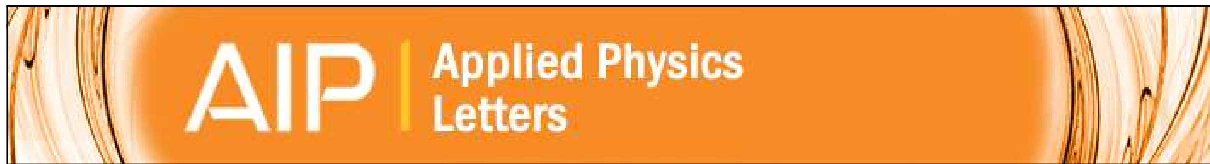

Studies of charge carrier trapping and recombination processes in Si ⁄ Si O 2 ⁄ Mg O structures using second-harmonic generation

Y. V. White, X. Lu, R. Pasternak, N. H. Tolk, A. Chatterjee, R. D. Schrimpf, D. M. Fleetwood, A. Ueda, and R. Mu

Citation: Applied Physics Letters **88**, 062102 (2006); doi: 10.1063/1.2172008
View online: http://dx.doi.org/10.1063/1.2172008
View Table of Contents: http://scitation.aip.org/content/aip/journal/apl/88/6?ver=pdfcov
Published by the AIP Publishing

Articles you may be interested in
Charge trapping defects in Si / SiO 2 / Hf (1 − x) Si x O 2 film stacks characterized by spectroscopic second-harmonic generation
J. Vac. Sci. Technol. B **29**, 04D101 (2011); 10.1116/1.3591433

Trapping-related recombination of charge carriers in silicon
Appl. Phys. Lett. **97**, 112111 (2010); 10.1063/1.3490240

Determination of spatially resolved trapping parameters in silicon with injection dependent carrier density imaging
J. Appl. Phys. **99**, 114908 (2006); 10.1063/1.2202729

Localized charge injection in SiO 2 films containing silicon nanocrystals
Appl. Phys. Lett. **79**, 791 (2001); 10.1063/1.1383574

Detection of gate oxide charge trapping by second-harmonic generation
Appl. Phys. Lett. **75**, 3506 (1999); 10.1063/1.125370

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 128.59.222.12 On: Sun, 30 Nov 2014 23:28:46

Studies of charge carrier trapping and recombination processes in $Si/SiO_2/MgO$ structures using second-harmonic generation

Y. V. White,[a] X. Lu, R. Pasternak, and N. H. Tolk
Department of Physics and Astronomy, Vanderbilt University, Nashville, Tennessee 37235

A. Chatterjee, R. D. Schrimpf, and D. M. Fleetwood
Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, Tennessee 37235

A. Ueda and R. Mu
Department of Physics, Fisk University, Nashville, Tennessee 37208

(Received 15 August 2005; accepted 16 December 2005; published online 6 February 2006)

Effects of MgO deposition on Si/SiO_2 system and charge carrier trapping and recombination in $Si/SiO_2/MgO$ structures are studied using second-harmonic generation (SHG). An ultrafast 800 nm laser was used both for multi-photon induced electron injection through the SiO_2 into a potential well in the MgO, and for monitoring the time-dependent SHG signal, which is sensitive to the electric field at the Si/SiO_2 interface. Our results indicate that the MgO deposition introduces new trap states, and electrons trapped in the MgO transport more readily through the SiO_2 than those in traps on the surface of SiO_2. We attribute this to differences in trap energy levels and/or differences in process damage-induced defect densities in the SiO_2. *© 2006 American Institute of Physics*. [DOI: 10.1063/1.2172008]

As feature sizes continue to be reduced in silicon-based technologies, conventional SiO_2-based gate dielectrics in metal-oxide-semiconductor (MOS) transistors are rapidly approaching the fundamental limits of their scaling. The reduction of SiO_2 gate dielectric thickness increases device tunneling current and dopant penetration. The quality of the Si/SiO_2 interface plays an important role in MOS device performance. Traditionally, characterization of Si/SiO_2 interfacial properties is accomplished with electrical methods such as capacitance-voltage (C-V) and current-voltage (I-V) measurements.[1,2] Recently, second-harmonic generation (SHG) has been demonstrated as a powerful tool for contactless noninvasive *in situ* monitoring of the dc field across the noncentrosymmetric Si/SiO_2 interface, resulting from changes in local charge distributions.[3,4] Incident ultrashort laser pulses, by virtue of multi-photon absorption, cause electron injection into the oxide and trapping on the SiO_2 surface due to ambient oxygen.[3,5,6] The time-dependent SHG (TD-SHG) signal is a direct measure of the electric field created by the charge separation at the Si-oxide interface.[6] This time-dependent electric field induced second-harmonic (EFISH) signal from Si/SiO_2 can be described in general by

