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I_{ON} degradation in Si devices in harsh radiation environments: modeling of damage-dopant interactions

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***Abstract*— Electronic devices operating in harsh radiation environments must withstand high radiation levels with minimal performance degradation. Recent experiments on the radiation hardness of a new vertical p-type JFET power switch have shown a significant reduction of forward drain current under non-ionizing conditions. In this work, atomistic simulations are used to study the impact of irradiation-induced displacement damage on forward characteristics. Damage models have been updated to produce a better description of damage-dopant interactions at RT. Our results show that excess self-interstitials produced by irradiation deactivate a significant amount of B atoms, thus reducing the effective dopant concentration.**

Keywords*— *current degradation, radiation, displacement damage, boron deactivation, silicon, atomistic modeling.

I. Introduction

Electronic devices operating in radiation environments such as High Energy Physics and aerospace applications may undergo performance degradation due to irradiation. Some of the detrimental effects attributed to irradiation are the reduction of charge collection efficiency in radiation detectors, the reduction of the output power of solar cells, the degradation of charge-coupled devices and the increase of the off-state power consumption [1-3]. These macroscopic effects are caused by the microscopic changes produced by the energy loss of the incident particle by means of two mechanisms: ionization, which generates electron-hole pairs, and non-ionizing interactions, which leads to the production of phonons and the displacement of lattice atoms.

In particular, displacement damage induced by irradiation is responsible for the degradation of the electronic and optical properties of materials and devices [2, 4]. The interaction of energetic particles with the Si lattice results in permanent damage in the form of Si interstitials (Is) and vacancies (Vs). Depending on particle mass and energy, generated damage may range from isolated defects to local regions of disorder known as clusters of defects. These defects may act as additional generation and recombination centers giving rise to new energy levels in the Si bandgap. Besides, the interaction of defects with dopants may cause their diffusion and deactivation, resulting in a lower effective dopant concentration. Several studies indicate that B diffusion and clustering observed after ion implantation at RT can be attributed to the interaction of Si Is with B atoms [5-7].

To prevent irradiation-induced defects from affecting device performance, radiation hardness techniques are a key element in the development of electronic devices intended to operate in harsh radiation environments. Recent experiments on the radiation hardness of a new vertical p-type JFET power switch under non-ionizing conditions (neutron irradiation), show a significant degradation of both forward and reverse characteristics, attributed to the irradiation-induced displacement damage [8]. This damage is well known to increase leakage currents in the off-state [1], but its impact on forward current (I_{DON}) is still unclear.

In this work, atomistic simulations are used to study the role of damage-dopant interactions on the reduction of I_{DON} under non-ionizing irradiation. Conventional models for dopants developed for the fabrication of ultra-shallow junctions (USJ) are explored in this new regime. We have also updated standard damage models to incorporate new diffusing species that may alter the effective dopant concentration and thus the forward current.

II. Experimental

A power switch was designed to fulfill the radiation hardness requirements for the future ATLAS-Upgrade experiment in the High-Luminosity-Large Hadron Collider (HL-LHC) at the European Organization for Nuclear Research (CERN), which consists of vertical JFET cells as shown in Fig. 1 [8]. Each cell comprises a low-doped p type substrate (~7.6×10^{13}cm^{-3} B) surrounded by a highly doped n type polysilicon gate. The switch is intended to operate at a temperature below 0 °C for a period of several years.

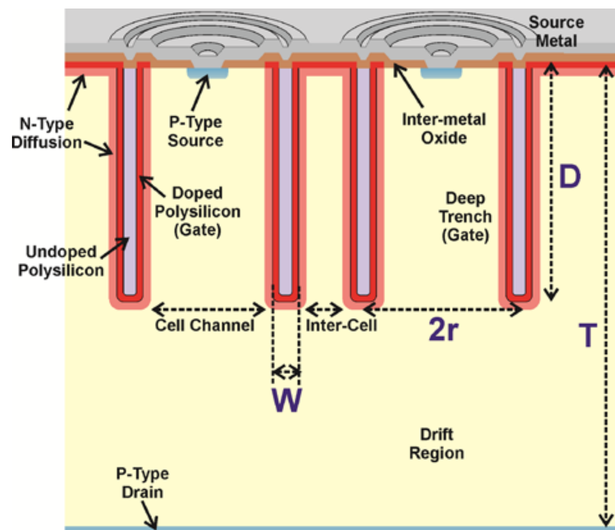

Fig. 1. Schematic cross section through the center of two adjacent vertical JFET cells (extracted from Ref. [8]).

