Electrical Conduction and Dielectric Breakdown in Aluminum Oxide Insulators on Silicon

James Kolodzey, Senior Member, IEEE, Enam Ahmed Chowdhury, Thomas N. Adam, Guohua Qui, I. Rau, Johnson Olufemi Olowolafe, John S. Suehle, Senior Member, IEEE, and Yuan Chen

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, Qox, was less than 1013 cm−2, and the interface trap density, Dita, was less than 1013 cm−2 eV−1. At an oxide electric field of 0.3 MV/cm, the leakage current density was less than 10−7 A/cm2, with a resistivity greater than 1012 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 Al2O3 is interesting for optical and electrical devices, but may contain residual arsenic [11], [12]. Tallantum pentoxide (Ta2O5) can be deposited at low process temperatures and has a dielectric constant above 25 depending on its structure, but may lack long-term stability against reactions with Si [13], [14]. Al2O3 deposited by sputtering is thermally stable and mechanically hard [15][16]. Simulations indicate that sputtered 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)
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 °C, for durations of 1–3 h. XRD measurements of the oxide showed relatively weak peaks corresponding to several phases including α-Al₂O₃ (sapphire), δ-Al₂O₃, and θ-Al₂O₃ [22], indicating that the oxide was microcrystalline and nearly amorphous. Table I shows the oxidation durations, temperatures, and the range of sublayer thickness. Shorter times and lower temperatures produced sublayers of incompletely oxidized AlN. Longer times and higher temperatures produced stronger Al₂O₃ peaks with fully oxidized AlN, and sometimes SiO₂ from the oxidation of the underlying Si substrate. The mechanism for the formation of SiO₂ at the Si interface is not understood because the diffusivity of O in sapphire is negligible at 1100 °C (D = 2 × 10⁻⁶ cm²·s⁻¹ at 1500 °C) [25]. It may be that the layers are porous.

The film composition was measured using Rutherford backscattering spectrometry (RBS), and secondary ion mass spectrometry (SIMS). The RBS data were analyzed using RUMP software simulations [26], which yielded thickness profiles with 10 nm accuracy for the layers reported here. RBS indicated that the as-deposited AlN was nearly stoichiometric with a few percent of oxygen, in agreement with the XRD data. The RUMP thickness values were calibrated by ellipsometry, profilometry and atomic force microscopy. To obtain the correct layer thickness using RUMP simulations, the density values for AlN and Al₂O₃ must be corrected manually by the user [27]. For samples in the 012 301 series and for samples 100 601d and e, there was no evidence for SiO₂.

The oxide was nearly stoichiometric Al₂O₃, with residual N less than 5% (the detection limit). As described previously [21], the thickness values given in Table I were simulated assuming three abrupt layers (Al₂O₃, AlN, and SiO₂) with no interface mixing. Therefore, the evidence for homogeneous layers thinner than 50 nm may not be physically valid because of interface roughness and composition mixing. AFM measurements indicated that the oxide surface roughness was about 1.2 nm rms.

Metal-insulator-silicon (MIS) capacitors were fabricated using standard optical lithography. Electrical contacts of 100-nm thick Al metal were evaporated onto the top of the oxide and onto the bottom of the Si substrate. Using photolithographic liftoff, the top contacts were patterned into circular dots with areas of 8 × 10⁻⁸ cm² for samples in the series 100 601, and 3.14 × 10⁻⁸ cm² for samples in the series 012 301.
total defect density. We emphasize that $Q_{\text{ox}}$ is not an interface parameter, but includes contributions from defects distributed throughout the oxide, and the defect density from the aluminum oxide would not be diminished even by the possibility of nearly ideal SiO$_2$ at the Si interface.

Comparisons between samples having the same thickness of AlN, but with different oxidation conditions, indicated that high temperatures and long times (sample 100 601) produced some SiO$_2$ at the Si interface and a low $Q_{\text{ox}}$. On the other hand, the under-oxidized sample (100 601) had a significantly higher defect density implying that the residual AlN at the Si interface is undesirable.

The density of interface traps, $D_{it}$, describes the quality of the Si surface. Due to their slower response time, interface traps produced a difference in the capacitances measured at low frequency $C_{it}$ and at high frequency $C_{hf}$, as shown in Fig. 1. Using a standard approach, the frequency dependence of capacitance yields $D_{it}$ at an energy in the gap determined by the total surface potential $\phi_s$ [30]

$$D_{it}(\phi_s) = \left(\frac{C_{\text{ox}}}{q}\frac{C_{hf}}{C_{\text{ox}} - C_{hf}} - C_{hf}ight) / (C_{\text{ox}} - C_{hf})$$

(1)

where the applied gate voltage is $V_G - V_{FB} = V_{\text{ox}} + \phi_s$, and $V_{\text{ox}}$ is the voltage drop across the oxide. The results in Table II are for $\phi_s$ near midgap where the defects have the most impact on device performance. $D_{it}$ densities below $10^{11}$ cm$^{-2}$ eV$^{-1}$ indicated excellent interfaces, similar to device-grade SiO$_2$.

