Tunneling Leakage Current in Oxynitride: Dependence on Oxygen/Nitrogen Content

Xin Guo, *Student Member, IEEE*, and T. P. Ma, *Fellow, IEEE*

Abstract—**It is widely known that the addition of nitrogen in silicon oxide, or the addition of oxygen in silicon nitride, affects its reliability as a gate dielectric. This letter examines the gate leakage current as a function of the oxygen and nitrogen contents in ultrathin silicon oxynitride films on Si substrates. It will be shown that, provided that electron tunneling is the dominant current conduction mechanism, the gate leakage current in the direct tunneling regime increases monotonically with the oxygen content for a given equivalent oxide thickness (EOT), such that pure silicon nitride passes the least amount of current while pure silicon oxide is the leakiest.**

I. Introduction

Silicon oxide, oxynitride, and silicon nitride have been extensively studied as dielectrics for both DRAM storage capacitors and field-effect transistors. Theoretical modeling of tunneling leakage current through thermal oxide has been carried out by the use of several approaches, including numerical integration of Airy function [1], semi-empirical WKB approximation [2], and quantum-mechanical calculation [3]. However, there has not been a systematic study of the dependence of the leakage current flowing through the oxynitride film on its oxygen/nitrogen ratio, despite its scientific interest as well as technological importance. One of the reasons for the lack of such a study, we believe, was due to the different conduction mechanisms that are operative in these dielectrics: ranging from electron tunneling in silicon oxide to Frenkel–Poole hopping in silicon nitride [4]–[6], which make the analysis very difficult.

It was recently demonstrated [7]–[10] that one can make silicon nitride and oxynitride films in which the current transport mechanism is predominantly electron tunneling, just like what has been observed in silicon oxide. The reason that Frenkel–Poole conduction does not play an important role in such dielectric films is believed to be due to the substantially lower trap density as compared to conventional CVD nitride and oxynitride films. This development makes the theoretical modeling and calculation of leakage currents in oxynitride films much more manageable, and this letter reports the results of such calculations on films covering the entire range of oxygen/nitrogen ratios.

Manuscript received December 7, 1997; revised February 12, 1998. This work was supported by grants from SRC, NSF, and ONR.

The authors are with the Center for Microelectronic Materials and Structures and the Department of Electrical Engineering, Yale University, New Haven, CT 06520 USA.

Publisher Item Identifier S 0741-3106(98)04187-1.

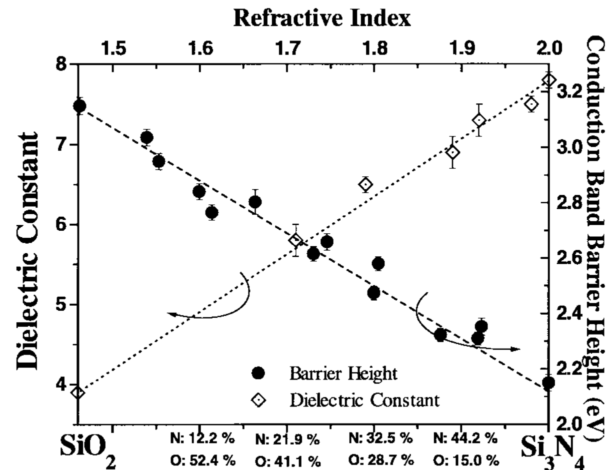

Fig. 1. Conduction band barrier heights and dielectric constants of oxynitride films [11]–[13].

II. Results and Discussion

To calculate the tunneling current one needs to know both the barrier height and the dielectric constant, in addition to the dielectric thickness. Fortunately, both of these parameters have been determined experimentally over a range of oxygen/nitrogen contents [11]–[13], and their results are very useful for this study.

