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Chemical bonding structure of TiO_2 thin films grown on n-type Si

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ABSTRACT

Titanium dioxide thin films were obtained by RF magnetron sputtering system with different Ar and O atmospheres. Chemical bonding structures of the thin films were investigated using the Fourier transform infrared spectroscopy (FTIR) in the range of 400–7500 cm^{-1} for as-deposited and conventionally thermal annealed films at different temperature in air. These structural characterizations of the films were carried out by describing the low-frequency fluctuations of the FTIR spectra using the noninvasive (i.e. error controllable) procedure of the optimal linear smoothing. This approach is based on the criterion of the minimal relative error in selection of the proper smoothing window. It allows the receiving an optimal separation of a possible trend from the high-frequency fluctuations, defined as a random sequence of the relative fluctuations possessing zero trends. Thus, the noise can be read and extra information about the structures was then obtained by comparing with the experimental results. In the film annealed at 900 °C, the rutile phase was the dominant crystalline phase as revealed by infrared spectroscopy. At the annealing temperatures lower than 900 °C, both the anatase and the rutile phases were coexisting. In addition, symmetric and asymmetric Si–O–Si vibrations modes were observed at around 1000 cm^{-1} and 800 cm^{-1}, respectively. These peaks suggest that a thin SiO_2 film was formed at the TiO_2/Si interface during the growth and the annealing of the TiO_2 films. It was also observed that the reactivity between TiO_2 film and Si substrate is increased with the increasing annealing temperature.

1. Introduction

Titanium dioxide thin films have been widely used in electronic and optoelectronic devices such as sensor and solar cells. TiO_2 thin films carry the rutile, anatase and brookite crystal phase structures which affect their optical and electrical characteristics. The desired phase structures can be obtained by changing the film deposition conditions and post-growth processes such as thermal annealing in different gas atmospheres. TiO_2 films can be grown on several substrates like Si and glass, by reactive sputtering, sol–gel spin coating and laser deposition techniques [1–3]. The improvement of TiO_2 technology and the extension of implementation areas are dependent on the development of better growth conditions and the detailed researches of film characteristics with all of their aspects. During the deposition process, the gas pressure and the substrate temperature affect the structural characteristics of TiO_2 films [4]. Additionally, post-growth thermal annealing can also strongly affect the structural and the optical characteristics of TiO_2 thin films [5]. The Fourier transform infrared spectroscopy (FTIR) technique plays a significant role in studies of the molecular ordering and orientations in the structures. FTIR spectroscopy gives beneficial information about the Si–O–Ti chains of SiO_2–TiO_2 oxide mixtures occurring during the deposition or the post-growth thermal annealing processes. Moreover, the existence of the crystal phases, the Ti–O bond and the other chemical bonds in TiO_2 films can be observed from the FTIR measurements.

In this study, two TiO_2 thin films were deposited on Si by RF magnetron sputtering system with different Ar and O atmospheres. The deposited films were annealed at different temperature by the conventional thermal annealing (CTA) procedure in air atmosphere. Chemical bonding structures in the thin films were investigated using FTIR spectroscopy in range from 400 to 7500 cm^{-1} for as-deposited and annealed films. The film characteristics were carried out by describing of the low-frequency fluctuations (that in our case coincide with FTIR spectra) with the usage of a procedure of the optimal linear smoothing (POLS). This procedure turned out to be very effective in

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