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The modelling of long-term damage after irradiation in silicon for uses at the LHC accelerator and in space mission, and its influence on detector performances

(Compilation)

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Abstract

The long-time annealing effects in silicon after irradiation are a major problem for the use of silicon detectors in HEP applications.
In some published papers, the authors have developed a theoretical model able to explain quantitatively the prfoduction of defects, their kinetics and influence on detector properties. These papers are grouped in the report, as reveiling different aspects of these phenomena.

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This report is a compilation of the authors' papers published in periodical journals, in the field of theoretical studies of the long-time annealing effects in silicon after irradiation.

The modelling of the effects of radiation in silicon is considered in a quantitative manner, and could be divided into three steps.

In the first one, the incident particle, having kinetic energy in the intermediate up to high energy range, interacts with the semiconductor material. The peculiarities of the incident particle interaction mechanisms in silicon must be explicitly considered for each particle and each kinetic energy – see, e.g. reference [1]. For other materials, details could be found in references [2, 3]

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 and authors' contributions [4].

Vacancies and interstitials, prior to any further rearrangement, are considered as primary point defects. 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.

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.

Vacancy-interstitial annihilation, interstitial migration to sinks, divacancy and vacancy - impurity complex formation (VP, VO, V_2 V_2O C_i, C_iO_i, C_iC_s) have been considered supposing the following chemical reaction scheme:

$$V + I \underset{G}{\overset{K_1}{\rightleftarrows}} 0 \qquad (1a)$$

$$I \overset{K_2}{\rightarrow} sinks \qquad (1b)$$

$$V + V \underset{K_4}{\overset{K_3}{\rightleftarrows}} V_2 \qquad (1c)$$

$$V + O \underset{K_6}{\overset{K_5}{\rightleftarrows}} VO$$

(VO is the A centre). (1d)

$$A + I \overset{K_7}{\rightarrow} O \qquad (1e)$$

$$V + P \underset{K_9}{\overset{K_8}{\rightleftarrows}} VP$$

(VP is the E centre). (1f)

$$VO + V \underset{K_{11}}{\overset{K_{10}}{\rightleftarrows}} V_2O \qquad (2a)$$

$$I + C_s \overset{K_{12}}{\rightarrow} C_i \qquad (3a)$$

$$C_i + O_i \overset{K_{11}}{\rightarrow} C_iO_i \qquad (3b)$$

$$C_i + C_s \overset{K_{13}}{\rightarrow} C_iC_s \qquad (3c)$$

where K_i with $i = 1,...13$ are the reaction constants.

In some particular hypothesis, the time evolution of the concentrations, found as a solution of the system of coupled equations, describing vacancy-interstitial annihilation, interstitial migration to sinks, divacancy formation as well as interstitial impurity complex formation (one impurity complex) can be solved analytically and this study is developed in the paper published in *Nuclear Instruments and Methods in Physics Research B 183, 383-390 (2001).*

Vacancy-interstitial annihilation, interstitial migration to sinks, vacancy-impurity complex (VP, VO and V_2O), and divacancy formation were considered in different irradiation conditions, for different concentrations of impurities in the initial semiconductor material and at different temperatures of irradiation are investigated in the paper *Physica Scripta. Vol. 66, 125-132, 2002.* In addition, the effects of carbon impurity in the annealing processes are explicitly studied in the paper *Nuclear Instruments and Methods in Physics Research B (in press).* The correlation between the initial material parameters, temperature, irradiation and annealing history is investigated in detail in the paper "Microscopic modelling of defects production and their annealing after irradiation in silicon for HEP particle detectors" *presented to RESMDD'2002 Florence, July 2002 and which will be published in Nucl. Instr. Meth. Phys. Res. A.*

The model predictions could be a useful clue in obtaining harder materials for detectors at the new generation of accelerators or for space missions. In the paper "Long-term damage induced by hadrons in silicon detectors for uses at the LHC-accelerator and in space missions", accepted to Physica Scripta and which will be published in 2003, some predictions about the structural silicon modifications as well as the expected leakage current of the detectors after long time operation in these radiation conditions are done.

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Nuclear Instruments and Methods in Physics Research B 183, 383-390 (2001)

Annealing of radiation induced defects in silicon in a simplified phenomenological model

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Abstract

The concentration of primary radiation induced defects has been previously estimated considering both the explicit mechanisms of the primary interaction between the incoming particle and the nuclei of the semiconductor lattice, and the recoil energy partition between ionisation and displacements, in the frame of the Lindhard theory. The primary displacement defects are vacancies and interstitials, that are essentially unstable in silicon. They interact via migration, recombination, annihilation or produce other defects.

In the present work, the time evolution of the concentration of defects induced by pions in medium and high resistivity silicon for detectors is modelled, after irradiation. In some approximations, the differential equations representing the time evolution processes could be decoupled. The theoretical equations so obtained are solved analytically in some particular cases, with one free parameter, for a wide range of particle fluences and/or for a wide energy range of the incident particles, for different temperatures; the corresponding stationary solutions are also presented.

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1. Introduction

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 [1] are used in relation to defects.

Vacancies and interstitials are produced in materials exposed to radiation in equal quantities; they are the primary radiation defects, being produced either by the incoming particle, or as a consequence of the subsequent collisions produced by the primary recoil.

In previous papers [2, 3], we calculated the concentration of radiation induced primary defects (CPD) in semiconductors exposed to hadron irradiation. Due to the important weight of annealing processes, as well as to their very short time scale, CPD is not a measurable physical quantity.

In silicon, vacancies and interstitials are essentially unstable and interact via migration, recombination, annihilation or produce other defects.

The problem of the annealing of radiation induced defects in semiconductor materials is not new. Several models, empirical or more theoretic, have been previously proposed to explain these phenomena. Damask and Dienes developed, in the sixties, a theoretical model that considers, as distinct cases, the kinetics of vacancy-interstitial annihilation with interstitial trapping at impurities [4], of vacancy-interstitial annihilation with interstitial trapping at impurities [5], and of vacancy-interstitial annihilation with diinterstitial formation [6]. In the first two cases, analytical solutions have been obtained by the authors, while in the last case only numerical solutions are possible. The escape of interstitials and vacancies from clusters and their subsequent interactions have been modelled by Tsveybak et al. [7]. Phenomenological approaches of the annealing could be found in Moll et al. [8] and Bates and co-workers [9] and references cited therein.

Most of the old studies were dedicated to electronic devices, made from low resistivity (in the Ωcm range) silicon. Recently, the behaviour of the silicon material with medium and high resistivity (tens Ωcm - kΩcm) in intense hadron fields started to present very much interest, these materials representing a major option for the detectors at the new generation of particle colliders and for space applications.

In the present paper, the time evolution of the concentration of primary defects induced by pion irradiation in silicon is studied in the frame of a simplified phenomenological model based on direct interactions between the primary induced defects and the impurities present in the material.

2. Equations for the kinetics of radiation induced defects. General formulation

The starting hypothesis of the physical model is that the irradiation process is unique at the determined particle fluence, and that the time of irradiation is shorter that all characteristics times of annealing.

In the frame of the model, equal concentrations of vacancies and interstitials are supposed to be produced by irradiation, in much greater concentrations than the corresponding thermal equilibrium values, characteristic to each temperature. Both the pre-existing defects and those produced by irradiation, as well as the impurities, are assumed to be randomly distributed in the solid. An important part of the vacancies and interstitials annihilate. The sample contains certain concentrations of impurities which can trap interstitials and vacancies respectively, and form stable defects.

In the present paper, vacancy-interstitial annihilation, interstitial migration to sinks, vacancy and interstitial impurity complex formation as well as divacancy formation are considered. The sample could contain more impurities that trap vacancies or interstitials, and in this case all processes are to be taken into account.

The following notations are used: V - monovacancy concentration; I - free interstitial concentration, J_1 - total impurity "1" concentration (impurity "1" traps interstitials and forms the complex C_1); C_1 - interstitial-impurity concentration: one interstitial trapped for one complex formed; J_2 - total impurity "2" concentration (impurity "2" traps vacancies and forms the complex C_2); C_2 - vacancy-impurity concentration: one vacancy trapped for one complex formed; V_2 - divacancy concentration. All concentrations are expressed as atomic fractions.

The chemical scheme for reaction rates has been used, and the differential equations corresponding to the above picture are:

$$\frac{dV}{dt} = -K_1 VI - K_5 V(J_{20} - C_2) + K_6 C_2 - K_7 V^2 + K_8 V_2 \tag{1}$$

$$\frac{dI}{dt} = -K_1VI - K_2I - K_3I(J_{10} - C_1) + K_4C_1 \quad (2)$$

$$\frac{dC_1}{dt} = K_3I(J_{10} - C_1) - K_4C_1 \quad (3)$$

$$\frac{dC_2}{dt} = K_5V(J_{20} - C_2) - K_6C_2 \quad (4)$$

$$\frac{dV_2}{dt} = \frac{1}{2}K_7V^2 - \frac{1}{2}K_8V_2 \quad (5)$$

The bimolecular recombination law of interstitials and vacancies is supposed to be a valid approximation for the present discussion, because at the concentrations of vacancies of interest, only a small fraction of defects anneal by correlated annihilation if their distribution is random (see the discussion in [10]).

If N is the total defect concentration, expressed as atomic fraction:

$$N = V + I + 2V_2 + C_1 + C_2 \quad (6)$$

then it satisfies the differential equation:

$$\frac{dN}{dt} = -2K_1VI \quad (7)$$

The initial conditions, at $t = 0$, are: at the end of the irradiation, there are equal concentrations of interstitials and vacancies: $I_0 = V_0$; the concentrations of impurities are J_{10} and J_{20} respectively, there are no complexes in the sample: $C_{10} = C_{20} = 0$ and no divacancies $V_{20} = 0$.

The reaction constants K_1 (corresponding to vacancy - interstitial annihilation), and K_3 (related to complex formation by interstitials) are determined by the diffusion coefficient of the interstitial atom to a substitutional trap, and therefore $K_1 = K_3$:

$$K_1 = 30\upsilon \exp(-E_{i1} / k_BT) \quad (8)$$

where E_{i1} is the activation energy of interstitial migration and υ the vibrational frequency. The reaction constant K_2 (related to interstitial migration to sinks) is proportional to the sink concentration α:

$$K_2 = \alpha \cdot \upsilon \cdot \lambda^2 \exp(-E_{i1} / k_BT) \quad (9)$$

with λ the jump distance.

K_4 characterises the decomposition of a complex into an impurity and an interstitial, and is given by:

$$K_4 = 5\upsilon \exp\left(-\frac{E_{i1} + B_1}{k_BT}\right) \quad (10)$$

K_5 and K_6 describe the formation and decomposition of vacancy - impurity complexes, while K_7 and K_8 the formation and decomposition of divacancies, and are given by:

$$K_5 = 30\upsilon \exp(-E_{i2} / k_BT) \quad (11)$$

with E_{i2} the activation energy for vacancy migration;

$$K_6 = 5\upsilon \exp\left(-\frac{E_{i2} + B_2}{k_BT}\right) \quad (12)$$

$$K_7 = 30\upsilon \exp(-E_{i2} / k_BT) \quad (13)$$

$$K_8 = 10\upsilon \exp\left(-\frac{E_{i2} + B_3}{k_BT}\right) \quad (14)$$

where B_1 is the binding energy of C_1, B_2 the binding energy of C_2, and B_3 is the corresponding binding energy of divacancies.

Due to the mathematical difficulties to solve analytically the complete differential equation system, some simplifications are necessary.

3. Hypothesis, approximations and discussions

The interstitials are much more mobile in silicon in respect to vacancies, and are characterised by an activation energy of migration a factor of 2 times smaller.

This difference between the activation energies E_{i1} and E_{i2} respectively justifies the introduction of two time scales, and the separate study of the processes involving interstitials and vacancies respectively. In the first stage, vacancy interstitial annihilation and interstitials migration to sinks are studied. The concentration of interstitials decays much rapidly than the concentration of vacancies. A cut-off condition for I is imposed (a p times decrease of interstitial concentration, p being an adjustable parameter of the model). The vacancy concentration determined by this procedure is the initial value for the processes comprised in the second stage, and will be denoted by $V_{initial}$. The formation of complexes by vacancies is considered less important, and is neglected in the following discussion.

So, for the "first stage", after some simple manipulations, from (1) and (2), the equation:

$$\frac{dI}{dV} = 1 + \frac{K_2}{K_1 V} \tag{15}$$

has been obtained, with the solution:

$$I = V + \frac{K_2}{K_1} \log \frac{V}{V_0} \tag{16}$$

and:

$$t = \frac{\log\left[1 + \frac{K_1 V(t)}{K_2 \log(V(t))}\right]}{K_2 \log(V(t))} \tag{17}$$

Imposing the cut-off condition for the concentration of interstitials, both $V_{initial}$ and the characteristic time could be found. As specified, $V_{initial}$ is used as initial vacancy concentration for the second step in the analysis, where the equations (4) and (5) are considered. $V_{initial}$ depends on V_0 and p, and it is temperature independent. This system of equations, expressing the kinetics of divacancy and vacancy-impurity formation, have no analytical solution. These processes are governed by the initial concentrations of vacancies and impurities, and by the temperature.

If the impurity that traps vacancies is phosphorus, the limiting cases correspond to low initial doping concentration (medium and high resistivity, uncompensated materials) and very high impurity concentration (low resistivity), respectively. In both cases the equations could be decoupled, and analytical solutions are possible.

So, if the formation of vacancy-impurity complexes is not so important, the main process responsible for the decay of vacancy concentration is divacancy production. In this case, the time evolution of the vacancy concentration is described by the equation:

$$V(t) = \frac{1}{4K_7}\left\{ -K_8 + R\,\frac{\frac{K_8 + 4K_7 V_i}{R} + \tanh\left(\frac{tR}{4}\right)}{1 + \frac{K_8 + 4K_7 V_i}{R}\tanh\left(\frac{tR}{4}\right)} \right\} \tag{18}$$

where:

$$R \equiv \sqrt{K_8\left(K_8 + 8K_7 V_i\right)} \tag{19}$$

while the increase of the divacancy concentration is given by:

$$V_2(t)=\frac{V_{initial}-V(t)}{2} \tag{20}$$

The stationary solution for $V(t)$ is given by:

$$\lim_{t\to\infty}V(t)=\frac{1}{4K_7}\cdot(R-K_8) \tag{21}$$

For n-type highly doped Si, vacancy-impurity complex formation is the most probable process. If J_0 is the initial concentration of impurities, and the initial concentration of complexes is zero, than:

$$V(t)=\frac{1}{2K_5}\left\{-K_6+K_5(V_i-J_0)+R^*\frac{\frac{K_6+K_5(V_i+J_0)}{R^*}+\tanh\left(\frac{tR^*}{2}\right)}{1+\frac{K_6+K_5(V_i+J_0)}{R^*}\tanh\left(\frac{tR^*}{2}\right)}\right\} \tag{22}$$

with:

$$R^*\equiv\sqrt{K_6^2+K_5^2(V_i-J_0)^2+2K_5K_6(V_i+J_0)} \tag{23}$$

and with the stationary solution:

$$\lim_{t\to\infty}V(t)=\frac{1}{2K_5}\left[K_5\cdot(V_i-J_0)+R^*-K_6\right] \tag{24}$$

and

$$C=V_{initial}-V \tag{25}$$

4. Results and physical interpretations

In Figure 1, the absolute value of the concentration of primary defects per unit fluence (CPD) induced by pions in silicon is presented as a function of the kinetic energy of the particle. This curve has been obtained in the hypothesis listed in references [11, 12]. In the kinetic energy range between 100 to 300 MeV, pion - nucleus interaction is resonant in all waves, the Δ_{33} resonance is produced and a pronounced maxima in the CPD is observed at approximately 150 MeV followed by a slight monotonic decrease at higher energies. Some local maxima are also presents at high energies, but with less importance.

