

Electrical Conduction and Dielectric Breakdown in Aluminum Oxide Insulators on Silicon

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Abstract—Leakage currents and dielectric breakdown were studied in MIS capacitors of metal—aluminum oxide—silicon. The aluminum oxide was produced by thermally oxidizing AlN at 800–1100 °C under dry O₂ conditions. The AlN films were deposited by RF magnetron sputtering on p-type Si (100) substrates. Thermal oxidation produced Al₂O₃ with a thickness and structure that depended on the process time and temperature. The MIS capacitors exhibited the charge regimes of accumulation, depletion, and inversion on the Si semiconductor surface. The best electrical properties were obtained when all of the AlN was fully oxidized to Al₂O₃ with no residual AlN. The MIS flatband voltage was near 0 V, the net oxide trapped charge density, Q_{ox} , was less than 10^{11} cm⁻², and the interface trap density, D_{it} , was less than 10^{11} cm⁻² eV⁻¹. At an oxide electric field of 0.3 MV/cm, the leakage current density was less than 10^{-7} A cm⁻², with a resistivity greater than 10^{12} Ω-cm. The critical field for dielectric breakdown ranged from 4 to 5 MV/cm. The temperature dependence of the current versus electric field indicated that the conduction mechanism was Frenkel–Poole emission, which has the interesting property that higher temperatures reduce the current. This may be important for the reliability of circuits operating under extreme conditions. The dielectric constant ranged from 3 to 9. The excellent electronic quality of aluminum oxide may be attractive for field effect transistor applications.

Index Terms—Dielectric breakdown, MIS capacitors, MOS capacitors, semiconductor-insulator interfaces.

I. INTRODUCTION

OVER the past decade, the gate oxides of field effect transistors in commercial integrated circuits have been scaled to below 4 nm thick to increase the gate capacitance and the transistor gain. In thin layers, the problems associated with gate electrode breakdown and leakage currents are crucial because of quantum mechanical tunneling. Under high electric field stressing, silicon dioxide degrades by the formation of traps, leading to lower breakdown fields [1]–[4]. After prolonged periods at relatively lower fields, SiO₂ may fail catastrophically by the mechanism of time dependent dielectric breakdown (TDDB), which is still not well understood [4]–[6]. Evidence indicates that the breakdown mechanism changes with the

strength of the applied electric field, casting doubt on the suitability of high field stressing alone to predict the long-term reliability of circuits normally operating at lower fields [7]. High tunneling currents cause heating and waste power [8], and SiO₂ may have difficulty sustaining further scaling reductions in thickness. Oxide scaling to zero thickness produces essentially a metal-semiconductor transistor (MESFET) [9] that may not be desirable because of the well-known limitations in drive currents and transconductance compared to MOSFET's [10]. A larger dielectric constant increases the transistor gate capacitance with higher transconductance for the same dielectric thickness, or it can be thicker for the same capacitance with less tunneling leakage current, which decreases exponentially with thickness.

For device applications, various dielectrics have been investigated as alternatives to SiO₂. Oxidized AlAs is interesting for optical and electrical devices, but may contain residual arsenic [11], [12]. Tantalum pentoxide (Ta₂O₅) thermally stable and mechanically hard [15][16]. Simulations indicate that sputtered Al

Al₂O₃ may be useful in the gates of flash memory circuits because its higher dielectric constant increases the capacitive coupling and increases circuit speed by three orders of magnitude, compared to using SiO₂ [17]. Unoxidized AlN has been used as a transistor gate dielectric on Si [18]. Previous studies of micron thick AlN films deposited by plasma enhanced chemical vapor deposition indicated resistance to oxidation up to 900 °C, with Al₂O₃ forming above 1100 °C [19]. In general, the defect density of deposited insulators is higher than that of thermally grown insulators.

