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HRBS/channeling studies of ultra-thin ITO films on Si

P. Malar, T.K. Chan, C.S. Ho, T. Osipowicz *

Centre for Ion Beam Applications, Physics Department, National University of Singapore, Singapore 119260, Singapore

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Abstract

High-resolution Rutherford backscattering spectroscopy (HRBS)/channeling techniques have been utilized for a detailed characterization of ultra-thin indium tin oxide (ITO) films and to probe the nature of the interface between the ITO film and the Si(0 0 1) substrate. Channeling studies provide a direct measure of the lattice strain distribution in the crystalline Si substrate in the case of amorphous over layers. The measurements on DC magnetron sputtered ITO films have been carried out using the recently installed HRBS facility at the Centre for Ion Beam Applications (CIBA). The thickness of the ultra-thin (~9.8 nm) ITO films was calculated from the HRBS spectra having an energy resolution of about 1.4 keV at the superimposed leading (In + Sn) edge of the ITO film. The films were near stoichiometric and the interface between ITO film and Si was found to include a thin SiO_x transition layer. The backscattering yields from (In + Sn) of ITO were equal in random and channeling directions, thereby revealing the non-crystalline nature of the film. Angular scans of HRBS spectra around the off-normal [1 1 1] axis clearly showed a shift in the channeling minimum indicative of compressive strain of the Si lattice at the SiO_x/Si interface. The observed strain was about 0.8% near the interface and decreased to values below our detection limits at a depth of ~3 nm from the SiO_x/Si interface.

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Keywords: High-resolution RBS; Ion channeling; Interfacial strain

1. Introduction

Growth and study of oxide films on Si substrates have acquired much attention because of their importance in microelectronics involving various oxides as functional or buffer layers. The modern device technologies seek downscaling of the devices by reducing the thicknesses to submicron or few tens of nanometer sizes. The realization of miniature devices necessitates elaborate characterization studies of ultra-thin structures using high-resolution techniques. High-resolution Rutherford backscattering spectroscopy (HRBS) offers near monolayer depth resolution [1], which is extremely useful in non-destructively extracting compositional depth profiles and interface characteristics of ultra-thin structures. The depth resolution of HRBS is one order of magnitude better when compared to conventional RBS, where the depth resolution is limited by the energy resolution of the Si detectors used. On the other hand, HRBS utilizes electrostatic or magnetic spectrometers equipped with position sensitive detectors as detection system [2–7] to improve the depth resolution. Recently, HRBS/channeling measurements equipped with magnetic spectrometers have been used for the study of ultra-thin HfO_2/Si(0 0 1) [8] Si(0 0 1)/HfSiON [9] and SiO_2/Si [10] structures.

In this paper, we report the results on HRBS characterization of ultra-thin indium tin oxide (ITO) films grown over Si(0 0 1) substrates. The HRBS detection system consisting of a 90° double focusing sector magnet and a 1D-MCP focal plane detector has demonstrated state of the art performance characteristics [11]. The HRBS spectra measured using this facility have shown sub 1 keV energy resolution for the leading Si edge in SiO_2/Si samples. Apart

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* Corresponding author. Tel.: +65 65166745; fax: +65 67776126.
E-mail address: phyto@nus.edu.sg (T. Osipowicz).

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from the determination of composition and interface properties, the strain induced on the Si substrate due to the over layer was estimated from channeling measurements. Ion channeling measurements along off-normal axes are sensitive to the substrate lattice strain [8,12,13], which causes an angular shift in the channeling directions between the strained and unstrained lattice. The amount and type of strain on the substrate is determined from the calculation of angular shift values as a function of depth from the interface.