Fig. 1 shows a compilation of barrier height and dielectric constant data taken from the literature [11]–[13] for a wide range of film compositions, all the way from pure oxide to pure nitride. It is apparent that the conduction band barrier height increases monotonically with increasing oxygen concentration while the dielectric constant decreases monotonically. The data also strongly suggest that both parameters vary linearly with the oxygen concentration, and may be represented by the following functional forms:

$$\epsilon_{\mathrm{ON}} = \epsilon_O + (1-\alpha)\times(\epsilon_N - \epsilon_O) = 3.9\times(2-\alpha) \quad (1)$$

and

$$\phi_{\mathrm{ON}} = \phi_O - (1-\alpha)\times(\phi_N - \phi_O) = 3.15 - (1-\alpha)\times 1.05 \quad (2)$$

where ϵ_O, ϵ_N, and ϵ_{ON} are the dielectric constant of oxide, nitride, and oxynitride, respectively, and ϕ_O, ϕ_N, and ϕ_{ON} are the corresponding conduction band barrier heights. The factor α is the equivalent percentage of silicon oxide in the oxynitride film; i.e., 100% for pure silicon oxide and 0% for pure silicon nitride. The atomic concentration of Si, O, and

0741–3106/98$10.00 © 1998 IEEE

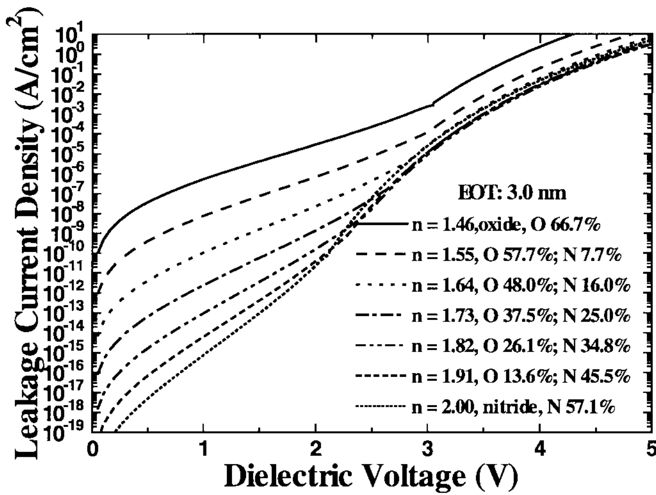

Fig. 2. Leakage current densities of dielectric films of 3.0-nm EOT as a function of refractive index and atomic concentrations of oxygen and nitrogen.

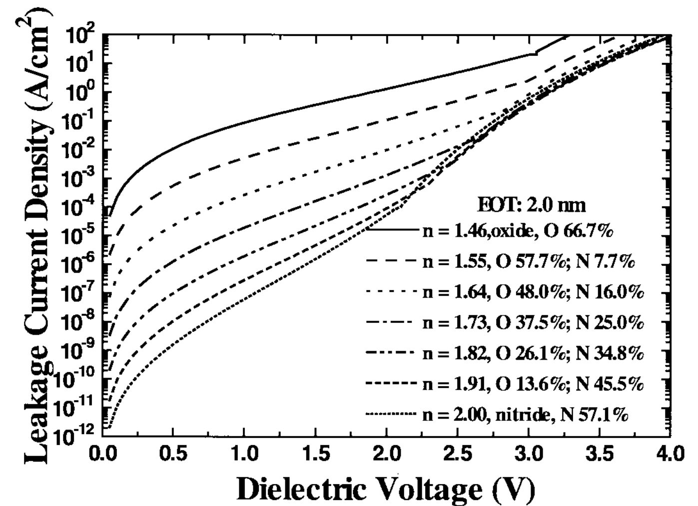

Fig. 3. Leakage current densities of dielectric films of 2.0-nm EOT as a function of refractive index and atomic concentrations of oxygen and nitrogen.

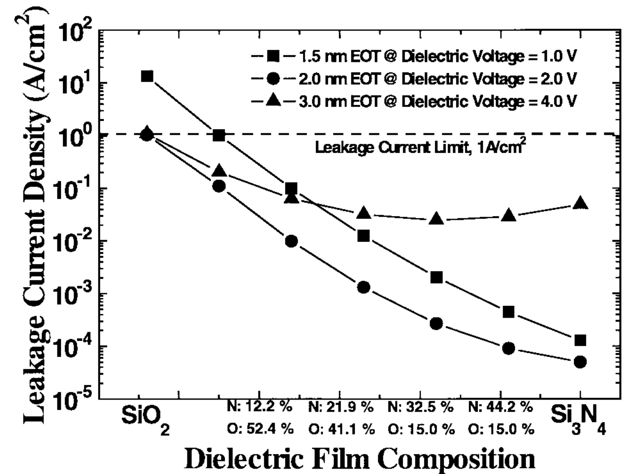

Fig. 4. Relationship between tunneling current and dielectric film composition: dependence on oxygen/nitrogen concentration.

