Long-term damage induced by hadrons in silicon detectors for uses at the LHC-accelerator and in space missions

I. Lazanu\textsuperscript{b} and S. Lazanu\textsuperscript{a,1},

\textsuperscript{a}National Institute for Materials Physics, POBox MG-7, Bucharest-Magurele, Romania
\textsuperscript{b}University of Bucharest, Department of Nuclear Physics, POBox MG-11, Bucharest-Magurele, Romania

Abstract

In the present paper, the phenomenological model developed by the authors in previous papers has been used to evaluate the degradation induced by hadron irradiation at the future accelerator facilities or by cosmic protons in high resistivity silicon detectors. The damage has been analysed at the microscopic (defects production and their evolution toward equilibrium) and at the macroscopic level (changes in the leakage current of the p-n junction). The rates of production of primary defects, as well as their evolution toward equilibrium have been evaluated considering explicitly the type of the projectile particle and its energy. Vacancy-interstitial annihilation, interstitial migration to sink, complex ($V_P$, $V_O$, $V_O^2$, $C_iO_i$ and $C_iC_s$) and divacancy formation are taken into account for different initial silicon material. The influence of these defects on the leakage detector current has been calculated in the frame of the Schokley-Read-Hall model.

PACS:
29: Experimental methods and instrumentation for elementary-particle and nuclear physics
81: Materials science
78: Optical properties, condensed-matter spectroscopy and other interactions of radiation and particles with condensed matter

Key words: silicon detectors, radiation damage, hadrons, LHC accelerator, space mission

\textsuperscript{1} corresponding author: fax: +40-21-4930267, e-mail:lazanu@alpha1.infim.ro

Preprint submitted to Elsevier Science 25 March 2022
1 Introduction

The use of silicon detectors at the new generation of accelerators or in space experiments poses severe problems due to changes in the properties of the material after long time irradiation, and consequently influences the performances of detectors.

The phenomenological model developed by the authors in previous papers has been used to evaluate the degradation induced by hadron irradiation at the future LHC accelerator facilities and by cosmic protons in high resistivity silicon detectors, in two types of silicon: ”standard” material (10^{14} \text{ cm}^{-3} \text{ atoms of phosphorus}, 2 \cdot 10^{15} \text{ cm}^{-3} \text{ atoms of oxygen}, and 5 \cdot 10^{15} \text{ cm}^{-3} \text{ atoms of carbon}), and ”oxygened” one (containing 10^{14} \text{ cm}^{-3} \text{ atoms of phosphorus}, 4 \cdot 10^{17} \text{ cm}^{-3} \text{ atoms of oxygen}, and 5 \cdot 10^{15} \text{ cm}^{-3} \text{ atoms of carbon}) respectively. The damage has been analysed at the microscopic (defect production and their evolution toward equilibrium) and at the macroscopic level (changes in the leakage current of the p-n junction).

These theoretical estimates permit to draw conclusions about the damages induced in silicon in various irradiation conditions and for different semiconductor materials.

2 Main hypothesis of the model

In the model, the effects of irradiation conditions and various initial impurities in the starting material are discussed in the a quantitative manner that the defect production and their evolution toward stable defects during and after irradiation in silicon is calculated. The model supposes three steps.

In the first step, the incident particle, having kinetic energy in the intermediate up to high energy range, interacts with the semiconductor material. The peculiarities of the interaction mechanisms are explicitly considered for each kinetic energy [1,2].

In the second step, the recoil nuclei resulting from these interactions lose their energy in the lattice. Their energy partition between displacements and ionisation is considered in accord with the Lindhard theory (see reference [3] and authors’ contributions [4]).

A point defect in a crystal is an entity that causes an interruption in the lattice periodicity. In this paper, the terminology and definitions in agreement with M. Lannoo and J. Bourgoin [5] are used in relation to defects.
We denote the displacement defects, vacancies and interstitials, as primary point defects, prior to any further rearrangement. After this step the concentration of primary defects is calculated.

