Amorphous Er_2O_3 films for antireflection coatings*

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This paper reports that stoichiometric, amorphous, and uniform Er_2O_3 films are deposited on Si(001) substrates by a radio frequency magnetron sputtering technique. Ellipsometry measurements show that the refractive index of the Er_2O_3 films is very close to that of a single layer antireflection coating for a solar cell with an air surrounding medium during its working wavelength. For the 90-nm-thick film, the reflectance has a minimum lower than 3% at the wavelength of 600 nm and the weighted average reflectances (400–1000 nm) is 11.6%. The obtained characteristics indicate that Er_2O_3 films could be a promising candidate for antireflection coatings in solar cells.

Keywords: Er_2O_3 film, optical constants, insulators, solar power
PACC: 7865, 7850E, 7820D, 7755

1. Introduction

To increase the convertible efficiency of solar energy into electricity, it is necessary to decrease the reflectance of the light-receiving surface of the solar device in the solar spectrum range. For this purpose, surface texturing or an antireflection (AR) coating is usually adopted.[1−3] Commercial solar cells fabricated on multicrystalline silicon (mc-Si) wafers exhibit poorer ability than their monocrystalline counterparts to adequately texture their surfaces which have randomly oriented grains. An alternate method of reducing the front surface reflection is using AR coatings.[4,5] The conventional AR coatings are dielectric materials such as SiO_2 or TiO_2. However, the refractive index of SiO_2 (1.46) is too low for optimal AR performance, while TiO_2 is a complex material, which has three crystalline phases as well as the amorphous one. It hereby has complicated physical, optical, electrical and chemical properties which depend greatly on the different phases.[6,7] Therefore, other AR coatings are widely investigated and the exploitation of new AR materials is still an open challenge now.

Thin films of erbium oxide (Er_2O_3) have been investigated with respect to different applications in recent years. Due to its high dielectric constant (1–14), it is a candidate material to replace the gate dielectric SiO_2 in the next generation of complementary metal oxide semiconductor devices with an oxide layer thickness below 2 nm.[8−10] Specifically, it may be used in optoelectronic devices because of its superior properties such as showing high transparentness in the working spectral range of solar cells, high chemical and thermal stability in contact with Si, high mechanical strength substantial hardness and possessing an optimum index of refraction for photovoltaic applications.[11−13]

Although, there are few papers reported on the results of AR coating of Er_2O_3 films recently, further investigations on the properties of Er_2O_3 AR coatings are needed because the structural, chemical, electrical properties of AR coatings are undoubtedly major issues which have direct relationship with the optical properties such as the refractive index and reflectivity.[13] In the previous work, we reported the chemical and electrical properties of Er_2O_3 films on Si(001).[9,14] Here, the structural and optical characteristics of Er_2O_3 films on Si(001) by radio frequency (RF) magnetron sputtering are investigated.

2. Experimental

The 3.8 cm p-type polished Si(001) wafers with resistivity of 2–10 Ω·cm were used as substrates. The Er_2O_3 films were deposited by RF sputtering with an Er_2O_3 target at room temperature. The base pres-

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sure of the sputtering chamber was about 10^{-5} Pa and the deposition was done in an Ar gas atmosphere. The substrates were rotated and placed parallel to the target surface. The Er_2O_3 films with thickness of about 90 nm were characterised using x-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES) measurements by a VG MICROLAB MKII system to identify the stoichiometric proportion. The film structures were studied by x-ray diffraction (XRD) $\theta - 2\theta$ scan. Film surface morphologies were obtained using atomic force microscopy (AFM). The optical properties of the films were measured at normal incidence in the wavelength range from 400 to 1000 nm using a WVA SE Spectroscopic Ellipsometry (SE) from J.A.Woollam Co., Inc.

3. Results and discussion

The composition of the prepared film was checked with an XPS and AES. Before XPS and AES measurements, Ar^+ ion sputtering was applied to remove the contamination formed by being stored in air.