This paper describes measurements of dielectric breakdown, leakage, and tunneling in Al₂O₃ produced by thermally oxidizing thin films of AlN on p-type Si substrates, as described previously [20]–[22]. We report on the defect density, dielectric constant, resistivity, and breakdown strength. In principle, aluminum oxide could be produced by other techniques including the reactive sputtering of Al metal in an oxygen atmosphere [23], and spray pyrolysis [24]. The optimum oxide process for applications is not clear, so it is valuable to compare methods. The best quality SiO₂ films are produced by thermal oxidation, which is the method explored here.

II. EXPERIMENTAL PREPARATION

The metal-insulator-silicon (MIS) capacitors were fabricated using the following procedure. First, p-type Si (100)

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TABLE I

PROCESS DATA FOR OXIDIZED AlN SAMPLES INCLUDING SAMPLE NUMBER, AS-GROWN THICKNESS OF THE AlN, AND OXIDATION TEMPERATURES AND TIMES. THE SUBLAYER THICKNESS (d) WAS DETERMINED FROM ELLIPSOMETRY, STYLUS PROFILOMETRY, AND RBS DATA SIMULATED WITH RUMP SOFTWARE, ASSUMING A STRUCTURE HAVING THREE STOICHIOMETRIC LAYERS WITH THE COMPOSITIONS SHOWN HERE. THE SUBSTRATES WERE Si (100) WITH 1 Ω -cm RESISTIVITY

as-deposited		after oxidation			
Sample	AlN thickness (nm)	temp. / time ($^{\circ}$ C) / (hr)	dAl ₂ O ₃ (nm)	dAlN (nm)	dSiO ₂ (nm)
100601a	250	1100 / 2	435	0	144
100601b	250	1100 / 1	452	0	76
100601c	250	1000 / 1	378	6	42
100601d	250	900 / 1	90	203	0
100601e	250	800 / 1	25	236	0
012301a	55	900 / 1	101	0	0
012301b	55	900 / 2	101	0	0
012301c	55	900 / 3	101	0	0
SO-9001	-	900 / 1	-	-	27
SO-9002	-	900 / 2	-	-	43
SO-9003	-	900 / 3	-	-	56

substrates having a resistivity of 1 Ω -cm were degreased and acid cleaned using an RCA etch and an HF dip. The substrates were Si pieces roughly 1 cm wide. Layers of AlN were deposited by RF magnetron reactive sputtering using an Al metal target and a mixture of N₂/Ar gases with 0–25% Ar. The RF magnetron power was varied from 200 to 400 W, and the substrates were not intentionally heated during deposition. The thickness of the AlN films, given in Table I, was measured by mechanical stylus profilometry, with an accuracy of 5 nm. Atomic force microscopy (AFM) indicated that the surface roughness of the as-deposited layers was about 1 nm rms. X-ray diffraction (XRD) measurements indicated that the AlN structure varied from microcrystalline (weak, broad XRD peaks), to polycrystalline depending on the sputtering parameters. Higher RF powers and low pressures produced stronger AlN peaks. The AlN samples reported here had relatively weak XRD peaks, indicating microcrystalline structure with multiple orientations, but with the (110) plane preferentially oriented parallel to the (100) substrate. Additional details of the processing were given previously [20]–[22].

Oxidation was performed in a horizontal quartz furnace tube with dry O₂ at temperatures ranging from 800 to 1100 $^{\circ}$ C, for durations of 1–3 h. XRD measurements of the oxide showed relatively weak peaks corresponding to several phases including α -Al₂O₃

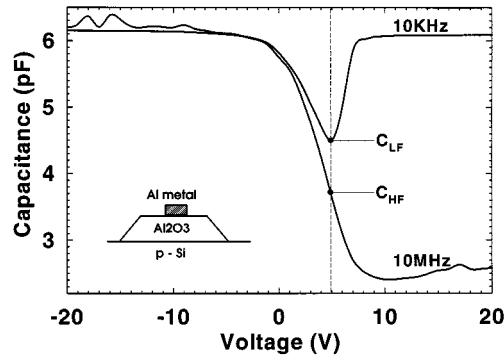


Fig. 1. The frequency dependence of the C - V characteristics at room temperature for an Al_2O_3 MIS capacitor with the AlN oxidized at 1000 °C for 1 h (sample 100 601c). The characteristics indicate the accumulation of holes at negative bias, the depletion of the Si surface at slightly positive bias, and the inversion of the Si surface at higher positive bias at low frequencies. The properties of the sample are given in Tables I and II. The relatively small flatband voltage corresponds to a low oxide defect density. The capacitances at low frequency C_{lf} and high frequency C_{hf} were used to calculate the interface trap density D_{it} . The inset shows the MIS structure with electrical contacts.