The concentration of the primary radiation induced defects per unit fluence ($CPD$) in silicon has been calculated as the sum of the concentration of defects resulting from all interaction processes, and all characteristic mechanisms corresponding to each interaction process, using the explicit formula (see details, e.g. in references [6,7]):

$$CPD(E) = \frac{N_{Si}}{2E_{Si}} \sum_{i} \left( \frac{d\sigma}{d\Omega} \right)_{i, Si} L(E_{Ri})_{Si} d\Omega = \frac{1}{N_{A}} \frac{N_{Si}A_{Si}}{2E_{Si}} NIEL(E)$$

where $E$ is the kinetic energy of the incident particle, $N_{Si}$ is the atomic density in silicon, $A_{Si}$ is the silicon atomic number, $E_{Si}$ is the average threshold energy for displacements in the semiconductor, $E_{Ri}$ is the recoil energy of the residual nucleus produced in interaction $i$, $L(E_{Ri})$ is the Lindhard factor that describes the partition of the recoil energy between ionisation and displacements and $(d\sigma/d\Omega)_{i}$ is the differential cross section of the interaction between the incident particle and the nucleus of the lattice for the process or mechanism $i$, responsible in defect production. $N_{A}$ is Avogadro’s number. The formula gives also the relation with the non ionising energy loss ($NIEL$), the rate of energy loss by displacement $(dE/dx)_{ni}$ [8,9].

The kinetic energy dependence of $CPD$ for pions (from reference [10]) and for protons [8,11] is used in the present calculations. $CPD$ versus the kinetic energy of pions and protons is presented, e.g., in Figure 1 of reference [12].

The basic assumption of the model is that primary defects, vacancies and interstitials, are produced in equal quantities and are uniformly distributed in the material bulk. They are produced by the incoming particle, or thermally - only Frenkel pairs are considered. The generation rate of primary defects is a sum of two components:

$$G = G_{R} + G_{T}$$

where $G_{R}$ accounts for the generation by irradiation, and is calculated as:

$$G_{R} = CPD(E) \times \Phi(E)$$

with $\Phi(E)$ the flux of considered incident particles, and $G_{T}$ for thermal generation.

In silicon, vacancies and interstitials are essentially unstable and interact via migration, recombination and annihilation or produce other defects. The concentration of primary defects represents the starting point for the following step of the model, the consideration of the annealing processes, treated in the
frame of the chemical rate theory. A review of previous works about the problem of the annealing of radiation induced defects in silicon can be found, e.g. in Reference [13].

After silicon irradiation, the following stable defects have been identified experimentally and confirmed: \( Si, VP, VO, V_2, V_2O, C_iO_i, C_i, C_iC_s \) (after the compilations from references [5,14]). Vacancy-interstitial annihilation, interstitial migration to sinks, divacancy and vacancy-impurity complex formation \( (VP, VO, V_2O, C_i, C_iO_i \) and \( C_iC_s \)) have been considered supposing the following chemical reaction scheme:

\[
V + I \xrightarrow{K_1/G} \text{annihilation} \quad (4)
\]

\[
I \xrightarrow{K_2} \text{sinks} \quad (5)
\]

\[
V + O \xrightarrow{K_3/K_4} VO \quad (6)
\]

\( VO \) is the \( A \) centre.

\[
V + P \xrightarrow{K_3/K_5} VP \quad (7)
\]

\( VP \) is the \( E \) centre.

\[
V + V \xrightarrow{K_3/K_6} V_2 \quad (8)
\]

\[
V + VO \xrightarrow{K_3/K_7} V_2O \quad (9)
\]

\[
I + C_s \xrightarrow{K_1} C_i \quad (10)
\]

\[
C_i + O_i \xrightarrow{K_8} C_iO_i \quad (11)
\]

\[
A + I \xrightarrow{K_s} O \quad (12)
\]

\[
C_i + C_s \xrightarrow{K_8} C_iC_s \quad (13)
\]

\( K_i \) with \( i = 1, 3 \div 8 \) are the reaction constants. Some considerations about the determination of the reaction constants are given in references [12,13] and their concrete values are given in reference [15], and [16]. Without free parameters, this model is able to predict the absolute values of the concentrations of defects and their time evolution toward stable defects, starting from the primary incident particle characterised by type and kinetic energy.
3 Radiation environment at the LHC accelerator and in the near Earth orbits

In the present paper, two types of applications of silicon detectors are emphasised: for the tracker of experiments at the LHC accelerator, and for space missions in the near Earth orbit, as, for example experiments at the International Space Station.