2. Experimental details

ITO films were grown by the DC magnetron sputtering method. An ITO target was reactively sputtered in the presence of a $(Ar + O_2)$ gas mixture onto Si(001) substrates held at room temperature. The Si substrates were treated with 1% HF solution prior to deposition to remove any native oxide present on the surface. Ultra-thin films suitable for HRBS studies were prepared by varying and optimizing the experimental conditions such as sputtering power and deposition time. The films used for the present studies were sputtered at a constant power level of 100 W for 20 s. The surface roughness of the samples was examined by atomic force microscopy (AFM). Random and channeling measurements were carried out using a 500 keV He^+ beam. More details of HRBS end station and its performance characteristics are presented elsewhere [11]. Briefly, a 500 keV He^+ beam ($I \sim 15$ nA) collimated by a series of two slit systems to 1×1 mm^2 was incident on the sample. The sample was mounted on a high-precision five-axis goniometer attached to the UHV chamber. The computer controlled goniometer enables sample translations in x, y and z as well rotations up to 90° and 30° around vertical and horizontal axes, respectively. The beam to target-normal angle was 60°. The particles backscattered at 65° were measured by the high-resolution detection system mentioned above. The random HRBS spectra were analyzed with the help of the simulation software XRUMP [14]. For the calculation of strain distribution, angular scan measurements were carried out around [111] axis of the Si (001) substrate along the $(1\bar{1}0)$ plane.

3. Results and discussion

Fig. 1 shows typical random HRBS spectra obtained for ITO/Si(001) structure along with the XRUMP simulation data. The inset to Fig. 1 shows a typical AFM image. The AFM image exhibits characteristic features expected for a continuous amorphous films. The presence of some crystallization seeds is also seen. The root mean square (RMS) roughness was about 1 nm. In the HRBS spectrum, the symbols correspond to the experimental data and the solid line denotes the simulated data. The peaks at ~480 keV and ~370 keV are due to (In + Sn) and oxygen, respectively. Initially, the simulated spectrum was calculated assuming the sample configuration of ITO (9.8 nm) on Si, without incorporating any oxide intermediate layer. For this sample configuration, the experimental (In + Sn) peak matched well with the calculated (In + Sn) peak. On the other hand, the calculated oxygen peak was much narrower than the experimental data and the calculated Si edge was much sharper than the observed edge. These features indicated the presence of an interfacial layer between ITO film and the Si(001) substrate consisting of Si and O. In order to accommodate these features, an interfacial layer between ITO and Si was included in the calculated spectrum. The calculated spectrum shown in Fig. 1 includes $a \sim 5$ nm thick SiO_x interfacial layer, which reproduces the experimental data well.

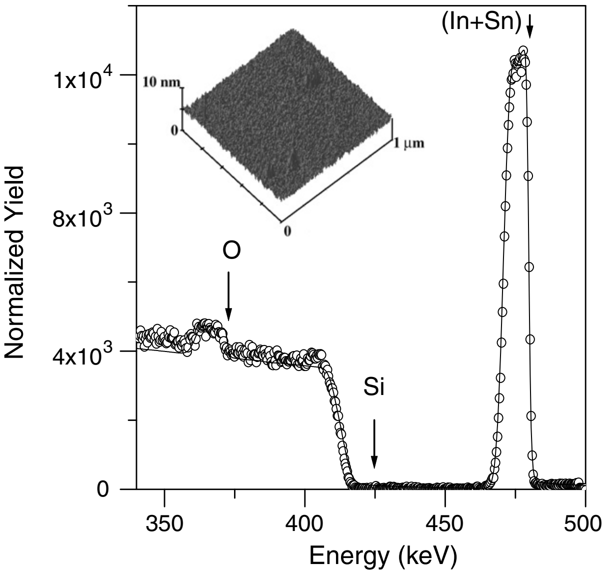

Fig. 1. Typical random HRBS spectra of ITO/Si(001) obtained using 500 keV He^+ beam and shown along with simulated data.

Fig. 2 shows the elemental depth profiles of In, Sn, O and Si in ITO/Si(001) structure. The depth profile data was extracted from the calculated spectrum shown in

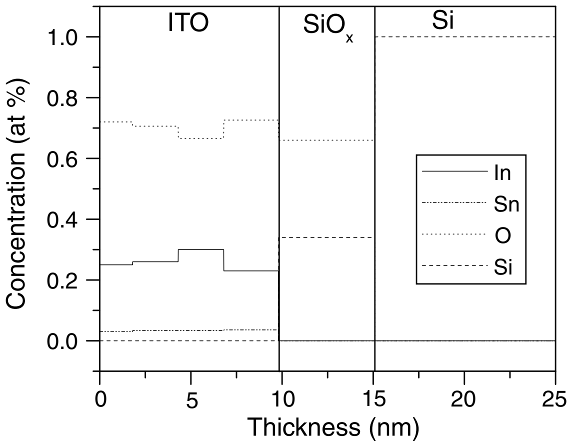

Fig. 2. Elemental depth profiles of In, Sn, O and Si in ITO/Si(001). The presence of oxygen in layer II indicates the formation of interfacial SiO_x layer between stoichiometric ITO and Si.