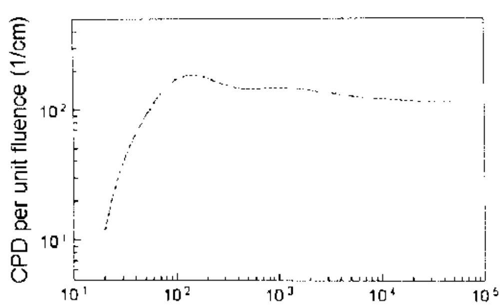


Figure 1

Energy dependence of the absolute value of the concentration of primary defects per unit fluence induced by pions in silicon.

The process of partitioning the energy of the recoil nuclei (produced due the interaction of the incident particle with the nucleus, placed in its lattice site) in new interaction processes, between electrons (ionisation) and atomic motion (displacements) has been considered in the frame of the Lindhard theory.

The CPD multiplied by the fluence is the initial value of the concentration of vacancies and interstitials, and in the forthcoming discussion it is expressed, as specified, as atomic fraction. Without loss of generality, will shall consider that the primary defects are produced by 150 MeV kinetic energy pions.

The following values of the parameters have been used: $E_{i1} = 0.4$ eV, $E_{i2} = 0.8$ eV, $B_1 = 0.2$ eV, $B_2 = 0.2$ eV, $B_3 = 0.4$ eV, $\upsilon = 10^{13}$ Hz, $\lambda^2 = 10^{15}$ cm^2, $\alpha = 10^{10}$ cm^{-2}. The value of the parameter p is taken 100.

The time evolution of the concentration of vacancies, normalised to the concentration of vacancies created by irradiation is represented in Figure 2. Fluences in the range 10^{11} - 10^{15} pions/cm^2 have been considered. The weight of the annihilation process in respect to interstitial migration to sinks increases abruptly with the fluence. At low fluences, up to 10^{11} pions/cm^2, the annihilation has a low importance. With a good approximation, it could be considered that after 0.2 sec. after irradiation the vacancy concentration is saturated. As could be seen from the figure, observable effects in V/V_0 appear for fluences higher than 10^{12} pions/cm^2. Experimentally, for silicon particle detectors irradiated with hadrons, some modifications in the electrical characteristics have been observed in the fluence range 10^{12} - 10^{13} cm^{-2}. [13, 14].

All the curves correspond to room temperature (20 °C) annealing.

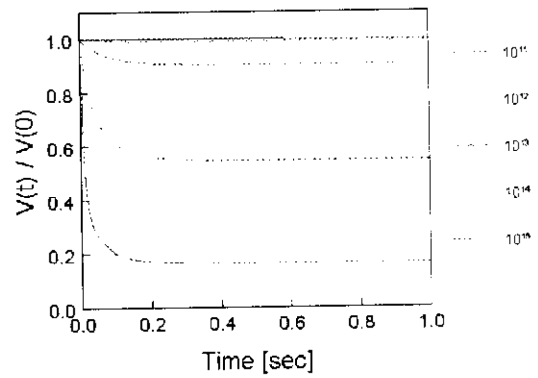


Figure 2
Concentration of vacancies created by irradiation versus time, normalised to the concentration of vacancies for the first stage, for different particle fluences, expressed in cm^{-2}.

The interval of time after which the concentration of interstitials decreases p times, given by eq. (17) with $V(t) = V_{initial}$ is a characteristic time of the processes in the first stage, and depends on temperature and fluence.

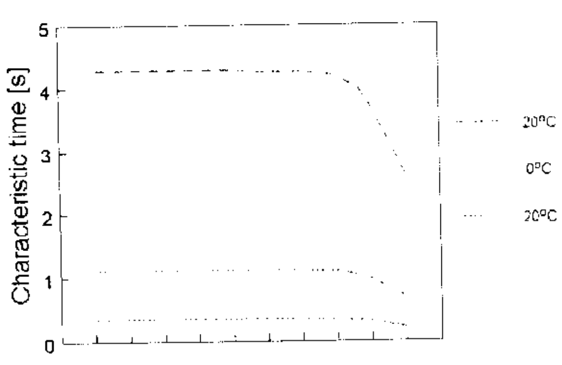


Figure 3
Characteristic time of the first stage versus the irradiation fluence, for -20 °C 0 °C and +20 °C temperature.

In Figure 3, this characteristic time is represented as a function of fluence, in the fluence range 10^{11} - 10^{15} pions/cm^2, for three temperatures of interest for high energy physics applications: -20^0, 0^0 and +20^0 C. It may be seen that, up to 10^{13} pions/cm^2, the characteristic time is independent on the fluence, and for higher fluences a decrease of the characteristic time is to be noted and a fluence dependence is obtained.

The initial concentration of vacancies for the second stage is $V_{initial}$ previously calculated. The second stage starts at a time equal to the characteristic time.

Two limiting cases have been studied, low doping concentration (high resistivity uncompensated material), and low resistivity, phosphorus doped silicon. The formation and decomposition of divacancies is a good approximation for the first, while the second is related to V-P complexes.

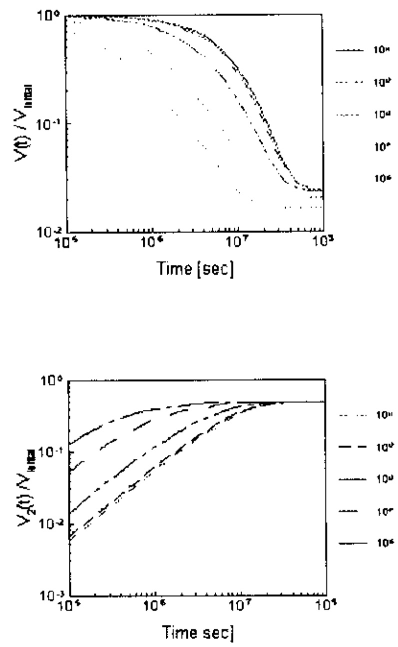


Figure 4

a) Time evolution of the concentration of vacancies, normalised to the concentration of vacancies remained after the first stage when divacancy formation and decomposition are considered, for different particle fluences, expressed in cm^{-2}. b)Same as Figure 4a) for the concentration of divacancies.

The time evolution of the concentration of vacancies when divacancy formation is considered is illustrated in Figure 4a. As underlined in Section 3, the time scale of this process is much longer in respect to the first stage. The origin of time in Figure 4a is the beginning of the second stage, this means a characteristic time after the start of the annealing.

The curves in this figure are normalised to the concentration of vacancies remained after the first stage. Values of the initial concentrations of vacancies that correspond to fluences in the same range as in the previous analysis have been considered. It could be observed that the time after which $V(t)/V_{initial}$ saturates is in the range 10^7 - 10^8 sec., and increases with the irradiation fluence. All curves have been calculated also for 20^0 C temperature.

The time evolution of divacancy concentration is represented in Figure 4b, also in a similar manner with the vacancy concentration in Figure 4a.

The case of high initial impurity (phosphorus) concentration, where divacancy formation is neglected in respect to complex formation, is presented in Figures 5a and 5b respectively.

Three initial concentrations for phosphorus in silicon (expressed as atomic fractions) have been considered: 10^{-5}, 10^{-7}, and 5 10^{-10}, corresponding to 0.1 Ωcm, 10 Ωcm, and 1 kΩcm resistivity respectively. The time evolution of the concentration of vacancies is represented in Figure 5a, while the corresponding one for the concentration of complexes in Figure 5b, both normalised to the concentration of vacancies remained after the first stage. An irradiation with 10^{13} pions/cm^2 has been considered.

The origin of time in Figures 5a and 5b is displaced in respect with the origin of the annealing, in the same way as in Figs. 4a and b.

The curves corresponding to 10^{11} - 10^{15} cm^{-2} are superimposed on the same curve, with the exception of the tail at times longer than 10^4 sec. where the values corresponding to higher fluences are slightly higher.

The time interval after which $V(t)/V_{initial}$ saturates is shorter than in the case of divacancy, and at room temperature is in the range 10^3 - 10^4 sec for the doping concentrations considered. It shortens with the increase of impurity concentration.

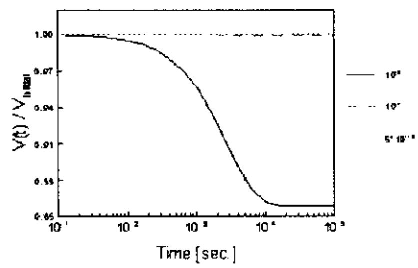
Some explicit considerations might be made about the formation of vacancy-impurity complexes. The mechanisms supposed above can be used both for boron and for phosphorus impurities. In this case, the corresponding processes are:

$$B_i + V \rightarrow [B_i - V] \qquad (26)$$

and respectively:

$$P_s + V \rightarrow [P_s - V] \qquad (27)$$

While the complex formed by boron is unstable and self anneals bellow room temperature, the interaction between a V and a P_s leads to the formation of an E centre which is stable in the same conditions [7].



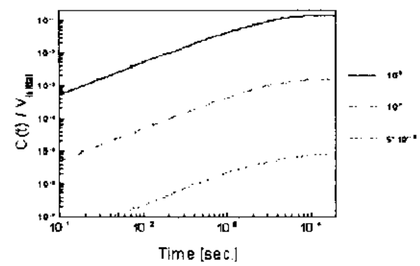


Figure 5
a)Time evolution of the concentration of vacancies, normalised to the concentration of vacancies remained after the first stage when V-P complex formation and decomposition are considered. The three curves correspond to different initial impurity concentrations, expressed in atomic fractions. b)Same as Figure 5a) for the concentration of complexes

Interactions between interstitial oxygen (another very studied impurity in the last time) and free vacancies is described as a higher order process (third order in reference [7] and fourth power in [15]). If the process is stopped as a first order one, the time evolution of the concentrations is not different from the case of phosphorus, studied before.

If two or more impurities that trap vacancies are considered as existing simultaneously in silicon, the system of coupled equations must be solved. Only numerical solutions for particular cases are possible.

So, in the frame of this model, three characteristic times have been found or 20 °C self annealing in silicon: one in the order of 0.2 sec., corresponding to vacancy - interstitial annihilation and interstitial migration to sinks, one around 10^4 sec, related to vacancy-phosphorous formation and decomposition, and another one around 10^7 sec, divacancy related.

The present model could be applied to the annealing of primary radiation defects induced in Si by any other hadron, the difference coming from the value of the CPD.

Experimentally, some material characteristics have been measured after irradiation. The effects of self annealing have been estimated phenomenologically, deconvoluting the radiation induced changes in the measured characteristics using an empirical parametrisation with a sum of exponential decreasing functions, corresponding to different possible annealing mechanisms [16, 17].

In spite of the great variability of material and irradiation characteristics (particles, energies), the present model predictions are in general agreement with the experimental results, and suggest a possible connection with the self annealing mechanisms. In the same time, this confirm the validity of the introduced hypothesis in the model.

5. Summary

The time evolution of the primary concentration of defects induced by pions after irradiation process has been modelled.

In this model, vacancy-interstitial annihilation, interstitial migration to sinks, vacancy and interstitial impurity complex formation as well as divacancy formation have been considered. In the considered hypothesis, the time evolution of impurity concentrations has been decoupled into two steps, the first one involving vacancy-interstitial annihilation and interstitial migration to sinks, the second vacancy-complex and divacancy formation.

The equations corresponding to the first step have been solved analytically for a wide range of particle fluences and for a wide energy range of incident particles, and for three different temperatures: $-20^0 C$, $0^0 C$ and $+20^0 C$.

The approximations that permit to decouple the differential equations representing the time evolution processes in the second step have been studied, and the processes have been treated separately. The simultaneous consideration of more processes in this last step of the model is possible only numerically.

The predictions of the model are in general agreement with the experimental results, and suggest a possible connection with the self annealing mechanisms.

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Radiation defects in silicon due to hadrons and leptons, their annealing and influence on detector performance

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Abstract

A phenomenological model was developed to explain quantitatively, without free parameters, the production of primary defects in silicon after particle irradiation, the kinetics of their evolution toward equilibrium and their influence on detector parameters. The type of the projectile particle and its energy is considered in the evaluation of the concentration of primary defects. Vacancy-interstitial annihilation, interstitial migration to sinks, vacancy - impurity complexes (VP, VO, V_2O), and divacancy (V_2) formation are taken into account in different irradiation conditions, for different concentrations of impurities in the semiconductor material, for 20 and 0°C. The model can be extended to include other vacancy and interstitial complexes. The density of the reverse current in the detector after irradiation is estimated. Comparison with experimental measurements is performed. A special application considered in the paper is the modelled case of the behaviour of silicon detectors operating in the pion field estimated for the LHC accelerator, under continuum generation and annealing.

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1. Introduction

The use of silicon detectors in high radiation environments, as to be expected in future high energy accelerators, poses severe problems due to changes in the properties of the material, and consequently influences the performances of detectors.

The incident particle, hadron or lepton, interacts with the electrons and with the nuclei of the semiconductor lattice. It losses its energy in several processes, which depend on the nature of the particle and on its energy. The effect of the interaction of the incident particle with the target atomic electrons is ionisation, and the characteristic quantity for this process is the

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energy loss or stopping power. The nuclear interaction between the incident particle and the lattice nuclei produces bulk defects and this phenomenon is studied in the present paper. As a result of this interaction, if the primary projectile is a particle, one or more light particles are formed, and usually one (or more) heavy recoil nuclei. This recoil nucleus has charge and mass numbers equal or lower than that of the medium. After this first interaction, the recoil nucleus or nuclei are displaced from the lattice positions into interstitials. Then, the primary knock-on nucleus, if its energy is large enough, can produce the displacement of a new nucleus, and the process continues as long as the energy of the colliding nucleus is higher than the threshold for atomic displacements. We denote these displacement defects, vacancies and interstitials, as primary defects, prior to any further rearrangement.

In silicon these defects are essentially unstable and interact via migration, recombination, annihilation or produce other defects.

As a consequence of the degradation to radiation of the semiconductor material, an increase of the reverse current due the reduction of the minority carrier lifetime, a reduction of the charge collection efficiency and a modification of the effective doping, due to the generation of trapping centres, are observed in the detector characteristics.

In this paper, for the first time, a phenomenological model was developed to explain quantitatively, without free parameters, the mechanisms of production of the primary defects during particle irradiation, the kinetics of their evolution toward stable defects and equilibrium and the influence of the defects on detector parameters. The effects of the incident particle type, of its kinetic energy and of the irradiation conditions on the concentration of defects are studied. Vacancy-interstitial annihilation, interstitial migration to sinks, vacancy - impurity complexes (VP, VO and V_2O), and divacancy (V_2) formation are considered in different irradiation conditions, for different concentrations of impurities in the semiconductor material and at different temperatures near room temperature. The model can be extended directly to include the effects of other mechanisms related to these, or other impurities in silicon, and of their interaction with the vacancy and/or interstitial. The density of the reverse current in the detector after irradiation is estimated. Comparison with experimental published data of the time evolution of the concentration of defects is performed, as well as with measurements of the density of the leakage current. For different discrepancies, some explanations are suggested. A special application considered in the paper is the simulated case of the behaviour of silicon detectors operating in the pion field simulated for the future conditions at the new LHC (Large Hadron Collider) accelerator.

2. Production of primary defects

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 [1] are used in relation to defects.

The basic assumption of the present model is that vacancies and interstitials are produced in materials exposed to radiation in equal quantities, uniformly in the bulk of the sample. They are the primary radiation defects, being produced either by the incoming particle, or as a consequence of the subsequent collisions of the primary recoil in the lattice.

