Numerical simulation of the influence of electron injections on the short-term annealing in pulse-neutron-irradiated $p$-type Si

Xiaoyan Bai, Yan Liu, Wei Chen, Chao Qi, Xiaoming Jin, Guizhen Wang, Ruibin Li, Chenhui Wang, and Junlin Li
Numerical simulation of the influence of electron injections on the short-term annealing in pulse-neutron-irradiated $p$-type Si

Cite as: AIP Advances 9, 115010 (2019); doi: 10.1063/1.5118750
Submitted: 4 July 2019 • Accepted: 29 October 2019 • Published Online: 14 November 2019

Xiaoyan Bai, Yan Liu, Wei Chen, Chao Qi, Xiaoming Jin, Guizhen Wang, Ruibin Li, Chenhui Wang, and Junlin Li

AFFILIATIONS
State Key Laboratory of Intense Pulsed Radiation Simulation and Effect, Northwest Institute of Nuclear Technology, Xi’an 710024, China

ABSTRACT
The physical reason behind the much more rapid short-term annealing progress in the presence of electrons in $P$-type silicon irradiated by pulse neutrons is investigated. Continuum equations coupled with defect reactions are used for the numerical simulation on the temporary evolutions of defects at different electron injection ratios. It is indicated that electron injections can significantly accelerate the creations of boron and carbon interstitials, but may have little influence on the creation of the vacancy-oxygen complex. The calculations on the relative concentrations of interstitials and vacancies in different charge states via the electron injection ratio show that more and more interstitials in the doubly positive charge state change into neutral ones, and neutral vacancies are always dominant with an increase in the electron concentration. The thermal diffusion coefficient of neutral interstitials is much larger than the ones of interstitials in other charge states. As a consequence, normal ionization enhanced diffusion for interstitials in the presence of electrons can significantly accelerate the short-term annealing progress in $P$-type silicon. Ionization enhanced diffusion coefficients for interstitials due to athermal diffusion are further estimated using the Bourgoin mechanism, and results indicate that the diffusion coefficients of positively charged interstitials are improved by several orders of magnitude when compared to their corresponding thermal diffusion coefficients. However, the production of boron and carbon interstitials is only accelerated by about one order of magnitude, which would be ascribed into such large thermal diffusion coefficients of neutral interstitials.

I. INTRODUCTION

When energetic particles are incident on semiconductor materials, a portion of their energy deposits into ionization and the remainder deposits into atomic displacements. The ionization energy loss results in electron-hole pair productions, while non-ionizing energy loss results in the displacement of lattice atoms. The initially created defects are vacancies and interstitials, where a vacancy is the absence of an atom from its normal lattice position and an interstitial is a dislodged atom that resides in a nonlattice position. For charged particle radiation, the primary modes of electronic device degradation result from ionization. For high-energy neutron radiation, the primary cause of device degradation is atomic displacement damage.

Extensive experimental data indicated that the damage in electronic devices from pulse neutron irradiation is considerably more severe immediately after the neutron pulse. The damage decreases with time on a time scale varying from milliseconds to seconds. This phenomenon is referred to as short-term, transient, or rapid annealing. The term annealing factor is introduced to describe the short-term annealing,

$$ AF = \frac{r^{-1}(t) - r^{-1}(0)}{r^{-1}(\infty) - r^{-1}(0)} $$

where $r(t)$ is the instantaneous effective lifetime, $r(0)$ is the lifetime before damage, and $r(\infty)$ is the stabilized lifetime long after
the neutron pulse. Short-term annealing following a neutron exposure has been studied extensively in transistors, solar cells, and other semiconductor devices. Experimental results indicated that the annealing factor is the function of dopant types, injection levels, and temperature. Minority carrier injection is much more important than temperature in governing the annealing progress. Injection of electrons into p-type is observed to significantly speed the annealing process, while hole injection in N-type causes an apparent decrease in the annealing rate. Moreover, injection has a much smaller effect in N-type in contrast to the P-type results.

