Analysis of Constitution and Characteristics of Lateral Nonuniformity Effects of MOS Devices Using QM-Based Terman Method

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Abstract—The Terman method for extracting interface trap density D_{it} has been used as a direct index of the lateral nonuniformity (LNU) distribution of charges in the dielectric layer of MOS capacitors. However, as dielectric layers become thin, reaching to 2–3 nm, quantum effects should be taken into consideration. The primitive Terman method has been modified with respect to quantum mechanisms, and both theoretical simulations and experimental data were examined to check the modified method's feasibility. The quantum-mechanism-based Terman method might obtain negative D_{it} if the high-frequency C – V curves are distorted by LNU charge distribution in the dielectric layer of MOS capacitors. To elucidate LNU effects, external constant voltage stress and water immersion were applied to clarify the roles of injected carriers in the LNU effects. Furthermore, the amount of effective oxide charge Q_{eff} has been found to be responsible to the LNU effects.

Index Terms—Constant voltage stress (CVS), C – V curve, D_{it} , effective oxide charge, lateral nonuniformity (LNU), Terman method, MOS.

I. INTRODUCTION

LATERAL nonuniformity (LNU) of effective oxide charges in gate dielectrics has been reported to be one significant factor influencing the electrical performance of all electronic devices [1]. In terms of gate dielectrics, these effective oxide charges can manifest as oxide trapped charges Q_{ot} , fixed oxide charges Q_f , interface trapped charges Q_{it} , or mobile ionic charges Q_m . Some electrical characteristics, such as flat-band voltage, carrier lifetime, and scattering of carriers, are also influenced by these effective oxide charges [2]–[4]. It has been reported that, the LNU distribution of Q_{ot} and Q_{it} along the channel direction affects carrier transport in the inversion layer of MOS transistors [2], [3] and stress-induced leakage current (SILC) in gate dielectrics. Therefore, the constitution of the LNU effects and the physical mechanism by which it operates requires a detailed investigation with the goal of improving instability in electronic devices.

In [1], LNU charges are attributed to the localized injection of avalanche hot carriers from the deep-depletion silicon substrate. In addition to hot carriers, Q_f and clustering of Q_m

(such as H^+ , Na^+ , and K^+ ions) are found to be correlated to the generation of LNU charges. In this paper, a more detailed investigation into the constitution of LNU by using the quantum-mechanism-based (QM-based) Terman method is explored. This new technique is proposed as a detection technique to watch the LNU profiles of effective oxide charges Q_{eff} in ultrathin oxides. Many extant techniques have been reported to ably determine the spatial distribution and lateral profile of Q_{ot} and Q_{it} , such as the charge pumping method [5], [6], the direct-current current–voltage method [7], and the gate-induced drain leakage current profiling method [8]. It is known that the existence of LNU effective oxide charges poses extra electrical potential, affects surface band bending ψ_s , and distorts the high-frequency capacitance–voltage (HFCV) curves of MOS capacitors. Making use of these characteristic oxide charges, the Terman method extracts interface trap density D_{it} by differentiating the distorted ψ_s – V_g curve in thick oxides [9]. However, excessive distortion of ψ_s – V_g curves may result in negative effective D_{it} (NED) [10], directly indicating the LNU effect in thick oxides [11]. However, with the trend of decreasing feature sizes, quantum mechanisms, such as direct tunneling, should be taken into consideration in ultrathin oxide (< 4 nm) when extracting oxide thickness or device modeling. In this paper, Hu *et al.*'s model [12] is cited as a reference for modifying the classical Terman method. The feasibility of the proposed QM-based Terman method is examined through both theoretical simulation (~ 2.2 nm) and experimental data.

All of the examined oxide charges Q_{ot} , Q_f , Q_m , and Q_{it} might be more or less responsible for the occurrence of LNU in ultrathin oxides. We simulated the actual spatial LNU distribution of effective oxide charges Q_{eff} with a simplified 2-D model consisting of two parallel MOS capacitors. The role of Q_{eff} in the LNU effect was examined through a series of experimental comparisons based on the proposed QM-based Terman method.

