

Estimated modifications of the characteristics of silicon detectors due to their use at the LHC-accelerator and in AMS space conditions

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Abstract: The phenomenological model developed by the authors in previous papers is used to evaluate the degradation induced in high resistivity silicon detectors by pion and proton irradiation at the future accelerator facilities or by cosmic protons considering the continuous irradiation for ten years of work. The equations governing the degradation of the semiconductor lattice are explicitly considered. The damage is analysed at the microscopic level (defects production and their evolution toward equilibrium) and at the macroscopic level (the changes in the leakage current of the p-n junction). The rates of production of primary defects, as well as their evolution toward equilibrium are evaluated considering explicitly the irradiation field characterising the specified applications, i.e. the type of the projectile particle and its energy. The influence of these defects on the leakage current density is 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 are done, in the frame of the Schokley-Read-Hall model.

INTRODUCTION

Silicon detectors are planned to be used for many applications in particle or astroparticle physics as, for example, at the CERN Large Hadron Collider (LHC) and Super-LHC or in space mission as, e.g. AMS. The detectors used in these environments will be exposed long-time and/or to high fluences of charged and neutral particles. Various systematic studies have been carried out to understand better the origins and consequences of radiation damage in silicon detectors. These cover the production of primary defects [1], their annealing mechanisms [2], [3], [4], [5], [6], [7], [8], [9], the correlation with the characteristics of the irradiation particle [10], [11], [12] and with initial material impurities [13], [14]. The microscopic modifications of the material characteristics produce changes in the detector parameters. The microscopic phenomena and their consequences at the device level are poorly understood.

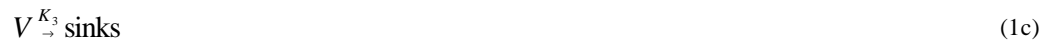
A point defect in a crystal is an entity that causes an interruption in the lattice periodicity. In this paper, the terminology and definitions in agreement with M. Lannoo and J. Bourgoin [15] are used in relation to defects. We denote the displacement defects, vacancies and interstitials, as primary point defects, prior to any further rearrangement.

The primary incident particle, having kinetic energy with values in the intermediate up to high-energy range, interacts with the semiconductor material. After this process, 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 [16] and authors' contributions [17] and after this step the concentration of primary defects is calculated. 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. The generation term (G) is the sum of two components: G_R accounting 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 concentrations of defects resulting from all interaction processes, and all characteristic mechanisms corresponding to each interaction process, using the explicit formula from reference [17] (see also concrete relations and details). 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, 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 product between the generation rate of defects and the flux of particles are the same.

THE MODEL

In some previous papers [18], [19], [20], the authors developed a quantitative phenomenological model to explain the production of primary defects and their time evolution toward stable defects, starting from silicon with different quantities of initial impurities, considering different rates of primary defects production and conditions of irradiation. 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, from the material characteristics: lattice bonds, lattice constant, impurities, keeping into account the temperature during and after irradiation. In the chemical reaction description, the formation and evolution of defects in silicon, around room temperature, could be described as follows:





The reaction constants K_i ($i = 1, 4 \div 16$) have the general form:

$$K_i = C \cdot \mathbf{n} \cdot \exp(-E_i / k_B T) \quad (7a)$$

with \mathbf{n} 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 and vacancies to sinks could be expressed as:

$$K_j = \mathbf{a}_j \mathbf{n} \cdot I^2 \exp(-E_j / k_B T) \quad (7b)$$

with $j = 2$ (interstitials) and 3 (vacancies), α_j - the sink concentration and λ - the jump distance.

The values of the activation energies are from the literature see for example reference [20].

The reactions have been grouped into four categories: the first is related only to primary defects and their reciprocal interactions (equations 1 and 2), the second involves the reactions of primary defects with impurities, as well as complex decomposition (equations 3, 4 and 5), while the interactions of complexes, and of complexes with primary defects are comprised into the group of reactions represented by equations 6. Other primary defects- impurities complexes could also be considered apart those formed with P, O and C. In the first group, only primary defects, vacancies and interstitials, are involved. They annihilate (1a) and migrate to sinks (1b and 1c). Both the interstitial and the vacancy are mobile at room temperature. More, the migration mechanisms of vacancies and interstitials are quite different: while interstitials undergo an athermal migration, being mobile even at 4.2K [21], vacancy motion occurs from near 160 K in p-type material and from 70K in n-type crystals, reflecting the effects of charge state on the migration process [21]. At room temperature, a migration energy of the vacancy twice that the corresponding one for interstitials has been estimated [2]. Due to the fact that interstitials are much faster, and they have not been identified even at the lowest irradiation temperatures, and also to the fact that in n-type silicon for detectors only carbon impurities trap interstitials, it is natural to consider interstitial migration to sinks (e.g. the surface and the edges of the sample). Contrary to this, the migration of vacancies to sinks (reaction 1c) plays no role in the time dependence of the concentrations, as seen from calculations [22]. It is thus justified to be neglected, as it really was in the previous calculations [18], [20]. During their migration, vacancies could form aggregates (divacancies – reaction 2a). Divacancy decomposition involving interstitials is also possible (2b) Type (3) reactions involve vacancies, interstitials and phosphorous, and the formation and decomposition of the VP complex is described. The following type of reactions is related to complexes of primary defects with oxygen (group 4) and carbon (group 5) respectively. While the substitutional carbon is fix, C_i has a high mobility. Due to this fact, the $C_i C_s$ complex could be formed. Higher order vacancy-oxygen, carbon-carbon and carbon-oxygen complexes are also important, and are described by reactions of type (6). Reactions of interstitials with vacancy-impurity complexes (2b, 3b and 4b), and of vacancies with interstitial-impurity complexes (5b) are natural to occur when there are interstitials and vacancies available. In spite of this, calculations [22] demonstrate that they play no role in the evolution of defect concentration during and after irradiation. In this respect, their neglect in previous papers [18], [19] and [20] is justified. A special mention must be made to the problem of reversible and irreversible processes. To obtain semiconductor materials with useful properties for the harder radiation detectors, the mechanisms is useful that the processes to be irreversible.

