Characterisation of reactively sputtered silicon oxide for thin-film transistor fabrication

S.-I. Jun, T.E. McKnight, A.V. Melechko, M.L. Simpson and P.D. Rack

To overcome deficiencies of sputtered silicon dioxide (SiO_2) films the RF magnetron sputtering process was optimised using a full factorial design of experiment. The optimised SiO_2 film has a 5.7 MV/cm breakdown field and a 6.2 nm/min deposition rate at 10 W/cm^2 RF power, 3 mTorr pressure, 300°C substrate temperature, and 56 V substrate bias. Thin-film transistors were also fabricated and characterised to show potential and prospective applications of the optimised SiO_2 films.

Introduction: Sputtered silicon dioxide (SiO_2) has been widely studied and used as a dielectric insulator of electronic switching and sensing devices such as thin-film transistors (TFTs) and metal-insulator-semiconductor (MIS) switching devices. Sputter deposition is a particularly attractive process as a low temperature large area fabrication process on transparent, flexible, and plastic substrates [1, 2]. In using SiO_2 as a gate dielectric thin film, however, there is a well-known trade-off between the quality of thin films and the throughput (deposition rate), which is dominated by the oxygen gas ratio in the sputtering. In this work, we evaluated and optimised the SiO_2 sputtering process with high breakdown voltage, high deposition rate, and ideal stoichiometric composition. The optimised SiO_2 film from this work has a ~5.7 MV/cm breakdown voltage and ~6.2 nm/min deposition rate which is comparable to the deposition rate of refractory metal films (tungsten and molybdenum) at the same conditions in our sputtering system. Lastly we fabricated and characterised thin-film transistors (TFTs) that were entirely processed by RF magnetron sputtering deposition; gate and source-drain electrodes, active layers (gate SiO_2, a-Si, n^+ a-Si), and passivation (SiO_2).

Experimental details: An AJA ATC2000 RF magnetron sputtering system equipped with four magnetron sources and heated and/or DC biased substrate holder was utilised for the deposition of SiO_2, a-Si, n^+ a-Si, and metal films. A pure silicon target (99.9995%) was used since its sputtering yield (S, atoms/ion) is much higher than that of quartz ($S_{Si} = 0.6$ against $S_{SiO2} = 0.13$ for 1 KeV argon). The dielectric breakdown strength (breakdown voltage) was evaluated by a HP 4156 A, precision semiconductor parameter analyser, and the reported values are an average of ten measurements over each sample. The patterns for measuring are lithographically patterned metal-SiO_2-metal structure.

Table 1: Experimental condition of variable factors and quantitative results of responses

Factors				Responses		
No.	Temp. [°]	Oxygen [$O_2/O_2 + Ar$]	Substrate bias [V]	Deposition rate [nm/min]	Breakdown field [MV/cm]	(3) Oxygen ratio in SiO_x, x
1	25	0.15	0	6.36	1.61	1.66
2	25	0.15	150	5.62	1.15	1.77
3	25	0.30	0	1.65	3.14	1.75
4	25	0.30	150	1.05	3.00	1.86
5	300	0.15	0	6.05	5.13	1.93
6	300	0.15	150	5.07	5.61	2.00
7	300	0.30	0	1.54	5.43	2.00
8	300	0.30	150	0.84	5.56	2.00
(1) 9	25	0.15	0	—	1.93	—
(2) 10	25	0.15	150	—	2.74	—

(1),(2) Post-annealed after deposition: 300°C, 5 h in vacuum

(3) Measured by X-ray photoelectoron spectroscopy (XPS)