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To test the radiation hardness in non-ionizing conditions the device was irradiated with neutrons to 1-MeV neutron equivalent fluences from 10^{12} to 10^{15} neqcm^{-2}. Electrical measurements when the switch is ON (undepleted substrate) reported a significant reduction of saturated drain current (I_{DON}) with fluence. This behavior is consistent with a lower effective dopant concentration, which increases the bulk resistance. Theoretical calculations indicate that the effective dopant concentration required to obtain the measured I_{DON} values is progressively reduced with neutron fluence, and saturates at approximately 10% of the initial value.

III. Simulation Scheme

We use an atomistic kinetic Monte Carlo (kMC) process simulator (DADOS) to model the evolution of the displacement damage induced by irradiation, as well as the interaction between defects and dopants [9-11]. In the kMC technique, system dynamics is modeled by performing random events whose probability is determined by the energetics of the defects and particles involved in the process. Contrary to continuum methods, atomistic simulators do not solve partial equations but interactions are considered at atomic level, which allows a more detailed description of the system. kMC simulators have been successfully used to study the phenomena of damage generation, amorphization, and dopant diffusion and clustering during ion implantation processes used for the fabrication of USJ.

Due to the relevance of B implants for USJ formation in Si, numerous studies were devoted to obtain fundamental information on parameters and interaction mechanisms between defects and dopants. The insight gained, in particular on the mechanisms of B deactivation by damage, can be applied to the system analyzed in this work. It must be noted that, while the fabrication of USJ is characterized by high local concentrations of defects and dopants, in our study damage is dilute and B concentration is low. Table I shows the main reactions involving defects and dopants that we have considered. It is well stablished that the interaction of Si Is generated by irradiation with electrically active B atoms (substitutional B) leads to the formation of mobile B-I pairs (Bi), which are responsible for B diffusion [12]. The migration of Bi pairs and their interaction with Si Is, B atoms or other Bi pairs causes B deactivation (eq. (7)-(9) in Table I), via the formation of immobile B-I clusters (BICs), i.e. B_nI_m complexes with n B atoms and m Si Is [13,14].

The interaction of Si Is with Vs produces their mutual annihilation. This is the main source of damage removal in bulk systems, in which recombination at surfaces is almost negligible. Equally, the interactions between defects of the same type result in the growth of defect clusters, which can be envisioned as immobile agglomerates of Vs or Is. Different values of the activation energies for clusters dissolution have been proposed, depending on defect configuration and the calculation method [15]. In our study, as system dynamics is analyzed under a low thermal budget, both BICs and defect clusters are stable, and therefore our results are somehow insensitive to the cluster energies used. Most models assume that all Si Is clusters are immobile, although several studies assign a significant mobility to the di-interstitial cluster (I_2) [16-18]. Calculated migration energies range between 0.2 eV and 1 eV depending on the simulation technique used, but in general it is considered that I_2 is a faster diffuser that the single interstitial. The role of the I_2 on surface recombination and Si Is clustering processes has already been analyzed [19], but not its possible effect on B deactivation. In this work, we explore the implications of I_2 diffusion on B deactivation, which opens new pathways for the growth and dissolution of clusters and BICs (see equations in italics in Table I), since they can also capture and emit I_2 clusters.

