Universal Analytic Model for Ionization Defect Dynamics in Silicon Dioxides

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A pair of analytical formulas is proposed to describe the irradiation-induced defect dynamics of oxide trapped charges (OT) and interface traps (IT) in silicon dioxides. It is shown that, the interplay between a direct creation of OT and an OT-IT interconversion plays an essential role in the defect dynamics. The perfect match between the model and experimental observations for both wet and dry processed oxides, which show strong process fingerprints, nonlinear dose dependence, dose rate sensitivity, and sample variability, is unprecedented, which not only clarifies the physical ambiguity, but also eliminates the computational difficulty encountered in previous standard approaches.

Silicon dioxide is the key material for modern silicon microelectronics. Usually, higher quality gate silicon dioxides are made by a dry oxidation process and used for complementary metal-oxide-semiconductor (CMOS) technology and lower quality base silicon dioxides are made by a wet oxidation process and used for bipolar technology. Under persistent ionizing irradiation, two kinds of ionization defects, i.e., oxide trapped charge (OT) and interface trap (IT) defects, are generated in the insulating dioxide and at its interface with silicon, which are responsible for the degradation of the electrical properties of silicon devices [1]. For both kinds of oxides, the irradiation induced dynamics have been described as a complex generation, transport, and reaction processes of charge carriers, oxygen vacancies, and hydrogen impurities [2, 3]. More specifically, it was believed that the OT is created as a result of an activation of defect precursors and the IT is generated due to the depassivation of interface Si-H bond through protons, which can be released from OT–H₂ interaction. Accordingly, a standard approach [4–9] have to use dozens of coupled nonlinear rate equations to describe the complex processes.

Although some important features of the defect dynamics, such as the time dependent effects [10] and rebound effect [11] in CMOS technology have been successfully explained within the current theoretical framework, this approach, due to the lack of transparency, has also encountered difficulty in explaining some physical observations. For example, an enhanced low-dose-rate sensitivity (ELDRS) of IT has been experimentally found in 1991 [12]. During the last 30 years, many possible mechanisms, such as Coulomb repulsion of space charge on protons [13, 14], hydrogen dimerization [5, 15], and competition between defect reactions [16, 17] have been proposed. However, it is still hard to confirm which mechanism is dominant. Recently, an abnormal non-monotonous dose dependence of OT at relatively low dose rate is also obtained [18], which cannot be explained within the current framework, unless a carrier-recombination-induced energy release is assumed only for the low dose rate case [18]. Finally, it has been widely realized that the wet base oxides and dry gate oxides respond differently under irradiation, especially for the dose rate sensitivity [19]. However, the physical origin for the difference is still not very clear. Besides these puzzling physical observations, the current standard approach also encounters computational difficulties because there are dozens of parameters in the stand approach, and many of them such as the initial concentrations of the neutral trap precursors and the reaction energies are either unknown or difficult to obtain with high certainty [8, 5]. Hence it is very difficult to numerically reproduce the experimental results.

In this Letter we propose a pair of analytical formulas for the irradiation defect dynamics of OT and IT by considering a generation-interconversion framework of the defects and including a creation mechanism of OT. Experimental data of gamma-ray-irradiated base oxide within an extremely wide dose rate range and available data for gate oxide in the literature are used to verify our derived formulas. The perfect match between the model and data under various conditions is unprecedented. The four parameters in the proposed formulas can be directly extracted from the fitting of data, which eliminates the computational difficulties encountered by the current standard approach. The physical ambiguity of the approach can also be clarified by using the verified formulas, because the puzzling ELDRS of IT and non-monotonous dose dependence of OT in base oxide, as well as the different irradiation responses of gate and base oxides can be explicitly explained in terms of the dose rate dependence of the generation and conversion rates.

The microscopic dynamics of the ionization-induced defects in silicon dioxides is very complex. In this work, we
consider the concentration of the defects (N) as the key parameter and extract a generation-interconversion framework from the generation, transport, and reaction processes,

\[
D^\frac{g}{k_f} \rightarrow OT \quad \frac{k_f}{k_b} \rightarrow IT.
\] (1)

The first part in Eq. (1) is an irreversible generation of OT in the silicon dioxide from the ionization irradiation dose \(D\). As obtained by Imai et al. [24,25] and Griscom et al. [23–25] in irradiation experiments of bulk silicon dioxides, the generation of OT is governed by a fractional power law of \(N_{OT}^g = gD^\Delta\), where \(\Delta\) is a fractional exponent between 0 and 1, and \(g\) is a dose-rate-dependent generation rate. The generation rate of OT as a function of dose reads

\[
\frac{\partial N_{OT}}{\partial D} = g\Delta D^{\Delta - 1}.
\] (2)

As indicated in previous works [23,26,28], this fundamental behavior happens due to two main reasons. The first is that the irradiation drives a Kohlrausch relaxation process [29] in the loosely packed and covalently bonded amorphous network, which leads to time-dependent defect production probabilities [30] and the fractional power law [26]. In existing models [2,9], only the activation process is considered and a linear dependence is usually assumed for small dose. However, this often leads to large error in effort to achieve a self-consistent description of the experimental data.