III. RESULTS

A. Capacitance–Voltage Measurements

The capacitance–voltage (C - V) characteristics yielded the bulk and interface defect densities of the oxide, and were

TABLE II

THE DIELECTRIC PROPERTIES OF OXIDIZED AlN THIN FILMS OBTAINED FROM $C-V$ AND $I-V$ MEASUREMENTS OF MIS CAPACITORS. PRESENTED ARE THE SAMPLE NUMBER, OXIDE CAPACITANCE PER AREA, DIELECTRIC CONSTANT, FLATBAND VOLTAGE, NET OXIDE TRAPPED CHARGE, DENSITY OF INTERFACE TRAPS, RESISTIVITY AT 0.3 MV/cm, AND BREAKDOWN FIELD OF THE ALUMINUM OXIDE

Sample	C_{ox} (nF-cm ⁻²)	κ_{ox}	V_{FB} (V)	$(Q_{ox})/q$ (cm ⁻²)	D_{it} (cm ⁻² eV ⁻¹)	ρ_{ox} (Ω -cm)	E_{BD} (MV/cm)
100601a	13.04	8.45	-1.67	1.46×10^{11}	2.26×10^{10}	2.2×10^{13}	4.6
100601b	13.2	7.9	-2.96	3.6×10^{11}	1.31×10^{10}	-	-
100601c	20.5	9.77	+1.13	6.6×10^{11}	1.59×10^{11}	4.2×10^{12}	4.23
100601d	27.5	9.1	-18.1	2.84×10^{12}	1.04×10^{10}	1.6×10^{13}	5.67
100601e	30	8.8	-19.4	2.85×10^{12}	-	-	-
012301a						2.9×10^{12}	4.99
012301b	53	6.0	-3	7.0×10^{11}	7.25×10^{10}	3.5×10^{12}	4.94
012301c						1.3×10^{12}	5.32
SO9001						1.9×10^{13}	10.3
SO9002						2.8×10^{13}	-
SO9003						3.5×10^{13}	8.27

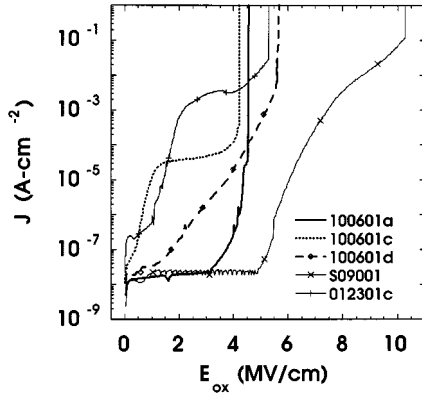


Fig. 2. The dependence of leakage current density on oxide electric field for MIS capacitors with AlN oxidized at 1100 °C for 2 h, 1000 °C for 1 h, and 900 °C for 1 h (samples 100 601a, c, and d, respectively), thinner AlN oxidized at 900 °C for 3 h (012 301c), and SiO₂ oxidized at 900 °C for 1 h (SO-9001). Properties are given in Tables I and II., and the shapes of the curves are discussed in the text. Dielectric breakdown occurred in the range from 4 to 5 MV/cm for the Al₂O₃, and near 10 MV/cm for the SiO₂.

A cm⁻² at fields under 0.3 MV/cm, corresponding to resistivities ρ_{ox} greater than 10^{12} Ω -cm. The resistivities agreed reasonably with the published value for sapphire (10^{14} Ω -cm) but the breakdown strength of the samples was higher than the value accepted for bulk sapphire (0.5 MV/cm) [31].