The concentration of the primary radiation induced defects per unit fluence (CPD) in the semiconductor material has been calculated using the explicit formula (see details, e.g. in references [2, 3]):

$$CPD(E) = \frac{N_{Si}}{2E_{Si}} \int \sum_i \left(\frac{d\sigma}{d\Omega}\right)_{i;Si} L(E_{Ri})_{Si} \, d\Omega = \frac{1}{N_A} \cdot \frac{N_{Si} A_{Si}}{2E_{Si}} \cdot NIEL(E) \quad (1)$$

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} - the average threshold energy for displacements in the semiconductor, E_{Ri} - the recoil energy of the residual nucleus produced in interaction i, $L(E_{Ri})$ - the Lindhard factor that describes the partition of the recoil energy between ionisation and displacements and $\left(d\sigma/d\Omega\right)_i$ - 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). It is important to observe that there exists a proportionality between the CPD and NIEL only for monoelement materials.

For CPD produced by pions, the pion - silicon interaction has been modelled [4] and the energy dependencies of the Lindhard factors have been calculated in the frame of analytical approximations for different recoils in Si [5].

The concentration of primary defects produced by protons, neutrons, electrons and photons have been obtained from the NIEL. The calculations of Summers and co-workers for proton and electron NIEL in silicon from reference [6], the calculations of proton, electron and photon NIEL of Van Ginneken [7] as well as those of Ougouang for neutrons [8] have been considered.

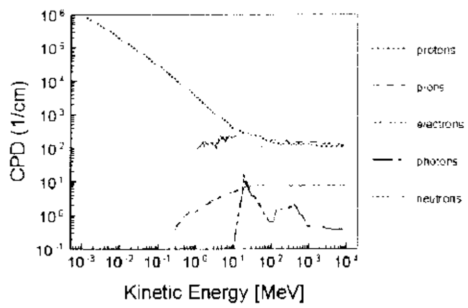

Figure 1
Energy dependence of the concentration of primary defects on unit fluence induced by protons, pions, electrons, photons and neutrons in silicon - see text for details.

In Figure 1, the dependence of the CPD on the particle kinetic energy is presented: for pions, our calculations from reference [9] have been used; for protons, in the energy range 10^{-3} - 1 MeV the calculations of Summers, in the range 1 - 200 MeV the average between those of Summers and of Van Ginneken, while in the range 200 - 10000 MeV, Van Ginneken's. The curve for electrons uses, up to 1 MeV only the values from reference [6], in the range 1 - 200 MeV an average between the values from references [6] and [7], and after 200 MeV only from [7]. The curves for photons and neutrons are calculated from Van Ginneken's [7] and Ougouang's [8] respectively.

The main source of errors in the calculated concentration of defects comes from the modelling of the particle - nucleus interaction and from the number and quality of the experimental data available for these processes.

Due to the important weight of annealing processes, as well as to their very short time scale, CPD is not a measurable physical quantity.

In silicon, vacancies and interstitials are essentially unstable and interact via migration, recombination, annihilation or produce other defects.

3. The kinetics of radiation induced defects

In the frame of the model, equal concentrations of vacancies and interstitials are supposed to be produced by irradiation, in much greater concentrations than the corresponding thermal equilibrium values, characteristic to each temperature. Both the pre-existing defects and those produced by irradiation, as well as the impurities, are assumed to be randomly distributed in the solid. An important part of the vacancies and interstitials annihilate. The sample contains certain concentrations of impurities which can trap interstitials and vacancies respectively, and form stable defects.

In the present paper, vacancy-interstitial annihilation, interstitial migration to sinks, divacancy and vacancy impurity complex formation (VP, VO, V_2O), are considered. The mechanisms of formation of higher order defects involving vacancy and oxygen can be added, as well as the effects of other impurities, e.g. carbon.

This picture could be described in terms of chemical reactions by the kinetic scheme:

$$V + I \underset{G}{\overset{K_1}{\rightleftarrows}} 0 \qquad (2)$$

$$I \xrightarrow{K_2} sinks \qquad (3)$$

$$V + O \underset{K_4}{\overset{K_3}{\rightleftarrows}} VO \qquad (4)$$

(VO is the A centre).

$$V + P \underset{K_6}{\overset{K_5}{\rightleftarrows}} VP \qquad (5)$$

(VP is the E centre).

$$V + V \underset{K_8}{\overset{K_7}{\rightleftarrows}} V_2 \qquad (6)$$

$$V + A \underset{K_{10}}{\overset{K_9}{\rightleftarrows}} V_2O \qquad (7)$$

The bimolecular recombination law of interstitials and vacancies is supposed to be a valid approximation for the present discussion, because at the concentrations of vacancies of interest, only a small fraction of defects anneals by correlated annihilation if their distribution is random (see the discussion in reference [10]).

The multivacancy oxygen defects as, e.g. V_3O, V_2O_2, V_3O_2, V_3O_3, are not considered in the model.

The reaction constant K_1 (corresponding to vacancy - interstitial annihilation) is determined by the diffusion coefficient of the interstitial atom to a substitutional trap:

$$K_1 = 30\upsilon \exp\left(-E_{i1} / k_B T\right) \quad (8)$$

where E_{i1} is the activation energy of interstitial migration and υ the vibrational frequency. The reaction constant K_2 (related to interstitial migration to sinks) is proportional to the sink concentration α:

$$K_2 = \alpha \cdot \upsilon \cdot \lambda^2 \exp\left(-E_{i1} / k_B T\right) \quad (9)$$

with λ the jump distance.

Lee and Corbett [11] argue that divacancies, vacancy-oxygen and divacancy-oxygen centres are equally probable below 350^0 C; thus, K_3, K_5, K_7 and K_9, that describe the formation of vacancy - impurity complexes and of divacancies, are determined by the activation energy of vacancy migration, E_{i2} and are given by:

$$K_3 = K_5 = K_7 = K_9 = 30\upsilon \exp\left(-E_{i2} / k_B T\right) \quad (10)$$

while K_4, K_6, K_8 and K_{10} are related to the activation energies of dissociation of the A, E, V_2 and V_2O centres respectively.

$$K_4 = 5\upsilon \exp\left(-\frac{E_A}{k_B T}\right) \quad (11)$$

$$K_6 = 5\upsilon \exp\left(-\frac{E_E}{k_B T}\right) \quad (12)$$

$$K_8 = 5\upsilon \exp\left(-\frac{E_{V_2}}{k_B T}\right) \quad (13)$$

$$K_{10} = 5\upsilon \exp\left(-\frac{E_{V_2O}}{k_B T}\right) \quad (14)$$

where E_A, E_E, E_{V_2} and E_{V_2O} are the dissociation energies of the A, E, V_2 and V_2O complexes respectively.

G is the generation rate of vacancy-interstitial pairs, and is given by the product of CPD by the irradiation flux. Thermal generation is neglected, this approximation corresponding to high irradiation fluxes.

In the simplifying hypothesis of random distribution of CPD for all particles, two different particles can produce the same generation rate for vacancy-interstitial pairs.

$$G = \left|(CPD)_{part\,a}(E_1)\right| \times \Phi_{part\,a}(E_1) = \left|(CPD)_{part\,b}(E_2)\right| \times \Phi_{part\,b}(E_2) \quad (15)$$

is fulfilled.

Here, Φ is the flux of particles (a) and (b) respectively, and E_1 and E_2 their corresponding kinetic energies.

The system of coupled differential equations corresponding to the reaction scheme (2) ÷ (7) cannot be solved analytically.

The following values of the parameters have been used: E_{i1} = 0.4 eV, E_{i2} = 0.8 eV, E_A = 1.4 eV, E_E = 1.1 eV, E_{V_2} = 1.3 eV, E_{V_2O} = 1.6 eV, $\upsilon = 10^{13}$ Hz, $\lambda = 10^{15}$ cm^2, $\alpha = 10^{10}$ cm^{-2}.

Defect concentrations, as well as their time evolution, have been calculated solving numerically the system of coupled differential equations.

We would like to underline the specific importance of the irradiation and annealing history (initial material parameters, type of irradiation particles, energetic source spectra, flux, irradiation temperature, measurement temperature, temperature and time between irradiation and measurement) on defect evolution.

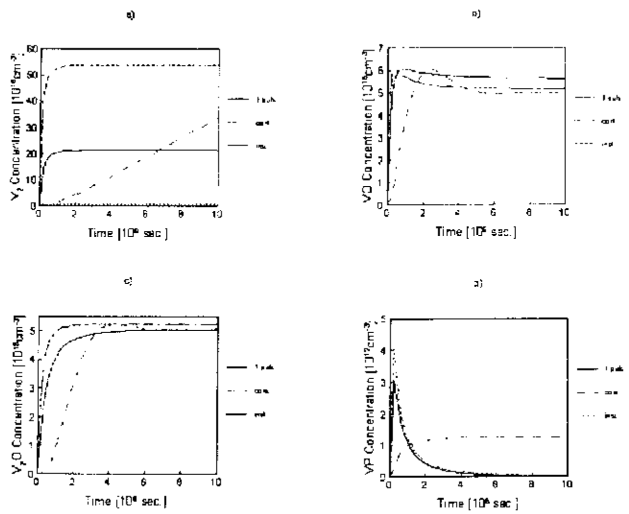

Figure 2

Time dependence of the concentrations of: a) V_2, b) VO, c) V_2O and d) VP, induced in silicon with 10^{14} P/cm^3 and $5{\cdot}10^{16}$ O /cm^3, irradiated with 200 MeV kinetic energy pions, at a total fluence of 10^{15} pions/cm^2 in different irradiation conditions - see text.

In Figures 2a ÷ d, the formation and time evolution of the divacancy, vacancy-oxygen, divacancy-oxygen, and vacancy-phosphorous is modelled in silicon containing the initial concentrations of impurities: 10^{14} P/cm^3 and $5{\cdot}10^{16}$ O /cm^3, and irradiated with pions with about 200 MeV kinetic energy (corresponding to the in their maximum of CPD in the energetic distribution), at a total fluence of 10^{15} pions/cm^2, in different irradiation conditions. The instantaneous irradiation process is an ideal case [12] where the total fluence is received by the material at time $t = 0$, and only the relaxation process is studied. This process supposes that the annealing effects are not present during irradiation. The second case considered is: the irradiation is performed in a single pulse for a $2{\times}10^4$ seconds, followed by relaxation, and the third case is a continuum irradiation process with a generation rate of defects equal with $5{\times}10^{10}$ pions/cm^2/s. In these last two cases, annealing takes place during irradiation. During and after irradiation, the temperature is kept at 293K.

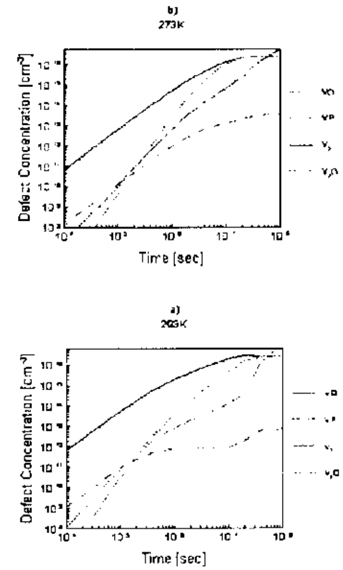

Figure 3

Time dependence of the concentrations of VO, VP, V_2 and V_2O induced in silicon with 10^{14} P/cm^3 and $5{\cdot}10^{16}$ O /cm^3, irradiated with 200 MeV kinetic energy pions a total fluence of 10^{15} pions/cm^2 with the flux esrimated for LHC, for: 293 and 273 K

As expected, after instantaneous irradiation the concentrations of defects are higher in respect with "gradual" irradiation. A special attention must be paid to the formation of VO and V_2O centres, for which the same concentration is attained both in the case of continuous and instantaneous irradiation.

The effect of the decrease of temperature, from 293 to 273 K during irradiation and annealing, is presented in Figures 3a and b. The material contains the same phosphorous and oxygen concentrations as in the modelled case presented in Figure 2, and was irradiated with pions of 200 MeV kinetic energy, receiving continuously a fluence of 10^{15} pions/cm^2 in ten years, in accord to the pions simulated radiation field at LHC [13, 14].

The increase of temperature increases the rate of all defect formation. In the case of VO and VP a plateau in the time dependencies is attained. Only for VP the plateau value is temperature sensitive.

The rate of generation of primary defects in silicon influences the concentrations of all stable defects. In Figure 4 a - c, the time evolution of the concentrations of VO, VP, V_2 and V_2O in silicon with 10^{14} P/cm^3 and $5{\cdot}10^{16}$ O/cm^3, irradiated with pions of 200 MeV with the flux estimated for LHC, 10 and 100 times higher respectively, is presented. It can be observed that at the LHC generation rate for CPD, after $3\text{x}10^7$ seconds an equilibrium is established for the VP complex: its rate of formation equals its rate of dissociation - Fig. 4a. This time is shorter for higher generation rate, as can be observed in Figures 4b and 4c. The value of the plateau concentration for the vacancy-oxygen complex is attained after around the same time as the plateau for the VP concentration, in conditions of the LHC generation rate, and a shorter time, about $2\text{x}10^6$ sec. for a rate hundred times higher than the LHC one. For other defects, as divacancies and divacancy-oxygen, the processes to established the equilibrium are very slow.

The formation of divacancy-oxygen in delayed in respect to vacancy oxygen, and for long exposure times, the same value for the concentration is obtained.

The effect of oxygen in irradiated silicon has been a subject of intensive studies in remote past. 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 [15, 16]. These impurities added to the silicon bulk modify the formation of electrically active defects, thus controlling the macroscopic device parameters. If silicon is enriched in oxygen, the capture of radiation-generated vacancies is favoured by the production of the pseudo-acceptor complex vacancy-oxygen. Interstitial oxygen acts as a sink of vacancies, thus reducing the probability of formation of the divacancy related complexes, associated with deeper levels inside the gap. For this purpose, in the model, the effects of the initial oxygen concentration in silicon was studied. In Figures 5 a, b, c, d the time dependencies of V_2, VO, V_2O and VP are presented, for silicon containing 10^{15}, 10^{16}, 10^{17}, and 10^{18} atoms/cm^3 initial oxygen concentrations.

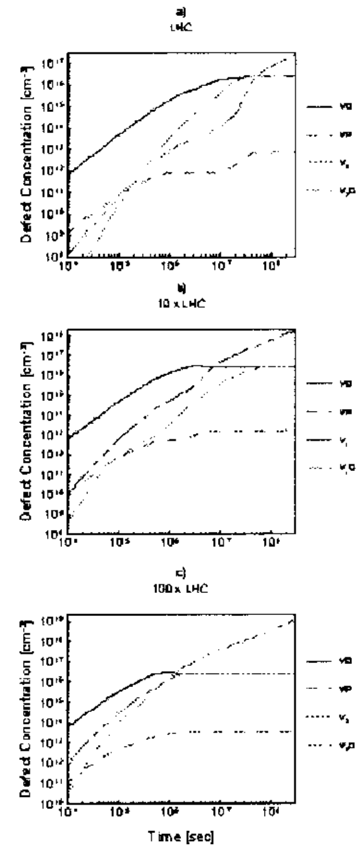

Figure 4
Time dependence of the concentrations of VO, VP, V_2 and V_2O induced in silicon with 10^{14} P/cm^3 and $5{\cdot}10^{16}$ O/cm^3, by continuous irradiation with 200 MeV kinetic energy pions with the flux: :a) estimated for LHC, b) 10 times the flux estimated for LHC, c) 100 times the flux estimated for LHC, at: 293 K

One can observe that vacancy-oxygen formation in oxygen enriched silicon is favoured in respect to the generation of V_2, V_2O and VP, confirming the considered hypothesis, so, for detector applications the leakage current is decreased. At high oxygen concentrations, the concentration of VO centres saturates starting from low fluences.

