Mechanism of charge transport of stress induced leakage current and trap nature in thermal oxide on silicon

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Abstract. We study the charge transport mechanism of electron via traps in thermal SiO₂ on silicon. Electron transport is limited by phonon-assisted tunnelling between traps. Charge flowing leads to oxygen vacancies generation, and the leakage current increases. Long-time annealing at high temperatures decreased the leakage current to initial values due to oxygen vacancies recombination with interstitial oxygen. Taking into account results of ab initio simulations, we found that the oxygen vacancies act as electron traps in SiO₂.

1. Introduction
Write/erase operations of flash memory with poly-Si-floating gates are driven by tunnelling injections of electrons and holes through thin 1.8–8.0 nm (tunnel) SiO₂ layer [1, 2]. The current through the tunnel oxide during erase/rewrite operations by applying high electric field ∼ 10 MV/cm in the oxide increases the conductivity of the layer at low electric fields ∼ 1 MV/cm. This is caused by the appearance of additional current components through the tunnel oxide compared to the current flowing in a strong electric field on the mechanism of Fowler-Nordheim [3]. This phenomenon is called Stress Induced Leakage Current, SILC. SILC limits reprogramming cycles number of the flash memory cells based on floating gate and the poly-silicon to 10⁴–10⁵. SILC also leads to accelerate the de-charging of the flash memory elements in the data storage mode, i.e., leads to memory characteristics degradation. In spite of SILC intensive study, the nature of this phenomenon is still a debatable question [2, 4–6]. The purposes of the present study are identification of the electron trap ionization and transport mechanisms in SiO₂ in external electric field and determination of the trap parameters (ionization energy, concentration).

2. Experiment details
SILC and transport measurements were performed for test structures based on FET transistors with n⁺-type poly-Si floating gate, manufactured using the 180-nm design rule technology. The
$p$-Si substrate with $n^+$-type channel ($n^+$-Si$_p$) was used as the bottom contact. The $n^+$-Si floating gate was used as the top contact. The 7.5-nm-thick SiO$_2$ was used as tunnel layers between contacts. Test samples were formed by 16 parallel-connected $n^+$-Si/SiO$_2$/n$^+$-Si$_p$ capacitors with the total area of the poly-Si electrode $S = 8 \times 10^4 \mu$m$^2$. Current-voltage ($J-V$) characteristics were measured at different temperatures 25–70°C before and after charge stress $\Sigma = (0.01–10)$ C/cm$^2$. The silicon electrode resistivity is much less than the one of SiO$_2$ layer, and the most part of the electric field falls on the oxide layer.

The electronic structure of oxygen vacancy in $\alpha$-SiO$_2$ was calculated within the spin polarized density functional theory using the ab initio simulation code QUANTUM ESPRESSO with B3LYP functional [7]. The oxygen vacancy was generated by the removal of an O atom, followed by relaxation of remaining atoms in 72-atom supercell. This method yields the $\alpha$-SiO$_2$ band gap of 8.0 eV.

3. Results and discussions

![Figure 1. Experimental current-voltage characteristics of $n^+$-Si/SiO$_2/n^+$-Si$_p$ structures at room temperature (25°C). Boxes (Ω) present results of measurements for “as deposited” samples before stress and annealing, rounds (⊙) — after stress and before annealing, crosses (×) represent data for stressed samples after long time annealing.](image)

Experimental current-voltage characteristics of the fresh (as deposited) SiO$_2$ are shown in Fig. 1 by boxes. The high-field ($|V| > 5$ V, $F > 6$ MV/cm) current through the structure was limited by Fowler-Nordheim tunnelling

$$J_{FN} = \frac{e^3 F^2}{8 \pi h \Phi_0} \exp \left( -\frac{8 \pi \sqrt{2m^*}}{3ehF} \Phi_0^{3/2} \right),$$

(1)

where $J_{FN}$ is the tunnel current density, $e$ is the elementary charge, $F$ is the electric field, $h$ is the Planck constant, $\Phi_0$ is the height of the triangular potential barrier for electrons at the Si/SiO$_2$ interface, $m^*$ is the electron effective tunnelling mass [3]. According to photoemission measurements, the height of the triangular potential barrier for electrons at the Si/SiO$_2$ interface is $\Phi = 3.14$ eV [8]. In high fields at the Si/SiO$_2$ interface the effective barrier height decreases to $\Phi_0 = 2.9$ eV due to quantization of electron energy spectrum [9]. Taking this into account, we obtained the electron effective mass in SiO$_2$ $m^*/m_0 = 0.5 \pm 0.02$ from simulations (1) at both positive and negative biases on the poly-Si electrode. These results are in consistent with the literature data [9,10]. Low-field ($|V| < 5$ V, $F < 6$ MV/cm) measured current values are determined by the sensitivity of the measuring devices and bulk properties of the substrate.

The experimental current-voltage characteristics after SILC (10 C/cm$^2$) are shown in Fig. 1 by rounds. High-field current through SiO$_2$ layer is limited by Fowler-Nordheim tunnelling (1). Low-field current is SILC. The characters in Fig. 2 represent the experimental $J-V$ characteristics of $n^+$-Si/SiO$_2/n^+$-Si$_p$ structures at room temperature after different stresses. The SILC currents ($2 < |V| < 5$ V) grow with increasing of the stress, while the slope of $J-V$ curves decreases. The temperature increase leads to growing SILC currents on 30–50%, but Fowler-Nordheim tunnelling remains the same level.
charge values.