The substrate doping is modeled by considering a concentration of 7.6×10^{13} cm^{-3} B atoms randomly distributed. We use a simulation cell of $2.36\times2.36\times2.36$ µm^3 with periodic boundary conditions in Y, Z directions and "mirror" surfaces on the X direction (depth), to analyze the kinetics in the bulk of the device. Neutron irradiation is known to generate dilute damage in the form of point defects or small defect clusters [2]. Thus, isolated Si Is and Vs concentrations in the range from 10^{13} to 10^{16} cm^{-3} are introduced to simulate the different amounts of displacement damage resulting from the exposure to increasing neutron fluences. The sample is then left to evolve at RT for a year.

At this temperature, once defect clusters and BICs are formed they will not dissolve during the simulated time. Therefore, system dynamics is controlled by the interactions that diffusing Si Is perform before they recombine or are trapped in defect or dopant clusters. As B deactivation occurs via the interaction with Si Is, it may be sensitive to the availability of diffusing Si Is. To explore the role that mobile Si Is play on dopant evolution, simulations were done with three different clustering models. In the standard model ("Immobile I_2 model"), Si Is can diffuse but all Is clusters are immobile. Our second model ("Mobile I_2 model") considers that I_2 can diffuse with an activation energy of 0.5 eV. In the third model ("Unstable I_2 model") the I_2 is not mobile but it is very unstable, which means that once formed it quickly dissolves. In this situation, although it is not based on a reported binding energy for I_2, we can explore system dynamics when defect cluster formation is practically inhibited.

TABLE I. Main equations in simulator DADOS describing defects and dopants interactions.

(1)	$I + V \rightarrow 0$	(7)	$B_i + I_m \leftrightarrow BI_{m+1}$
(2)	$I + I \leftrightarrow I_2$	(8)	$B_i + B \leftrightarrow B_2I$
(3)	$I + I_m \leftrightarrow I_{m+1}$	(9)	$B_i + B_i \leftrightarrow B_2I_2$
(4)	***$I_2 + I_m \leftrightarrow I_{m+2}$***	(10)	$I + B_nI_m \leftrightarrow B_nI_{m+1}$
(5)	$I + B \leftrightarrow B_i$	(11)	***$I_2 + B_nI_m \leftrightarrow B_nI_{m+2}$***
(6)	***$I_2 + B \leftrightarrow BI_2$***	(12)	$B_i + B_nI_m \leftrightarrow B_{n+1}I_{m+1}$

IV. Results

Simulation results presented here correspond to a concentration of 10^{15} cm^{-3} Si Is and Vs, higher than that of B (7.6×10^{13} cm^{-3}), which results in a significant B deactivation. This allows us analyze the role of the diffusion and clustering of defects on dopant evolution. Fig. 2 shows the fraction of active B (substitutional B), Bi pairs and B atoms in BICs after annealing at RT for a year, obtained with the three different clustering models described above. As can be seen, the highest activation corresponds to the model where the I_2 cluster is immobile and stable, and only the single Si

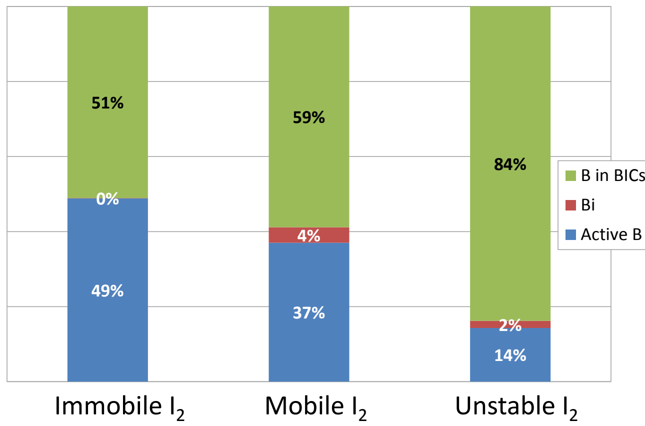

Fig. 2. Fraction of active B (blue), Bi pairs (red) and B belonging to BICs (green) after annealing at RT for a year for the three different models considering that the I_2 cluster cannot diffuse, that the I_2 cluster is mobile and that the I_2 cluster is unstable.