From the measured oxide capacitance and thickness, the dielectric constants in Table II ranged from 3 to 9, compared to 3.9 for SiO$_2$ [29]. The dielectric constant of sapphire (c-Al$_2$O$_3$) is 10.6 [31], but it is well know that the dielectric constants vary with microstructure for many materials. It may also be that the Al$_2$O$_3$ produced by thermally oxidizing AlN is less dense than sapphire.

**B. Current–Voltage Measurements**

Current–voltage ($I$–$V$) measurements were used to determine the dielectric breakdown strength and the electrical conduction mechanisms in the oxide. Using a voltage stress probe station described elsewhere [28], [32], the capacitors were biased into accumulation with the top metal contacts negative (–). The applied voltage was ramped at the relatively slow rate of 100 mV/s for better accuracy. In principle, a faster ramp rate would yield a higher breakdown field.

Fig. 2 shows the current density versus electric field ($J$–$E$) characteristics of several aluminum oxide samples, including the sample of Fig. 1 and an SiO$_2$ sample oxidized under similar conditions. The physical parameters of the samples are given in Table I. The electric field in the aluminum oxide was determined from the applied voltage using the thickness and the dielectric constants of the other layers ($\kappa = 9.1$ for AlN and 3.9 for SiO$_2$) [33]. The variation in $J$–$E$ characteristics from sample to sample were attributed to differences in oxidation conditions, sublayer composition, and structure.

Table II summarizes the electrical results. The aluminum oxide had dielectric breakdown at fields ranging from 4 to 5 MV/cm. The leakage current densities were below $1.2 \times 10^{-7}$
TABLE II  
THE DIELECTRIC PROPERTIES OF OXIDIZED AlN THIN FILMS OBTAINED FROM C–V AND J–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.

<table>
<thead>
<tr>
<th>Sample</th>
<th>C_ox (nF-cm^2)</th>
<th>e_ox</th>
<th>V_FB (V)</th>
<th>(Qox)/q (cm^-2)</th>
<th>D_t (cm^-2 eV^-1)</th>
<th>P_ox (G2-cm)</th>
<th>E_BD (MV/cm)</th>
</tr>
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<tbody>
<tr>
<td>100601a</td>
<td>13.04</td>
<td>8.45</td>
<td>-1.67</td>
<td>1.46x10^11</td>
<td>2.26x10^10</td>
<td>2.2x10^13</td>
<td>4.6</td>
</tr>
<tr>
<td>100601b</td>
<td>13.2</td>
<td>7.9</td>
<td>-2.96</td>
<td>3.6x10^11</td>
<td>1.31x10^10</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>100601c</td>
<td>20.5</td>
<td>9.77</td>
<td>+1.13</td>
<td>6.6x10^11</td>
<td>1.59x10^11</td>
<td>4.2x10^12</td>
<td>4.23</td>
</tr>
<tr>
<td>100601d</td>
<td>27.5</td>
<td>9.1</td>
<td>-18.1</td>
<td>2.84x10^12</td>
<td>1.04x10^10</td>
<td>1.6x10^13</td>
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</tr>
<tr>
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<td>30</td>
<td>8.8</td>
<td>-19.4</td>
<td>2.85x10^12</td>
<td>-</td>
<td>-</td>
<td>-</td>
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<tr>
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<td>-3</td>
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<tr>
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<td>3.5x10^13</td>
<td>8.27</td>
</tr>
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</table>

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 \( \rho_{ox} \) greater than 10^12 \( \Omega \)-cm. The resistivities agreed reasonably with the published value for sapphire (10^14 \( \Omega \)-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 \times 10^{-6} 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]

\[
J_{FN} = aE_{ox}^2 \exp\left[-b/E_{ox}\right],
\]

The constants \( a \) and \( b \) are

\[
a = q^2 / (8\pi\hbar\phi_k) = 1.338 \times 10^{-6}(\phi_k)^{-1}\text{A-V}^{-2}
\]

and

\[
b = 8\pi(2m^*)^{1/2}(q\phi_k)^{3/2} / (3\hbar q)
\]

\[
= 68(m^*/m_0)^{1/2}(\phi_k)^{3/2}\text{MV/cm}
\]

where
Fig. 3. The current density versus electric field characteristics at room temperature for two aluminum oxide MIS capacitors (sample 100 601c oxidized at 1000°C for 1 h and sample 012 301c 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 Al₂O₃.

Fig. 4. The current density versus electric field characteristics of a SiO₂ 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 SiO₂.

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 100 601c oxidized at 1000°C for 1 h). Linear slopes and the strong dependence on temperature imply Frenkel–Poole emission.

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, $E_{act} = q(dE_{ox})^{1/2} - \phi_b$.