Results and conclusions: To evaluate the effects of the process factors in an efficient way, we performed a design of experiment (DOE) with 2-level and 4-factor factorial design as shown in Table 1. Our process target is high deposition rate with higher than 5 MV/cm breakdown field. Prior to the DOE, we analysed the hysteresis of the magnetron target voltage against the oxygen fraction in the sputtering gas to determine the ranges of 'metallic' and 'covered or oxide' sputtering modes that provide a proper range of oxygen fraction in the gas to achieve both modes of sputtering [3]. The abrupt decrease in target voltage, as shown in Fig. 1, shows that the plasma impedance increases with oxygen addition as the silicon oxide starts to form on the silicon sputtering target (oxide sputtering mode). The hysteresis did not changed with the sputtering temperature and substrate bias but changed with sputtering pressure. This indicates higher pressure causes the target to oxidise at lower oxygen flow rate because the effective oxygen partial pressure is higher even for lower flow rates because the throttle valve decreases the effective conductance of the pumping system. Therefore, the pressure was fixed at a low total pressure of 3 mTorr for all subsequent depositions. In addition to pressure, RF power can also shift the hysteresis loop to lower oxygen flow rates so the power was also fixed at 200 W (10 W/cm^2) for each deposition. Previous literature has shown that the oxygen flow rate significantly affects the SiO_2 properties, and has shown that higher oxygen partial pressures resulted in higher quality SiO_2 with high breakdown voltage and low current density [4]. On the other hand, the deposition rate decreases with increasing oxygen partial pressure. To analyse both sputtering modes, the oxygen ratios ($O_2/O_2 + Ar$) were set to 0.15 and 0.30; metallic and oxide sputtering modes from the hysteresis, respectively. From the results of Table 1 showing experimental conditions of variable factors and quantitative results of responses, firstly, deposition rate, as we mentioned previously, depends mainly on the oxygen fraction in the sputtering gas. The deposition rate drastically decreases as the oxygen partial pressure increases as there is a concomitant change from metal to oxide sputtering mode. The other factors, temperature and substrate bias, only slightly affect the deposition rate as the rate slightly decreases with temperature and substrate bias. It is suggested that densification of SiO_2 film with increase of temperature and substrate bias causes the effectively lower deposition rate. As the temperature increases from room temperature to 300°C, the breakdown field increases up to ~5.5 MV/cm. Also, as we expected, higher oxygen in the sputtering gas mixture has a positive factor on the breakdown voltage. Both higher temperature and oxygen fraction reduce the defect densities in the films; dangling bonds, vacancies and non-stoichiometric defects, etc. Counter to our expectation, the substrate bias does not affect the breakdown voltage. We speculate that substrate bias densifies the thin film by energetic ion bombardment; however, these energetic ions can also produce ion-irradiated defects such as dislocation loops, point defects, and can change the stoichiometry by preferentially sputtering either the cation or anion species [4]. These defects induced by substrate bias can be released by post-annealing as shown in the results for sputtering condition (10) of Table 1, which has almost same breakdown voltage as the unbiased sample after post-annealing. This result shows that the substrate bias in sputtering provides densification and ion-radiated defects in the films at the same time. The ion-radiated defects can be easily released by post-annealing and its electrical properties are improved by the annealing resulting from relaxation of the bias-originated defects and more densified films by substrate bias. The SiO_2 film becomes more stoichiometric with increasing temperature, oxygen fraction, and substrate bias. From the results of Table 1, the SiO_2 film is denser and more stoichiometric with applying substrate bias but, contrarily, the breakdown voltage is almost unchanged with substrate bias. We can conjecture that the substrate bias provides ideal SiO_2 films with good stoichiometry and very dense. However, it causes micro-structural defects, e.g. dislocations, owing to the highly energised ion bombardment [5]. Table 2 shows the optimised individual factors with higher deposition rate, higher breakdown voltage, and stoichiometric SiO_2 films by statistical software, MINITAB®. By doing the additional statistical approach, as shown in Table 3, we obtained the optimised process conditions; 300°C temperature, 0.15 oxygen ratio, and 56 V substrate bias. We also compared the predicted value done by the statistical program with the actual value by depositing the optimised film condition as shown in Table 3. The actual values are slightly higher than the predicted in the deposition rate and breakdown voltage but are within an acceptable value of 10% of the predicted values. Fig. 2 demonstrates electrical characteristics and SEM image of the TFT by our sputtered SiO_2, a-Si, and n^+ a-Si in order to show the prospective of using these sputtered films. A TFT is composed of gate electrodes (MoW) [4], a gate insulator (SiO_2), a-Si, n^+ a-Si, source-drain electrodes, and passivation (SiO_2). The MoW gate and active layer (a-Si, n^+ a-Si) were patterned by conventional lithography and reactive ion etching (RIE) using $SF_6 + CF_4 + O_2$ plasma gas. The deposition condition of the sputtered gate insulator is 200 W RF power, 3 mTorr pressure, 300°C temperature, 25.0/4.4 sccm Ar/O2 gas flow rate ($O_2/Ar + O_2 = 0.15$), and 57 V substrate bias. The a-Si, n^+ a-Si, and passivation (SiO_2) were also deposited via the RF sputtering. The TFT shows excellent and dynamic transfer curves and it has ~0.25 cm^2/Vs field effect mobility and $\sim 10^{3.5}$ on/off current ratio. From the results mentioned, we can conclude the optimised SiO_2 film has very reasonable characteristics, high deposition rate and high enough breakdown voltage for fabricating microelectronic devices at relatively low temperature.