$$I^{2\omega}(t) = |\chi^{(2)} + \chi^{(3)}E(t)|^2(I^{\varpi})^2, \tag{1}$$

where $I^{(\omega)}$ is the intensity of the incident laser light, $E(t)$ is the varying time-dependent electric field at the interface, and $\chi^{(2)}$ and $\chi^{(3)}$ are the interfacial second- and third-order susceptibilities, respectively. EFISH measurements provide information about electronic structure, carrier dynamics, local fields, symmetry, and quality of interfaces.[4,7,8]

Different approaches have been made in order to study the Si/SiO_2 system and improve device performance. Bias application and its effect on the SHG signal in Si/SiO_2 structures have been reported.[9–12] It has been shown that the deposition of an additional layer of Cr on native and thermally grown SiO_2 drastically changes the SHG response of the system.[13] In this work we present TD-SHG measurements of $Si/SiO_2/MgO$ structures. The MgO material has been a subject of research due to its wide band gap ($\sim$7.8 eV),[14] its ionic bonding properties (in contrast to the covalent bonding in SiO_2), and attractive dopant properties.[15–17] In our experiments, we demonstrate that the deposition of a MgO layer on SiO_2 creates a potential well that leads to new electronic states that significantly change the SHG response of the system, and may also lead to defect formation in the SiO_2, e.g., via chemical reactions between the Mg and hydrogen-related species in the SiO_2, or via soft x-ray or ultraviolet photon interactions during the electron beam deposition.[18] Hence, measurements of TD-SHG can provide insight into the electronic processes in the SiO_2/MgO layers.

The TD-SHG experiments performed here used the following experimental configuration: 150 fs p-polarized pulses ($\lambda = 800$ nm) from a mode locked Ti:sapphire laser (Coherent Mira 900) were focused on the sample at a 45° angle of incidence. The samples were mounted on an aluminum plate to reduce heating effects. The diameter of the laser spot was $\sim$50 μm. The experiments were carried out at room temperature in air. Four sets of samples were used in the experiment: the first one was a 2.4 nm Si/SiO_2 sample [thermally grown oxide film on Si (100)]. The second, third, and fourth samples had thin MgO layers of 5, 10, and 15 nm deposited on otherwise identical 2.4 nm Si/SiO_2. The MgO films were deposited by electron-beam evaporation under a base vacuum of $\sim 5 \times 10^{-7}$ Torr at an average deposition rate of 0.1 Å/s; the electron beam energy was 4 keV.

TD-SHG measurements for the $Si/SiO_2/MgO$ system at low and high laser intensities are shown in Fig. 1. Each time the laser was blocked for 100 s to monitor electron transport

[a]Author to whom correspondence should be addressed; electronic mail: yelena.v.rogachyova@vanderbilt.edu

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 128.59.222.12 On: Sun, 30 Nov 2014 23:28:46