An empirical relationship between base-emitter bias, electron density, annealing factor, and time after exposure for a constant room temperature was formulated in the nomograph form by Sander and Gregory. McMurray and Messenger devised an analytical expression from the nomograph, and Wrobel and Evans modified this expression and expressed the annealing factor directly as the function of base-emitter bias. These expressions were suitable for use in circuit simulation codes for prediction of the circuit transient response. A compact model including the dependence of neutron fluence on the relevant SPICE parameters was developed by Deng et al., in which a single time constant was used in an exponential time dependence of the anneal.

Physical modeling on the short-term annealing generally started from continuum equations. Leadon presented a physical model describing the damage cluster resulting from neutron radiation in P-type silicon in 1970. Because of the lack of knowledge on the defects, this model is greatly simpler and the disordered core was only characterized by vacancies and divacancies. Sandia National Laboratories developed a computer code Charon to simulate a silicon semiconductor device at the carrier-concentration level, including the transport of the numerous defect complexes created by neutron radiation at the short time scales and high fluence levels. The influence of clustering in pulse-neutron irradiated silicon was simulated by Myers et al. in a unified mechanistic fashion.

Hjalmarson et al. mainly discussed the effects of combined transient neutron and ionizing radiation on silicon diodes and bipolar junction transistors using REOs software. Keiter et al. coupled a localized defect reaction model, a carrier model, and an integration term with a normal environment transistor model to develop a physics-based compact model of transient neutron damage.

Although empirical expressions and numerical simulations showed some agreement with the dependence of the annealing factor on the injection level in the experiment, there are no further investigations on the physical reasons behind this dependence. The speculation given by McMurray and Messenger in 1981 was that the much more rapid annealing process in the presence of electrons was due to the much higher diffusion constant of vacancies in the charged state compared to the one in the neutral state. However, this speculation is the lack of validation. In this paper, we try to find the physical reasons behind this dependence by using the simulation on the temporary evolution of defects in P-type silicon irradiated by pulse neutrons.

In essence, the short-term annealing process can be understood as the reaction processes of primal interstitials and vacancies with dopants and impurities. Generally, these reactions are assumed to be diffusion-limited and the rate constants are linear with the diffusion coefficients of the reacting species. Since the dopants and impurities are generally assumed to be immobile, the diffusion coefficients of interstitials and vacancies are important for the production of defect complexes. Conventionally, the diffusion is considered to be thermally activated. However, various investigations indicated that the mobility of the same defects may increase significantly when a concentration of electrons, of holes, or of electron-hole pairs is present in the crystal, which is due to the ionization enhanced diffusion (IED) in essence. Based on the numerical simulation presented in this paper, we connect the dependence of the short-term annealing process on injection levels with the IED.

II. THE MODEL CONTINUUM MODEL AND DEFECT REACTIONS

Continuum equations were used to simulate the density evolution of defect species. With the assumptions of primal interstitials and vacancies generated uniformly and no electric fields, the complete continuum equations can be simplified as

\[
\frac{\partial n_Y}{\partial t} = G - R,
\]

where \(Y\) denotes a particular defect, electron or hole; \(n_Y\) is the number density of species \(Y\); \(t\) is time; and \(G\) and \(R\) are the bulk sources of creation and recombination of species \(Y\), respectively. With this simplification, we can focus on the temporary evolution of different defects.

