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Materials Research Bulletin 40 (2005) 1303–1307
Materials Research Bulletin
www.elsevier.com/locate/matresbu

Structural properties of indium tin oxide thin films prepared for application in solar cells

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Received 29 August 2004; received in revised form 22 January 2005; accepted 8 April 2005

Abstract

Indium tin oxide (ITO) thin films prepared by rf sputtering were annealed in several temperatures. The electrical, optical and structural properties of these films are systematically investigated. The post annealing of the samples lead to considerably higher electrical conductivity, better optical transparency and larger grain size for the films. In an optimum annealing temperature of 400 °C, we have found that a maximized conductivity of films is achieved without a remarkable loss in their transparency. The sheet resistance of 2.3 Ω/□ and average grain size of 30 nm, are the results of the optimized post processing of films. The investigation for microstructure of films investigated by X-ray diffraction measurement (XRD) shows that a preferential crystal growth toward the (2 2 2) orientation takes place when the annealing temperature increases to 400 °C.

Keyword: C. X-ray diffraction; ITO; C. XRD; Structure; Transmission; Resistivity

1. Introduction

Indium tin oxide (ITO), an n-type degenerate wide gap semiconductor with an optical band gap of 3.7 eV, is transparent in the visible and reflective in the infrared spectral regions [1–4]. This

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0025-5408/$ – see front matter
doi:10.1016/j.materresbull.2005.04.007

material has a relatively high electrical conductivity, which makes it an excellent transparent conductive oxide (TCO) for various electronic applications [5–10]. Because of these various sensitive physical properties, thin films of this material must be processed very carefully. Recently, many groups have investigated ITO deposition and post processing by a number of techniques [1–10]. ITO has also excellent applications in solar cells [11–13]. Microstructure of ITO is investigated by different researcher groups by X-ray diffraction (XRD) measurement [14–17].

The optimized condition for preparation of high quality ITO films is investigated for this study. For the annealing temperature of 400 °C, we have found that the conductivity of films has a maximized value without a remarkable loss in their transparency. The sheet resistance of the so prepared ITO films was 2.3 Ω/□. Structural properties of these films ITO are also investigated by XRD measurement method. These measurements were made on a Philips diffractometer. The results from XRD are in excellent agreement with those of electro-optical characterization.

2. Experimental

For deposition of Indium tin oxide films, we used soda lime glass substrates. The substrates were first cleaned and than thin films of ITO are deposited using RF sputtering. By utilization of a rotary/diffusion pumping system we reached a vacuum better than 8×10^{-6} Torr. After this a mixture of argon–oxygen (90% Ar, 10% O_2) as sputtering gas was introduced to the chamber through a mass flow controller (MFC). The sputtering target was a hot pressed oxide and the constant distance to the substrate was 3.5 cm.

Various films of ITO are fabricated at room temperature with a deposition pressure of 27 mTorr by varying the flow of Ar/O_2 sputtering gas. A pre-sputtering of ITO target for 10–15 min played an important role for preparation of homogeneous films. We then prepared thin films of ITO under the same condition only with a difference in their post-deposition annealing. The electrical properties of the films are concluded from electrical conductivity measurements and the optical properties from their transmission spectra. The structural properties of these films are then investigated by XRD measurement method. XRD measurements were made on a Philips diffractometer.

3. Results and discussion

Fig. 1 shows the electrical resistivity and an average transparency at high transmission of films as a function of post annealing temperature. The annealing temperature of 400 °C seems to be the most suitable temperature for post processing of our ITO films prepared by rf sputtering. At this temperature, the out diffusion of oxygen atoms of ITO leads to an increase in the electrical conductivity of films without a remarkable change in their transparency. We believe that any change in the concentration of oxygen in the film will lead to a change of the electrical conductivity of the film since ITO is a non-stoichiometric oxide. In other words, the conductivity of ITO is related to the oxygen vacancies in the film and film structure (grain formation, grain size, form and quantity of disorders). One oxygen vacancy generates two electrons on the conduction band because of

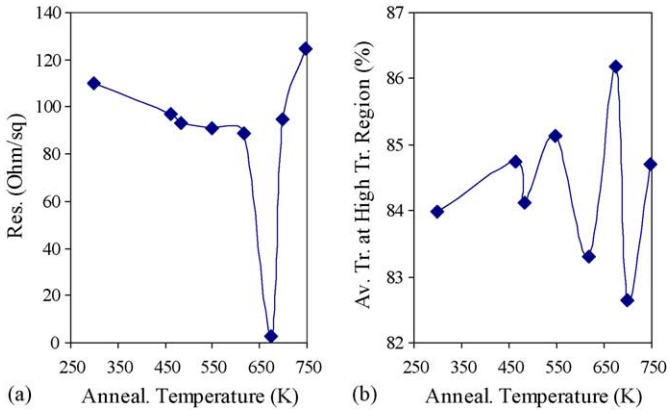

Fig. 1. Electrical resistivity and average transparency at high transmission of films as a function of post annealing temperature.

charge neutrality. This means that carrier concentration increases with decreasing of oxygen in the film.