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 $\phi_b$, of the oxide traps and the square
The dielectric constant of Al₂O₃ is generally higher than SiO₂, so that gate dielectrics can be thicker for the same gate capacitance. Prior to breakdown, the conduction mechanism in Al₂O₃ was Frenkel–Poole emission, which is qualitatively different from breakdown in SiO₂. The results showed that Al₂O₃ has device-grade characteristics and holds great promise for applications including gate dielectrics for field effect transistors.

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**IV. DISCUSSION**

At fields below breakdown, the Frenkel–Poole emission in Al₂O₃ is fundamentally different from conduction in SiO₂, which exhibits FN tunneling. The decrease in current with increasing temperature in Al₂O₃ may be important for circuit reliability under extreme conditions.

The dielectric constant of Al₂O₃ is generally higher than SiO₂, 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 SiO₂ in an N ambient reduces the defect density [29], and that the nitriding of SiO₂ using N₂O improves circuit reliability [42], [43]. The carrier confinement properties of Al₂O₃ are expected to be similar to those of SiO₂ because the bandgap of Al₂O₃ is 8.7 eV [44], close to the 8–9 eV bandgap of SiO₂.

**V. CONCLUSIONS**

Aluminum oxide (Al₂O₃) was produced by thermally oxidizing AlN on Si substrates using oxidation conditions similar to those for SiO₂. 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 10¹¹ cm⁻², similar to device-grade SiO₂. The dielectric constants ranged from 3 to 9, implying that properly prepared Al₂O₃ can be thicker than SiO₂ for the same gate capacitance. Prior to breakdown, the conduction mechanism in Al₂O₃ was Frenkel–Poole emission, which is qualitatively different from breakdown in SiO₂. The results showed that Al₂O₃ has device-grade characteristics and holds great promise for applications including gate dielectrics for field effect transistors.

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Guohua Qiu received the B.S. and M.S. degrees in material science from Shanghai Jiao Tong University, Shanghai, China, in 1987 and 1990, respectively. He received the M.S. degree in electrical engineering from the University of Delaware, Newark, in 1997. His M.S. dissertation was on the investigation on Al$_x$In$_{1-x}$N and AlO$_x$N$_{1-x}$ thin films.

From 1990 to 1995, he was a Lecturer and Research Associate at Shanghai Jiao Tong University and engaged in research of intermetallic composite materials. He served as a Research Assistant at the University of Delaware from 1995 to 1997. He is currently a Product Engineer at Dallas Semiconductor, Dallas, TX.

I. Rau was born in Karl-Marx-Stadt, Germany, in 1975. He was admitted to the undergraduate program in physics at the Chemnitz University of Technology, Chemnitz, Germany, in 1993, where he is currently finishing his thesis to achieve the Dipl.-Phys. degree. His current research is focused on epitaxial silicide formation.

From 1997 to 1998, he was with the Department of Electrical and Computer Engineering, University of Delaware, Newark.

Johnson Olufemi Olowolafe received the Ph.D. degree in applied physics from the California Institute of Technology, Pasadena.

He was a World Trade Postdoctoral Fellow at the IBM T. J. Watson Research Center, Yorktown Heights immediately after graduation. After the postdoctoral training, he was a Senior Lecturer and Associate Professor at the University of Ife, Nigeria, from 1978 to 1989. During this period, he was a Visiting Research Associate Professor at Cornell University, Ithaca, NY, for a total of two years. From 1990 to 1995, he was with Motorola, Inc., Austin, TX, where he developed the copper interconnect metallization. Since 1995, he has been an Associate Professor of Electrical and Computer Engineering at the University of Delaware, Newark. His research interests include interaction of metals with elemental and compound semiconductors, Cu and Al interconnect metallization on microelectronic devices, development of novel gate electrode materials, and fabrication of semiconductor devices. He has coauthored over 100 journal articles and seven patents.

Yuan Chen received the B.S. and M.S. degrees in electrical engineering from Xi’an Jiaotong University, Xi’an, China, in 1989 and 1992, respectively, and the Ph.D. degree in reliability engineering from the University of Maryland, College Park, in 1998. She conducted her postdoctoral research with NIST/UMCP and is currently with Bell Labs, Lucent Technologies, as a Member of Technical Staff. Her present research and projects cover wafer-level reliability testing and modeling, oxide reliability measurement, ultra-thin oxide characterization, hot-carrier aging, and failure analysis.

John S. Suehle (S’81–M’82–SM’95) received the B.S., M.S., and Ph.D. degrees in electrical engineering from the University of Maryland, College Park, in 1980, 1982, and 1988, respectively. In 1981, he received a Graduate Research Fellowship with the National Institute of Standards and Technology (NIST), Gaithersburg, MD.

Since 1982, he has been with the Semiconductor Electronics Division at NIST, where he is Leader of the Dielectric Reliability Metrology project. His research activities include failure and wear-out mechanisms of semiconductor devices and CMOS-compatible MEMS devices for in situ process monitoring. He serves as the chairman of the Oxide Integrity Working Group of the EIA/JEDEC 14.2 Standards Committee.

Dr. Suehle is a member of Eta Kappa Nu.