Sample 100 601c has a current density that increased and then saturated at about 4×10^{-5} A cm⁻² at fields near 1–3 MV/cm, and then increased again. This behavior is under study, but has been observed in ultrathin SiO₂ layers for which the constant current plateaus were attributed to phonon-assisted tunneling in neutral traps [2]. Another possibility for the current plateaus is series resistance in the test structure. For sample 100 601c, the increase in current at low fields may be due to breakdown at defects or weak spots in the dielectric, followed by a mechanism of self-healing [34], [35]. Small dark spots were observed by

visual microscopy on the metal surface, and it is possible that localized current surges evaporated small regions of the Al metal contact from the surface, preventing further conduction through that spot.

In comparison, the SiO₂ sample had relatively low current up to 5 MV/cm, followed by increasing current with dielectric breakdown near 10 MV/cm, in agreement with the accepted breakdown field of 10 MV/cm for thick SiO₂ [10]. Although the breakdown field of aluminum oxide was lower than for SiO₂, the breakdown voltage may be similar for optimized MIS devices having the same capacitance because of the higher dielectric constant of aluminum oxide.

C. Analysis of Leakage Current and Dielectric Breakdown

To determine the physical mechanisms responsible for leakage, the dependence of current on electric field was compared for two transport mechanisms known to be important for tunneling in insulators: Fowler–Nordheim (FN) tunneling and Frenkel–Poole emission.

The FN mechanism describes the tunneling of electrons from the metal into the conduction band of an insulator, with a dependence of current density on oxide electric field strength E_{ox} given by [10]

$$J_{FN} = aE_{ox}^2 \exp[-b/E_{ox}]. \quad (2)$$

The constants a and b are

$$a = q^2/(8\pi\hbar\phi_b) = 1.538 \times 10^{-6}(\phi_b)^{-1} \text{ A-V}^{-2} \quad (3)$$

and

$$\begin{aligned} b &= 8\pi(2m^*)^{1/2}(q\phi_b)^{3/2}/(3\hbar q) \\ &= 68(m^*/m_o)^{1/2}(\phi_b)^{3/2} \text{ MV/cm} \end{aligned} \quad (4)$$

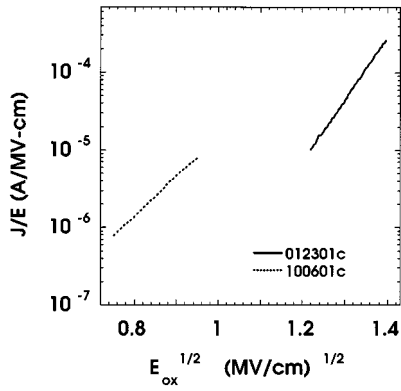


Fig. 3. The current density versus electric field characteristics at room temperature for two aluminum oxide MIS capacitors (sample 100601c oxidized at 1000 °C for 1 h and sample 012301c oxidized at 900 °C for 3 h). Data are presented as a Frenkel–Poole plot showing the dependence of the leakage current density divided by the oxide electric field versus the square root of electric field. The linear slopes imply Frenkel–Poole emission in the Al_2O_3 .

- h Planck's constant;
- q magnitude of the electron charge;
- $q\phi_b$ energy barrier height between the oxide and the metal contact (about 3.19 eV for Al on SiO_2 [36]);
- m^* electron effective mass for tunneling;
- m_o electron rest mass.

For SiO_2 , the effective mass of a tunneling electron ranges from $m^* = 0.3m_o$ [37] to $0.5 m_o$ [1].

Frenkel–Poole emission describes the field enhanced thermal excitation of trapped electrons into the oxide conduction band, with a dependence of current density on oxide electric field given by [10]

$$J_{\text{FP}} = cE_{\text{ox}} \exp\left[\left((dE_{\text{ox}})^{1/2} - \phi_t\right)q/k_bT\right] \quad (5)$$

where

- k_b Boltzmann's constant;
- T measurement temperature;
- c a constant that depends on the trap density N_t [38][39];
- d $q/\pi\epsilon_i$;
- ϵ_i total electric permittivity of the insulator.