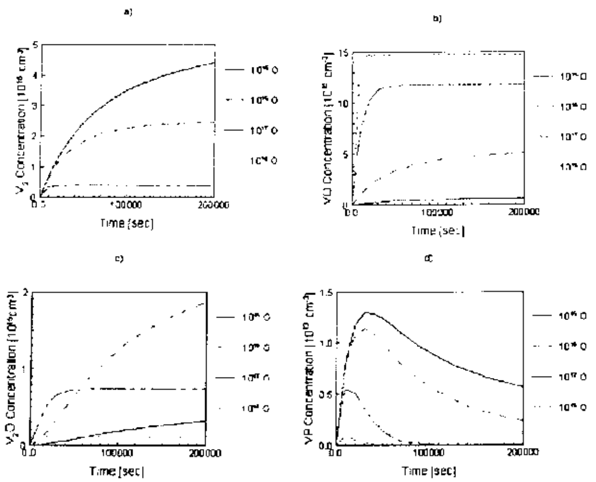

Figure 5
Effect of oxygen doping concentration on the time dependence of the concentrations of: a) V_2, b) VO, c) V_2O and d) VP, induced in silicon with 10^{14} P/cm^3 irradiated with 200 MeV kinetic energy pions at total fluence of 10^{14} pions/cm^2 in one pulse.

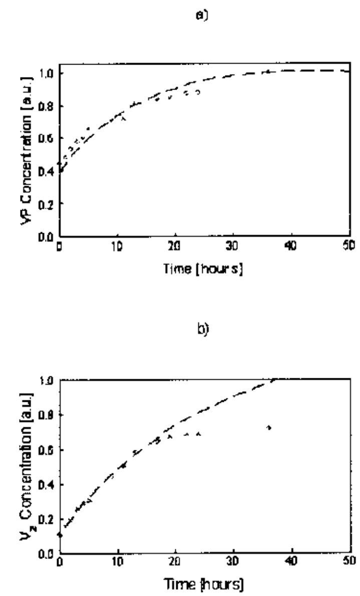

Figure 6
Time dependence of a) VP and b) V_2 concentrations after electron irradiation; points: experimental data from reference [17] and dashed line: model calculations.

A difficulty in the comparison of model predictions with experimental data is the insufficient information in published papers regarding the characterisation of silicon, and on the irradiation (flux, temperature during irradiation and measurement, irradiation time, time and temperature between irradiation and measurement) for most of the data.

For electron irradiation, our simulations are in agreement with the measurements presented in reference [17], where defect concentrations are presented as a function of the time after irradiation. In Figure 6, both measured and calculated dependencies of the VP and V_2 concentrations are given. The irradiation was performed with 2.5 MeV electrons, up to a fluence of 10^{16} cm^{-2}. A good agreement can be observed for the concentration of VP, see Figure 6a, while for the divacancy, Figure 6b, the experimental data attain a plateau faster, and at smaller values than the calculations. The relative values are imposed by the arbitrary units of experimental data.

A good agreement has also been obtained for hadron irradiation. For example, the sum of the calculated VP and V_2 concentrations (8×10^{12} cm^{-3}) induced in silicon by 5.67 10^{13} cm^{-2} 1 MeV neutrons, are in accord with the experimental value by 11.2×10^{12} cm^{-3} reported in reference [18].

4. Correlation with detector parameters

It is well known that the dark current in a $p-n$ junction is composed by three different terms: the diffusion current, caused by the diffusion of the minority charge carriers inside the depleted region; the generation current, created by the presence of lattice defects inside the bulk of the detector; and surface and perimetral currents, dependent on the environmental conditions of the surface and the perimeter of the diode. The appearance of the defects after irradiation corresponds therefore in an increase of the leakage current of the detector by its generational term.

Inside the depleted zone, $n, p << n_i$ (n_i is the intrinsic free carrier concentration), each defect with a bulk concentration N_T causes a generation current per unit of volume of the form [19]:

$$I = qU = q\rangle v_t \langle n_i \frac{\sigma_n \sigma_p N_T}{\sigma_n \gamma_n e^{(E_t - E_i)/kT} + \sigma_p \gamma_p e^{(E_i - E_t)/kT}} \qquad (16)$$

where γ_n and γ_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 $\rangle v_t \langle$ is the average between electron and hole thermal velocities.

In the case of E and A centres and V_2^- and $V_2^=$ defects, the current concentration can be expressed in the simple form:

$$I = q\langle v_t \rangle n_i \frac{\sigma_n}{\sigma_p} N_T e^{(E_t - E_i)/kT} \qquad (17)$$

The primary effect in the recombination process is the change the charge state of the defect. The different charge states of the same deep centre may have different barriers for migration or for reacting with other centres. Thus, carrier capture can either enhance or retard defect migration or particular defect reactions. As a characteristics for detectors (as diode junction), the defect kinetics is dependent to the reverse - bias voltage during the irradiation [20].

The comparison between theoretical and experimental generation current densities after irradiation shows a general accord between experiment and the model results for the lepton irradiation and large discrepancies for the hadron case.

There could be several reasons for the observed discrepancies.

The model hypothesis of defects distributed randomly in semiconductors exclude the possibility of cluster defects. For this case, other mechanisms of defect formation are necessary, which suppose different reaction rates and correlation between the constituent defects of the cluster.

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. In fact, the defects could have more levels, and charge states, as is the case of the divacancy, and also could be coupled, as in the case of clusters. As shown in the literature [21, 22], both cases can produces modifications of the generation rate.

Also the multivacancy oxygen defects as, e.g. V_3O, V_2O_2, V_3O_2, V_3O_3, are not considered in the model.

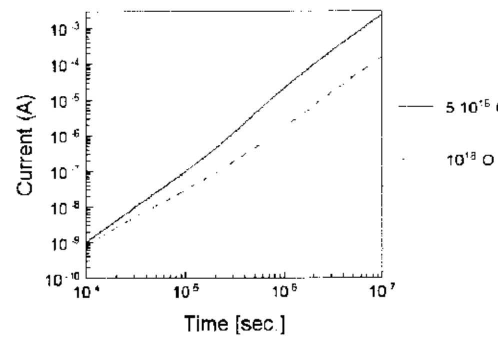

Figure 7
Time dependence of the reverse current after 200 MeV kinetic energy pions irradiation, with the rate estimated for LHC, at 293K, for silicon containing a) 5 10^{16} cm^{-3} and b) 10^{18} cm^{-3} oxygen.

A model estimation of the time dependence of the leakage current, in conditions of continuous irradiations with pions of 200 MeV kinetic energy, in the conditions of the LHC [13, 14] and at 293K is presented in Figure 7, for two concentrations of oxygen in silicon: 5 10^{16} cm^{-3} and 10^{18} cm^{-3}, respectively. As underlined before, oxygen incorporation in silicon has beneficial effects, decreasing the reverse current. This conclusion is valid in the hypothesis of random distribution of defects inside the depleted zone of the p-n junction. These values are probably underestimated.

5. Summary

A phenomenological model that describes silicon degradation due to irradiation, the kinetics of defects toward equilibrium, and the influence on the reverse current of detectors was developed.

The production of primary defects (vacancies and interstitials) in the silicon bulk was considered in the frame of the Lindhard theory, and considering the peculiarities of the particle - silicon nuclei interaction.

The mechanisms of formation of stable defects and their evolution toward equilibrium was modelled, and the concentrations of defects were calculated solving numerically the system of coupled differential equations for these processes. Vacancy-interstitial annihilation, interstitial migration to sinks, vacancy-impurities complexes (VP, VO and V_2O), and divacancy formation were considered in different irradiation conditions, for different concentrations of impurities in the initial semiconductor material and at different temperatures of irradiation. The calculated results suggest the importance of the conditions of irradiation, temperature and annealing history. The model supports the experimental studies performed to investigate the influence of oxygen in the enhancement of the radiation hardness of silicon for detectors. The VO defects in oxygen enriched silicon is favoured in respect to the other stable defects, so, for detector applications it is expected that the leakage current decreases after irradiation. The second result in the model is that at high oxygen concentrations, this defect saturates starting from low fluences.

Most of the model calculations simulates some of the pion field estimated at the new LHC accelerator, where the silicon detector will operate under continuum generation and annealing.

The density of the reverse current in detectors after irradiation is estimated, compared with experimental available data and for discrepancies some explanations are suggested.

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The influence of initial impurities and irradiation conditions on defect production and annealing in silicon for particle detectors

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Abstract

Silicon detectors in particle physics experiments at the new accelerators or in space missions for physics goals will be exposed to extreme radiation conditions. The principal obstacles to long-term operation in these environments are the changes in detector parameters, consequence of the modifications in material properties after irradiation.
The phenomenological model developed in the present paper is able to explain quantitatively, without free parameters, the production of primary defects in silicon after particle irradiation and their evolution toward equilibrium, for a large range of generation rates of primary defects. Vacancy-interstitial annihilation, interstitial migration to sinks, divacancy and vacancy-impurity complex (VP, VO, V_2O, *and* C_iO_i, C_iC_s) formation are taken into account. The effects of different initial impurity concentrations of phosphorus, oxygen and carbon, as well as of irradiation conditions are systematically studied. The correlation between the rate of defect production, the temperature and the time evolution of defect concentrations is also investigated.

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1. Introduction

The use of silicon detectors in high radiation environments, as to be expected in future high energy accelerators or in space missions, poses severe problems due to changes in the properties of the material, and influences the performances of detectors.

As a consequence of the degradation to radiation of the semiconductor material, an increase of the reverse current due the reduction of the minority carrier lifetime, a reduction of the charge collection efficiency and a modification of the effective doping, due to the generation of trapping centres, are observed in the detector characteristics.

In this paper, the effects of irradiation conditions and various initial impurities in the starting material are discussed in the frame of the phenomenological model able to explain quantitatively defect production and evolution toward stable defects during and after irradiation in silicon. The model supposes three steps.

In the first step, the incident particle, having kinetic energies with values 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.

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 ([1] and authors' contributions [2]).

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 [3] 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 mechanisms of interaction of the incident particle with the semiconductor lattice, accompanied by displacement defect production have been discussed in some papers, see, e.g. references [4, 5, 6]. The incident particle produces, as a consequence of its interaction with ions of the semiconductor lattice, cascades of displacements.

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 [7].

Without free parameters, the 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.

The first two steps have been treated extensively in previous papers [4, 5, 6], where the concentration of primary defects has been calculated. In this paper, the third step is discussed extensively and represents a generalisation of the previous results published in references [7, 8] including also the carbon contributions to defect kinetics.

The influence and the effects of different initial impurity concentrations of phosphorus, oxygen and carbon as well as of the irradiation conditions were systematically studied. Vacancy-interstitial annihilation, interstitial migration to sinks, vacancy - impurity complexes (VP, VO, V_2 V_2O C_i, C_iO_i, C_iC_s) - only the stable defects confirmed experimentally in silicon for high energy physics applications were considered. The correlation between the rate of defect productions, the temperature and the time evolution of the defect concentrations was also investigated. Some conclusions about the possibilities to obtain semiconductor materials harder to radiation are given.

2. Production of primary defects

The basic assumption of the present model is that the 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, as a consequence of the subsequent collisions of the primary recoil in the lattice, or thermally (only Frenkel pairs are considered). The generation term (G) is the sum of two components:

$$G = G_R + G_T \tag{1}$$

where G_R accounts for the generation by irradiation, and G_T for thermal generation.

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 [9, 10]):

$$CPD(E)=\frac{N_{Si}}{2E_{Si}}\int\sum_i\left(\frac{d\sigma}{d\Omega}\right)_{i,Si} L(E_{Ri})_{Si}\,d\Omega=\frac{1}{N_A}\cdot\frac{N_{Si}A_{Si}}{2E_{Si}}\cdot NIEL(E) \qquad (2)$$

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} - the average threshold energy for displacements in the semiconductor, E_{Ri} - the recoil energy of the residual nucleus produced in interaction i, $L(E_{Ri})$ - the Lindhard factor that describes the partition of the recoil energy between ionisation and displacements and $\left(d\sigma/d\Omega\right)_i$ - 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 $\left(\frac{dE}{dx}\right)_{n.i.}$ ([3], [11]).

In Figure 1, the kinetic energy dependence of CPD for different particles is presented: for pions the values are calculated in accord with equation (1) and are from reference [12], and for the other particles these are evaluated from the published NIEL calculations, as follows: for protons - reference [6, 13], for neutrons – reference [14], for electrons – reference [6, 13] and for photons from [6].

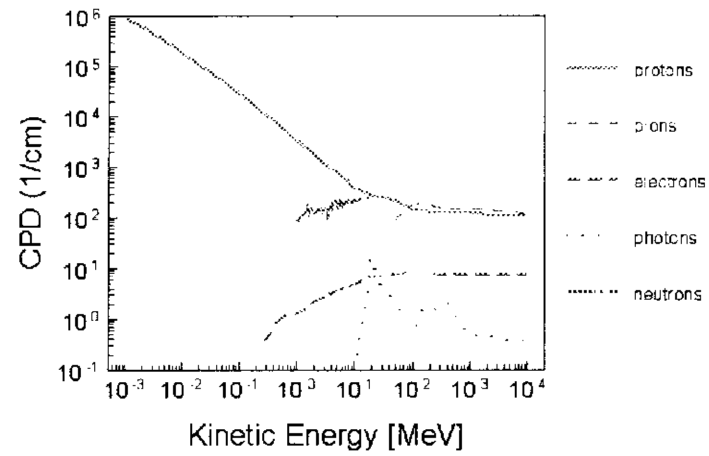

Figure 1
Energy dependence of the concentration of primary defects on unit fluence induced by protons, pions, electrons, photons and neutrons in silicon - see text for details.

The main source of errors in the calculated concentration of primary defects comes from the modelling of the particle - nucleus interaction and from the number and quality of the experimental data available for these processes.

Due to the important weight of annealing processes, as well as to their very short time scale, CPD is not a measurable physical quantity. In silicon, vacancies and interstitials are essentially unstable and interact via migration, recombination, and annihilation or produce other defects.

In the simplifying hypothesis of random distribution of CPD for all particles, used in the present paper, the identity of the particle is lost after the primary interaction, and two different particles could produce the same generation rate (G_R) for vacancy-interstitial pairs if the following condition:.

$$G_R=\left|(CPD)_{part.a}(E_1)\right|\times\Phi_{part.a}(E_1)=\left|(CPD)_{part.b}(E_2)\right|\times\Phi_{part.b}(E_2) \qquad (3)$$

is fulfilled. Here, Φ is the flux of particles of type a and b respectively, and E_1 and E_2 their corresponding kinetic energy.

3. The kinetics of radiation induced defects

Silicon used in high energy physics detectors is n-type high resistivity ($1 \div 6\ K\Omega cm$) phosphorus doped FZ material.

The effect of oxygen in irradiated silicon has been a subject of intensive studies in remote past. 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 [15, 16]. Some people consider that these impurities added to the silicon bulk modify the formation of electrically active defects. thus controlling the macroscopic device parameters. Empirically, it is considered that if the silicon is enriched in oxygen, the capture of radiation-generated vacancies is favoured by the production of the pseudo-acceptor complex vacancy-oxygen. Interstitial oxygen acts as a sink for vacancies, thus reducing the probability of formation of the divacancy related complexes, associated with deeper levels inside the gap.

The concentrations of interstitial oxygen O_i and substitutional carbon C_s in 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 Czochralski Si these concentrations can reach values as high as $10^{18}\ cm^{-3}$. Because Czochralski silicon is not available in detector grade quality, an oxygenation technique developed at BNL produces Diffusion Oxygenated Float Zone in silicon, obtaining a O_i concentration of the order $5 \times 10^{17}\ cm^{-3}$. These materials can be enriched in substitutional carbon up to $[C_s] \approx 1.8 \times 10^{16}\ cm^{-3}$.

After the irradiation of silicon, the following stable defects have been identified (see References [3, 17]): Si_i, VP, VO, V_2, V_2O, C_iO_i, C_i, C_iC_S.