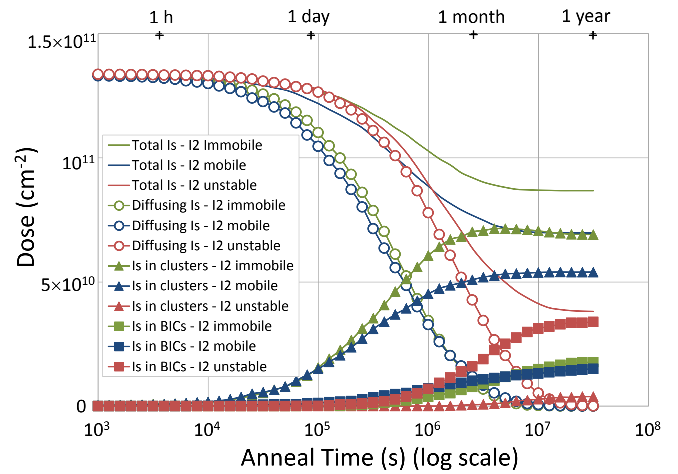

Fig. 3. Evolution of the total dose of Si Is (solid lines), and the dose of diffusing Si Is (open circles), Si Is in clusters (solid triangles) and Si Is in BICs (solid squares) during annealing at RT for a year. Results correspond to three different models considering the I2 cluster immobile (green lines and symbols), the I2 cluster mobile (blue lines and symbols) and the I2 cluster unstable (red lines and symbols).

interstitial can diffuse. A reduction of 12% in B activation, and therefore an increase of the B dose trapped in BICs, occurs when the di-interstitial cluster can also diffuse. Both effects are greatly enhanced when the I_2 cluster is unstable and quickly dissolves, releasing two mobile single interstitials. These data indicate that the fraction of active B strongly depends on the availability of diffusing Si Is, which may reach B atoms causing their deactivation, and therefore on the formation and growth of interstitial defects.

In order to clarify the availability of Si Is, the total dose of Si Is, the dose of diffusing Si Is, and the dose of Si Is trapped in clusters and BICs is reported in Fig. 3. As the starting dose of both Si Is and Vs is relatively high (2.36×10^{11}cm^{-2}) there is an initial decay on the total dose of Si Is (not shown in Fig. 3), due to the recombination with diffusing Vs (a faster diffuser than Si Is), that ends up when the remaining Vs are immobilized in Vs clusters. As the annealing proceeds, significant differences on defect population can be observed with the three models considered. The total amount of Si Is and the dose of Si Is in clusters is notably reduced when the I_2 cluster can diffuse, and these effects are much more pronounced when the I_2 cluster is unstable.

When damage concentration is high, diffusing Si Is are likely to interact with other Si Is forming I_2 clusters. In the standard model this cluster is immobile and stable and hence it will not dissolve during the RT annealing, which means that a significant dose of Si Is are trapped in I_2 clusters, and therefore they are no longer available for diffusion. In the model where I_2 clusters can diffuse, they can also be recombined with Vs increasing defect annihilation, or form larger Is clusters by interacting with other Si Is. In addition, some of them reach B atoms and form BICs, contributing to an enhanced B deactivation as reported in Fig. 2. It must be noted that in the unstable I_2 model, as I_2 clusters quickly dissolve, the trapping of Si Is in clusters is almost inhibited, as evidenced by the residual dose of Si Is in clusters in Fig. 3. Therefore, single Si Is survive longer since they will diffuse until they are recombined with Vs or interact with B atoms, leading to a very high dopant deactivation.