N can then be obtained from the "stoichiometric" oxynitride (SiO_xN_y) composition relationship [13] as in the following form:

$$2x + 3y = 4. \tag{3}$$

Although somewhat fortuitous, the linear relationships of (1) and (2) provide very convenient means for interpolating, which is necessary to fill in the data points which are not available experimentally.

Having obtained the composition-dependent values of the barrier height and the dielectric constant, we then calculated the tunneling $I-V$ characteristics for sets of oxide, nitride, and oxynitride films with various equivalent oxide thicknesses (EOT's) in both direct tunneling (DT) regime and Fowler–Nordheim (FN) regime. WKB approximation was used to calculate the tunneling probability. The direct tunneling current calculation is derived from an earlier study by Simmons [14] on tunneling current through thin insulating films. An electron effective mass of $0.5m_0$ is used throughout the entire calculation. The calculated leakage current agrees well in both the FN and the DT regimes. In the case of pure thermal oxide, the calculated results obtained from this model are consistent with previously published quantum-mechanical calculations [3].

The calculated results are shown in Fig. 2 for films of 3.0 nm EOT, and in Fig. 3 for films of 2.0 nm EOT. In the DT regime, it is obvious that the pure silicon nitride film gives the lowest leakage current density because of its larger physical thickness, despite its lower barrier height, and the leakage current increases monotonically with the oxygen content. However, in the FN regime, there is a clear turnaround, showing that some oxynitride can give us lower leakage current than pure nitride. These two effects can be seen more clearly in Fig. 4, where the leakage current densities of the 1.5-nm, 2-nm, and 3-nm films are plotted at dielectric voltages of 1 V (DT), 2 V (DT), and 4 V (FN), respectively.

One striking aspect of the theoretical results is that, with as little as 10% of nitrogen in the film, the direct tunneling current below 1 V can be reduced by more than two orders of magnitude compared to its pure oxide counterpart. The previously proposed 1 A/cm^2 scaling limit [3] is also plotted on Fig. 4. One can see that, while the scaling limit for thermal oxide is about 2.0 nm, with oxynitride of high nitrogen content or pure nitride, the scaling limit can be much thinner at the projected operating dielectric voltage of 1 V.

While it is not easy to determine accurately the film composition in the ultrathin regime, the preliminary experimental results that we have obtained do agree well with the theoretical calculations. Fig. 5 shows the experimental data of oxynitride films of 1.82-nm EOT to 2.18-nm EOT with $\sim$10% to $\sim$18% of nitrogen, deposited by the JVD technique [7]–[10]. The EOT was obtained from $C-V$ measurement with extrapolation based on a fully-quantum-mechanical scheme [15]. One can see that the data fit the theory quite well. The nitrogen concentrations extracted from the data fitting procedure agree with

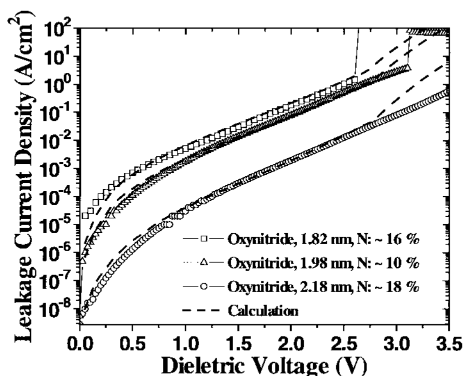

Fig. 5. Comparison of experimental data and theoretical calculation of oxynitride films of three different EOT's containing ∼10% to ∼18% nitrogen.

the film compositions obtained from AES measurements with about 5% error, which we believe is within the measurement error of the AES method.