The pre-existing thermal defects and those produced by irradiation, as well as the impurities, are assumed to be randomly distributed in the solid. An important part of the vacancies and interstitials annihilate. The sample contains certain concentrations of impurities, which can trap interstitials and vacancies respectively, and form stable defects.

Vacancy-interstitial annihilation, interstitial migration to sinks, divacancy, vacancy and interstitial impurity complex formation are considered. The role of phosphorus, oxygen and carbon is taken into account, and the following stable defects : VP, VO, V_2 V_2O C_i, C_iO_i, C_iC_s,, are considered. Other possible defects as V_3O, V_2O_2, V_3O_3 [18], are not included in the present model.

The following picture describes in terms of chemical reactions the mechanisms of production and evolution of the defects considered in the present paper:

$$V + I \underset{G}{\overset{K_1}{\rightleftarrows}} 0 \tag{4}$$

$$I \overset{K_2}{\rightarrow} sinks \tag{5}$$

$$V + O \underset{K_4}{\overset{K_3}{\rightleftarrows}} VO \tag{6}$$

(VO is the A centre).

$$V + P \underset{K_6}{\overset{K_5}{\rightleftarrows}} VP \tag{7}$$

(VP is the E centre).

$$V + V \underset{K_8}{\overset{K_7}{\rightleftarrows}} V_2 \tag{8}$$

$$VO + V \underset{K_{10}}{\overset{K_9}{\rightleftarrows}} V_2O \tag{9}$$

$$I + C_s \overset{K_1}{\rightarrow} C_i \tag{10}$$

$$C_i + O_i \overset{K_{11}}{\rightarrow} C_iO_i \tag{11}$$

$$A + I \overset{K_{12}}{\rightarrow} O \tag{12}$$

$$C_i + C_s \overset{K_{13}}{\rightarrow} C_iC_s \tag{13}$$

Some considerations about the determination of the reaction constants are given in references [7, 8].

The reaction constants K_i (i = 1, 3 ÷ 10) have the general form:

$$K_i = C \cdot \upsilon \cdot \exp(-E_i / k_B T) \qquad (14)$$

with ν the vibration frequency of the lattice, E_i the associated activation energy and C a numerical constant that accounts for the symmetry of the defect in the lattice.

The reaction constant related to the migration of interstitials to sinks could be expressed as:

$$K_2 = \alpha \cdot \upsilon \cdot \lambda^2 \exp(-E_2 / k_B T) \qquad (15)$$

with α: the sink concentration and λ the jump distance.

The system of coupled differential equations corresponding to the reaction scheme (4) ÷ (13) cannot be solved analytically and a numerical procedure was used.

The following values of the parameters have been used: $E_1 = E_2 = 0.4$ eV, $E_3 = 0.8$ eV, $E_4 = 1.4$ eV, $E_6 = 1.1$ eV, $E_8 = 1.3$ eV, $E_{10} = 1.6$ eV, $E_{11} = 1.3$ eV, $E_{12} = 1.7$ eV, $\upsilon = 10^{13}$ Hz, $\lambda = 10^{15}$ cm^2, $\alpha = 10^{10}$ cm^{-2}, in accord with standard constants characterising the silicon material, see for example the books of Lannoo and Bourgoin [3] or Damask and Dienes [19].

4. Results, discussion, comparison with experimental data and predictions

The formation and time evolution of stable defects depends on various factors, e.g. the concentrations of impurities pre-existent in the sample, the rate of generation, and the temperature.

In Figures 2 a) ÷ f), and 3 a) ÷ 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 modelled in silicon containing different initial concentrations of phosphorus, oxygen and carbon, and for two very different rates of generation.

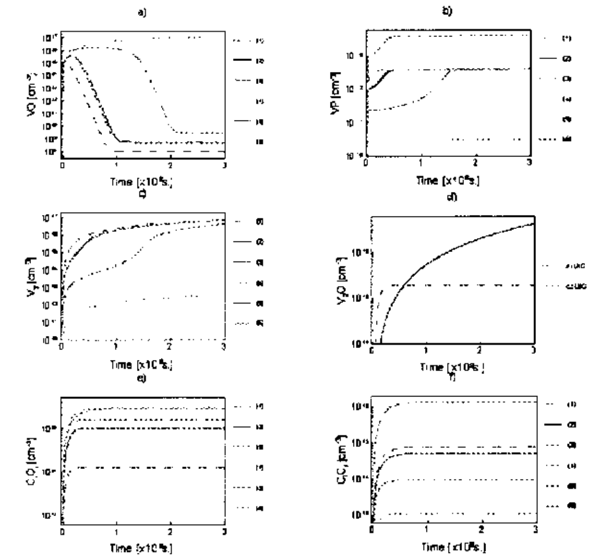

Figure 2
Time dependence of the concentrations of a) VO, b) VP, c) V_2, d) V_2O, e) C_iO_i and f) C_iC_s induced in silicon with the following concentrations of impurities: (1): 10^{14} P/cm^3, $2 \cdot 10^{15}$ O/cm^3, and 3×10^{15} C /cm^3 ; (2): 10^{14} P/cm^3, 10^{16} O/cm^3 and 3×10^{15} C/cm^3; (3) 10^{14} P/cm^3, 5×10^{16} O/cm^3 and 3×10^{15} C/cm^3;.(4): 10^{14} P/cm^3, 4×10^{17} O/cm^3 and 3×10^{15} C/cm^3; (5): 10^{15} P/cm^3, 10^{16} O/cm^3 and 3×10^{15} C/cm^3,.(6): 10^{14} P/cm^3, 10^{16} O/cm^3 and 3×10^{16} C/cm^3; by a generation rate $G_R = 7 \times 10^8$ VI pairs/cm^3/s, at 20°C.

In Figure 2, the evolution of defect concentrations during high rate irradiation ($G_R = 7 \cdot 10^8$ $VI - pairs/cm^3 s$) is presented. This corresponds, in the model hypothesis, to order of magnitude of the radiation levels estimated for the forward tracker region at the future LHC accelerator.

The increase of the initial oxygen concentration in silicon, from $2 \cdot 10^{15}$ cm^{-3} to $4 \cdot 10^{17}$ cm^{-3}, conduces, after ten years of operation in the field 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, a variation of the V_2O generation rate is observed, so that, from the studied cases, the maximum concentration for this defect is obtained for $5 \cdot 10^{16}\ cm^{-3}$ initial oxygen. The increase of initial phosphorus is seen in the increase of concentration of VP centres, while the increase of initial carbon concentration has important consequences on the concentrations of C_iC_s centres. 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. This is an important feature that could be used for detector applications, determining the decrease of the leakage current [8]. At high oxygen concentrations, the concentration of VO centres attains a plateau during the 10 years period considered.

The other extreme situation corresponds to a generation rate $G_R = 200\ \ VI - pairs/cm^3 s$, equivalent with a rate of defect production by protons from the cosmic ray spectra in the orbit near the Earth, at about400 Km, as will be the position of the International Space Station. The same concentrations of P, O and C have been considered as pre-existent in silicon as in Figure 2. 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, it is not influenced by the oxygen content, and of the C_iO_i concentration, where an increase is observed.. As could be seen from Figure 3, as a consequence of the small rate of generation rate of vacancy - interstitial pairs, after ten years of operation 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 curves, both from Fig. 2 and Fig. 3, have been calculated for 20^0C temperature. Thermal generation has been taken into account in both cases, although it is important only for the silicon exposed to low rates of defect production.

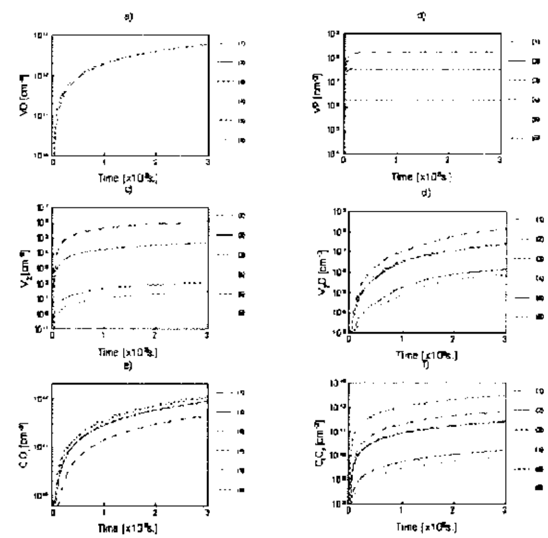

Figure 3

Same as Figure 2, $G_R = 200\ \ VI\ \ pairs/cm^3\ s$.

The influence of the generation rate of primary defects on the concentration of stable defects and on their time evolution has also been investigated. In Figure 4 a) – f), the time evolution of the VO, VP, V_2, V_2O, C_iO_i and C_iC_S concentrations is presented for six decades of generation rates of defects ($G_R = 7 \cdot 10^5 \div 7 \cdot 10^{10}\ \ VI - pairs/cm^3 s$), for silicon containing the following concentrations of impurities: $10^{14}\ \ P/cm^3$, $10^{16}\ \ O/cm^3$, $3 \times 10^{15}\ \ C/cm^3$, at 20^0C temperature. At small times, the curves corresponding to different generation rates are all parallel and equidistant in a log-log representation. Starting from the highest generation rates, they start to increase slower $(V_2,\ VP)$, attain a plateau (V_2O), or event start to decrease $(VO,\ C_iO_i,\ C_iC_s)$. The maximum attained can be the same, independent on the generation rate as is the case of VO concentration, or could be generation dependent $(C_iC_S,\ C_iC_S)$.

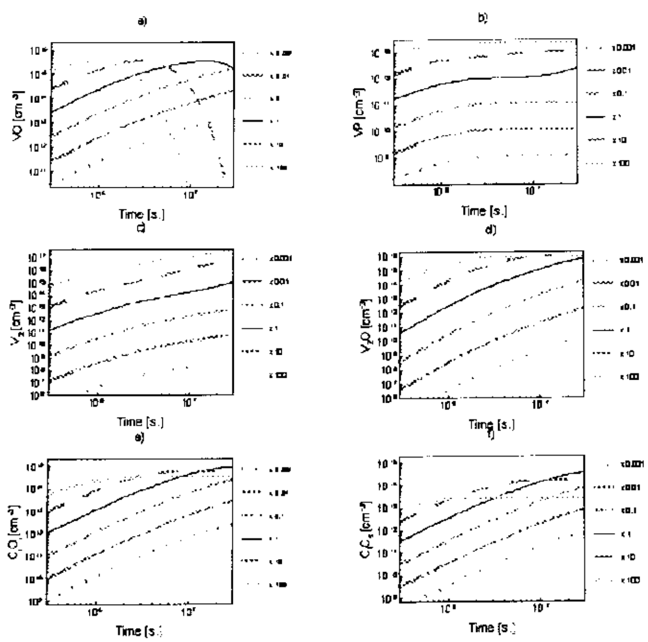

Figure 4
Time dependence of the concentrations of a) VO, b) VP, c) V_2, d) V_2O, e) C_iO_i and f) C_iC_s induced in silicon with: 10^{14} P/cm^3, 10^{16} O/cm^3, and 3x10^{15} C, by continuous irradiation.

The temperature is another important factor determining the time evolution of defects. In Figure 5 a) – f) and 6 a) – f), the effect of the temperature is studied for the same generation rates of primary defects as in Figures 2 and 3 respectively, for five temperatures: $+20^0C$, $+10^0C$, 0^0C, -10^0C and -20^0C. The concentrations of pre-existing impurities in silicon are as follows: $10^{14}\ cm^{-3}\ P$, $10^{16}\ cm^{-3}\ O$ and $3\times10^{15}\ cm^{-3}\ C$. The decrease of the temperature decreases the generation rate of stable defects, with the exception of VP. Where the highest values correspond to the lowest temperature. The maximum values of the VO concentration are temperature independent; the values of the concentration on the plateau decrease with the decrease of temperature for C_iO_i and C_iC_S and increase for V_2O.

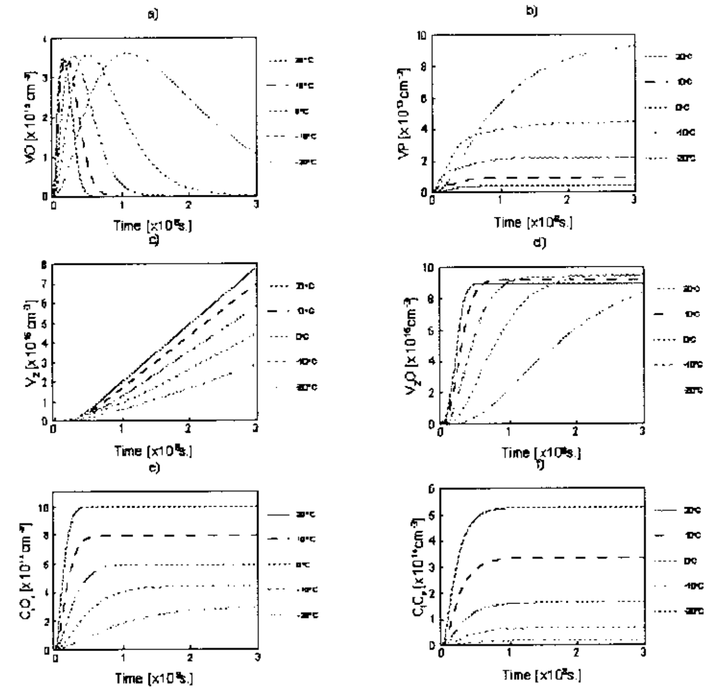

Figure 5
Time dependence of the concentrations of a) VO, b) VP, c) V_2, d) V_2O, e) C_iO_i and f) C_iC_s induced in silicon with: 10^{14} P/cm^3, 10^{16} O/cm^3, and 3x10^{15} C, by continuous irradiation. in the same conditions as in Figure 2, at 20^0C, 10^0C, 0^0C, -10^0C, and -20°C.

For silicon exposed to low rates of defect production the same amount of time (Figure 6), the process of defect production in slowed down. The most unexpected time dependence is for V_2, that has the highest values at the lowest temperature.

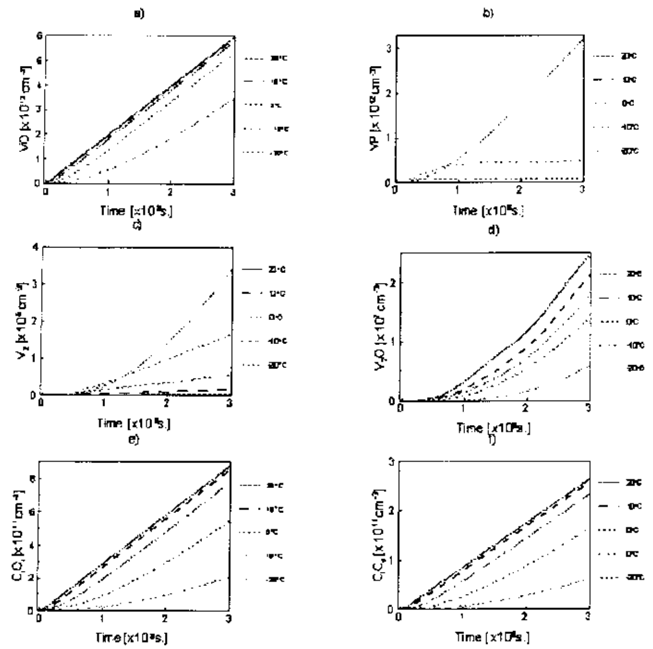

Figure 6

Time dependence of the concentrations of a) VO, b) VP, c) V_2, d) V_2O, e) C_iO_i and f) C_iC_s induced in silicon with: 10^{14} P/cm^3, 10^{16} O/cm^3, and 3×10^{15} C, by continuous irradiation. in the same conditions as in Figure 3, at 20°C, 10°C, 0°C, -10°C and –20°C.