II. EXPERIMENTS

The devices that were used in this paper are MOS capacitors with aluminum gate electrodes fabricated on 3-in (100)-oriented p-type substrates with resistivity in the range of $1\text{--}5\ \Omega \cdot \text{cm}$. First, the standard Radio Corporation of America (RCA) cleaning, followed by dipping in 50:1 (H_2O : HF), was performed, and then rinsing with deionized water was carried out. After the RCA cleaning step, the p-type wafers were oxidized in the rapid thermal processor at $> 760^\circ\text{C}$ for 5–10 s at the oxygen ambient of 40 torr. After the thermal

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Fig. 1. Illustrative interpolation of surface band bending plots for theoretical (QM and classical) 2.2-nm CV curves and imperfect experimental CV.

oxidation process, a 300-nm aluminum film was evaporated onto the oxide layer. Next, photolithography and wet etching were used to fabricate the MOS capacitor with the area size of $150 \times 150 \mu\text{m}$.

After rear oxide removal, aluminum was also evaporated for 200-nm back contact. The 1-MHz high-frequency C - V measurements were performed with an HP-4284 inductance-capacitance-resistance (LCR) meter.

III. RESULTS AND DISCUSSION

A. Comparison of the Terman Method to Theoretical QM C - V

1) *Classical Terman Method*: The Terman method makes use of the excessive distortion of HFCV curves, which is caused by the existence of D_{it} charges to obtain the D_{it} value [9]

$$D_{it}(\psi_S) = \frac{C_{it}(\psi_S)}{q} = \frac{1}{q} \left[C_{ox} \left(\left(\frac{d\psi_S}{dV_G} \right)^{-1} - 1 \right) - C_S \right] \quad (1)$$

where C_S is the surface capacitance of silicon, ψ_S is the surface band bending of silicon, and q is the elementary charge. By comparing the experimental and theoretical ($d\psi_S/dV_G$) in (1), one can obtain the D_{it} of the C - V curves, without taking QM into consideration [11]. Later, the classical Terman method will be compared with the proposed QM-based Terman method based on a theoretical QM C - V curve (2.2 nm).

2) *QM-Based Terman Method*: However, for ultrathin oxides, the derivation of ψ_S should take quantum effects into consideration. Therefore, we focus on the derivation of ψ_S and C_S based on quantum mechanisms.

By using the correlation of ψ_S with the theoretical QM C - ψ_S curve, the ψ_S - V_G curves for theoretical (both QM and classical) and experimental MOS capacitors can be obtained by interpolating the same capacitance value that exactly mapped to one definite ψ_S , as shown in Fig. 1. The V_G values corresponding to classical and experimental QM are denoted as $V_{G(Q.M.)}$, $V_{G(classical)}$, and $V_{G(exp)}$, respectively, as shown in Fig. 1. The

Fig. 2. Surface band bending versus gate voltage plots for theoretical 2.2-nm CV through both classical calculation (ψ_S - $V_{G(Classical)}$) and QM (ψ_S - $V_{G(Q.M.)}$), and experimental 2.2-nm CV (ψ_S - $V_{G(Experimental)}$).

ψ_S - V_G curves corresponding to the preceding three cases are plotted in Fig. 2. As shown in Fig. 2, the ψ_S - $V_{G(classical)}$ and ψ_S - $V_{G(exp)}$ curves are not coincident with the ψ_S - $V_{G(Q.M.)}$ curve. The D_{it} calculations based on (1), according to various ψ_S - V_G curves, are therefore derived from one case to another. Generally, the C_S of the QM-based C - V curves can be derived from the definition equation as follows:

$$C = -\frac{dQ_S}{dV_G} = -\frac{dQ_S}{d\psi_S} \frac{d\psi_S}{dV_G} \quad (2)$$

or

$$C_S = -\frac{dQ_S}{d\psi_S} = C \times \frac{dV_G}{d\psi_S} \quad (3)$$

where Q_S is the surface charge of silicon taken from the 2.2-nm QM C - V curve based on Hu *et al.*'s model, and $(dV_G/d\psi_S)$ can be calculated from the QM-interpolated ψ_S - $V_{G(Q.M.)}$ curve, as shown in Fig. 2. The C_S values that were calculated from (3) are denoted as $C_{S(Q.M.)}$ and are plotted in Fig. 3. The classical C_S value (i.e., $C_{S(classical)}$) according to the following equation is also shown for comparison [9]:

$$C_S = -\text{sgn}(u_B - u_S) \frac{\epsilon_S}{\lambda_i} \times \frac{\sinh u_S - \sinh u_B}{\sqrt{2} [(u_B - u_S) \sinh u_B - \cosh u_B + \cosh u_S]^{1/2}} \quad (4)$$

where $\lambda_i = (\epsilon_s kT / (2q^2 n_i))^{1/2}$ is the intrinsic Debye length, $u_S = q\Phi_S / kT$ is the dimensionless potential difference from the Si/SiO₂ surface Fermi level to the intrinsic Fermi level, and $u_B = q\Phi_B / kT$ is dimensionless bulk potential. As shown in Fig. 3, it was observed that, with the exception of the accumulation and inversion regions, the two C_S curves are identical within the marked region. This marked region is subject to Terman calculation. C_S increases exponentially in the accumulation region, and the capacitance value maintains C_{min} for high-frequency capacitance in the inversion region for the maximum of the expanded depletion width [13]. Hence,

Fig. 3. Surface capacitance on silicon versus gate voltage plots for classical calculation ($C_{S(\text{Classical})}$) and QM derivation ($C_{S(\text{Q.M.})}$).

Fig. 4. Interface defect density versus surface band bending plots extracted from theoretical 2.2-nm $C-V$ curve with and without QM concern and experimental 2.2-nm $C-V$.

the QM-derived C_S of (3) and the interpolated $\psi_S-V_{G(\text{Q.M.})}$ curve are adopted as the reference parameters in the QM-based Terman method.

3) *Effective D_{it} Results Based on the QM $C-V$ Curve:* The Terman method is applied to the ψ_S-V_G curves, as shown in Fig. 2, based on the theoretical QM $C-V$ curve, and the results are plotted in Fig. 4. The D_{it} value of an ideal QM $C-V$ curve is expected to be zero. For the QM-based Terman method, the resultant D_{it} values are nearly zero, indicating that our numerical analysis of differential calculations is correct. However, the D_{it} that fails to take quantum mechanisms into consideration deviates significantly from the ideal zero D_{it} curve. One should use the QM curve as a reference for D_{it} calculation by the Terman method for ultrathin oxide samples.

An experimental $C-V$ curve (2.2 nm) was also examined by using this QM-based Terman method. According to the $\psi_S-V_{G(\text{exp})}$ curve in Fig. 2 and the $C_S-\psi_S$ curve in Fig. 3, one can obtain the D_{it} value based on (1). Then, the calculated D_{it} curve is also shown in Fig. 4 as the hollow square curve. Apparently, this D_{it} curve partially contains NED as a result of

Fig. 5. Simulation of distorted $C-V$ curves that resulted from LNU distribution of charges in the dielectric layer of MOS structure.

LNU effective oxide charges. The origin of NED due to LNU is described as follows.

B. LNU Effective Oxide Charge Model

The actual LNU distribution of charges in the gate dielectric is more complicated than expected. The LNU region might exist in 3-D space and the composition of Q_{eff} might contain different species and different electrical polarities. For the ultrathin oxide, the LNU effect was considered by a two-capacitor model [11]. It was assumed that two subcapacitors with equivalent oxide thicknesses but different flatband voltages V_{FB} were shunt in parallel. One subcapacitor was neutral, and the other possesses more positive oxide charges and, thus, a more negative V_{FB} shift. As shown in Fig. 5, the flatband voltages of one ideal subcapacitor and one shifted subcapacitor were set as -0.9 V (i.e., according to the ideal value of the work function difference between the Al gate and the silicon substrate) and -1.1 V, respectively. In order to simulate different LNU effects, the area ratios of the two subcapacitors were varied. The area ratios of shifted versus original subcapacitors were 1/9, 3/7, 5/5, 7/3, and 9/1 in Fig. 5. Accordingly, five $C-V$ curves with different LNU extents were obtained, as shown in Fig. 5, and the synthesized $C-V$ curves had different V_G values at the same ψ_S that leads to different $d\psi_S/dV_G$ values. So far, it was observed that the five distorted $C-V$ curves in Fig. 5 were quite similar in shape to the HFCV deformation caused by real D_{it} . However, the distorted $C-V$ curves were simulated by two subcapacitors with no real D_{it} but with different V_{FB} 's. Any calculation of D_{it} from the distorted $C-V$ due to LNU is considered to be the effective D_{it} in this paper.