At the luminosity of $10^{34} \text{cm}^{-2}\text{s}^{-1}$, and assuming an inelastic non-diffractive cross section of 80 mb, the LHC will produce on average $8 \cdot 10^8$ inelastic p-p events per second, creating an extremely hostile radiation environment. For radiation studies, the bunch structure of LHC is not significant. The only scaling parameter for doses and fluences is the inelastic interaction rate.

The central tracker is expected to be exposed to a primary particle flux from the interaction region, and the main concern is radiation damage of silicon detectors. Without loss of generality, the radiation field simulated for the CMS silicon tracker geometry is considered in the following calculations [17]. The high magnetic field imposes a $p_T$ cut-off on charged particles, so that a significant proportion of the most damaging low energy particles never reach the outer tracker layers. In addition, the average kinetic energy rises with increasing pseudorapidity. The spectra of charged hadrons (pions, kaons and protons) simulated for the positions of the silicon layers are taken from Reference [17]. The flux decreases by a factor 50 going from $r = 20$ cm to $r = 100$ cm, and most of the low energy particles disappear. The hadrons are predominantly low-energy charged pions and protons, that are present in different amounts and have different energy spectra as a function of the distance in respect to the interaction point, and of the pseudorapidity. In all cases, the pions are the dominant particles.

In figure 1 the energetic differential generation rate of defects is presented. Each spectrum has been obtained as a convolution of the simulated hadron flux in the tracker cavity for CMS experiment and the energetic dependence of concentration of primary defects (CPD) for protons and pions in the same energy range.

The calculations have been performed for two extreme positions in the tracker cavity: (1): $r = 20$ cm, $z = 0 \div 140$ cm, and (2): $r = 100$ cm, $z = 140 \div 280$ cm.

In the figure, the area under each curve represents the integral generation rate of vacancy-interstitials pairs. The values obtained for the first position (1) are: $6.2 \cdot 10^8$ VI pairs/cm$^3$/s for pions and $5.6 \cdot 10^7$ VI pairs/cm$^3$/s for protons, while for the second one (2) these are $8.1 \cdot 10^6$ VI pairs/cm$^3$/s and $3.1 \cdot 10^6$ VI pairs/cm$^3$/s for pions and protons respectively.
Fig. 1. Differential energetic generation of vacancy-interstitial pairs for pions and protons, for two positions (1): $r = 20$ cm, $z = 0 \div 140$ cm, and (2): $r = 100$ cm, $z = 140 \div 280$ cm. in the tracking cavity of LHC.

We would like to mention that the main contribution for protons comes from the lowest energy region, while for pions the maximum shifts from around 200 MeV to 800 MeV passing from position (1) to position (2). For pions, the $CPD$ dependence is cut at 20 MeV.

The second type of application discussed in the present paper refers to the radiation field produced by cosmic rays. From these particles, the most important contribution comes from protons. The primary proton spectrum in the kinetic range 0.2 to 200 GeV, in the neighbourhood of the Earth, at an altitude of about 380 km, was measured by the Alpha Magnetic Spectrometer (AMS) during space shuttle flight STS-91. The complete data set combining three shuttle altitudes and including all known systematic effects is given in reference [18]. The convolution of this spectrum with the CPD for protons is presented in Figure 2, and it corresponds to a generation rate of vacancy-interstitial pairs of $2 \cdot 10^2$ VI pairs/cm$^3$/s. This represents a nearly seven order of magnitude lower generation rate in respect to the higher one calculated for the tracking cavity of the LHC experiments.
Fig. 2. Differential energetic generation rate of vacancy-interstitial pairs by cosmic protons in the space near the Earth.