We define q, as a parameter which characterizes the electro-optical properties of the films. Q is the ratio of normalized transmission to normalized resistivity at high transmission range of ITO films. Fig. 2 shows q as a function of the post annealing temperature. It shows that the annealing temperature of 400 °C is the most suitable temperature for post processing of our ITO films.

Fig. 3 shows the results of XRD measurements. In Fig. 3a, the representative X-ray diffraction profiles of ITO films annealed at different temperatures are shown. The films have two strong (2 2 2) and (4 0 0) crystal orientations. The (4 0 0) diffraction intensity decreases accompanied by the large increase of the (2 2 2) intensity when the annealing temperature increases to 400 °C and then starts to decrease. Fig. 3b demonstrates the ratio of (2 2 2) to (4 0 0) intensities. This ratio is higher than 7 for the optimized sample. This indicates that a preferential crystal growth toward the (2 2 2) orientation takes place when the annealing temperature increases to 400 °C.

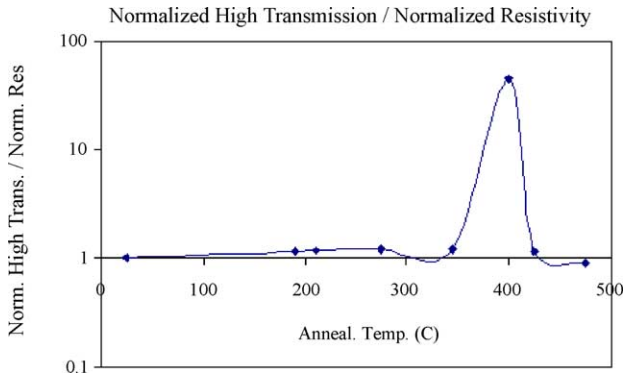

Fig. 2. The variation of q as a function of the post annealing temperature.

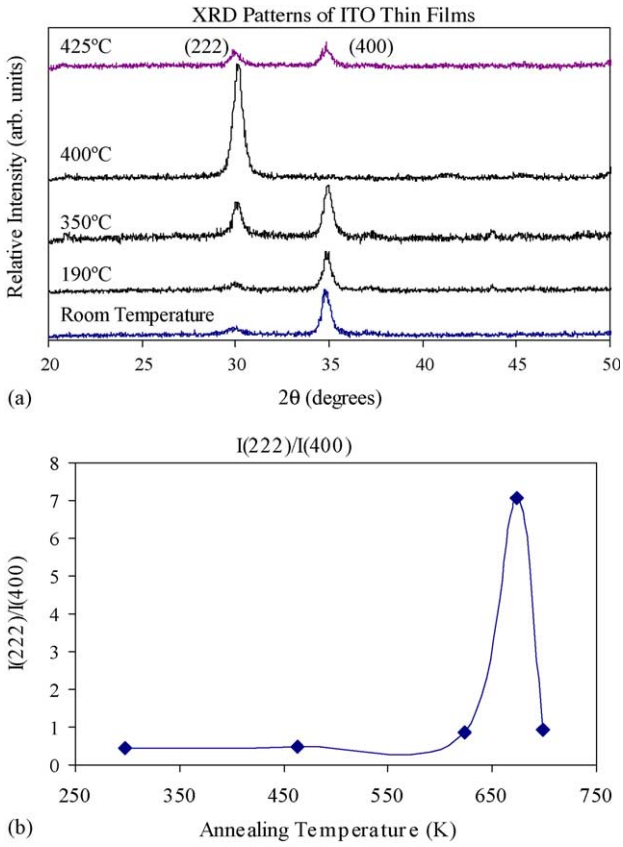

Fig. 3. (a) X-ray diffraction profiles of ITO films annealed at different temperatures. (b) The ratio of (2 2 2) to (4 0 0) intensities.

4. Summary

Electrical, optical and structural properties of ITO thin films prepared by rf sputtering, annealed at temperatures up to 500 °C are systematically investigated. Post annealing of the samples lead to high electrical conductivity, better optical transparency and large grain size for the films. The optimum annealing temperature is 400 °C resulting in a sheet resistance of 2.3 Ω/□ and an average grain size of 30 nm. We believe that a preferential crystal growth toward the (2 2 2) orientation takes place by annealing, and it has its highest value for annealing temperatures close to 400 °C.

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