Subsequently, those five deformed $C-V$ curves were subjected to QM-based Terman treatment, and from those were derived the five $D_{it}-\psi_S$ curves that are shown in Fig. 6. Portions of curves still displayed NED values near the midgap region. Notably, these $C-V$ curves were based on the theoretical $C-V$ curves, which were themselves modeled on ideal defect-free oxides. Therefore, we suppose that the $C-V$ distortion in

Fig. 6. Analyses of effective D_{it} curves of the simulated distorted $C-V$ curves through the QM-based Terman method.

Fig. 7. Effective D_{it} versus surface band bending of experimental data through the QM-based Terman method.

Fig. 5 can be totally attributed to the LNU oxide charges, thus resulting in the abnormal NED in Fig. 6.

In addition to the simulated LNU effects of theoretical $C-V$ curves, the QM-based Terman method was also applied to experimental HFCV, and some of the selected $D_{it}-\psi_S$ curves were plotted in Fig. 7. A series of experiments were carried out, and the oxidation conditions are listed in Table I. All the $D_{it}-\psi_S$ curves in Fig. 7 are identically shaped to those of the aforementioned LNU two-capacitor model. Despite the simplification of the proposed LNU two-capacitor model, the LNU charge effect is adequately described by the curves. Nevertheless, two $D_{it}-\psi_S$ curves of no NED occurrence, i.e., 750 °C and 775 °C, are also observed in Fig. 7. It was supposed that a higher temperature could produce oxides of better quality and thus of lesser real positive interface traps. Furthermore, the calculated effective D_{it} consists of the real positive D_{it} and the LNU-induced NED. Therefore, it is easier for the higher tem-

TABLE I
RECIPES FOR THERMAL OXIDATION TEMPERATURE AND THE RESULTANT AVERAGE OXIDE THICKNESS OF EACH CONDITION

	Oxidation Conditions	Average Oxide Thickness
1	75	2.05 nm
2	775	1.99 nm
3	800	2.15 nm
4	825	2.23 nm
5	850	2.48 nm
6	875	2.84 nm

Fig. 8. Minimum of effective D_{it} versus Q_{eff} plot shows the trend that a larger amount of Q_{eff} leads to more NED.

perature oxides to be deducted from NED due to the existence of LNU charges. So, it can be concluded that the experimental oxides do not all suffer serious LNU effects. In some cases, the distribution of effective oxide charges might not distort the HFCV enough to result in NED occurrence.

C. Investigation Into the Origins of LNU Charges

To gain a deeper understanding of the constitutions of oxides that result in LNU effects, a series of experiments were carried out in order to obtain various oxide thicknesses of $\sim 2-3$ nm. The temperature conditions under which those oxides were formed are listed in Table I.

1) *Oxide Charge Distribution of LNU Effect:* In this section, 120 MOS(P) devices of different SiO_2 thicknesses (shown in Table I) were chosen. After QM-based Terman method calculation, the minimum of each resultant $D_{it}-\psi_S$ curve was obtained and denoted as $D_{it,min}$. The observed V_{FB} shifts of the $C-V$ curves can be mainly attributed to the contribution of Q_{eff} of each device. The correlation of $D_{it,min}$ and Q_{eff} is plotted in Fig. 8.

There is an obvious correlation between the amount of Q_{eff} and NED occurrence. More Q_{eff} appears to lead to greater

Fig. 9. Gate capacitance versus gate voltage plot with CVS time. The CV curves keep shifting to the positive end with increasing CVS time.

Fig. 11. Plots of gate capacitance and gate current density versus gate voltage before and after water immersion treatment.

Fig. 10. Effective D_{it} curves of experimental data shifts upward with CVS time.