In a previous paper [8], we demonstrated in concrete cases the importance of the sequence of irradiation process, considering that the same total fluence can be attained in different situations: the ideal case of instantaneous irradiation, irradiation in a single pulse followed by relaxation, and respectively continuos irradiation process. As expected, after instantaneous irradiation the concentrations of defects are higher in respect with "gradual" irradiation.

After this analysis, the specific importance of the irradiation and annealing history (initial material parameters, type of irradiation particles, energetic source spectra, flux, irradiation temperature, measurement temperature, temperature and time between irradiation and measurement) on defect evolution must be underlined.

The model predictions have been compared with experimental measurements. A difficulty in this comparison is the insufficient information in published papers regarding the characterisation of silicon, and on the irradiation parameters and conditions for most of the data.

It was underlined in the literature [20] that the ratio of VO to VP centres in electron irradiated silicon is proportional to the ratio between the concentrations of oxygen and phosphorus in the sample. For electron irradiation, in Ref. [21] a linear dependence of the V_2 versus VO centre concentration has been found experimentally. In the present paper, the ratio of concentrations of V_2 to VO centres and VO to VP ones has been calculated in the frame of the model, for the material with the characteristics specified in Ref. [21], and irradiated with 12 MeV electrons, in the conditions of the above mentioned article. The time dependence of these two ratios is represented in Figure 7. Annealing is considered both during and after irradiation. It could be seen that for the ratio of V_2 and VO concentrations the curves corresponding to different irradiation fluences are parallel, while the ratio of VO to VP concentrations is fluence independent, in the interval $2\times10^{13} \div 5.5\times10^{14}\ cm^{-2}$, in good agreement with the experimental evidence. The ratio between V_2 and VO concentrations is determined by the generation of primary defects by irradiation, while the ratio between VO and VP concentrations is determined by the concentrations of oxygen and phosphorus in silicon.

Our estimations are also in agreement with the measurements presented in reference [22], after electron irradiation, where defect concentrations are presented as a function of the time after irradiation. In Figure 8, both measured and calculated dependencies of the VO and VP concentrations are given. The irradiation was performed with 2.5 MeV electrons, up to a fluence of $3\cdot10^{16}\ cm^{-2}$. A good agreement can be observed for these concentrations. The dependencies put in evidence the important role played by the carbon-related defects. The relative values are imposed by the arbitrary units of experimental data.

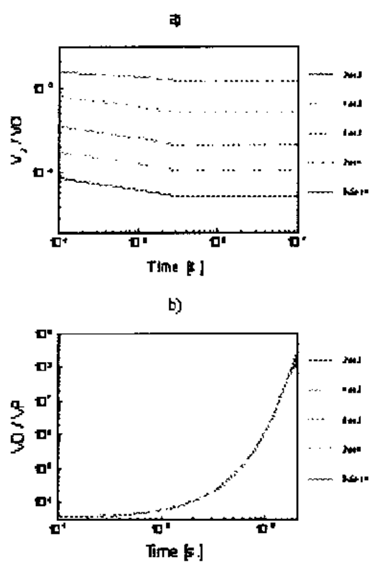

Figure 7
Time dependence for a) V_2/VO and b) VO/VP concentrations calculated for silicon with 1.4x10^{14} P/cm^3, 5x10^{17} O/cm^3, and 3x10^{15} C/cm^3, by 12 MeV electron irradiation, with the flux 5.8x10^{10} e/cm^2/s, up to the fluences: 2x10^{13} e/cm^2, 4x10^{13} e/cm^2, 8x10^{13} e/cm^2, 2x10^{14} e/cm^{2}and 5.5x10^{14} e/cm^2, followed by relaxation (see reference [21]).

Also, a good agreement has been obtained between the absolute values of concentrations of $VP+V_2$ and C_iC_s predicted by the model, and the experimental results after 1 MeV neutron irradiation at a total fluence of 5.67×10^{13} cm^{-2}, reported in reference [23]. The calculated $1.5\cdot10^{13}$ cm^{-3} and $4.1\cdot10^{12}$ cm^{-3}concentrations for $VP+V_2$ and C_iC_s respectively, are in accord with the values of $1.1\cdot10^{13}$ cm^{-3} and $3.8\cdot10^{12}$ cm^{-3}, measured experimentally. For the VO concentration, a poorer concordance has been obtained.

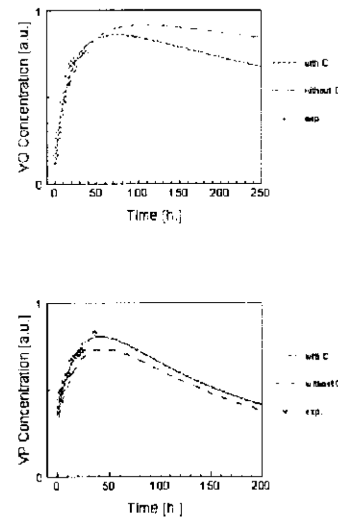

Figure 8
Time dependence of VO and VP concentrations after electron irradiation: crosses - experimental data from reference [22]; continuous line present model calculations; dashed line - without the consideration of carbon contribution to defect formation.

5. Summary

A phenomenological model that describes silicon degradation due to irradiation from the point of view of the kinetics of produced defects toward equilibrium was developed.

The production of primary defects (vacancies and interstitials) in the silicon bulk was considered in the frame of the Lindhard theory, and the peculiarities of the particle - silicon nuclei interaction were taken into account.

The mechanisms of formation of stable defects and their evolution toward equilibrium was modelled, and the concentrations of defects were calculated solving numerically the system of coupled differential equations for these processes. Vacancy-interstitial annihilation, interstitial migration to sinks, vacancy-impurities complexes (VP, VO, V_2O, C_iO_i, C_iC_S), and divacancy formation were considered in different irradiation conditions, for different concentrations of impurities in the initial semiconductor, in the temperature range $-20 \div 20°C$.

The calculated results suggest the importance of the conditions of irradiation, temperature and annealing history.

The model supports the experimental studies performed to investigate the influence of oxygen in the enhancement of the radiation hardness of silicon for detectors. The VO defects in oxygen enriched silicon are favoured in respect to the other stable defects, so, for detector applications it is expected that the leakage current decreases after irradiation. At high oxygen concentrations, this defect saturates starting from low fluences at high generation rates of defects.

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Microscopic modelling of defects production and their annealing after irradiation in silicon for HEP particle detectors

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Abstract

In this contribution, the production of defects in radiation fields and their evolution toward equilibrium in silicon for detector uses has been modelled. In the quantitative model developed, the generation rate of primary defects is calculated starting from the projectile - silicon interaction and from recoil energy redistribution in the lattice. Vacancy-interstitial annihilation, interstitial migration to sinks, divacancy and vacancy-impurity complex (VP; VO; V_2O, C_iO_i and C_iC_s) formation are considered.

The results of the model support the experimental available data.

The correlation between the initial material parameters, temperature, irradiation and annealing history is established. The model predictions could be a useful clue in obtaining harder materials for detectors at the new generation of accelerators or for space missions.

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Key words: radiation damage, bulk defects, defect concentrations, kinetics of defects, annealing processes.

1. Introduction

Silicon is the most used semiconductor material for detectors in particle physics experiments. The principal obstacles to long term operation in the extreme radiation conditions are the changes in detector parameters, consequence of the modifications in material properties during and after irradiation, ultimately related to the defects induced this way in the lattice.

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 [1] are used in relation to defects.

We denote the displacement defects, vacancies and interstitials, as primary point defects, prior to any further rearrangement.

The microscopic model developed in this contribution is able to explain quantitatively, without free parameters, the production of primary defects in silicon, and their evolution toward equilibrium because in silicon, these defects are essentially unstable and interact via migration, recombination, and annihilation or produce other defects.

The generation rate of primary defects is considered in a large range of values, and is calculated starting from the projectile – silicon nucleus interaction, and from the analytical extensions of the Lindhard theory [2].

Silicon used for detectors in high energy physics is n-type high resistivity ($1 \div 6\ K\Omega cm$) phosphorus doped FZ material. The concentrations of interstitial oxygen O_i and substitutional carbon C_s in 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 Czochralski Si these concentrations can reach values as high as $10^{18}\ cm^{-3}$. Because Czochralski silicon is not available in detector grade quality, an oxygenation technique developed at BNL produces Diffusion Oxygenated Float Zone in silicon, obtaining a O_i concentration of the order $5 \times 10^{17}\ cm^{-3}$. These materials can be enriched in substitutional carbon up to $[C_i] \approx 1.8 \cdot 10^{16}$ cm^{-3}.

Vacancy-interstitial annihilation, interstitial migration to sinks, divacancy and vacancy-impurity complex (VP; VO; V_2O, C_iO_i and C_iC_s) formation are considered.

Model predictions are compared with experimental data.

The correlation between the initial material parameters, temperature, irradiation and annealing history is established.

2. Production of primary defects and their kinetics

The basic assumption of the present model is that the 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 as a consequence of the subsequent collisions of the primary recoil in the lattice.

Prior to the irradiation process, in silicon there are thermally generated defects (only Frenkel pairs are considered).

After the irradiation, the following stable defects have been identified in silicon (see References [1, 3]): Si_i, VP, VO, V_2, V_2O, C_iO_i, C_i, C_iC_S.

The pre-existing thermal defects and those produced by irradiation, as well as the impurities, are assumed to be randomly distributed in the solid. An important part of the vacancies and interstitials annihilate. The sample contains certain concentrations of impurities, which can trap interstitials and vacancies respectively, and form stable defects.

Vacancy-interstitial annihilation, interstitial migration to sinks, divacancy, vacancy and interstitial impurity complex formation are considered. The role of phosphorus, oxygen and carbon is taken into account, and the following stable defects: VP, VO, V_2 V_2O C_i, C_iO_i, C_iC_s, are considered. Other possible defects as V_3O, V_2O_2, V_3O_3 [4], are not included in the present model.

The following picture describes in terms of chemical reactions the mechanisms of production and evolution of the defects considered in the present paper:

$$V + I \underset{G}{\overset{K_1}{\rightleftharpoons}} 0 \tag{1}$$

$$I \xrightarrow{K_2} sinks \quad (2)$$

$$V + O \underset{K_4}{\overset{K_3}{\rightleftarrows}} VO \quad (3)$$

(VO is the A centre).

$$V + P \underset{K_6}{\overset{K_5}{\rightleftarrows}} VP \quad (4)$$

(VP is the E centre).

$$V + V \underset{K_8}{\overset{K_7}{\rightleftarrows}} V_2 \quad (5)$$

$$VO + V \underset{K_{10}}{\overset{K_3}{\rightleftarrows}} V_2O \quad (6)$$

$$I + C_s \xrightarrow{K_1} C_i \quad (7)$$

$$C_i + O_i \xrightarrow{K_8} C_iO_i \quad (8)$$

$$A + I \xrightarrow{K_{12}} O \quad (9)$$

$$C_i + C_s \xrightarrow{K_9} C_iC_s \quad (10)$$

The reaction constants K_i (i = 1, 3 ÷ 9) have the general form:

$$K_i = C \cdot \upsilon \cdot \exp(-E_i / k_B T) \quad (11)$$

with ν the vibration frequency of the lattice, E_i the associated activation energy and C a numerical constant that accounts for the symmetry of the defect in the lattice.

The reaction constant related to the migration of interstitials to sinks could be expressed as:

$$K_2 = \alpha \cdot \upsilon \cdot \lambda^2 \exp(-E_2 / k_B T) \quad (12)$$

with α: the sink concentration and λ the jump distance.

The system of coupled differential equations corresponding to the reaction scheme (1) ÷ (10) cannot be solved analytically and a numerical procedure was used.

The following values of the parameters have been used: $E_1 = E_2 = 0.4$ eV, $E_3 = 0.8$ eV, $E_4 = 1.4$ eV, $E_6 = 1.1$ eV, $E_8 = 1.3$ eV, $E_{10} = 1.6$ eV, $E_{11} = 0.8$ eV, $E_9 = 1.7$ eV, $\upsilon = 10^{13}$ Hz, $\lambda = 10^{15}$ cm^2, $\alpha = 10^{10}$ cm^{-2}.

The generation term (G) is the sum of two components:

$$G = G_R + G_T \quad (13)$$

where G_R accounts for the generation by irradiation, and G_T for thermal generation.

The concentration of the primary radiation induced defects per unit fluence (CPD) in silicon has been calculated using the explicit formula (see details, e.g. in references [5, 6]):

$$CPD(E) = \frac{N_{Si}}{2E_{Si}} \int \sum_i \left(\frac{d\sigma}{d\Omega}\right)_{i,Si} L(E_{Ri})_{Si} d\Omega = \frac{1}{N_A} \cdot \frac{N_{Si} A_{Si}}{2E_{Si}} \cdot NIEL(E) \quad (14)$$

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} - the average threshold energy for displacements in the semiconductor, E_{Ri} - the recoil energy of the residual nucleus produced in interaction i, $L(E_{Ri})$ - the Lindhard factor that describes the partition of the recoil energy between ionisation and displacements and $\left(d\sigma/d\Omega\right)_i$ - 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).

Due to the important weight of annealing processes, as well as to their very short time scale, CPD is not a measurable physical quantity.

If the anisotropy of the silicon lattice is not considered, the simplifying hypothesis of random distribution of CPD for all particles could be introduced: the identity of the particle is lost after the primary interaction, and two different particles could produce the same generation rate (G_R) of vacancy-interstitial pairs if the following condition:

$$G_R = \left|(CPD)_{part.a}(E_1)\right| \times \Phi_{part.a}(E_1) = \left|(CPD)_{part.b}(E_2)\right| \times \Phi_{part.b}(E_2) \qquad (15)$$

is fulfilled. Here, Φ is the flux of particles of type a and b respectively, and E_1 and E_2 their corresponding kinetic energy.

3. Results and discussion

a. Comparison between model predictions and experimental data

The model predictions have been compared with experimental measurements. A difficulty in this comparison is the insufficient information in published papers regarding the characterisation of silicon, and the irradiation parameters and conditions for most of the data.

It was underlined in the literature [7] that the ratio of VO to VP centres in electron irradiated silicon is proportional to the ratio between the concentrations of oxygen and phosphorus in the sample. For electron irradiation, in Reference [8] a linear dependence of the V_2 versus VO centre concentration has been found experimentally. In the present paper, the ratios of concentrations of V_2 to VO centres and VO to VP ones has been calculated respectively in the frame of the model, for the material with the characteristics specified in Reference [8], and irradiated with 12 MeV electrons, in the conditions of the above mentioned article. The time dependence of these two ratios is represented in Figures 1a and 1b; annealing is considered both during and after irradiation. It could be seen that for the ratio of V_2 and VO concentrations, the curves corresponding to different irradiation fluences are parallel, while the ratio of VO to VP concentrations is fluence independent, in the interval $2 \times 10^{13} \div 5.5 \times 10^{14}\ cm^{-2}$, in good agreement with the experimental evidence. The ratio between V_2 and VO concentrations is determined by the generation of primary defects by irradiation, while the ratio between VO and VP concentrations is determined by the concentrations of oxygen and phosphorus in silicon.