 © 2006 American Institute of Physics

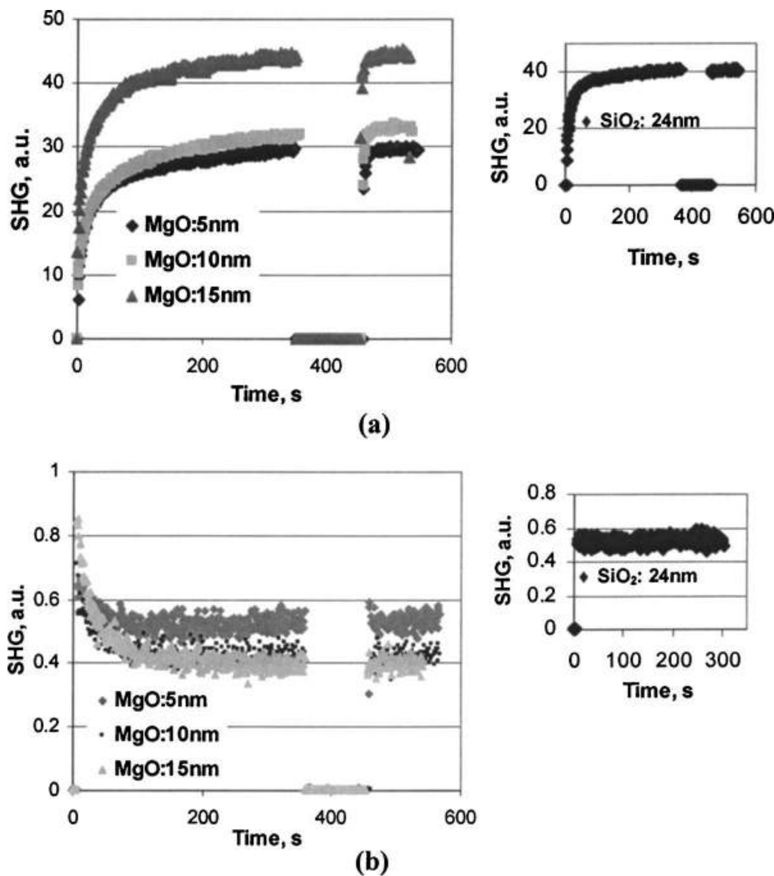

FIG. 1. Time-dependent SHG signals from $Si/SiO_2/MgO$ structures at laser powers of (a) 620 mW and (b) 240 mW. The insets show TD-SHG signals from a Si/SiO_2 sample with a thickness of 2.4 nm.

and electron-hole recombination processes. For high average laser intensity [Fig. 1(a)], the SHG signal increased with increasing MgO layer thickness. After the laser was unblocked, we observed a rapid rise of the TD-SHG signals, beginning at a level lower than the level at the time of blocking. In comparison, the inset of Fig. 1(a) shows the data taken from a Si/SiO_2 sample without the MgO. This structure did not show any decrease in SHG signal after the laser was unblocked, consistent with previous work.[19,20] It is clear that the additional MgO layer significantly changes the TD-SHG.

Next, we performed similar TD-SHG experiments on the same $Si/SiO_2/MgO$ structure but at a much lower average laser power of 240 mW [Fig. 1(b)]. In this case we observed an initial decrease in the SHG signal, followed by saturation. This decrease was greater for increasing MgO thickness. In addition, the Si/SiO_2 structure without MgO did not show any time dependence at this intensity [see the inset in Fig. 1(b)].

To understand the results of Fig. 1, please consider the diagrams of the two structures used in this work shown in Fig. 2. For the structures with MgO overlayers, electron potential-well states become available in or near the MgO conduction band, which are at a lower energy than the SiO_2 conduction band. This provides a higher density of states than is otherwise available for the SiO_2 structures with no overlayers. The data of Fig. 1 suggest that the electron-trap states on the surface of SiO_2 have a higher potential barrier for transport than the available electronic states in the MgO, and/or that defects have been introduced into the SiO_2 during the electron-beam stimulated MgO deposition.[18] These defects can facilitate trap-assisted tunneling of the electrons across the SiO_2, leading to a decrease in the TD-SHG.[21] One defect known to enhance electron tunneling through SiO_2 is

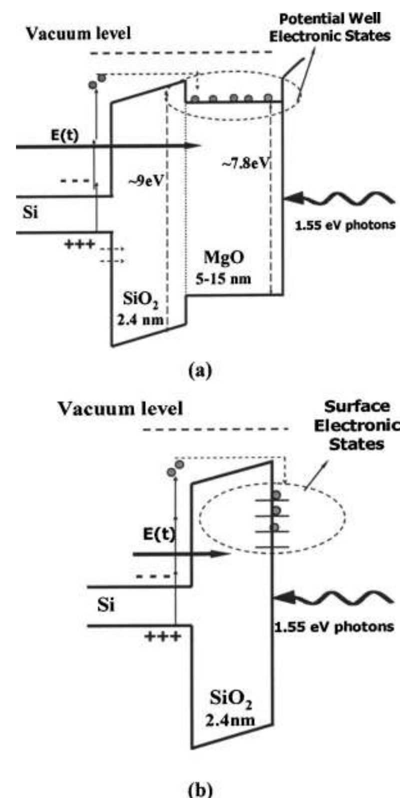

FIG. 2. Schematic band diagrams of (a) $Si/SiO_2/MgO$ and (b) Si/SiO_2 systems.