Figures 1(a) and 1(b) show the XPS spectrum taken from the Er_2O_3 film. Only Er 4d and O 1s signals at 168 and 531 eV, respectively, could be detected within the detection limit of XPS. Since both the peak energy and peak shape of Er 4d and O 1s peaks are consistent with those of Er_2O_3 films by other method,[15,16] we suggest that the Er_2O_3 films grown by this RF magnetron sputtering method are basically stoichiometric, which is one of basic requirements for a solar cell in order to act as a metallization mask to electroless metal plating solutions.

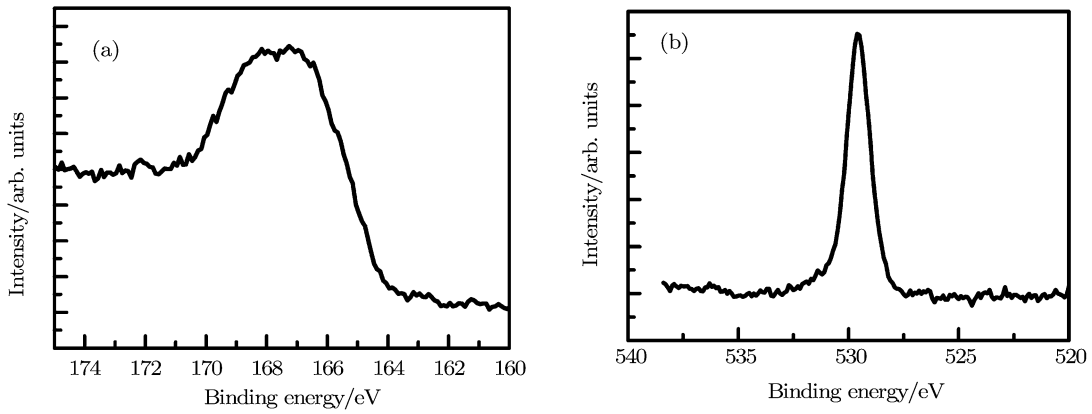


Fig. 1. The XPS spectra of (a) Er 4d peak and (b) O 1s peak for the Er_2O_3 film deposited on Si(001) substrate by RF magnetron sputtering.

The corresponding AES spectrum is shown in Fig. 2.

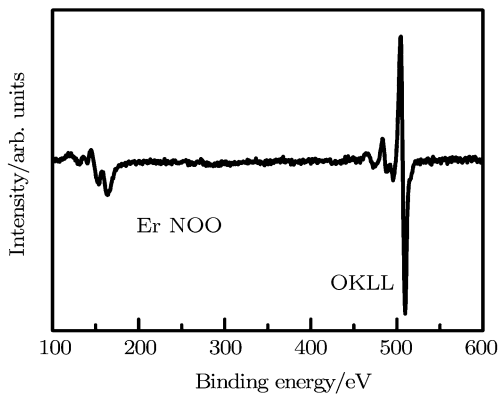


Fig. 2. The AES spectrum of the Er_2O_3 film deposited on Si(001) substrate by RF magnetron sputtering.

It can be found that there are only Er NOO peak at 165 eV and O KLL peak at 510 eV. From the peak intensities (peak to peak heights) of O KLL and Er NOO, the O to Er atomic ratio is estimated to be 1.5 by using their relative atomic sensitivity factors, which also indicates that the Er_2O_3 film is stoichiometric. Furthermore, the same stoichiometric characteristic is observed on the Er_2O_3 films with different thicknesses prepared by the same RF magnetron sputtering method.[14]

The structure of the Er_2O_3 film is checked by XRD. Figure 3 shows the XRD pattern collected between 20° and 60°. No peak is observed at all angles being scanned, indicating that the film is mainly amorphous. The use of a non-crystalline material is important in AR coating design of a silicon PV de-

vice because the grain boundaries in polycrystalline films cause many problems such as increasing scattering and decreasing transparency. Although, this problem could be prevented if the material is prepared in single crystalline form by using epitaxial growth techniques, there is still no clear evidence of superior characteristics in comparison with that of amorphous ones. In addition, the epitaxial growth of oxides is difficult in technology and expensive in price. Therefore, amorphous AR films are the best choice nowadays. Furthermore, it has been established that amorphous Er_2O_3 films have superior thermal and chemical stability,[14] which are also desired for AR films in solar cell devices.

