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, V₂O), and divacancy (V₂) 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 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

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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 to 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 (VN, VO and VN2), and divacancy (V2) 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 [3, 4]):

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

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 $(d\sigma/d\Omega)_i$ - 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 and the energy dependencies of the Lindhard factors have been calculated in the frame of analytical approximations for different recoils in Si.

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 [4], the calculations of proton, electron and photon $NIEL$ of Van Ginneken [5] as well as those of Ougouang for neutrons [6] have been considered.

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 $10^{-3} \div 1$ MeV the calculations of Summers, in the range $1 \div 200$ MeV the average between those of Summers and of Van Ginneken, while in the range $200 \div 10000$ MeV, Van Ginneken’s. The curve for electrons uses, up to 1 MeV only the values from reference [6], in the range $1 \div 200$ MeV an average between the values from references [5] and [6], and after 200 MeV only from [6]. 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:

$$V + I \xrightarrow{K_1} \text{annihilation} \quad (2)$$

$$I \xrightarrow{K_2} \text{sinks} \quad (3)$$
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.

\[ V + P \frac{K_4}{K_5} VP \]  \hspace{1cm} (4)

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

\[ V + O \frac{K_4}{K_5} VO \] \hspace{1cm} (5)

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

\[ V + V \frac{K_4}{K_6} V_2 \] \hspace{1cm} (6)

\[ V + A \frac{K_9}{K_{10}} V_2 O \] \hspace{1cm} (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:

\[ K_1 = 30\nu \exp \left(-\frac{E_{i1}}{k_B T}\right) \] \hspace{1cm} (8)

where \( E_{i1} \) is the activation energy of interstitial migration and \( \nu \) the vibrational frequency. The reaction constant in process (2) is proportional to the sink concentration \( \alpha \):
\[ K_2 = \alpha \nu \lambda^2 \exp \left(-E_{i1}/k_BT\right) \]  

with \( \lambda \) the jump distance.

Lee and Corbett \[11\] argue that divacancies, vacancy-oxygen and divacancy-oxygen centres are equally probable below 350 °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:

\[ K_3 = K_5 = K_7 = K_9 = 30 \nu \exp \left(-E_{i2}/k_BT\right) \]  

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.

\[ K_4 = 5 \nu \exp \left(-E_A/k_BT\right) \]  
\[ K_6 = 5 \nu \exp \left(-E_E/k_BT\right) \]  
\[ K_8 = 5 \nu \exp \left(-E_{V2}/k_BT\right) \]  
\[ K_{10} = 5 \nu \exp \left(-E_{V2O}/k_BT\right) \]

where \( E_A, E_E, E_{V2} \) and \( E_{V2O} \) 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.

\[ G = [(CPD)_{part.a}(E_1)] \cdot \Phi_{part.a}(E_1) = [(CPD)_{part.b}(E_2)] \cdot \Phi_{part.2}(E_2) \]

is fulfilled.

Here, \( \Phi \) 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: \( E_{i1} = 0.4 \text{ eV}, E_{i2} = 0.8 \text{ eV}, E_A = 1.4 \text{ eV}, E_E = 1.1 \text{ eV}, E_{V2} = 1.3 \text{ eV}, E_{V2O} = 1.6 \text{ eV}, E_{V2O} = 10^{13} \text{ Hz}, \lambda = 10^{13} \text{ cm}^2, \alpha = 10^{10} \text{ cm}^{-2}. \)

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.

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: \( 10^{14} \text{ P/cm}^3 \) and \( 5 \times 10^{16} \text{ O/cm}^3 \), 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 \( 10^{15} \).
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 $5\times10^{16}$ 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.

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 Figures 4a ÷ c, the time evolution of the concentrations...
Figure 3: Time dependence of the concentrations of $V O$, $V P$, $V_2$ and $V_2O$ induced in silicon with $10^{14}$ P/cm$^3$ and $5\times10^{16}$ O/cm$^3$, irradiated with 200 MeV kinetic energy pions a total fluence of $10^{15}$ pions/cm$^2$ with the flux estimated for LHC, for 293 and 273 K.

of $V O$, $V P$, $V_2$ and $V_2O$ in silicon with $10^{14}$ P/cm$^3$ and $5\times10^{16}$ 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 $3\times10^7$ 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 concentration, in conditions of the LHC generation rate, and a shorter time, about $2\times10^6$ 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 is 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.

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 4: Time dependence of the concentrations of $VO$, $VP$, $V_2$ and $V_2O$ induced in silicon with $10^{14}$ P/cm$^3$ and $5 \times 10^{16}$ 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.
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$^2$ irradiated with 200 MeV kinetic energy pions at total fluence of $10^{14}$ pions/cm$^2$ in one pulse.

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 ($8 \times 10^{12}$ cm$^{-3}$) induced in silicon by $5.67 \times 10^{13}$ cm$^{-2}$ 1 MeV neutrons, are in accord with the experimental value of $11.2 \times 10^{12}$ 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, \( n_e < n_i \) (\( n_i \) 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 \([19]\):

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

(16)

where \( \gamma_n \) and \( gamma_p \) are degeneration factors, \( \sigma_n \) (\( \sigma_p \)) are the cross sections for majority (minority) carriers of the trap, \( E_i = (E_C - E_V)/2 \) and \( < v_t > \) is the average between electron and hole thermal velocities. In the case of \( E \) and \( A \) centres and \( V_2^- \) and \( V_2^+ \) defects, the current concentration can be expressed in the simple
form:
\[ I = qU = q < v_t > n_i \frac{\sigma_n}{\sigma_p} N_T e^{(E_t - E_i) / k_B T} \]  

(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 [21].

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.

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: \( 5 \times 10^{16} \text{ cm}^{-3} \) and \( 10^{16} \text{ cm}^{-3} \) 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 \( (VP, VO \text{ and } V_2O) \), 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
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) $5 \times 10^{16}$ cm$^{-3}$ and b) $10^{16}$ cm$^{-3}$ oxygen. 

silicon for detectors. The $V\text{O}$ 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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