B deactivation is triggered by the formation of Bi pairs when mobile Si Is interact with B atoms. As Bi pairs diffuse they are more likely to interact with Si Is or Is clusters (since they are abundant) resulting in BICs with one B atom (B_1I_m) (eq. (7) in Table I). Only when Bi concentration is high, BICs with 2 B atoms are formed, as it requires the interaction of Bi pairs with B atoms, Bi pairs or B_1I_m BICs (eq. (8), (9) and (12) in Table I). To clarify the differences on B deactivation between the standard model and the improved model with mobile I_2 clusters, we have analyzed the evolution and composition of BICs. Fig. 4 shows the dose of Bi pairs, the total dose of B in BICs and the dose of B in BICs with one B atom (B_1I_m) and with two or more B atoms ($B_{>=2}I_m$) during annealing.

In the standard model B_1I_m clusters are initially formed, and when Bi concentration is high, BICs with a larger B content start growing. In the improved model, mobile I_2 clusters can interact with B atoms forming a B_1I_2 cluster (eq. (6) in Table I), a precursor for the growth of bigger BICs. This opens a new pathway for the formation of B_1I_m clusters

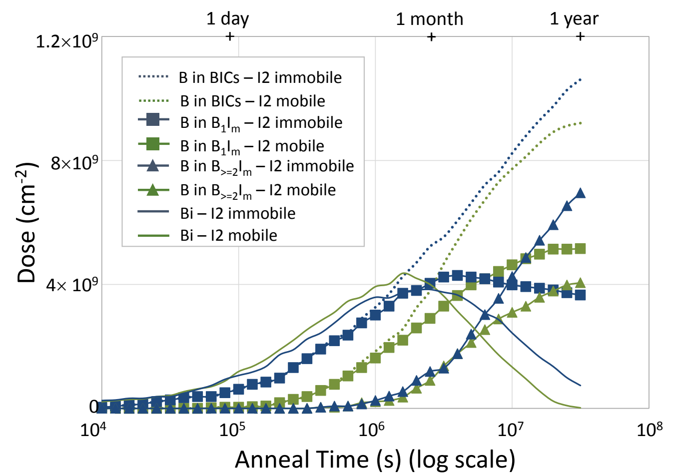

Fig. 4. Total dose of B in BICs (dotted lines), dose of B atoms in BICs with one B atom (B_1I_m) (solid squares), in BICs with two or more B atoms ($B_{>=2}I_m$) (solid triangles) and dose of Bi pairs during annealing at RT, for the standard (green lines and symbols) and the mobile (blue lines and symbols) I_2 models.

that does not require the intervention of Bi pairs. For this reason, in the first stages of the annealing there is a larger dose of B_1I_m clusters than in the standard model.

As can be seen in Fig. 4, the higher deactivation reported for the mobile I_2 model is mainly due to the large number of BICs with two or more B atoms. These BICs start forming under high Bi concentrations, but their growth takes place at a higher pace than in the standard model. The increase on the number of BICs with at least two B atoms is fueled by the large Bi dose maintained during the annealing. One of the implications of I_2 diffusion is an enhanced defect annihilation (as shown in Fig. 3), which reduces the amount of recombination and trapping defects (Vs and Is clusters, respectively) for diffusing Si Is. This favors the formation of Bi pairs through the interaction of Si Is with B atoms. In summary, the rapid formation of B_1I_2 clusters, together with the steep increase in the population of BICs with a higher B content, can explain the enhanced B deactivation reported for the mobile I_2 model.

Dopant deactivation induced by defects can contribute to explain the degradation of forward current in devices exposed to non-ionizing radiation, as in the vertical JFET switch presented above. However, simulation results indicate that a high dose of both Vs and Is clusters is still present after the annealing, comparable or even larger than that of B. Defect clusters have been reported to introduce new energy levels in the Si bandgap [3], that could also reduce the effective dopant concentration and degrade forward current.

V. CONCLUSIONS

An acceptor removal effect due to B deactivation by displacement damage can contribute to the reduction of I_{DON} with irradiation fluence. Our results show that the availability of diffusing Si Is has a strong effect on both defect clustering and dopant deactivation. Atomistic simulations are a suitable tool to analyze the effect of irradiation-induced damage on device performance, and to explain the physical mechanisms that underlie the experimental observations.

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