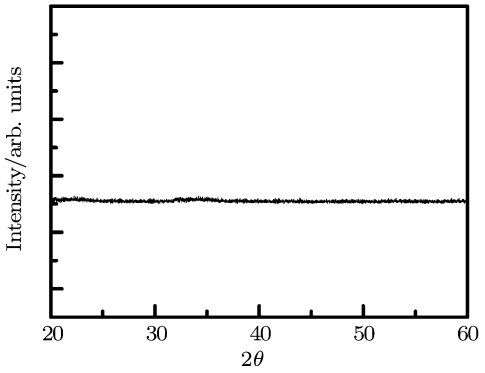


Fig. 3. The XRD curve of the Er_2O_3 films on Si(001) substrate.

It is well known that optical materials are described by the complex refractive index

$$N(\lambda) = n(\lambda) - \mathrm{i}\,k(\lambda), \tag{1}$$

where n is the real part of the refractive index and k is the extinction coefficient. Ellipsometry is a very powerful tool to determine the optical properties such as refractive index and reflectance by fitting with some specific models. Transparent materials can often be fitted by a Cauchy relation.[17] Therefore, Cauchy type dependence has been applied on optical parameters when the transparent Er_2O_3 films were measured by SE.

Figure 4 displays the refractive index n and extinction coefficient k as a function of incident photon energy obtained from the Er_2O_3 film by SE. The refractive index n is 1.66–1.79 in the photon energy region of 1–4 eV, which is very close to the index range of a single layer AR coating for a solar cell with an air surrounding medium during its working incident energy. On the other hand, from the curve n in Fig. 4(b), normal energy dispersion of the refractive index n is evident. Data n monotonically and slowly increases with increasing the photon energy. Nevertheless, no peak is seen in n curve. As the extinction coefficient k, the data is maintained at very low values which is close to zero and can be negligible in the whole spectral range and, noteworthily, there is no discrepancy as shown in Fig. 4(a). Therefore, the direct energy gap of the Er_2O_3 film must be larger than the maximum of the incident photon energy of 4.0 eV in the SE measurement, where there is no peak found in either k or n curves in Figs. 4(a) and 4(b), due to the peaks in curves of both n and k versus photon energy correspond to the direct optical band gap, or in other words, a direct photoexcitation process where electrons excited from the valence band to the conduction band. This result supports, to some extent, the energy gap value of the Er_2O_3 film by other methods.[10] The large energy gap of Er_2O_3 films indicates that they could be promising AR coatings for solar cells because of the high transparentness in the whole working spectral range of solar cells.

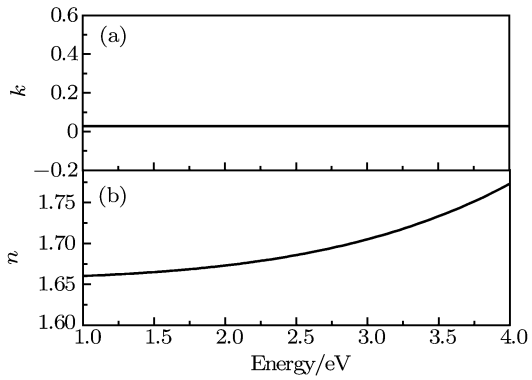


Fig. 4. Refractive index n and extinction coefficient k as a function of photon energy of incidence obtained from the Er_2O_3 film on Si (001) substrate by SE measurements.

The thickness dependence on the reflectance is also studied. The reflectance of the Er_2O_3 films with different thicknesses of 90, 60 and 20 nm is shown in Fig. 5. Since polished Si(001) wafers are used in this paper, all the incidence were measured to be reflected. It is seen from Fig. 5 that the reflectance of all the Er_2O_3 films with different thicknesses decreased at all of wavelengths with respect to that of the uncoated Si. The weighted average reflectances (400–1000 nm) for the three Er_2O_3 films with different thicknesses of 20, 60, 90 nm are 30.2%, 30.7% and 11.6%, respectively. The reflectance of the Er_2O_3 film with the thickness of 90 nm is lowest which has a minimum below 3%.