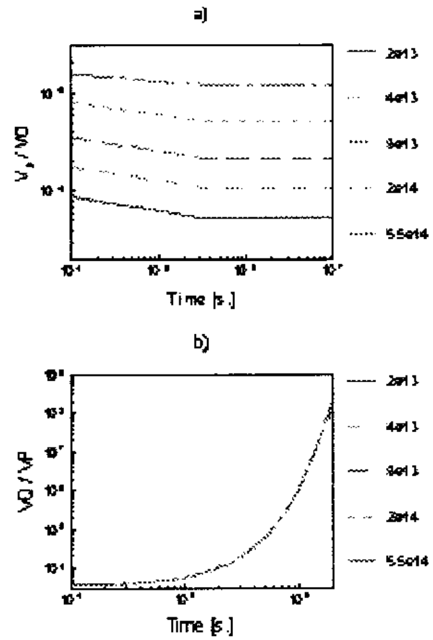

Figure 1

Time dependence for a) V_2/VO and b) VO/VP concentrations calculated for silicon with 1.4 10^{14} P/cm^3, 5 10^{17} O/cm^3 and 3 10^{15}C/cm^3, after 12 MeV electron irradiation, with the flux 5.8 10^{10} e/cm^3/s, up to the fluences: 2 10^{13} e/cm^2, 4 10^{13} e/cm^2, 8 10^{13} e/cm^2, 2 10^{14} e/cm^2 and 5.5 10^{14} e/cm^2, followed by relaxation (see reference [8]).

Our estimations are also in agreement with the measurements presented in reference [9], after electron irradiation, where defect concentrations are presented as a function of the time after irradiation. In Figure 2, both measured and calculated dependencies of the VO and VP concentrations are given. The irradiation was performed with 2.5 MeV electrons, up to a fluence of 3 10^{16} cm^{-2}.

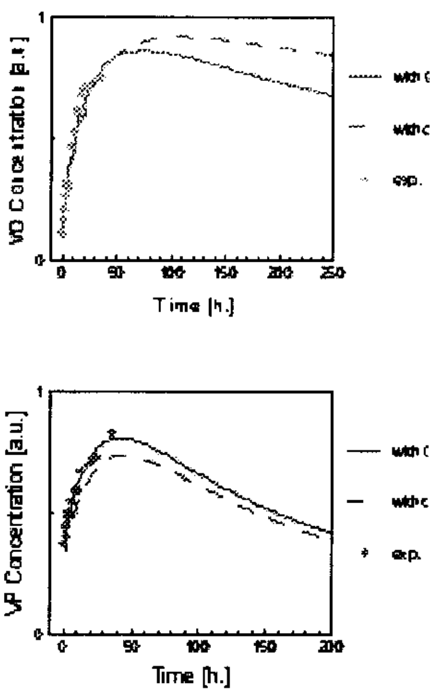

Figure 2
Time dependence of VO and VP concentrations after electron irradiation: crosses - experimental data from reference [9]; continuous line present model calculations; dashed line - without the consideration of carbon contribution to defect formation.

The dependencies put in evidence the important role played by the carbon-related defects. The relative values are imposed by the arbitrary units of experimental data.

A good agreement has also been obtained between the absolute values of concentrations of $VP+V_2$ and C_iC_s centres predicted by the model, and the experimental results after 1 MeV neutron irradiation at a total fluence of 5.67×10^{13} cm^{-2}, reported in reference [10]. The calculated $1.5\cdot10^{13}$ cm^{-3} and $4.1\cdot10^{12}$ cm^{-3} concentrations for $VP+V_2$ and C_iC_s respectively, are in accord with the values of $1.1\cdot10^{13}$ cm^{-3} and $3.8\cdot10^{12}$ cm^{-3}, measured experimentally. For the VO concentration, a poorer concordance has been obtained.

The formation and time evolution of stable defects depends on various factors, e.g. the concentrations of impurities pre-existent in the sample, the rate of generation, and the temperature and the irradiation history.

b. The variation of the concentration of stable defects in respect to the irradiation rate and the influence of oxygen

The effect of oxygen in irradiated silicon has been a subject of intensive studies in remote past. 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 [11, 12]. Some authors consider that these impurities added to the silicon bulk modify the formation of electrically active defects, thus controlling the macroscopic device parameters. Empirically, it is considered that if the silicon is enriched in oxygen, the capture of radiation-generated vacancies is favoured by the production of the pseudo-acceptor complex vacancy-oxygen. Interstitial oxygen acts as a sink for vacancies, thus reducing the probability of formation of the divacancy related complexes, associated with deeper levels inside the gap.

Two types of silicon have been considered in the model calculations: "standard" material, with the following doping concentrations: 10^{14} cm^{-3} phosphorous content, $2\text{x}10^{15}$ cm^{-3} oxygen, and $3\text{x}10^{15}$ cm^{-3} carbon, and "oxygenated" material, with the same concentrations of phosphorous and carbon, but with 200 higher oxygen content, $4\text{x}10^{17}$ cm^{-3}.

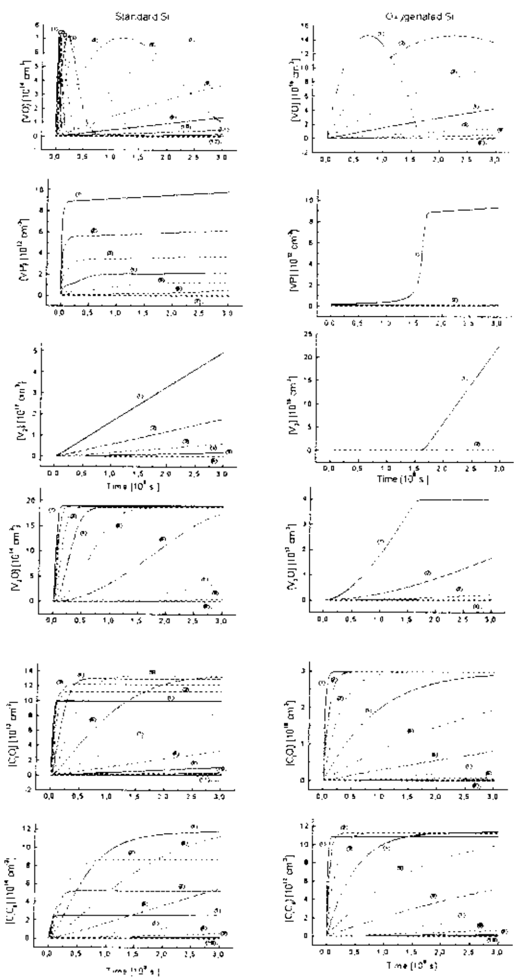

Figure 3
Influence of irradiation rate on the time evolution of defect concentrations. The values of G_R are decreasing from $5{\cdot}10^9$ VI pairs/s - curve (1) to 50 VI pairs/s - curve (17), from half to half order of magnitude

These two types of materials are considered to be exposed to continuous irradiation, with G_R varying from 5×10^9 $(VI)-pairs/cm^3/s$, to 50 $(VI)-pairs/cm^3/s$, from half to half order of magnitude, at 20°C, during 10 years. Thermal generation has been considered each time in the calculations. The results are illustrated in Figure 3.

The highest generation rate corresponds here to a value 10 times higher than that estimated for the forward position in the tracker silicon detector at the new LHC hadron accelerator (determined from integration over the energy range of interest of the convoluted function between simulated hadron flux spectra [13] and the CPD), while the smallest generation rate corresponds to a value 10 times smaller than the rate produced by protons from cosmic rays, in an orbit near the Earth, at about 380 Km, as measured by the AMS Collaboration [14].

It could be seen that the presence of oxygen slows down the formation of all defects related to oxygen and vacancy, i.e. VO, VP, V_2, V_2O and C_iO_i, and increases the rate of formation of C_iC_s centres. It could also be observed that the highest concentrations attained by the VO centres during this period, as well as those corresponding to the V_2O ones increases, from "standard" to "oxygenated" silicon, in the same ratio as the corresponding oxygen content. Because the process of formation of both divacancies and V_2O centres is, in an important measure, slowed down in oxygenated silicon, and the maximum values of divacancy concentrations are reduced with the increase of oxygen concentration, the generation current in the depleted regions of p-n junction detectors could be decreased by oxygen addition, especially at smaller rates than those associated with curves (1).

c. The effect of the temperature

Both "standard" and "oxygenated" silicon are considered to be exposed to similar continuous irradiations, characterised by a generation rate $G_R = 5\times10^7$ VI $pairs/s$, during ten years, at temperatures between -20^0 C and 20^0 C. Thermal generation has been considered for each temperature. The results are represented in Figure 4 for the concentrations of VO, V_2 and V_2O centres respectively.

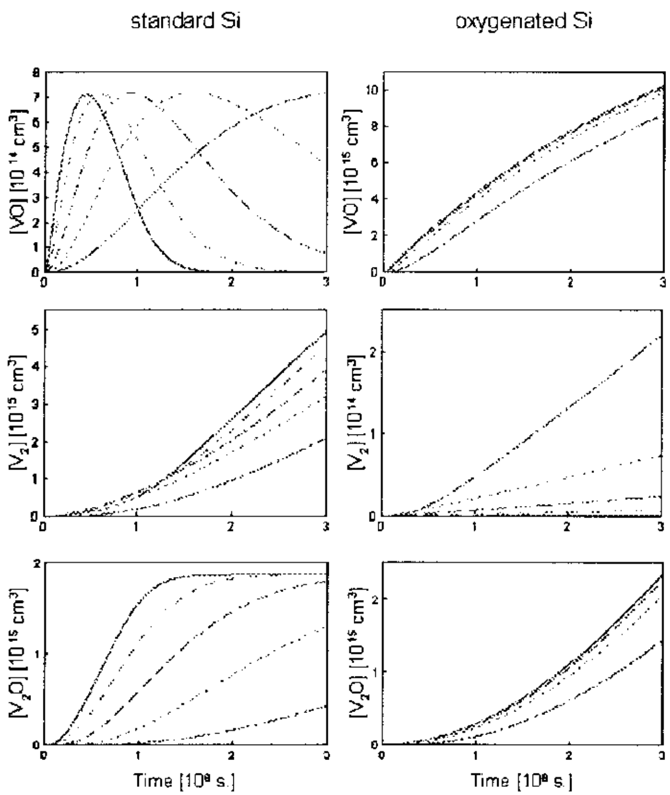

Figure 4

Time dependence of the concentrations VO, V_2 and V_2O centres, in the conditions of continuous irradiation with $G_R = 5\cdot10^7$ VI pairs/s, in "standard" and "oxygenated" silicon, for 20°C, 10°C, 0°C, - 10°C and -20°C respectively.

While in "standard" silicon the decrease of the temperature slows down the rate of VO formation, a much weaker dependence has been found in silicon enriched in oxygen.

For the V_2O centres, the maximum concentrations correspond to the highest temperature, 20 °C, and similar values are found at the end of the time interval considered, although the introduction rate of this defect has different behaviours in the two types of silicon considered.

In contrast to oxygen related centres, the V_2 concentration is more sensitive to temperature in "oxygenated" silicon, where its values are much lower in respect to the corresponding ones for "standard" material. More, the concentration of V_2 centres increases with the decrease of the temperature from 20 to -20°C in "oxygenated" silicon, and decreases in the "standard" material.

d. The correlation between the history of the irradiation process and defect concentrations

In some previous papers [15, 16], we demonstrated in concrete cases the importance of the sequence of irradiation processes, considering that the same total fluence can be attained in different situations: the ideal case of instantaneous irradiation, irradiation in a single pulse followed by relaxation, and respectively continuos irradiation process. As expected, after instantaneous irradiation the concentrations of defects are higher in respect with "gradual" irradiation.

After this analysis, the specific importance of the irradiation and annealing history (initial material parameters, type of irradiation particles, energetic source spectra, flux, irradiation temperature, measurement temperature, temperature and time between irradiation and measurement) on defect evolution must be underlined.

Now, we present comparatively in Figure 5 the time evolution of stable defects in standard silicon, irradiated during $10^7\ s$, when $5\times10^7\ (VI)-pairs/cm^3/s$ have been generated (continuous line), and during $2\times10^7\ s$, with $2.5\times10^7\ (VI)-pairs/cm^3/s$ (dashed line), respectively. The values have been chosen to produce the same amount of vacancy - interstitial pairs. The behaviour of stable defect concentrations is analysed after irradiation. It could be seen that a shorter and stronger irradiation conduces to higher concentrations of V_2 and VP centres in the asymptotic limit, with important consequences for the leakage current, due to the position in the band gap of silicon of these defect levels.

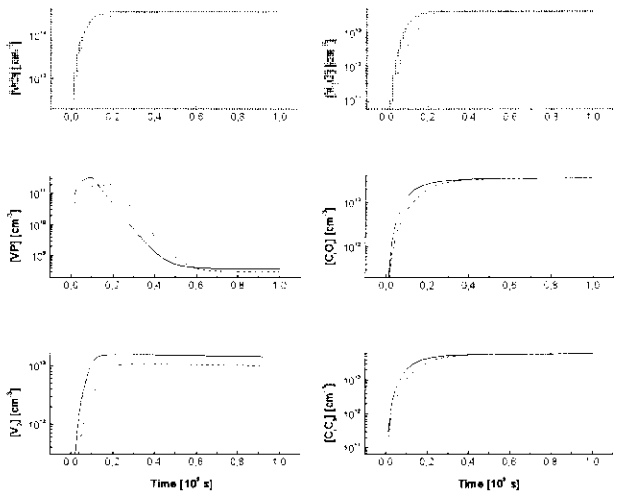

Figure 5

Time evolution of the concentrations of (up to down): VO, VP, V_2, V_2O, C_iO_i, and C_iC_s concentrations in "standard" Si, al 20°C, for two types of irradiation: 10^7 s. irradiation with $G_R = 5{\cdot}10^7$ VI pairs/s (continuous line), and $2{\cdot}10^7$ s. $G_R = 2.5{\cdot}10^7$ VI pairs/s (dashed line) respectively.

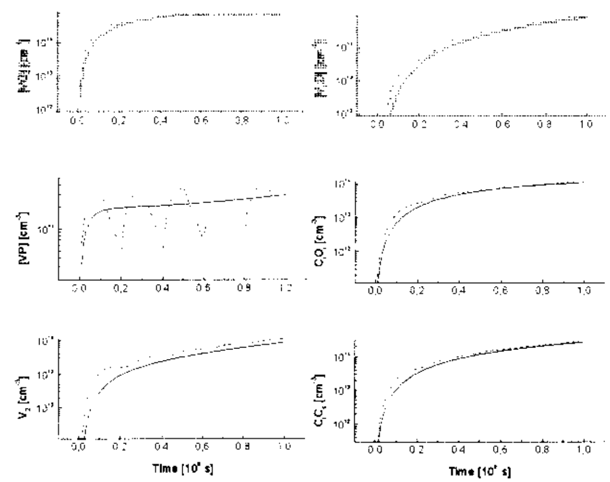

Figure 6

Time evolution of the concentrations of (up to down): VO, VP, V_2, V_2O, C_iO_i, and C_iC_s for two types of irradiation: continuous line - continuous irradiation with $2.5{\cdot}10^7$ VI pairs/s during 10^8 sec, (continuous line), and rectangular pulses 10^7 s. irradiation with $G_R = 5{\cdot}10^7$ VI/s, and 10^7 s relaxation.

Another scenario that could be of interest is the comparison of the effects of continuous and pulsed irradiation, with the same integral rate of primary defect production. The time evolution of the concentrations of stable defects is represented in Figure 6. The effects of continuous irradiation of standard silicon, at 20°C, with a rate of $5\times10^7\ (VI)-pairs/cm^3/s$ (continuous line) are compared with pulsed one: $10^7\ s$ irradiation, with $5\times10^7\ (VI)-pairs/cm^3/s$, and $10^7\ s$ relaxation. As in the previous case (Figure 5), the concentration of VP centres follows the best the irradiation type, while for the other defects the succession irradiation - relaxation is almost not observable.

4. Summary and conclusions

The production of defects in radiation fields, in silicon for detector uses, and their evolution toward equilibrium, has been microscopically modelled in the frame of a quantitative model, without free parameters. Vacancy-interstitial annihilation, interstitial migration to sinks, divacancy and vacancy-impurity complexes (VP; VO; V_2O, C_iO_i and C_iC_s) formation is considered.