III. Summary

In summary, we have shown that an oxynitride film is generally less leaky than its thermal SiO_2 counterpart of the same EOT, provided the dominant current conduction mechanism is electron tunneling. In the direct tunneling regime, a higher nitrogen concentration leads to a less leaky film, and in the extreme case of a pure silicon nitride film, the leakage current may be as much as seven to eight orders of magnitude lower than its pure thermal SiO_2 counterpart. This comes about due to the nitride's larger physical thickness for a given EOT, despite the fact that it has a lower barrier height.

Acknowledgment

The authors would like to thank the Jet Process Corporation for making a JVD machine available for silicon nitride deposition.

References

[1] K. H. Gundlach, "Zur Berechnung ds Tunnelstroms Durch eine Trapezformige Potentialstufe," *Solid-State Electron.*, vol. 9, p. 949, 1966.
[2] K. F. Schuegraf, C. C. King, and C. Hu, "Ultrathin silicon dioxide leakage current and scaling limit," in *Dig. Tech. Papers, 1992 Symp. VLSI Technol.*, p. 18.
[3] S. H. Lo, D. A. Buchanan, Y. Taur, and W. Wang, "Quantum-mechanical modeling of electron tunneling current from the inversion layer of ultra-thin-oxide nMOSFET's," *IEEE Electron Device Lett.*, vol. 18, p. 209, May 1997.
[4] L. D. Yau, "Arguments for electron conduction in silicon nitride," *IEEE Electron Device Lett.*, vol. EDL-5, p. 318, Aug. 1984.
[5] Z. A. Weinberg, "Hole conduction in Si_3N_4 films on Si," in *Appl. Phys. Lett.*, vol. 29, p. 617, 1976.
[6] D. K. Schroder and M. H. White, "Characterization of current transport in MNOS structures with complementary tunneling emitter bipolar transistors," *IEEE Trans. Electron Devices*, vol. ED–26, p. 899, June 1979.
[7] X. W. Wang, T. P. Ma, G. J. Cui, T. Tamagawa, J. W. Golz, S. Kareci, B. L. Halpern, and J. J. Schmitt, "High reliable silicon nitride films made by jet vapor deposition," *Jpn. J. Appl. Phys.*, vol. 34, pt. 1, no. 2B, p. 955, 1995.
[8] M. Khare, X. Guo, X. W. Wang, T. P. Ma, G. J. Cui, T. Tamagawa, B. L. Halpern, and J. J. Schmitt, "Ultrathin, silicon nitride gate dielectric for deep-sub-micron CMOS devices," in *Dig. Tech. Papers, 1997 IEEE Symp. VLSI Technol.*, vol. 5A-4, p. 51.
[9] Y. Shi, X. W. Wang, T. P. Ma, G. J. Cui, T. Tamagawa, B. L. Halpern, and J. J. Schmitt, "Current transport in ultrathin JVD silicon nitride films," in *26th IEEE Semicond. Interface Specialist Conf.*, Abstr. 7.2, Dec. 7–9, 1995.
[10] T. P. Ma, "Making silicon nitride film a viable gate dielectric," *IEEE Trans. Electron Devices*, vol. 45, pp. 680–690, Mar. 1998.
[11] D. M. Brown, P. V. Gary, F. K. Heumann, H. R. Philipp, and E. A. Taft, "Properties, of $Si_xO_yN_z$ films on Si,"*J. Electrochem. Soc.*, vol. 115, no. 3, p. 311, Mar. 1968.
[12] L. He, T. Inokuma, and S. Hasegawa, "Properties of 'Stoichiometric' silicon oxynitride films," *Jpn. J. Appl. Phys.*, vol. 35, pt. 1, no. 2B, p. 1503, Feb. 1996.
[13] V. A. Gritsenko, N. D. Dikovskaja, and K. P. Mogilnikov, "Band diagram and conductivity of silicon oxynitride films," *Thin Solid Films*, vol. 51, p. 353, Feb. 1978.
[14] R. Rios and N. D. Arora, "Determination of ultrathin gate oxide thicknesses for CMOS structures using quantum effects," in *IEDM Tech. Dig.*, 1994, p. 612.
[15] J. G. Simmons, "Generalized formula for the electric tunnel effect between similar electrodes seperated by a thin insulating film," *J. Appl. Phys.*, vol. 34, no. 6, p. 173, 1963.