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 128.59.222.12 On: Sun, 30 Nov 2014 23:28:46

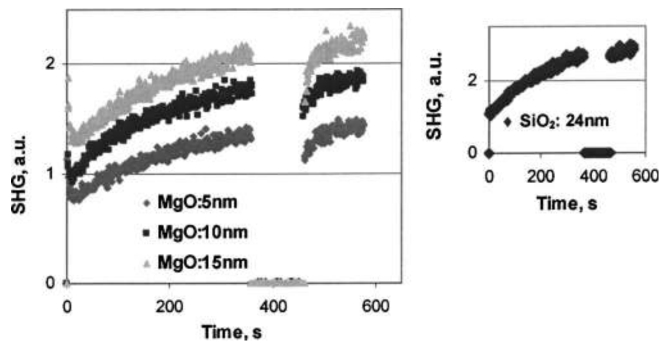

FIG. 3. Time-dependent SHG signal from the $Si/SiO_2/MgO$ structure at laser power of 300 mW.

the hydrogen bridge.[22] The inset of Fig. 1(a) indicates that there is no electron transport through the thin SiO_2 with no MgO overlayer. The electrons remain trapped on the surface of the oxide even after substantial dark time (>100 s).

Electron injection from the silicon into the MgO and/or the surface of the SiO_2 is a three-photon process.[3] When the laser intensity is low [Fig. 1(b)], the probability of three-photon processes is greatly reduced over its probability when the intensity is increased. Hence, at low intensity, no significant electron injection is observed. The inset in Fig. 1(b) shows the SHG signal from the Si/SiO_2 system. At low intensity the SHG signal from the Si/SiO_2 system is time independent, and due mostly to bulk and interface $\chi^{(2)}$ contributions. For MgO coated samples, at low laser intensity, a slight decrease in SHG signal is observed, which we attribute to hole trapping in the SiO_2.[23] "Hot" holes are generated during the SHG measurements via one- and/or two-photon processes. These holes can be trapped in discrete levels, which are most likely associated with O vacancies, distributed in space and energy in the near-interfacial SiO_2, below the Si valence band.[24] After ~100 s of laser irradiation, the hole trapping saturates, as evidenced by the SHG.

Next, we increased the laser power to 300 mW (Fig. 3). In this case the initial decrease of the TD-SHG signal was followed by a rapid rise. The initial drop is once again due to hole injection into near interfacial oxide (border) traps in SiO_2. The onset of electron injection first annihilates the trapped holes,[25] and then leads to the net buildup of trapped electrons, as observed in Fig. 1(a). This causes an initial decrease in SHG magnitude, followed by an increase, observed in Fig. 3. The minimum magnitude of the SHG signal corresponds to reversal of the electric field. These results are similar to those commonly observed in high-field stressing experiments,[25,26] but in this case the trapping responses are observed in a contactless and noninvasive manner—one that is suitable for *in situ* diagnostics, and requiring no gate metallization. Moreover, the localized nature of the charge injection during the SHG does not lead to permanent damage of the insulating layers, as one often observes during high-field stress.

In summary, we have shown that thin MgO layers deposited onto Si/SiO_2 provide new insight into charge carrier injection and trapping in thin oxide films. At low laser intensity, hole injection into the interfacial SiO_2 appears to dominate the trapping response. At higher laser intensities, three-photon processes lead to electron injection that first annihilates the trapped holes, and then leads to excess electron trapping. For 2.4 nm SiO_2, electron traps are relatively stable. In contrast, electrons trapped in MgO overlayers can quickly transport through the SiO_2 when the injection processes are interrupted. This is attributed to differences in energy levels of the trapped electrons and/or process induced damage (e.g., associated with hydrogen complexes) in the SiO_2. We conclude that SHG offers significant advantages for studying charge carrier dynamics in thin oxides and multi-interface semiconductor structures.

This work was supported in part by DARPA/ORN, ARO, NFS-CREST, NREL-DOE, and Air Force Office of Scientific Research through the MURI program.