The generation and recombination items in Eq. (1) are mainly dependent on the defect reactions. In general, there are mainly two types of reactions: carrier-defect reactions and defect-defect reactions. Carrier-defect reactions mainly include electron/hole capture and emission. Defect-defect reactions mainly include the reactions of primal interstitials and vacancies with dopants and impurities. The following three defect-defect reactions are included in the simulation:

\[
O_i + V \rightarrow VO_i, \quad (2.1)
\]
\[
B_i + I \rightarrow B_I, \quad (2.2)
\]
\[
C_i + I \rightarrow C_I. \quad (2.3)
\]

In Eq. (2.1), a vacancy \(V\) reacts with interstitial oxygen \(O_i\) to create an oxygen-vacancy pair \(VO_i\) in Eqs. (2.2) and (2.3), an interstitial \(I\) reacts with substitutional boron \(B_i\) and substitutional carbon \(C_i\) to create a boron interstitial \(B_I\) and a carbon interstitial \(C_I\) respectively. The divacancies \(VV\) did not undergo reactions, and the starting vacancies were apportioned between \(VV\) and \(V\) in the ratio \([VV]/[V] = 0.4\). It has been confirmed that there are five charge states for \(V\) and \(I\) from \(-2\) to \(+2\), four for divacancies from \(-2\) to \(+1\), two for \(VO\) from \(-1\) to 0, and three for \(B_I\) and \(C_I\) from \(-1\) to \(+1\).

The calculations of the rate constants for electron/hole capture and emission were elaborated in Ref. 12. The activation energies for carrier emission and the cross sections for carrier suggested in Ref. 13 are employed here. The state degeneracies for all defect species employed here are suggested to be 1.0.

Defect-defect reactions are generally assumed to be diffusion-limited, and then, the von Smoluchowski approach leads to a rate constant given by

\[
k_{DD} = 4 \pi a^2 \langle D_1 + D_2 \rangle. \quad (3)
\]
The symbols $D_1$ and $D_2$ stand for the diffusion coefficients of the reacting species; $a^0$ stands for the capture or reaction radius. Defect-defect reactions with species of like charge are currently neglected (very small cross sections). In the absence of electrostatic interaction, the reaction distance is approximately in the order of the lattice parameter within Si ($a^0 \approx 5.43 \times 10^{-8}$ cm). In the case of attractive interaction, the reaction distance is that at which the attractive potential is equal to $kT$ and can be approximated as 

$$a = \frac{|m \cdot n| \left(1.4 \times 10^{-4} \text{cm K}\right)}{T[K]},$$

(4)

where $m$ and $n$ are the number of electron charges carried by the two reacting species.

Diffusion in solids can occur via a number of different mechanisms. Traditionally, the diffusion is considered to be thermally stimulated and the temperature dependence of thermal diffusion coefficients determined from experiments is usually found to obey an Arrhenius relation:

$$D = D_0 \exp\left(-\frac{E_A}{kT}\right),$$

(5)

characterized by the prefactor $D_0$ and the activation energy $E_A$. The corresponding values for vacancies and interstitials in different charge states are listed in Table I.13,17

Various investigations indicated that the mobility of the same defects may increase significantly under some conditions such as electron injection or stimulation with light.17 Bourgoin and Corbett termed it as ionization-enhanced diffusion (IED) and gave a comprehensive discussion on it.18 Two kinds of IED mechanisms were mainly discussed by them: normal ionization enhanced diffusion (NIED) and the Bourgoin mechanism. The former process occurs when two different charge states have different activation energies for thermally activated diffusion, while the latter process occurs when two different charge states have different activation energies for high dopant concentration, it increases with an increase in the injection ratio. For low dopant concentrations in $n$-type silicon, the enhanced migration of generated vacancies and interstitials is very likely to speed the short-term annealing process. We try to calculate the influence of the enhanced diffusion on the temporary evolution of the defects by numerical simulation.

For electron injections into $p$-type silicon irradiated by pulse neutrons, the enhanced migration of generated vacancies and interstitials is very likely to speed the short-term annealing process. We try to calculate the influence of the enhanced diffusion on the temporary evolution of the defects by numerical simulation.

The $p$-type silicon was assumed to be doped with $2 \times 10^{16} \text{ cm}^{-3}$ boron acceptors. Oxygen and carbon impurities were assumed to have the concentrations of $1 \times 10^{17} \text{ cm}^{-3}$ and $1 \times 10^{16} \text{ cm}^{-3}$, respectively.