Fig. 1. Atomic concentrations of In, Sn and O in Layer I indicate near stoichiometry of the ITO film. The formation of an interfacial layer due to oxidation of Si substrate during the film growth process has been reported often [8,9]. However, the thickness of SiO_x (~5.0 nm) observed in the present study is higher when compared to the values reported in the HRBS study of HfO_2/Si(001) [8]. This difference can be attributed to the oxygen rich growth environment in DC magnetron reactive sputtering process.

An angular scan of the HRBS spectrum around [111] axis of the Si (001) substrate in the $(1\bar{1}0)$ plane was performed for strain calculations. The scattering yield of Si was lowest for the incident angle 54.74° corresponding to the [111] axis of Si (001). For incident angles away from the channeling direction, the scattering yield of Si changed markedly towards the random yield. However, the scattering yield from (In + Sn) did not show any difference with change in angle of incidence. This is indicative of amorphous nature of the ITO film. Each of the observed HRBS spectra in the angular scan measurements were divided into a number of narrow strips corresponding to different depth regions of 0.98 nm width beginning from the ITO/SiO_x interface into the Si substrate. The integrated scattering yield from each individual depth region was extracted as a function of angle of incidence. Fig. 3 shows variation of integrated scattering yield as a function of angle of incidence for various depth regions. The [111] channeling dip was clearly seen for regions deep inside the Si substrate and the dip position was found to agree with bulk [111] Si (curves D and E). However, the region corresponding to the SiO_x interface layer exhibited a much shallower channeling dip (curve A). In addition, the position of the channeling dips (curves C, B and A) shifted toward larger incident angles indicating the change in channeling directions. This angular shift in the channeling directions towards larger angle is suggestive of vertical lattice compression.

Fig. 4 is a sketch of the connection between compressive lattice strain and the angular shift seen in channeling. In the figure, the bulk lattice parameters are denoted as a and b. The strain causes a change in the lattice parameter resulting in a', assuming that only vertical compression is present.

The compressive strain in terms of lattice parameter can be written as

$$\varepsilon = \frac{(a - a')}{a} = \frac{\Delta a}{a}. \tag{1}$$

The off-normal channeling axis for the unstrained Si lattice makes angle θ with the normal [001] axis, whereas the off-normal axis for the strained Si lattice increases from θ to θ' causing an angular shift of $\Delta\theta$, and the incident angle θ in terms of lattice parameters can be written as

$$\tan\theta = \frac{a}{b}. \tag{2}$$

For any change in the lattice parameter due to strain there is a change in θ, which is determined by differentiating Eq. (2)

$$\sec^2\theta(\Delta\theta) = \frac{b(\Delta a) - a(\Delta b)}{b^2} = \tan\theta\varepsilon, \tag{3}$$

$$\Rightarrow \varepsilon = \frac{2\Delta\theta}{\sin 2\theta}. \tag{4}$$

The angular shift ($\Delta\theta$) values for different depth regions (curves A, B, C and D in Fig. 4) with respect to the unstrained Si lattice (curve E in Fig. 4) were determined and substituted in Eq. (4) to calculate the local compressive

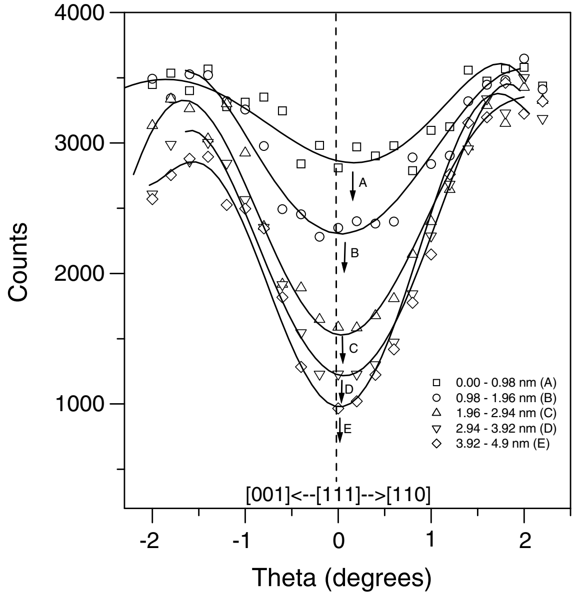

Fig. 3. Scattering yield of Si from different depth regions from the ITO/SiO_x interface as a function of angle of incidence around the [111] axis. The angles of incidence increase for shallower regions.