4 Estimated damage in silicon detectors

Silicon used in high energy physics detectors is n-type high resistivity ($1 \div 6$ KΩ·cm) phosphorus doped FZ material. In the last decade a lot of studies have been performed to investigate the influence of different impurities, especially oxygen and carbon, as possible ways to enhance the radiation hardness of silicon for detectors in the future generation of experiments in high energy physics - see, e.g. references [19,20]. Some peoples consider that these impurities added to the silicon bulk modify the formation of electrically active defects, thus controlling the macroscopic device parameters. The effect of oxygen in irradiated silicon has been a subject of intensive studies in remote past. Empirically, it is considered that if the silicon is enriched in oxygen, the capture of radiation generated vacancies is favoured by the production of pseudo-acceptor complex vacancy-oxygen. Interstitial oxygen acts as a sink for vacancies, thus reducing the probability of formation of divacancy related complexes, associated with deeper levels inside the gap. These conclusions are confirmed by the present model.

The concentrations of interstitial oxygen and substitutional carbon are silicon
are strongly dependent on the growth technique. In high purity Float Zone Si, oxygen interstitial concentrations are around $10^{15}$ cm$^{-3}$, while in the oxygenation technique developed at BNL, an interstitial oxygen concentration of the order $5 \cdot 10^{17}$ cm$^{-3}$ is obtained. These materials can be enriched in substitutional carbon up to $[C_i] \approx 1.8 \cdot 10^{16}$ cm$^{-3}$.

4.1 Changes in the microscopic material properties

In Figure 3 a) to f), the formation and time evolution of the vacancy-oxygen, vacancy-phosphorus, divacancy, divacancy-oxygen, carbon interstitial-oxygen interstitial and carbon interstitial-carbon substitutional are presented. Two types of silicon have been considered: the "standard" material, containing the following impurities concentrations: $10^{14}$ cm$^{-3}$ atoms of phosphorus, $2 \cdot 10^{15}$ cm$^{-3}$ atoms of oxygen, and $5 \cdot 10^{15}$ cm$^{-3}$ atoms of carbon; and the "oxygened" one, containing $10^{14}$ cm$^{-3}$ atoms of phosphorus, $4 \cdot 10^{17}$ cm$^{-3}$ atoms of oxygen, and $5 \cdot 10^{15}$ cm$^{-3}$ atoms of carbon respectively, and for the two generation rates of $VI$ pairs discussed above, namely $7 \cdot 10^8$ and $2 \cdot 10^2$ $VI$ pairs/cm$^3$/s. The curves in the figures are labelled as follows: (1): standard silicon, LHC irradiation rate, (2): oxygenated silicon, LHC irradiation; (3): standard silicon, cosmic irradiation rate; and (4): oxygenated silicon, cosmic exposure. As could be observed from the figure, the content of oxygen in silicon influences especially defects formation in the case of high rates of generation of vacancy-interstitial pairs. The increase of the initial oxygen concentration in silicon, conduces, after ten years of operation in the LHC environment, characterised by a high and constant generation rate, to the increase of the concentrations of $VO$ and $C_iO_i$ centres, and to the decrease of the concentrations of $V_2$, $VP$ and $C_iC_s$ ones. With the increase of oxygen concentration, an increase of the $V_2O$ generation rate is observed. It is interesting to observe that in almost all cases, an equilibrium in reached between generation and annealing, and a plateau is obtained in the time dependence of the concentrations. The slowest is, in this respect, $V_2O$, that has the highest binding energy.

As underlined above, vacancy-oxygen formation in oxygen, enriched silicon is favoured in respect to the generation of $V_2$, $V_2O$ and $VP$ centres. At high oxygen concentrations, the concentrations of $VO$ centres attain a plateau during the 10 years period considered.

After cosmic proton irradiation, the effects are strongly different. For this generation rate, the increase of the oxygen concentration produces the decrease of the concentration of all centres, with the exception of the $VO$ concentration, that, at these rates, is not influenced by the oxygen content, and of the $C_iO_i$ concentration, where an increase is observed. As a consequence of the small rate of generation of vacancy-interstitial pairs, after ten years of operation,
Fig. 3. Time dependence of the concentrations of a): VO, b): VP, c): V$_2$, d): V$_2$O, e): ClO$_i$ and f): Cl$_i$C$_s$ induced in standard and oxygenated silicon, in conditions of LHC and cosmic continuous irradiation rates (see text).

the equilibrium between generation and annealing is not reached, the concentrations of defects being, with the exception of VP (that has a relatively low binding energy), slightly increasing functions of time.