The second part in Eq. (1) is a reversible interconversion between OT and IT. As indicated by literatures, this process can be realized through the generation of proton from the irradiation generated ones [35,36]; meanwhile, only the generated defects (\(\Delta N\)) are important for the irradiation response of devices. So, we can resolve the coupled equations (3) with initial conditions of \(N_{OT}(0) = N_{IT}(0) = 0\). The results read

\[
\Delta N_{OT}(D) = (1 - \lambda)gD^\Delta + \lambda g\tau^\Delta D^{-\Delta / \tau}\Gamma[\Delta, 0, D / \tau],
\] (4a)

\[
\Delta N_{IT}(D) = \lambda gD^\Delta - \lambda g\tau^\Delta D^{-\Delta / \tau}\Gamma[\Delta, 0, D / \tau].
\] (4b)

Here \(\lambda = k_f/(k_f + k_b)\) and \(\tau = (k_f + k_b)^{-1}R\) are a proportion factor and a half-life of the interconversion, respectively. \(\Gamma(\Delta, 0, D / \tau) = \int_0^{D / \tau} x^\Delta e^{-x}dx\) is a generalized incomplete gamma function in terms of \(\Delta\) and \(D / \tau\); it is a convolution of a power generation and an exponential conversion terms, which reflects the interplay between the two mechanisms in the irradiation defect dynamics.

The proposed formulas predict nonlinear and coupled dynamic behaviors of the two defects under irradiation. First, it predicts that the total concentration of them follows a fractional power law dependence of the irradiation dose, \(gD^\Delta\). Second, it predicts OT and IT share a ratio of \(k_b/(k_f + k_b)\) and \(k_f/(k_f + k_b)\) of such a growth term, respectively. Third, OT and IT also display an addition and deduction of an interconversion term, respectively. The interference term is a product of a power growth function, an exponential decay function, and a \(\Gamma\) function, hence first increases and then decreases with increasing dose.

To test the predictions of the proposed formulas Eq. (4), we first check the available data of dry processed oxides (DPO). In Ref. [37] the shift of threshold voltage of p-channel MOS field-effect transistors is separated into shifts due to OT and IT using the subthreshold-operating method. The obtained \(\Delta V_{OT}\) and \(\Delta V_{IT}\) hence can be regarded as \(\Delta N_{OT}\) and \(\Delta N_{IT}\) (only differ by a constant capacitance), respectively, which is investigated as a function of the ionization dose and dose rate. The dose rate varies in 3 orders of magnitude, from 0.05 rad(Si)/s to 51.4 rad(Si)/s. The total concentration is first checked and found to exactly follow the predicted fractional power law. From the model fitting the parameters of \(g\) and \(\Delta\) in Eq. (4) are extracted. The separated data are shown in Fig. 1 as the dots. It is seen that, the two defects show very different nonlinearity on the dose, which is sub-linear for OT and super-linear for IT. The two defects also show clear different dose-rate dependence, which is the ELDRS for IT and the inverse for OT. These data of OT and IT are straightforwardly fitted using the two proposed formulas Eq. (4) with the already extracted parameters \(g\) and \(\Delta\), respectively. The
fitting curves are plotted in the Figs. (1a) and (1b) as solid curves, respectively. It is seen that, all data of both OT and IT can be uniformly and quantitatively described by the proposed OT and IT formulas, suggesting the physical models underlying the Eq. (4) is correct, that is, the different nonlinearity of OT and IT stems from the addition or deduction of the interference terms, respectively, and the dose-rate sensitivity stems from the dose rate behavior of the parameters, which will be further analyzed below.

To check if the proposed physical process and formulas also work for wet processed oxides (WPO), we prepare high quality data of OT and IT in WPO by carrying out gamma ray irradiation experiments on a large number of samples of gated lateral PNP structure in an extremely wide range of dose rate. The total concentration is extracted from the shift of sub-threshold sweep curves of the structure [40]. The value of $\Delta N_{OT}$ is read out from the peak position of the gate sweep curves [40]. The value of $\Delta N_{IT}$ is simply calculated by their difference. The dose rate varies from 1 rad/s to 58 $\mu$rad/s, which spend 5 order of magnitudes. For each dose rate, 3 samples are adopted for sample-to-sample variability [41,42].

