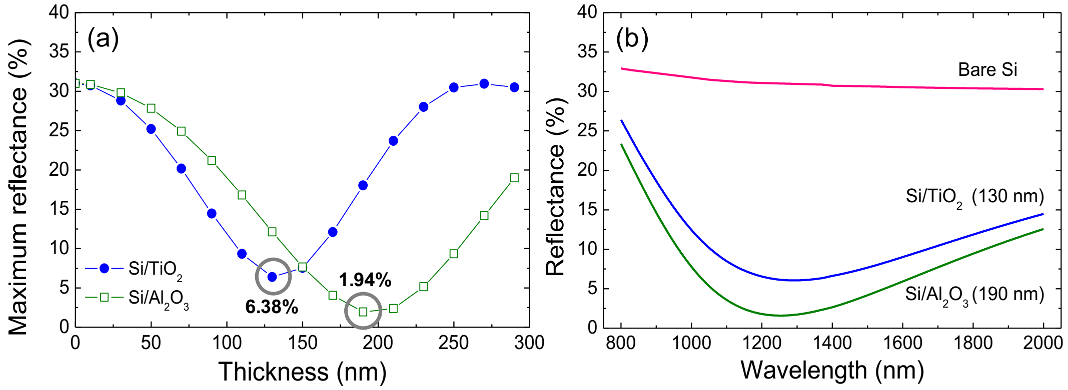

Fig. 1. (a) The maximum reflectance of single-layer AR structure for wavelength from 1270 to 1330 nm is 6.38% for the Si/TiO_2 structure and 1.94% for the Si/Al_2O_3 structure. The variation of thickness was from 10 to 290 nm. (b) Full reflectance spectra from 800 to 2000 nm for Si/TiO_2 and Si/Al_2O_3 structures at the optimized thickness.