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Characterization and simulation on antireflective coating of amorphous silicon oxide thin films with gradient refractive index

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ABSTRACT

The optical reflective properties of silicon oxide (Si_xO_y) thin films with gradient refractive index are studied both theoretically and experimentally. The thin films are widely used in photovoltaic as antireflective coatings (ARCs). An effective finite difference time domain (FDTD) model is built to find the optimized reflection spectra corresponding to structure of Si_xO_y ARCs with gradient refractive index. Based on the simulation analysis, it shows the variation of reflection spectra with gradient refractive index distribution. The gradient refractive index of Si_xO_y ARCs can be obtained in adjustment of SiH_4 to N_2O ratio by plasma-enhanced chemical vapor deposition (PECVD) system. The optimized reflection spectra measured by UV–visible spectroscopy confirms to agree well with that simulated by FDTD method.

1. Introduction

In the recent years, amorphous silicon (α-Si) thin films on glass substrates have attracted a great deal of attention in photovoltaics, microelectronics and display technologies because of its potential applications for electronic devices, especially thin film solar cells [1–3]. Efficient solar cells must satisfy two kinds of requirements: both strongly optical absorption and effectively electrical transportation. To enhance performance of antireflection and passivation, dielectric oxide layers must be selected to deposit on the surface of α-Si thin films. The antireflective coatings (ARCs) have been widely used in manufacturing process of conventional crystalline solar cells (c-Si) to benefit optical absorption, such as silicon nitride (Si_xN_y) deposited on the surface of n-type c-Si [4–6] and aluminum oxide (Al_xO_y) prepared on the surface of p-type c-Si [7–9]. Because of the match of lattice to α-Si substrates, amorphous silicon oxide (Si_xO_y) thin films have been used to prepare ARCs by plasma-enhanced chemical vapor deposition (PECVD) [10,11], magnetron sputtering [12,13] and sol-gel methods [14–16]. Compared to physical vapor deposition (PVD) method, it is more suitable to prepare multilayer films with different refractive index by PECVD method. The average reflectance for double-layer ARCs are lower over a broader wavelength range than for a single-layer ARC, because single-layer ARC has only minimal point of reflectance [17,18]. With these requirements, double-layer Si_xO_y ARCs with gradient refractive index not only decrease electrical recombination effectively, but also enhance

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optical antireflection strongly [19,20]. However, it is worth discussing how to enhance antireflective effect of α-Si thin film solar cells through different distribution structures of Si_xO_y ARCs.

In this paper, we present theoretical and experimental study of optical reflective properties of Si_xO_y ARCs with gradient refractive index. The finite difference time domain (FDTD) method is used to study the light-modulated characteristics of ARCs with gradient refractive index. Reflection spectra for different distribution structures of Si_xO_y ARCs with gradient refractive index are simulated by FDTD method. This experimental work aims to focus on the correlation between reflection spectra and gradient refractive index distribution. Surface characterization and FDTD simulation analysis of Si_xO_y ARCs with gradient refractive index are investigated simultaneously.

2. Experimental details

The hydrogenated amorphous silicon oxide (Si_xO_y:H) thin films are prepared by the following procedure. First, Si_xO_y:H films as a layer is deposited on the glass substrates using PECVD by silane (SiH_4), nitrous oxide (N_2O) and hydrogen (H_2). The experimental parameters of deposited Si_xO_y:H thin films are shown in Table 1. The PECVD system is HLF-400 made in Beijing Beiyi Innovation Vacuum Technology Co. Ltd. Before the thin films are deposited on glass substrate, heat-resistant tape has been adhered to the corner of glass substrate. After we finish depositing Si_xO_y:H thin films and uncover tape from the substrate, the thickness of thin film is measured on the step between glass substrate and thin films by stylus profiler. Thickness measurement of stylus profiler is Vecco Dektak 150. Then double-layer structures are formed on the surface of first layer according to above procedure again. All of samples have been dehydrogenated, after thin films were annealed in vacuum condition at 200 °C for 30 min.

The structural orientation of Si_xO_y films are measured by a D/Max-2200 X-ray diffractometer (XRD) of Rigaku using the Cu Kα radiation. The cross-section morphology and element composition of thin films is characterized respectively by scanning electron microscope (SEM) and energy dispersive spectrometer (EDS) made by JEOL JSM-6700F. The refractive index and thickness are measured by spectroscopic ellipsometer of Sentech SE-400adv. UV–visible reflection spectra are performed by Hitachi U-2910 spectrophotometer.

3. Results and discussion

3.1. Structural modeling

In this paper, the software of FDTD Solution is used as analysis for simulating different distribution structures of Si_xO_y ARCs with gradient refractive index. The size of rectangular model is that the length, width and height are 2.5 μm, 2.5 μm and 0.1 μm respectively. The physical and optical values of silicon oxide materials are used as parameters in the simulation. Different structures of Si_xO_y ARCs with gradient refractive index are selected to simulate the properties of optical reflection. The optimal results can be analyzed to obtain the lowest average reflectance in the wavelength range of visible light.

The basic cross-section structures of single ARC and double ARCs on the substrate have been shown in Fig. 1(A) and Fig. 1(B) respectively. The reflectance of incident light of wavelength λ from the surface of substrate covered by a single non-absorbing layer is given by Eq. (1):

$$R = \frac{r_1^2 + r_2^2 + 2r_1r_2\cos 2\theta}{1 + r_1^2r_2^2 + 2r_1r_2\cos 2\theta} \quad [1]$$

where r_1 and r_2 are the individual Fresnel reflectance given by Eq. (2):

$$r_1 = \frac{n_0 - n_1}{n_0 + n_1}, r_2 = \frac{n_1 - n_s}{n_1 + n_s} \quad [2]$$

and θ is the phase difference of the single layer, β is refractive angle given by Eq. (3):

$$2\theta = \frac{4\pi n_1 d_1}{\lambda \cos\beta} \quad [3]$$

Table 1
Experimental parameters of Si_xO_y:H thin film samples deposited by PECVD system.

Parameters of deposited Si_xO_y:H thin film	Specific values
Pressure (Torr)	0.4–0.6
Temperature (°C)	200–250
The Ar_2 flow of pretreatment (sccm)	30
Frequency (MHz)	13.56
RF power (W)	60–80