The typical results of obtained $\Delta N_{OT}$ and $\Delta N_{IT}$ as a function of the gamma ray dose are plotted as the dots in Figs. 2 (a) and 2 (b), respectively. The dose rates are indicated in the figure. It is seen that, the nonlinear dose dependence and dose-rate sensitivity obtained in the DPO are also observed; the latter becomes even stronger for WPO. The most remarkable feature is a non-monotonous dose dependence of OT for dose rate lower than 1 mrad/s. This abnormal behavior was also observed by Li et al. for their 10 mrad/s case [18]. Besides the two features, a big sample-to-sample variability is also obtained in the data for both defects, as seen in Fig. 3. The larger the irradiation dose the larger the variability. Again, these data of $\Delta N_{OT}$ and $\Delta N_{IT}$ are straightforwardly fitted using the two proposed formulas Eq. (4), respectively. It is first found that the sum of them satisfies exactly the predicted fractional power law. The fitting curves of the separated defects are plotted in the Figs. 2 and 3 as solid curves. It is seen that, all data of both OT and IT, which although show strong dose nonlinearity, dose rate sensitivity, and sample-to-sample variability, can be quantitatively and uniformly described by the proposed OT and IT formulas, suggesting the correct physical model behind the formulas. The OT data of Li can also be well fitted by the proposed model; see the insert of Fig. 3 (a).

The excellent agreement between our theoretical model and experiments under various conditions proves the validity and universality of the proposed formulas. The ‘validity’ means the realization of quantitative description of both OT and IT, which are closely related and show strong dose nonlinearity and sample-to-sample variability. The ‘universality’ means the quantitative description can be done simultaneously, not only for both DPO and WPO which show process fingerprints, but also for extremely wide dose rate range which show very different behaviors. The verified formulas uncover that the interplay between the direct creation of OT and the reversible OT-IT interconversion is the dominating mechanism of the complex ionization defect dynamics in silicon dioxides.

Our finding show that the computational difficulty encountered by the standard approach can be totally eliminated by the proposed formulas. It is seen that to quantitatively describe the data, no parameters in the proposed formulas need to be assumed in advance; instead, all the 4 parameters ($g$, $\Delta$, $\lambda$, and $\tau$) can be directly extracted from the fitting of the data. The forward and backward conversion rates $k_f$ and $k_b$ can be further calculated through the relations of $k_f = \lambda R \tau^{-1}$ and $k_b = (1 - \lambda) R \tau^{-1}$. For the DPO and WPO, the results are shown in Figs. 4 and 5 as the blue and red dots, respectively. As seen in Fig. 4 (b), the fractional exponent $\Delta$ is about 2/3 for the DPO but varies between 0.5 and 0.9 for the WPO. The former was also observed in early experiments on MOS capacitors [43,44]. In Fig. 4 (a) the generation rate decreases slightly for DPO but increases rather strongly for the WPO as
mechanisms have been speculated for this important effect in rate, which readily leads to the ELDRS of IT. While several 
crease of present a clear and explicit explanation. On the other hand, 
reason is that, both 
for DPO are about one order larger than the one for the WPO. 
parameters extracted from Li et al’s data [18] are shown by the magenta dots. 
monotonous dose dependence of OT arises. It is noticed that, 
by the dose rate sensitivity of the generation and interconversion rates, the totally different but deeply related dose rate dependencies of OT and IT can be explained self-consistently. 
From the above analysis, it is also clear that, as the generation rate and proportion factor are almost insensitive to dose rate, there was no physical trouble for DPO even using the stand approach. Actually, the extracted parameters indicate that, the main reason for the dose rate effects of DPO is the change of half-life, which is very different from the WPO case. 

In summary, we have proposed a universal analytical model for the two dominant irradiation-induced ionization defects in silicon oxides. The key in our model is the consideration of a generation-interconversion framework and a defect creation mechanism. The model predicts a combined fractional power law and exponential decay function of the irradiation dose. Experimental data for both wet processed base oxides and dry processed gate oxides are used to verify the proposed mechanism and formulas. It is unprecedented that, the strong process fingerprints, nonlinear dose dependence, dose rate sensitivity, and sample variability displayed in the experimental data, can all be quantitatively and consistently described, which reflects the validity and universality of our proposed formulas. It is demonstrated that by using the proposed formulas, the computational difficulty and physical ambiguity encountered by the standard approach can be completely eliminated. Especially, the important but long-time unsettled mechanism of the low-dose-rate sensitivity of IT and the confusing non-monotonic dose dependence of OT at relatively low dose rate for wet processed oxides can be clearly and uniformly explained in terms of the dose rate dependence of the generation and interconversion rates. Our proposed mechanism and formulas, hence, provide a powerful tool for understanding the physics of the irradiation-induced ionization defect dynamics in technically important silicon and silicon dioxide electronic devices.

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FIG. 4. Extracted model parameters (a) \( g \), (b) \( \Delta \), (c) \( \lambda \), and (d) \( \tau \) as a function of dose rate for both DPO (blue color) and WPO (red color). The parameters extracted from Li et al’s data [18] are shown by the magenta dots.

FIG. 5. Calculated forward and backward conversion rates from Figs. 4 (c) and (d) as a function of irradiation dose rate.