[1] S. A. Mitchell, T. R. Ward, D. M. Wayner, and G. P. Lopinski, J. Phys. Chem. B **106**, 9873 (2002).
[2] N. L. Cohen, R. E. Paulsen, and M. H. White, IEEE Trans. Electron Devices **42**, 2004 (1995).
[3] J. Bloch, J. G. Mihaychuk, and H. M. van Driel, Phys. Rev. Lett. **77**, 920 (1996).
[4] G. Lüpke, Surf. Sci. Rep. **35**, 75 (1999).
[5] N. Shamir, J. G. Mihaychuk, and H. M. van Driel, Phys. Rev. Lett. **82**, 359 (1999).
[6] J. G. Mihaychuk, J. Bloch, and H. M. van Driel, Opt. Lett. **20**, 2063 (1995).
[7] J. F. McGilp, J. Phys. D **29**, 1812 (1996).
[8] T. Scheidt, E. G. Rohwer, H. M. von Bergmann, and H. Stafast, Phys. Rev. B **69**, 165314 (2004).
[9] C. Ohlhoff, G. Lupke, C. Meyer, and H. Kurz, Phys. Rev. B **55**, 4596 (1997).
[10] O. A. Aktsipetrov, A. A. Fedyanin, A. V. Melnikov, E. D. Mishina, A. N. Rubtsov, M. H. Anderson, P. T. Wilson, H. ter Beek, X. F. Hu, J. I. Dadap, and M. C. Downer, Phys. Rev. B **60**, 8924 (1999).
[11] B. Jun, R. D. Schrimpf, D. M. Fleetwood, Y. V. White, R. Pasternak, S. N. Rashkeev, F. Brunier, N. Bresson, M. Fouillat, S. Cristoloveanu, and N. H. Tolk, IEEE Trans. Nucl. Sci. **51**, 3231 (2004).
[12] B. Jun, Y. V. White, R. D. Schrimpf, D. M. Fleetwood, F. Brunier, N. Bresson, S. Cristoloveanu, and N. H. Tolk, Appl. Phys. Lett. **85**, 3095 (2004).
[13] Y. Q. An and S. T. Cundiff, J. Appl. Phys. **96**, 2638 (2004).
[14] Y. M. Chiang, D. Birnie III, and W. D. Kingery, *Physical Ceramics* (Wiley, New York, 1997), p. 120 (Table 2.3).
[15] Y. Furukawa, M. Sato, F. Nitanda, and K. Ito, J. Cryst. Growth **99**, 832 (1990).
[16] E. Tokizaki, K. Terashima, and S. Kimura, J. Cryst. Growth **123**, 121 (1992).
[17] P. Sen, P. K. Sen, R. Bhatt, S. Kar, V. Shukla, and K. S. Bartwal, Solid State Commun. **129**, 747 (2004).
[18] G. F. Derbenwick and B. L. Gregory, IEEE Trans. Nucl. Sci. **22**, 2151 (1975).
[19] R. Pasternak, Y. V. Shirokaya, Z. Marka, J. K. Miller, S. N. Rashkeev, S. T. Pantelides, N. H. Tolk, B. K. Choi, R. D. Schrimpf, and D. M. Fleetwood, Nucl. Instrum. Methods Phys. Res. A **514**, 150 (2003).
[20] Yu. D. Glinka, W. Wang, S. K. Singh, Z. Marka, S. N. Rashkeev, Y. Shirokaya, R. Albridge, S. T. Pantelides, N. H. Tolk, and G. Lucovsky, Phys. Rev. B **65**, 193103 (2002).
[21] Z. Marka, S. K. Singh, W. Wang, S. C. Lee, J. Kavich, B. Glebov, S. N. Rashkeev, A. P. Karmarkar, R. G. Albright, S. T. Pantelides, R. D. Schrimpf, D. M. Fleetwood, and N. H. Tolk, IEEE Trans. Nucl. Sci. **47**, 2256 (2000).
[22] P. E. Blöchl and J. E. Stathis, Phys. Rev. Lett. **83**, 372 (1999).
[23] D. M. Fleetwood and N. S. Saks, J. Appl. Phys. **79**, 1583 (1996).
[24] S. L. Miller, D. M. Fleetwood, and P. J. McWhorter, Phys. Rev. Lett. **69**, 820 (1992).
[25] D. M. Fleetwood, H. D. Xiong, Z.-Y. Lu, C. J. Nicklaw, J. A. Felix, R. D. Schrimpf, and S. T. Pantelides, IEEE Trans. Nucl. Sci. **49**, 2674 (2002).
[26] D. J. DiMaria, E. Cartier, and D. Arnold, J. Appl. Phys. **73**, 3367 (1993).

This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to IP: 128.59.222.12 On: Sun, 30 Nov 2014 23:28:46