The model supports the experimental data and confirms the different studies performed to investigate the influence of oxygen in the enhancement of the radiation hardness of silicon for detectors. The VO defects in oxygen enriched silicon are favoured in respect to the other stable defects, so, for detector applications it is expected that the leakage current decreases after irradiation. At high oxygen concentrations, this defect saturates starting from low fluences at high generation rates of defects.

The generation rate of primary defects, calculated starting from the projectile – silicon nucleus interaction and from the extended Lindhard theory, is considered in a large range of values.

The obtained results suggest the importance of the conditions of irradiation, temperature and annealing history on defect kinetics.

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

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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, divacancy and complex (VP, VO, V_2O, C_iO_i, C_iC_s) formation are taken into account for differently doped initial silicon material. The influence of these defects on the leakage current density has been compared with experimental data from the literature, and predictions for the LHC radiation fields, as well as for space missions in the near Earth orbits have been done, 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

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

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} cm^{-3} atoms of phosphorus, 2×10^{15} cm^{-3} atoms of oxygen, and 5×10^{15} cm^{-3} atoms of carbon;), and "oxygened" one (containing 10^{14} cm^{-3} atoms of phosphorus, 4×10^{17} cm^{-3} atoms of oxygen, and 5×10^{15} cm^{-3} 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. The main hypothesis of the model

In the model, the effects of irradiation conditions and various initial impurities in the starting material are discussed in a quantitative manner: 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 obtained.

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]):

$$CPD(E)=\frac{N_{Si}}{2E_{Si}}\int\sum_i\left(\frac{d\sigma}{d\Omega}\right)_{i,Si} L(E_{Ri})_{Si}\,d\Omega=\frac{1}{N_A}\cdot\frac{N_{Si}A_{Si}}{2E_{Si}}\cdot NIEL(E) \qquad (1)$$

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} - the average threshold energy for displacements in the semiconductor, E_{Ri} - the recoil energy of the residual nucleus produced in interaction i, $L(E_{Ri})$ - the Lindhard factor that describes the partition of the recoil energy between ionisation and displacements and $\left(d\sigma/d\Omega\right)_i$ - 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 $\left(\frac{dE}{dx}\right)_{n.i.}$ [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 can be found, 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:

$$G = G_R + G_T \qquad (2)$$

where G_R accounts for the generation by irradiation, and is calculated as

$$G_R(E) = CPD(E) \times \Phi(E) \qquad (3)$$

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: Si_i, VP, VO, V_2, V_2O, C_iO_i, C_i, C_iC_s, using one or more of the following techniques: electron paramagnetic resonance, infrared absorption spectroscopy, thermally stimulated currents, deep level transient spectroscopy, photoluminescence analysis (see, e.g., the compilations from references [5], [14]).

Vacancy-interstitial annihilation, interstitial migration to sinks, divacancy and vacancy - impurity complex formation (VP, VO, V_2 V_2O C_i, C_iO_i, C_iC_s) have been considered supposing the following chemical reaction scheme:

$$V + I \underset{G}{\overset{K_1}{\rightleftarrows}} 0 \qquad (4a)$$

$$I \overset{K_2}{\rightarrow} sinks \qquad (4b)$$

$$V + O \underset{K_4}{\overset{K_3}{\rightleftarrows}} VO$$

(VO is the A centre). (4c)

$$V + P \underset{K_6}{\overset{K_5}{\rightleftarrows}} VP$$

(VP is the E centre). (4d)

$$V + V \underset{K_8}{\overset{K_7}{\rightleftarrows}} V_2 \qquad (4c)$$

$$VO + V \underset{K_{10}}{\overset{K_9}{\rightleftarrows}} V_2O \qquad (4f)$$

$$I + C_s \overset{K_1}{\rightarrow} C_i \qquad (4g)$$

$$C_i + O_i \overset{K_{11}}{\rightarrow} C_iO_i \qquad (4h)$$

$$A + I \overset{K_{12}}{\rightarrow} O \qquad (4i)$$

$$C_i + C_s \overset{K_9}{\rightarrow} C_iC_s \qquad (4j)$$

where K_i with $i = 1,...8$ 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 references [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 $10^{34}\ cm^{-2}s^{-1}$, and assuming an inelastic non-diffractive cross section of $80\ mb$, the LHC will produce on average 8×10^8 inelastic p-p events per second, creating an extremely hostile radiation environment. For radiation studies, the bunch structure of LHC is not significant.

The central tracker is expected to be exposed to the primary particle flux from the interaction region, and the main concern is radiation damage of the silicon detectors. Without loss of generality, the radiation field simulated for the CMS silicon tracker geometry [17] is considered in the following calculations. 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.

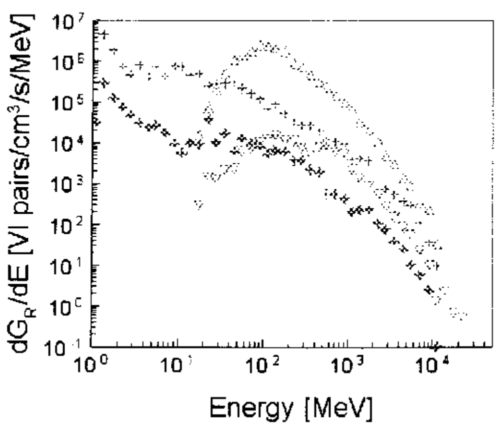

Figure 1
Differential energetic generation rate of vacancy-interstitial pairs for pions and protons, for two positions (1): r = 20 cm, z = 0 ÷ 140 cm , and (2): z = 100 cm, z = 140 ÷ 280 cm , in the tracking cavity of LHC.

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 and the energetic dependence of concentration of primary defects (CPD) for pions and protons 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-interstitial pairs. The values obtained for the first position (1) are: $6.2 \times 10^8\ VI\ pairs/cm^3/s$ for pions and $5.6 \times 10^7\ VI\ pairs/cm^3/s$ for protons, while for the second one (2) these are $8.1 \times 10^6\ VI\ pairs/cm^3/s$ and $3.1 \times 10^6\ VI\ pairs/cm^3/s$ for pions and protons respectively.

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

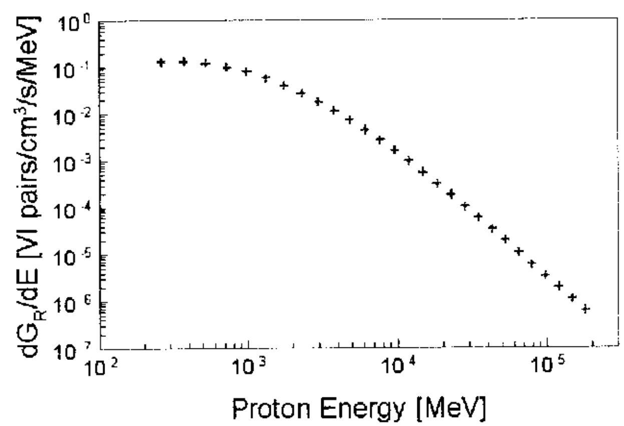

Figure 2
Differential energetic generation rate of vacancy-interstitial pairs by cosmic protons in the space near the Earth.

800 MeV passing from position (1) to position (2). For pions, the $CPD(E)$ 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 energy range 0.2 to 200 GeV, in the neighbourhood of the Earth, at an altitude about 380 km, has been 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 2×10^2 VI $pairs/cm^3/s$. This represents nearly seven orders of magnitude lower generation rate in respect to the higher one calculated for the tracking cavity of the LHC experiments.

4. Estimated damage in silicon detectors

Silicon used in high energy physics detectors is n-type high resistivity ($1\div6$ $k\Omega\cdot cm$) 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 people 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 in 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 5×10^{17} cm^{-3} is obtained. These materials can be enriched in substitutional carbon up to

$[C_i]\approx1.8\times10^{16}$ cm^{-3}.

4a. Changes in the microscopic material properties

The model explains well the experimental data of defect production and evolution in silicon after irradiation [12], [15], and [21].

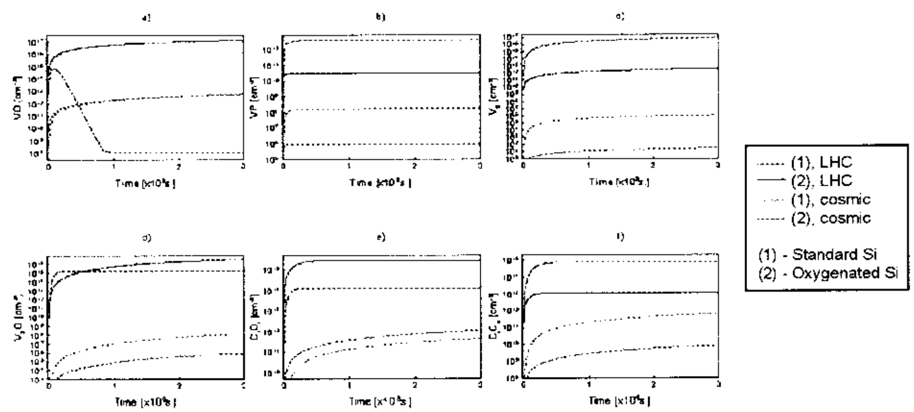

Figure 3
Time dependence of the concentrations of VO, VP, V_2, V_2O, C_iO_i and: C_iC_s induced in standard and oxygenated silicon, in conditions of LHC and cosmic continuous irradiation rates (see text).

In Figure 3, 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, 2×10^{15} cm^{-3} atoms of oxygen, and

5×10^{15} cm^{-3} atoms of carbon; and the "oxygened" one, containing 10^{14} cm^{-3} atoms of phosphorus, 4×10^{17} cm^{-3} atoms of oxygen, and 5×10^{15} cm^{-3} atoms of carbon respectively, and for the two generation rates of VI -pairs discussed above, namely 7×10^{8} and 2×10^{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, 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.

In addition, 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].

4b. 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 perimetral 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, $n, p << n_i$ (n_i is the intrinsic free carrier concentration); each defect with a bulk concentration (N_T) causes a generation current per unit volume of the form [22]:

$$I = qU = q\langle v_t\rangle n_i \frac{\sigma_n\sigma_p N_T}{\sigma_n\gamma_n e^{(E_t-E_i)/kT} + \sigma_p\gamma_p e^{(E_i-E_t)/kT}} \tag{5}$$

where γ_n and γ_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 $\langle v_t\rangle$ 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.

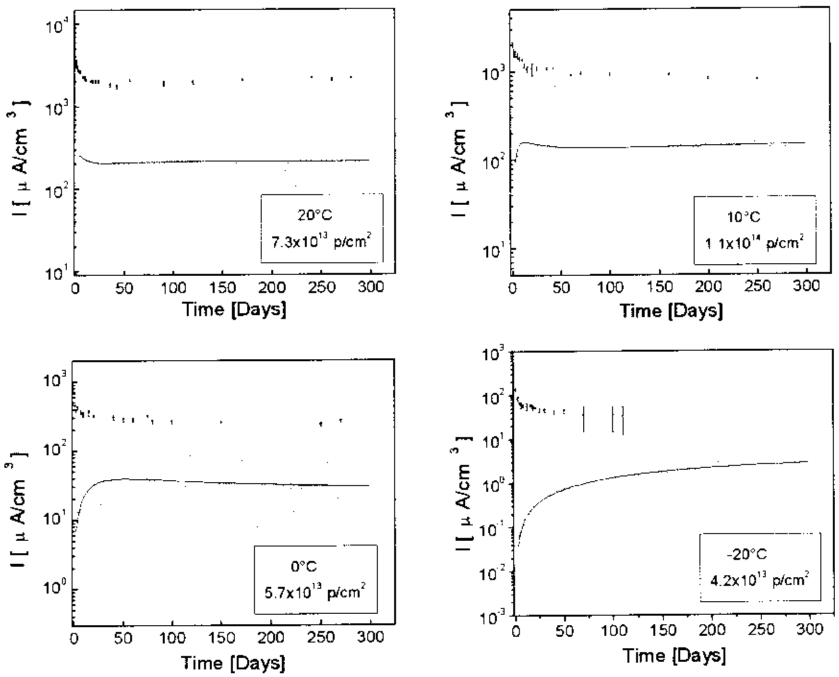

Figure 4
Time dependence of the leakage current density induced by 24 GeV/c proton irradiation in silicon detectors at 20°C, 10°C, 0°C and –20°C respectively. Experimental data: points, calculations: line. The band indicates the imprecision in the model calculations, due to the uncertainty in the values associated to the energy positions and cross sections of the defects.

The validity of the model in relation to leakage current data has been tested using some measurements from the literature, for silicon detectors irradiated with hadrons, at different fluences and temperatures. The measurements of the time dependence of the leakage current in high resistivity silicon pad detectors irradiated at +20°C (reference temperature), +10°C, 0°C and -20°C with 24 GeV/c protons at a flux of about 5×10^{9} $cm^{-2}s^{-1}$, up to the fluence 1.1×10^{14} cm^{-2} [23] were used to investigate model predictions. In Figure 4, the comparison between theoretical and experimental time dependencies of current densities for these silicon diodes is presented. In the figure, the bands represent maximal uncertainties in leakage current calculations due to the unsatisfactory knowledge of energy positions of the defects and of their cross sections.

This comparison put in evidence the following aspects:

The model reproduces in a satisfactory manner the time dependence of the current density at long time after irradiation for +20°C, +10°C and 0°C. At short time after irradiation, the calculated density of the leakage current increases slower than the data and this effect is more pronounced with the decrease of the temperature.

The calculated values of current densities are lower with up to one order of magnitude in respect to the data. Discrepancies between values of leakage currents measured and calculated from measured concentrations of defects respectively have been reported by other authors, see, e.g. references [24] and [25].

A poorer concordance with the data has been found at -20°C.

Explanations for the discrepancies could be related to the possible existence of other defects, that have not been considered in the model, and that could be sources of generation - recombination currents. 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's affirmation [26] that the independent and interacting energy level cases are indistinguishable if the energy levels are more than a few k_BT apart). At lower temperature, other defects and annealing mechanisms must probably be considered.

In Figure 5, 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 have the same significance as in Figure 4, representing the maximal uncertainties due to the energy position of the defects and to their cross sections. They are also drawn as dotted lines.

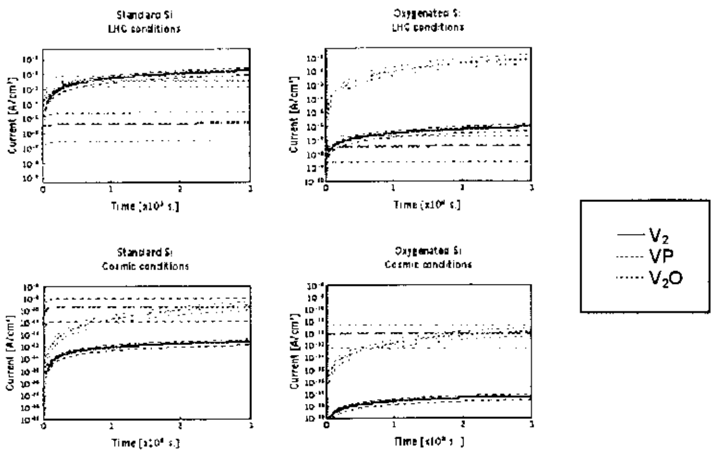

Figure 6
Time dependence of the generation current due to divacancy (continuous line), VP (dashed line) and V_2O (dashed dotted line).

One 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, C_iO_i and V_2O, and to the decrease of the V_2, VP and C_iC_s ones.

The influence of these defects on the leakage current density has been investigated. The calculated time dependencies of the leakage current have been compared with experimental data, and a reasonably good agreement has been found for temperatures in the range $0 \div +20$°C, in the hypothesis of the model.

Predictions for the leakage current densities of silicon detectors, operating in the radiation field of LHC and in the cosmic proton field in the neighbourhood of Earth have been done.

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.

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