Charge transport in dielectrics is determined by traps. When the trap density is high and the distance between them is short, trapped electrons (or holes) can tunnel between the neighbouring traps without ionisation to the conduction band [11]. Due to the external electric field electrons on the neighbouring traps have different energy levels, e.g. phonon emission and phonon absorption. According to phonon-assisted tunnelling model, the rate of such transitions is given as

\[ P_{\text{PAT}} = \frac{2\sqrt{\pi}hW_t}{m^*a^2Q_0\sqrt{kT}} \exp\left( -\frac{2a\sqrt{2m^*W_t}}{h} \right) \exp\left( -\frac{W_{\text{opt}} - W_t}{2kT} \right) \sinh\left( \frac{eFa}{2kT} \right). \] (2)

where \( h = h/2\pi \), \( Q_0 = \sqrt{2(W_{\text{opt}} - W_t)} \), \( W_{\text{opt}} \) and \( W_t \) are thermal and optical trap energies, \( k \) in the Boltzmann constant, \( T \) is the temperature. In the static one-dimensional case, the charge transport through the dielectrics is described current-voltage characteristics, including Fowler-Nordheim tunnelling (1)

\[ J = \frac{s}{S} \frac{e}{a^2} \frac{n_t}{N} \left( 1 - \frac{n_t}{N} \right) P_{\text{PAT}} + J_{\text{FN}}. \] (3)

Here \( J \) is the current density, \( n_t \) is the filled trap density, \( N = a^{-3} \) is the trap density. Here we assume that the stress generated new defects on some part of test sample, creating a filament-like structures. The total area of the stressed part is \( s \) (SILC area). Recently it was show that in spite of high trap density, trapped charge density in dielectric does not exceed \( 5 \times 10^{18} \text{ cm}^{-3} \) due to strong electron-electron (Coulomb) interaction, while the charge carriers form Wigner-like glass hexagonal lattice [12–14].

Experimental data is described quantitatively using thermal and optical trap energies of \( W_t = 1.6 \text{ eV} \) and \( W_{\text{opt}} = 3.2 \text{ eV} \). Obtained value of \( W_t \) is equal to a half of Stokes shift of photoluminescence near 4.4 eV exited by 7.6-eV-photons on oxygen vacancy in SiO\(_2\) [15] and equal to calculated trap energy for trapped electrons and holes on oxygen vacancies. The \( W_{\text{opt}} \) is close to measured electron trap energy in SiO\(_2\) [16]. Simulations of experimental current-voltage characteristics measures at 70°C gives the same trap energy values. These results confirm correctness of using the phonon-assisted tunnelling between traps model to describe SILC. The obtained values of trap densities and the squares of SILC area \( s \) depending on the total stress charge \( \Sigma \) are given in table 1. Charge trap density before stress was less than \( 10^{20} \text{ cm}^{-3} \). Charge stress caused arising of the trap density up to \( 7 \times 10^{21} \text{ cm}^{-3} \) depending on the stress. The SILC area increases with the stress up to \( 10 \mu\text{m}^2 \) (i.e. \( \sim 3 \mu\text{m} \times 3 \mu\text{m} \)). Note, that obtained SILC area in our experiments is less than 0.01% of total sample area.

After the charge stress some samples were treated by annealing at the temperature of 250°C during 120 hours. A comparison of the current-voltage characteristics measures for the “as deposited”, after the stress and after annealing structures are shown in Fig. 1. One can see
that J-V curves, after annealing, are almost identical to the “as deposited” control ones. I.e., long-time annealing leads to the electronic structure of the tunnel SiO\textsubscript{2}, which is identical to one of the “as deposited” films. This means that the trap density decreases with annealing to initial values. Since charge stress leads to generation of Frenkel pairs of oxygen vacancies and interstitial oxygen atoms, annealing leads to recombination of oxygen vacancies with interstitial oxygen. This phenomenon makes it possible to controllably suppress the leakage currents caused by the tunnel SiO\textsubscript{2} degradation due to the charge stress.

4. Summary
In conclusion, we demonstrated that charge transport via traps in thermal SiO\textsubscript{2} is phonon-assisted tunnelling between traps. This transport model in SILC is analytical and much easier than previously proposed multiphonon model of charge transport that requires complicate numerical calculations to describe transport in SILC. Furthermore, phonon-assisted tunnelling between traps model shows that oxygen vacancies are the charge traps in SiO\textsubscript{2}, whereas recently proposed multiphonon model does not clarify the nature of the traps responsible for SILC [4,6]. Obtained thermal and optical trap energies are $W_t = 1.6$ eV and $W_{opt} = 3.2$ eV, respectively. Charge flowing leads to oxygen vacancies generation, and the leakage current increases. Long-time annealing at high temperatures decreased the leakage current to initial values due to oxygen vacancies recombination with interstitial oxygen. Taking into account results of \textit{ab initio} simulations we found that the oxygen vacancies act as electron traps in SiO\textsubscript{2}.

Acknowledgments
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\begin{table}[h]
\centering
\caption{Obtained values of fitting parameters.}
\begin{tabular}{|c|ccccc|}
\hline
$\Sigma$ (C/cm$^2$) & 0 & 0.01 & 0.1 & 1 & 3 & 10 \\
\hline
$N$ (cm$^{-3}$) & $\ll 10^{20}$ & $1 \times 10^{21}$ & $2 \times 10^{21}$ & $4 \times 10^{21}$ & $5 \times 10^{21}$ & $7 \times 10^{21}$ \\
$s$ ($\mu$m$^2$) & 0 & 0.1 & 0.8 & 3 & 5 & 10 \\
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