The energy $q\phi_t$ is the depth of the oxide trap potential well, which differs from the barrier height for FN tunneling in (2).

Unlike FN tunneling, Frenkel–Poole emission is explicitly temperature dependent; higher temperatures reduce the current and the effect of the field on the current. Both tunneling mechanisms, however, are affected by the temperature dependence of the bandgap, the barrier heights, and the carrier occupation statistics.

Fig. 3 shows a Frenkel–Poole plot [40] of current density versus oxide electric field for two aluminum oxide samples of different thicknesses at room temperature. Linear slopes imply Frenkel–Poole emission, which occurs at higher fields for the thinner aluminum oxide sample (012301c). Frenkel–Poole emission is responsible for tunneling in Si_3N_4 [40]. Included purely for comparison, Fig. 4 shows a FN plot [28], [41] of current density versus oxide field for a conventional MOS

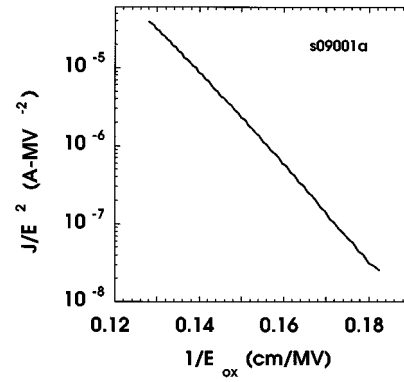


Fig. 4. The current density versus electric field characteristics of a SiO_2 MOS capacitor (sample SO-9001 oxidized at 900 °C for 1 h). Data are presented as a FN plot showing the dependence of leakage current density divided by the oxide electric field squared versus the reciprocal electric field. The linear slope implies FN tunneling in SiO_2 .

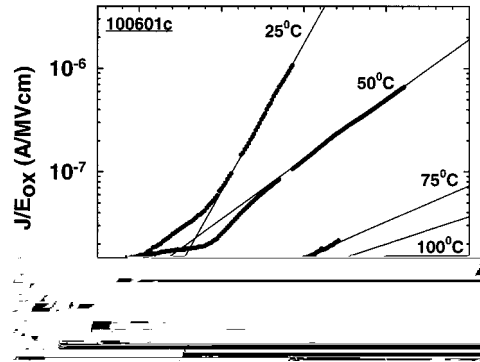


Fig. 5. Frenkel–Poole plot showing the current density versus oxide electric field characteristics at four measurement temperatures for an aluminum oxide MIS capacitor (sample 100601c oxidized at 1000 °C for 1 h). Linear slopes and the strong dependence on temperature imply Frenkel–Poole emission.

capacitor of aluminum metal— SiO_2 —Si. The linear slope covering several orders of magnitude corroborates FN tunneling in SiO_2 . When presented as a FN plot, the aluminum oxide data was not linear, implying that FN tunneling did not occur in the aluminum oxide.

D. Temperature Dependence of Current–Voltage Characteristics

For further insight into the aluminum oxide conduction, the temperature variation of the J – E characteristics is presented as a Frenkel–Poole plot in Fig. 5. Linear regions imply Frenkel–Poole emission, with the current decreasing exponentially with temperature, as given by (5), with the effect of the electric field on the current being opposite to the effect of the trap depth. The terms in the numerator of the exponent in (5) can be considered as a field dependent effective activation energy, $E_{\text{act}} = q(dE_{\text{ox}})^{1/2} - q\phi_t$.

