GROWTH OF SiO_2 AT THE Sc_2O_3/Si(100) INTERFACE DURING ANNEALING

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Thermodynamic calculations suggest that Sc_2O_3 should be stable on Si at 1000 K, although the formation of silicates could not be ruled out due to the lack of free energy data[1]. The measured dielectric constant[2], κ=13, also makes it a candidate replacement for SiO_2 as the gate insulator in future generations of CMOS devices. However, this material has not been extensively investigated. This paper describes the deposition and analysis of Sc_2O_3 layers on Si(100) by e-beam evaporation and the growth of the interfacial layer during subsequent annealing. The films were analysed by *x*-ray photoelectron spectroscopy (XPS), high resolution transmission electron microscopy (HRTEM), and other advanced TEM techniques.

The Si(100) substrates were given an HF last-RCA clean and introduced into the ultra high vacuum (UHV) system which consisted of a deposition chamber connected by a UHV tunnel to an XPS spectrometer. This had an Al K_α *x*-ray source in a standard 54° geometry. Films were deposited with a rod-fed e-beam evaporator using a pressed powder target of Sc_2O_3. The substrates were held at ambient temperature (20 °C) or heated to 500 °C using a quartz-halogen heater. Apart from hydrogen, the main gases liberated during the deposition, O_2 and CO, had partial pressures of ~1-3×10^{-6} Pa. During some depositions molecular oxygen was introduced into the chamber at a pressure of 1.0-1.3×10^{-5} Torr (1.3-1.7 mPa).

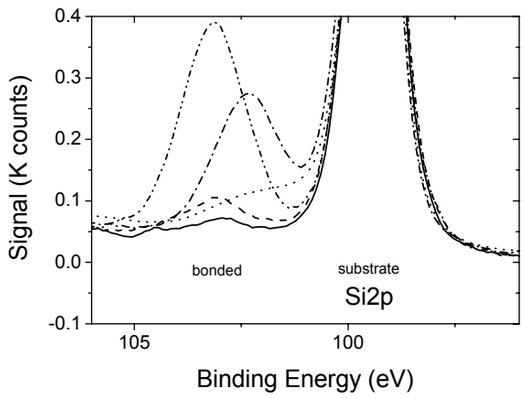

Figure 1. Si *2p* XPS peak for Sc_2O_3 films: (——) deposited at 20 °C without O_2, (----) at 500 °C without O_2, (·-·-·) at 500 °C with 1.3 mPa O_2, (·····) wafer deposited at 20 °C without O_2 exposed to air, (·····) bare Si(100) heated in 1.3 mPa O_2 for 42 min.

Fig. 1 shows the Si *2p* XPS peak of films 4.5-4.8 nm thick deposited at 20 °C or 500 °C with and without O_2 introduction. These spectra were used to determine a nominal thickness assuming the interfacial layer to be SiO_2. The Si *2p* peaks were fit to the spectra using a single gaussian-lorenzian for the bonded peak and a doublet for the substrate peak. The areas were used to calculate the thickness of an SiO_2 layer that would give rise to this Si *2p* (bonded) feature using the standard expression and the parameters derived for SiO_2 by Lu *et al*[3]. The sample deposited at ambient without O_2 (—) had a peak area corresponding to a nominal thickness of 0.08 nm of SiO_2. The films deposited in O_2 at 20 °C (----) and 500 °C (·---·) had a thickness of 0.4 and 0.6 nm, respectively. Also shown (····) in Fig. 1 is the spectrum for a bare silicon substrate annealed for 42 min in 1.3 mPa.

The film deposited without O_2 at 20 °C was brought out of the system for several hours and reintroduced for subsequent XPS analysis. The spectrum shown in Fig. 1 (··-··-) indicated that the interfacial layer had grown to a thickness of 0.8 nm. Since a layer this thick would not be formed by oxidizing silicon in ambient O_2 or H_2O, it can be deduced that the film was formed by a catalytic process, most likely through the diffusion of atomic oxygen liberated through reaction with the Sc_2O_3 film. The HRTEM analysis of the cross-section of this film revealed it to be amorphous with an amorphous interfacial layer ~0.8 nm thick, in agreement with the XPS result.

The result of ex-situ annealing of these films in O_2 and N_2 will be discussed. Further analysis was done to determine the amount of Sc present in the interfacial layers.

Advanced techniques used for the characterization of these thin dielectric films will be presented and compared with results obtained on ultrathin Si oxynitride films. These include energy filtered transmission electron microscopy, near edge structures analysis, electron nanodiffraction and high angle annular dark field scanning transmission electron microscopy with near nanometer to 0.2 nm spatial resolution.

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References

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