All the processes have been calculated for 20°C temperature. Thermal generation has been taken into account in all cases, although it is important only for the silicon exposed to cosmic protons.
Also, it is necessary to emphasise the importance of the irradiation and annealing conditions (initial material parameters, type of irradiation particles, energetic incident particle spectra and their flux, temperature) on defect evolution. These aspects have been discussed in previous papers [13,16].

4.2 Macroscopic modifications of detector parameters - the leakage current

The dark current of a reverse biased $p - n$ junction is composed of the following terms: the drift current, due to the drift of minority carriers, the generation current, due to carrier generation on the midgap energy levels inside the depleted region and surface and perimetal currents, dependent on the environmental conditions of the surface and the perimeter of the diode. The formation, during and after irradiation, of defects with associated energy levels inside the gap conduces to the increase of the generation current, since the ease with which a mobile carrier can traverse the gap is greatly enhanced by intermediate levels.

Inside the depleted zone, $n, p \ll n_t$ ($n_t$ is the intrinsic free carrier concentration); each defect with a bulk concentration $N_T$ causes a generation current per unit volume of the form [21]:

$$I = qU = q < v_t > n_i \frac{\sigma_n \sigma_p N_T}{\sigma_n \gamma_n e^{(E_T - E_i)/k_B T} + \sigma_p \gamma_p e^{(E_i - E_T)/k_B T}}$$

(14)

where $\gamma_n$ and $\gamma_p$ are degeneration factors, $\sigma_n$ ($\sigma_p$) are the cross sections for majority (minority) carriers of the trap, $E_i = (E_c - E_v)/2$ and $< v_T >$ is the average between electron and hole thermal velocities. In the Shockley-Read-Hall model used for the calculation of the reverse current, each defect has one level in the gap, and the defect levels are uncoupled, thus the current is simply the sum of the contributions of different defects. Two parameters characterising the defects enter in the calculation of the generation current: their energy position in respect to the intrinsic level, and their cross section. Only near midgap energy levels are important, and in this paper the contributions coming from $V_2O$, $V_2$ and $VP$ have been taken into account. An average between the values of the energy levels and cross sections reported in the literature (see compilations [5,14]) for $V_2$ and $VP$ have been introduced in the calculations, and averaged while for $V_2O$ this is true only for the energy level. In the lack of reported data for the cross section, for the $V_2O$ centre, the value $10^{-16}$ cm$^{-2}$ has been used.

Divacancy has three energy levels in the band gap. The equilibrium statistics for this case is formally different for this case from that for the same number of independent levels, since the occupancy of the levels is now interdependent. In the present calculations, the interaction of the $V_2$ energy levels has been
neglected (in accord with Sah and Schotkley affirmation [22] that the independent and interacting energy level cases are indistinguishable if the energy levels are more than a few $k_B T$ apart).

In Figure 4, the separate contributions of $V_2O$, $V_2$ and $VP$ defects to leakage current for ”standard” and ”oxygenated” silicon, in the irradiation conditions supposed for LHC and in the cosmic near Earth orbits, are represented. The calculations have been performed for 20°C, under continuous irradiation. The bands representing the maximal uncertainties due to the energy position of the defects and to their cross sections are also drawn as dotted lines. On can observe that in the conditions of LHC generation rate, the values of the total current are nearly the same for standard and oxygenated silicon: the higher contributions from the $V_2$ and $VP$ centres (standard silicon) are counterbalanced by the increase of the $V_2O$ concentration (oxygenated silicon), that is the nearest to the midgap. For smaller generation rates, oxygenated silicon is a better choice from the point of view of the leakage current, as could be seen from the case of cosmic irradiation.

5 Summary

The phenomenological model developed previously to explain defect generation and evolution in silicon has been used to evaluate the damage induced by hadron fields, for two classes of applications in high energy physics: at the new generation of colliders and in space applications. The generation rates of vacancy-interstitial pairs have been calculated as convolutions of the hadron spectra with the energy dependencies of the CPD. The time dependence of the concentrations of stable defects has been calculated for ”standard” and ”oxygenated” silicon, in conditions of continuous irradiation during 10 years, at 20°C, for generation rates of vacancy interstitial pairs corresponding to the applications mentioned before. The increase of the oxygen content in irradiated silicon conduces to the increase of the concentrations of oxygen related defects, $VO$, $CiOi$, and $V_2O$, and to the decrease of the $V_2$, $VP$ and $CiCs$ ones. For long term operation and high generation rates of VI pairs, comparable leakage currents are expected in standard and oxygenated silicon p-n junctions. The beneficial influence of a higher oxygen content in silicon becomes visible with the decrease of the generation rate.