Fig. 6 presents an Arrhenius plot for the sample of Fig. 5, for currents at several electric fields below breakdown. The thermally activated behavior is consistent with Frenkel–Poole emission. The effective activation energy is related to the potential well depth $q\phi_t$ of the oxide traps and the square

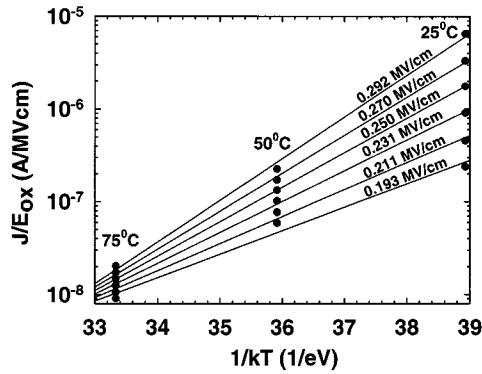


Fig. 6. Arrhenius plot of the aluminum oxide current at different values of electric field below breakdown for the sample of Fig. 5 (100 601c). Solid lines are the best fits to the experimental points. The slope implies thermally activated behavior, as discussed in the text.

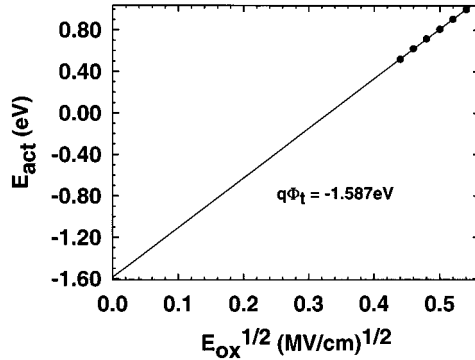


Fig. 7. Graphical determination of the Frenkel-Poole trap depth from the dependence of the effective activation energy on the square root of the electric field. By fitting the data to (5), the energy $q\phi_t = 1.6$ eV was obtained for the depth of the oxide trap potential well.

root of electric field. Fig. 7 show a graphical determination yielding $q\phi_t = 1.6$ eV. It is not yet clear if this energy is valid generally for aluminum oxide, or just for the particular samples measured here. For comparison, a 1.3 eV trap energy is reported for Si_3N_4 [40].

IV. DISCUSSION

At fields below breakdown, the Frenkel-Poole emission in Al_2O_3 is fundamentally different from conduction in SiO_2 , which exhibits FN tunneling. The decrease in current with increasing temperature in Al_2O_3 may be important for circuit reliability under extreme conditions.

The dielectric constant of Al_2O_3 is generally higher than for SiO_2 , so that gate dielectrics can be thicker for the same stored charge. For insulators less than 3 nm thick, tunneling occurs directly through the oxide with a probability that decreases exponentially with thickness. Thicker high dielectric gate insulators may be less susceptible to catastrophic failure and breakdown.

In principle, epitaxial techniques such as molecular beam epitaxy and chemical vapor deposition could be used to produce the

starting layers of AlN for oxidation. The role of small amounts of N in oxidized AlN is unclear, but may be beneficial. It is well known that annealing SiO_2 in an N ambient reduces the defect density [29], and that the nitriding of SiO_2 using N_2O improves circuit reliability [42], [43]. The carrier confinement properties of Al_2O_3 are expected to be similar to those of SiO_2 because the bandgap of Al_2O_3 is 8.7 eV [44], close to the 8–9 eV bandgap of SiO_2 .

V. CONCLUSIONS

Aluminum oxide (Al_2O_3) was produced by thermally oxidizing AlN on Si substrates using oxidation conditions similar to those for SiO_2 . MIS devices were fabricated and had C - V characteristics that exhibited the voltage-controlled charge regimes of accumulation, depletion and inversion on Si surfaces, with low defect densities. The best samples had net oxide trapped charge densities below 10^{11} cm^{-2} , similar to device-grade SiO_2 . The dielectric constants ranged from 3 to 9, implying that properly prepared Al_2O_3 can be thicker than SiO_2 for the same gate capacitance. Prior to breakdown, the conduction mechanism in Al_2O_3 was Frenkel-Poole emission, which is qualitatively different from breakdown in SiO_2 . The results showed that Al_2O_3 has device-grade characteristics and holds great promise for applications including gate dielectrics for field effect transistors.

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