This 90 nm Er_2O_3 film used for AR coating is appropriate because of the fact that a single-layer AR coating should exhibit a minimum reflectance at about 600 nm in order to take full advantage of the peak in working spectral range of the Si solar cells (550–750 nm).[6] According to the theory of interference of quarter-wave coatings, the positions of the reflectance minima give the optical thicknesses *nd*. The optical thickness of the Er_2O_3 film is then 600/4 nm=150 nm. With the refractive index of n of about 1.68 at 600 nm (or 2.0 eV), the thickness d of the Er_2O_3 film is about 90 nm. If there are some specific requirements in reflectance, the position of the minimum can be shifted to the desired wavelength by varying the thickness of the Er_2O_3 film.

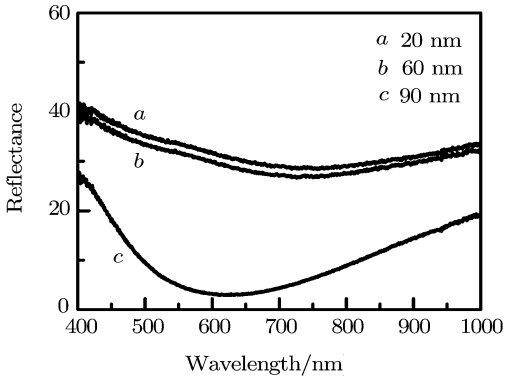


Fig. 5. Reflectance spectra versus the incident wavelengths of the Er_2O_3 films with different thicknesses.

It is known that pinholes or micro-cracks can affect measurements of the extinction coefficient and the reflectance. Therefore, the surface morphology of the film with the thickness of 90 nm is observed by AFM, as shown in Fig. 6. The Er_2O_3 film was found to have a root-mean-square surface roughness of 2.1 nm, which is larger than the desired value of below 1 nm for future CMOS structures.[18,19] However, no pinholes or micro-cracks are observed from the AFM image. The rough and uniform surface is also reflected in Figs. 5 and 4. The reflectance curves have no interference fringes, which indicate a relatively large surface roughness while the extinction coefficient datum k has no discrepancy, indicating that the surface roughness of these Er_2O_3 films is uniform. For these reasons, the ellipsometry measurement of coefficient datum k and the following refractive index n, reflectance as well, is believed to provide the best estimate of the behaviours of the Er_2O_3 films prepared by RF magnetron in this paper.

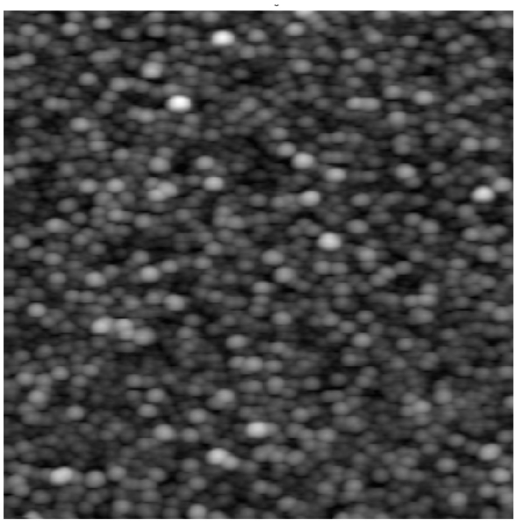


Fig. 6. The 3.8 μm×3.8 μm AFM image for the Er_2O_3 film with the thickness of 90 nm.

4. Conclusions

In summary, the amorphous and stoichiometric Er_2O_3 film has been achieved on Si(001) substrate by RF sputtering method at room temperature. The refractive index of as-deposited Er_2O_3 film in the photon energy region of 1–4 eV is between 1.66–1.79. For the 90-nm-thick film, the reflectance has a minimum lower than 3% at the wavelength of 600 nm and the weighted average reflectances (400–1000 nm) is 11.6%. The obtained characteristics indicate that the Er_2O_3 film could be a promising candidate for AR coatings in a solar cell.

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