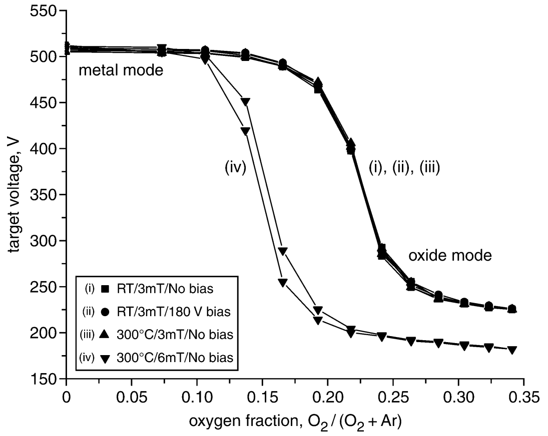

Fig. 1 *Hysteresis of magnetron target voltage for silicon target sputtered in Ar/O_2 mixed against oxygen fraction*

Table 2: Optimised process conditions of individual and mixed factors: optimisation of individual factors

Process target	Temp. [°C]	O_2 fraction	Bias [V]	Results
Max. deposition rate	25	0.15	0	6.36 nm/min
Max. breakdown voltage	300	0.15	150	5.61 MV/cm
Optimum stoichiometry $x = 2.0$ in SiO_x	300	0.30	150	2.0

Table 3: Optimised process conditions of individual and mixed factors: by statistical analysis and comparison of predicted and actual factors

	Process target	Temp. [°C]	O_2 fraction	Substrate bias [V]	Predicted	Actual
Deposition rate	Maximum				5.68	6.26
Breakdown voltage	Maximum	300	0.15	56	5.31	5.70
x, SiO_x	2.0				1.95	—

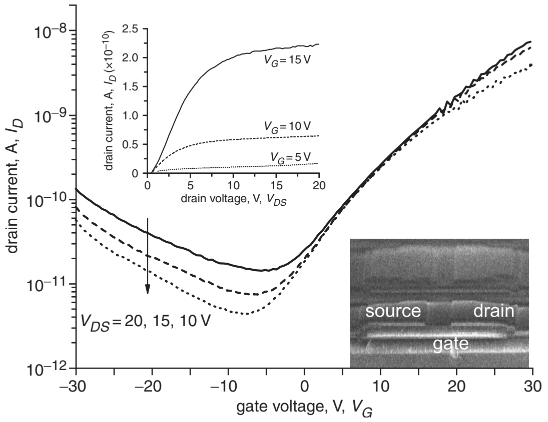

Fig. 2 *Current-voltage transfer characteristics and SEM image of TFT fabricated by entirely sputtered thin films (gate electrodes, gate SiO_2, a-Si, n^+ a-Si, source-drain electrodes, and passivation SiO_2)*

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S.-I. Jun and P.D. Rack (*Department of Materials Science and Engineering, The University of Tennessee, Knoxville, TN, 37996-2200, USA*)

E-mail: sjun3@utk.edu

T.E. McKnight, A.V. Melechko and M.L. Simpson (*Molecular Scale Engineering and Nanoscale Technologies Research Group, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*)

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