The transient neutron radiation was assumed to be uniform with a time duration of 10 ns. The density of surviving prinal vacancies was $1.0 \times 10^{11} \text{ cm}^{-3}$, the density of divacancies was $4.0 \times 10^{10} \text{ cm}^{-3}$, and then, the density of surviving prinal interstitials is $1.8 \times 10^{11} \text{ cm}^{-3}$. The temporary evolutions of different defects were simulated under the following four injection ratios (IR): (1) $IR = 5 \times 10^{-5}$, (2) $IR = 5 \times 10^{-4}$, (3) $IR = 5 \times 10^{-3}$, and (4) $IR = 5 \times 10^{-2}$. The IR is the ratio of the concentrations of the injected excess electrons and the majority holes.

### III. RESULTS AND DISCUSSION

At first, the temporary evolutions of $V$, $I$, $VO$, $B_I$, and $C_I$ at the four different injection ratios were simulated with the consideration of normal ionization enhanced diffusion (Fig. 1). It was clearly shown that the evolutions of $B_I$ and $C_I$ in $P$-type silicon were significantly accelerated by electron injections, while the evolution of $VO$ was basically unaffected. The evolutions of interstitials in five charge states at the four different injection ratios are illustrated in Fig. 2. At lower injection, interstitials in the doubly positive charge state are absolutely dominated. As the electron injection ratios increase, more and more interstitials in the doubly positive charge state change to interstitials in single positive and neutral charge states. In contrast, there is nearly no change of charge states for vacancies and neutral vacancies almost comprised more than 90% of the total vacancies with the electron injections.

In general, the charge states of defects are mainly controlled by the charge-carrier concentrations. Figures 3(a) and 3(b) give the relative concentrations of interstitials in the doubly positive charge state and of neutral vacancies via the electron injection ratio at different dopant concentrations in $P$-type silicon, respectively. The former is mainly controlled by the electron injection ratio and decreases with an increase in the injection ratio. For low dopant concentrations, the relative concentration of neutral vacancies is not significantly affected by the electron injection ratio and is nearly 1.0; for high dopant concentration, it increases with an increase in the injection ratio.

The thermal diffusion coefficients of interstitials in singly positive and neutral charge states are more than 10 orders of magnitude

| TABLE I. Species and parameter values for thermal diffusion. |
|------------------|------------------|------------------|------------------|
| Species | $D_0$ (cm$^2$/s) | $E_A$ (eV) | Species | $D_0$ (cm$^2$/s) | $E_A$ (eV) |
|------------------|------------------|------------------|------------------|------------------|------------------|
| $V^{-2}$ | $1.5 \times 10^{-2}$ | 0.18 | $Si_2^{-2}$ | $10^{-3}$ | 0.33 |
| $V^{-1}$ | $1.3 \times 10^{-3}$ | 0.45 | $Si_2^{-1}$ | $10^{-3}$ | 0.29 |
| $V^0$ | $1.3 \times 10^{-3}$ | 0.45 | $Si_0^0$ | $10^{-3}$ | 0.17 |
| $V^+$ | $9.6 \times 10^{-3}$ | 0.32 | $Si_2^1$ | $10^{-3}$ | 0.50 |
| $V^{+2}$ | $9.6 \times 10^{-3}$ | 0.32 | $Si_2^2$ | $10^{-3}$ | 1.17 |

\[ D_B = \left( \frac{1}{Q} + \frac{1}{R} \right) \frac{(\Delta x)^2}{4}, \]

(7)

where $\Delta x$ is the jump distance, provisionally equated to the lattice parameter of silicon.
FIG. 1. The temporary evolutions of different defects at four different injection ratios (IR). (a) IR = 5 × 10^{-5}. (b) IR = 5 × 10^{-4}. (c) IR = 5 × 10^{-3}. (d) IR = 5 × 10^{-2}.