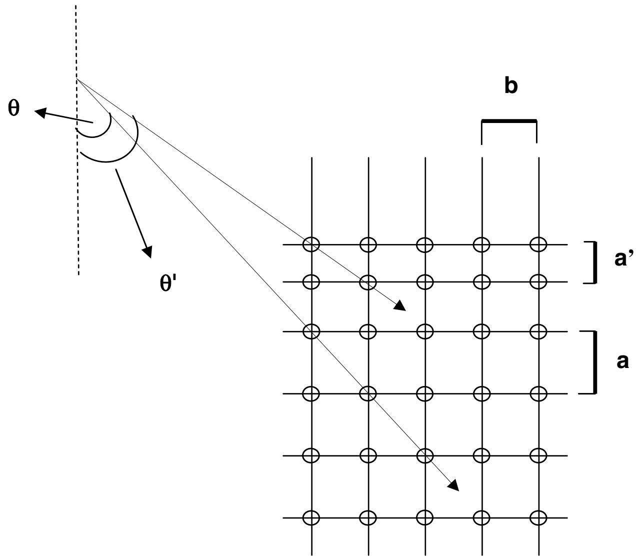

Fig. 4. Schematic illustration of how the strain in Si(001) substrate causes an angular shift in channeling directions for strained and unstrained lattices.

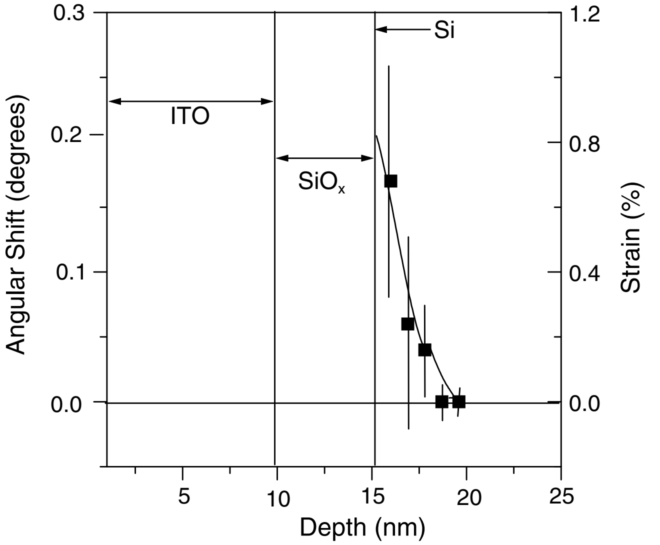

Fig. 5. Plot of angular shift in the [1 1 1] channeling direction in the strained Si lattice. The axis on the right shows the local compressive strain estimated from the observed angular shift using Eq. (4).

strain as a function of depth from the interface. Fig. 5 shows the angular shift (axis on the left) and local compressive strain (axis on the right) as a function of depth. The maximum observed strain was about 0.8% at the interface. The strain values decreased to values below the detection limits at a depth of ∼ nm from the interface. Similar results on formation of SiO_x and strained Si lattice near the SiO_x/Si interface have been reported, which were observed using the techniques such as spectroscopic ellipsometry [15] and nonlinear optical spectroscopy [16].

4. Conclusions

Ultra-thin ITO (9.8 nm) films grown on Si(0 0 1) substrates were characterized using HRBS. Analysis of the random spectra showed that the ITO films were near stoichiometric. An interfacial SiO_x layer (∼5 nm) has formed at the interface during the growth process. Channeling studies of local strain on Si substrate lattice due to SiO_x indicated a maximum vertical compressive strain of about 0.8% at the interface and the strain decreases with increase in depth. The strain extends down to ∼3 nm in the Si lattice from the interface.

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