References

[1] I. Lazanu, S. Lazanu, U. Biggeri, E. Borchi, M. Bruzzi, Nucl. Instr. Meth.Phys. Res. A 388, (1997) 370.
Fig. 4. Time dependence of the generation current due to divacancy (continuous line), $VP$ (dashed line) and $V_2O$ (dashed dotted line).

[2] I. Lazanu, S. Lazanu, Nucl. Instr. Meth. Phys. Res. A 432, (1999) 374.

[3] J. Lindhard, V. Nielsen, M. Scharff, P. V. Thomsen, Mat. Phys. Medd. Dan Vid. Sesk. 33 (1963) 1.

[4] S. Lazanu, I. Lazanu, Nucl. Instr. Meth. Phys. Res. A 462, (1999) 530.

[5] M. Lannoo and J. Bourgoin, ”Point Defects in Semiconductors”, (edited by M. Cardona, P. Fulde, H. J. Quisser), (Springer Verlag, Berlin, 1983) Springer
[6] I. Lazanu, S. Lazanu, U. Biggeri, E. Borchi, M. Bruzzi, Nucl. Phys. 61B (1998) 409c.

[7] S. Lazanu, I. Lazanu, U. Biggeri, S. Sciortino, Nucl. Instr. Meth. Phys. Res. A 413 (1998) 242.

[8] A. Van Ginneken, Preprint Fermi National Accelerator Laboratory, FN-522, 1989.

[9] E. A. Burke, IEEE Trans. Nucl. Sci., NS-33, 6 (1986) 1276-1281; G. P. Summers, E. A. Burke, C. J. Dale, E. A. Wolicki, P. W. Marshall, M. A. Gehlhauser, IEEE Trans. Nucl. Sci., NS-34, 6 (1987) 1134-1139; C. J. Dale, P. W. Marshall, E. A. Burke, G. P. Summers, E. A. Wolicki, IEEE Trans. Nucl. Sci., NS-35, 6 (1988) 1208-1214.

[10] S. Lazanu, I. Lazanu, Nucl. Instr. Meth. Phys. Res. A 419 (1998) 570.

[11] G. P. Summers, E. A. Burke, Ph. Shapiro, S. R. Messenger, R. J. Walters IEEE Trans. Nucl. Sci., NS 40 (1993) 1372.

[12] I. Lazanu, S. Lazanu, Physica Scripta 66 (2002) 125.

[13] S. Lazanu, I. Lazanu, Nucl. Instr. Meth. Phys. Res. B 183 (2001) 383.

[14] M. Bruzzi, IEEE Trans. Nucl. Sci, NS-48 (2001) 960.

[15] I. Lazanu, S. Lazanu, “The influence of initial impurities and irradiation conditions on defect production and annealing in silicon for particle detectors”, submitted for publication to Nucl. Instr. Meth. Phys. Res. B, arXiv physics/0208027.

[16] S. Lazanu, I. Lazanu, M. Bruzzi, ”Microscopic modelling of defects production and their annealing after irradiation in silicon for HEP particle detectors”, presented to RESMDD 2002, to be published in Nucl. Instr. Meth. Phys. Res. A.

[17] Compact Muon Solenoid, - Technical Proposal CERN/LHCC 94-38 (1994)

[18] J. Alcaraz et al, Phys. Lett. B 490 (2000) 27.

[19] M. Moll, E. Fretwurst, G. Lindstrom, Nucl. Instrum. Meth. Phys. Res. A 439 (2000) 282.

[20] B. C. Mac Evoy, A. Santacchia, G. Hall, Physica B 273-274 (1999) 1054.

[21] E. Borchi, M. Bruzzi, M. S. Mazzoni, Nucl. Instrum. Meth. Phys. Res. A 310, 273 (1991).

[22] C. T. Sah, W. Schotkley, Phys. Rev. 109, 1101 (1958).