FIG. 2. The evolutions of interstitials in five charge states at four different injection ratios. (a) IR = 5 × 10^{-5}. (b) IR = 5 × 10^{-4}. (c) IR = 5 × 10^{-3}. (d) IR = 5 × 10^{-2}.
higher than the one of interstitials in the doubly positive charge state (Table I). The latter is absolutely dominated at the intrinsic carrier concentration and will change into the former two types of interstitials with the electron injections. Hence, the migration of interstitials is significantly enhanced by the electron injections. The thermal diffusion coefficient of vacancies in the doubly negative charge state is far larger than the one in other charge states (Table I). However, their relative concentration can be omitted even at high electron injection ratios for p-type silicon. It can be seen from Fig. 3(b) that neutral vacancies always comprise more than 90% of the total vacancies when the dopant concentration is not larger than $2 \times 10^{16}$ cm$^{-3}$, and hence, the migration of vacancies would not be affected by electron injections. When the dopant concentration becomes larger, the vacancies in positive charge states become dominant at the intrinsic carrier concentration, which will change into neutral vacancies with the injection of electrons. As the diffusion coefficient of neutral vacancies is a little larger than the ones in positive charge states, the migration of vacancies can be enhanced. However, the enhancement in vacancies is much smaller than that in interstitials. McMurray and Messenger speculated that the much more rapid annealing process in the presence of electrons was due to the much higher diffusion constant of vacancies in charge states compared to the one in the neutral state. However, their speculation was not supported by our simulation. The much more rapid annealing in the presence of electrons in P-type silicon may be ascribed to the enhanced diffusion of interstitials by NIED.

Incidentally, the fast decrease in the concentration of interstitials in the singly positive charge state that appears at the time scale of $10^{-8}$ s in Fig. 2 is due to the change of interstitials in the singly positive charge state into that in the doubly positive charge state. Because of the much higher mobility of charge carriers than of atoms, capturing of charge carriers at defects can be very fast in comparison to the time constants of their reactions with dopants or impurities.

Next, we discuss the influence of athermal diffusion on the temporary evolution of defects. The Bourgoin mechanism was used for the calculation of the athermal diffusion coefficients for interstitials. As this mechanism occurs between the change of two charge states, the enhanced athermal diffusion coefficients for interstitials as the function of electron injection ratios were estimated under the following two cases: (a) $D_B^1$: $\text{Si}_1^0 \leftrightarrow \text{Si}_1^1$ and (b) $D_B^2$: $\text{Si}_1^1 \leftrightarrow \text{Si}_1^2$ (Fig. 4). The migration of interstitials in some charge state is characterized by the sum of its athermal and thermal diffusion coefficients. Due to such a large thermal diffusion coefficient of neutral interstitials, the athermal diffusion has a little influence on their migration. Instead, athermal diffusion can improve the migration of interstitials in singly and doubly positive charge states by several orders of magnitude.

The evolutions of $B_I$ with and without the consideration of athermal diffusion are illustrated in Fig. 5. When $IR = 5 \times 10^{-5}$, the evolution of $B_I$ in case (b) is significantly faster than the ones in the other two cases. With an increase in the injection ratio, the evolution curves of $B_I$ in cases (a) and (b) come closer. When $IR = 5 \times 10^{-2}$, these two curves nearly coincide with each other. As more and more interstitials in the doubly positive charge state change into ones in singly positive and neutral charge states with the
electron injections, the enhanced diffusion coefficients of interstitials in the doubly positive charge state in case (b) have less and less influence on the evolutions of interstitial complexes. Although the migration of interstitials in singly and doubly positive charge states is enhanced by several orders of magnitude by athermal diffusion, the evolution of $B_I$ is accelerated by only about one order of magnitude. It can be seen in Fig. 4 that the thermal diffusion coefficient of neutral interstitials is still about one order of magnitude larger than the enhanced diffusion coefficients of interstitials in singly and doubly positive charge states even when the electron injection ratio goes as high as $5 \times 10^{-2}$. Thus, neutral interstitials play an important role in the creation of interstitial complexes.