Fig. 12. Plot of experimental effective D_{it} versus surface band bending before and after water immersion treatment through the QM-based Terman method and the high-frequency-low-frequency method.

possibility of NED occurrence. Still, some devices possess NED with only slight amounts of Q_{eff} , while some possess positive $D_{it,min}$. Based on this fact, it is concluded that the amount of oxide charge is responsible for the LNU effect.

2) *External Constant Voltage Stress (CVS) Treatment:* As shown in Fig. 9, CVS (+10 MV/cm) was applied to a MOS capacitor. The $C-V$ curve in Fig. 9 keeps shifting toward the positive end with the increasing CVS time, as expected. This is because positive gate bias attracts negative charges in oxide and causes the $C-V$ curve to shift rightward. Afterward, each $D_{it}-\psi_S$ curve was extracted, as shown in Fig. 10. It was observed that the initial minimum NED ($-13.3 \times 10^{11} \text{ cm}^{-2} \text{ eV}^{-1}$) gradually shifted upward and finally becomes positive. Not until the CVS time reached 10 s did the D_{it} curve become steady. Therefore, the LNU effect seems to be compensated for by the external electrical field. Clustering mobile charges or some localized oxide charges might be compensated for due to the self-rearrangement of spatial distribution or the

generation of charges under external CVS treatment. It is also inferred that, under an external CVS, some clustering Q_m are able to move to the emptier neighboring regions to maintain the potential equilibrium, thus lessening the LNU effect. These carriers must be easy to move, particularly, with the assistance of an external electrical field. From the preceding observation, it can be concluded that the LNU effects can be modified by CVS stress.

3) *Water Immersion Treatment:* It has been reported that hydrogen plays a major role in controlling several characteristics of ultrathin oxide layers and silicon substrates in MOS structures. Hydrogen can migrate as H^+ ("bare" protons) near the Si-SiO₂ interfaces and even intrude into the silicon substrate and the near-interface oxide. H can passivate and two-step depassivate the Si-SiO₂ interface dangling bonds [14] and suboxide bonds [15]. In addition, H affects the positive charge trapping in the gate oxide [16]. Thus, H greatly influences Q_{eff} .

As such, one of the samples was examined in an environment of ambient H^+ ; water immersion is carried out to observe changes of LNU effect.

One sample with NED present was chosen and immersed in a cup of water for 10 000 s. Fig. 11 shows that the HFCV significant changes after water immersion and that the originally lowered HFCV was compensated for, while the low-frequency C - V curves remained almost identical. In the accumulation region of MOS capacitors, the frequency dispersion of gate capacitance is mainly due to the effect of series resistance R_s in the equivalent circuit model. It was supposed that the treatment of water immersion lessened the effect of R_s or enhanced the conductivity of device due to possible ion intrusion. However, the detailed mechanism is still under investigation. The significant reduction in frequency dispersion after water immersion is of interest. On the other hand, the right part of Fig. 11 shows that there was a current bump in the current density versus V_G (J - V_G) curve under the low-field region, which is similar to the SILC after water immersion. This might imply that some trap-assisted tunneling current occurs when hydrogen intrudes the oxide and detraps occupied states [17], [18]. Finally, the D_{it} - ψ_S curves are plotted in Fig. 12. The initial effective D_{it} curve rises from NED to the positive region, while the compared D_{it} curve, which was extracted by the high-low capacitance method, maintains the same level. Again, it was observed that the LNU was compensated for due to water immersion. It is believed that the hydrogen helps to rebuild a more uniform electrical equilibrium by detrapping occupied states or providing its own positive charge.

IV. CONCLUSION

In this paper, the classical high-frequency Terman method was modified to extract D_{it} with concern for QM, and feasibility was investigated through theoretical simulation and experimental data. The original Terman method was adopted to QM C - V curves with the parameters C_S and ψ_S extracted from the model with respect to the QM effect. The Terman method was proven to be useful to detect the existence of LNU oxide charges. By plotting the correlation of $D_{it,min}$ and Q_{eff} , and examining several external treatments, such as CVS and water immersion, it was concluded that the LNU effect might be altered by the existing and injected charges. Finally, it has been noted that LNU effects can even be reduced by controlling the behavior of the charges through external treatments.

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