IV. CONCLUSION

A numerical simulation on the temporary evolutions of defects in $P$-type silicon irradiated by pulse neutrons was presented. It was indicated that ionization enhanced diffusion for interstitials was the underlying physical reason behind the much more rapid annealing process in the presence of electrons for $P$-type silicon. Two types of ionization enhanced ionization were discussed. Normal ionization enhanced ionization were discussed. Normal ionization enhanced diffusion can significantly accelerate the evolution of $B_I$ and $C_I$ under the condition of electron injections by the change of interstitials in positive charged states into neutral ones. Athermal diffusion can further improve the evolutions of interstitial complexes by about one order of magnitude when compared to normal ionization enhanced diffusion. Although athermal diffusion can accelerate the migration of interstitials in positive charged states by several orders of magnitude, they are still about one order of magnitude smaller than the thermal diffusion coefficient of neutral interstitials, which play an important role in the evolutions of interstitial complexes in $P$-type silicon.

ACKNOWLEDGMENTS

This work was supported by the Fund of the State Key Laboratory of Intense Pulsed Radiation Simulation and Effect (Grant Nos. SKLIPR1804 and SKLIPR18017) and the Foundation of the Science and Technology on Analog Integrated Circuit Laboratory (Grant No. 6142802180304).

REFERENCES

1. B. L. Gregory and H. H. Sander, IEEE Trans. Nucl. Sci. 14, 116 (1967).
2. H. H. Sander and B. L. Gregory, IEEE Trans. Nucl. Sci. 13, 53 (1966).
3. J. W. Harrity and C. E. Mallon, IEEE Trans. Nucl. Sci. 17, 100 (1970).
4. C. E. Mallon and J. W. Harrity, IEEE Trans. Nucl. Sci. 18, 45 (1971).
5. H. H. Sander, ”Room temperature annealing of silicon transistor parameters degraded by a burst of neutrons,” Report No. SC-R-64-192, Sandia National Laboratories, 1964.
6 R. F. Rieden, IEEE Trans. Nucl. Sci. 26, 4775 (1979).
7 T. F. Wrobel and D. C. Evans, IEEE Trans. Nucl. Sci. 29, 1721 (1982).
8 H. H. Sander and B. L. Gregory, IEEE Trans. Nucl. Sci. 18, 250 (1971).
9 L. R. McMurray and G. C. Messenger, IEEE Trans. Nucl. Sci. 28, 4392 (1981).
10 Y. Q. Deng, T. A. Fjeldly, T. Ytterdal, and M. S. Shur, IEEE Trans. Nucl. Sci. 50, 1873 (2003).
11 R. E. Leadon, IEEE Trans. Nucl. Sci. 17, 110 (1970).
12 G. L. Hennigan, R. J. Hoekstra, J. P. Castro, D. A. Fixel, and J. N. Shadid, “Simulation of neutron radiation damage in silicon semiconductor devices,” Report No. SAND2007-7137, Sandia National Laboratories, 2007.
13 S. M. Myers, P. J. Cooper, and W. R. Wampler, J. Appl. Phys. 104, 044507 (2008).
14 S. M. Myers, W. R. Wampler, P. J. Cooper, and D. B. King, Physica B 401–402, 473 (2007).
15 H. P. Hjalmarson, R. L. Pease, R. M. Van Ginhoven, P. A. Schultz, and N. A. Modine, Nucl. Instrum. Methods Phys. Res., Sect. B 255, 114 (2007).
16 E. R. Keiter, T. V. Russo, C. E. Hembree, and K. E. Kambour, IEEE Trans. Nucl. Sci. 57, 3303 (2010).
17 P. Pichler, Intrinsic Point Defects, Impurities, and Their Diffusion in Silicon (Springer, New York, 2004).
18 J. C. Bougoin and J. W. Corbett, Radiat. Eff. 36, 157 (1978).