Radiation environment at the LHC accelerator and in the near Earth orbits.

In the present paper, two types of applications of silicon detectors are emphasised: for the tracker of experiments at the LHC accelerator, and for space missions in the near Earth orbit, as, for example, experiments at the International Space Station. At the luminosity of $10^{34} \text{ cm}^{-2} \text{ s}^{-1}$, and assuming an inelastic non-diffractive cross section of 80 mb , the LHC will produce on average 8×10^8 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 [23] 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 [23]. The flux decreases by a factor 50 going from $r = 20 \text{ cm}$ to $r = 100 \text{ cm}$, and most of the low energy particles disappear. The hadrons are predominantly low-energy charged pions and protons, which are present in different amounts and have different energy spectra as a function of the distance in respect to the interaction point, and of the pseudorapidity. In all cases, the pions are the dominant particles. In figure 1, the energetic differential generation rate of defects is presented. Each spectrum has been obtained as a convolution of the simulated hadron flux in the tracker cavity and the energetic dependence of concentration of primary defects (CPD) for pions and protons in the same energy range.

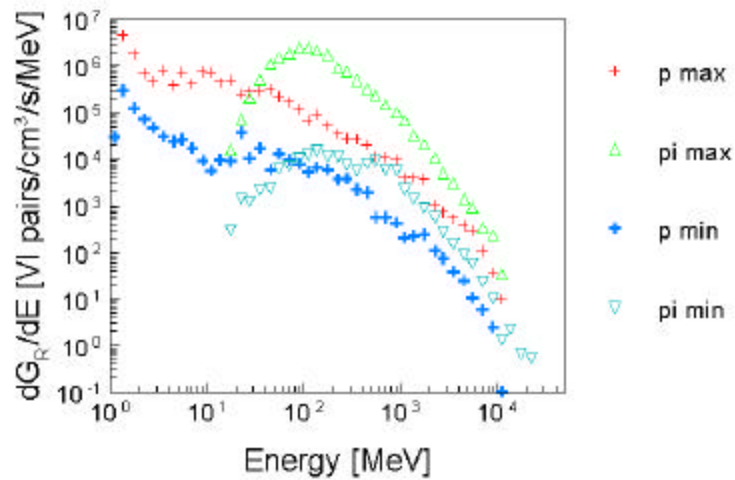


Fig. 1- Differential energetic generation rate of vacancy-interstitial pairs for pions and protons, for two positions (1): $r = 20 \text{ cm}$, $z = 0 \div 140 \text{ cm}$ and (2): $r = 100 \text{ cm}$, $z = 140 \div 280 \text{ cm}$ in the tracking cavity of LHC.

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

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: $6.2 \times 10^8 \text{ VI pairs/cm}^3/\text{s}$ for pions and $5.6 \times 10^7 \text{ VI pairs/cm}^3/\text{s}$ for protons, while for the second one (2) these are $8.1 \times 10^6 \text{ VI pairs/cm}^3/\text{s}$ and $3.1 \times 10^6 \text{ VI pairs/cm}^3/\text{s}$ 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 800 MeV passing from position (1) to position (2). For pions, the $CPD(E)$ dependence is cut at 20 MeV .

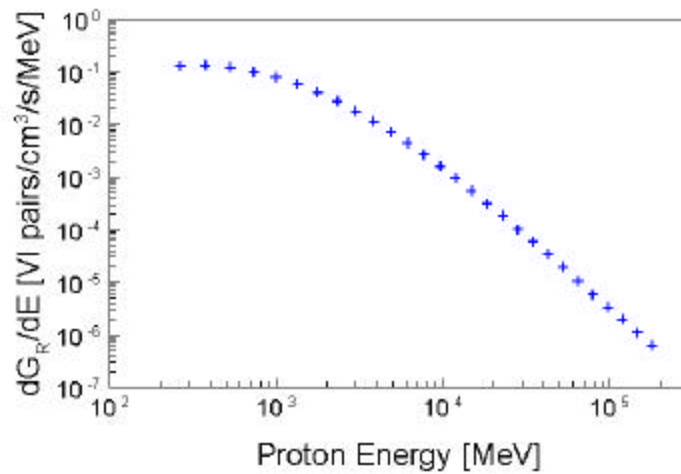


Fig. 2- Differential energetic generation rate of vacancy-interstitial pairs by cosmic protons in the space near the Earth.

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 [24]. 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/cm³/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.

Estimated damage in silicon detectors

Silicon used in high-energy physics detectors is n-type high resistivity ($1 \div 6$ 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 [25], [26]. 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. The present model confirms these conclusions. 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 1.8×10^{16} cm⁻³.

The model explains well the experimental data of defect production and evolution in silicon after irradiation [18] [19], and [27].

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

"oxygenating" one, containing 10^{14} cm^{-3} atoms of phosphorus, $4 \times 10^{17} \text{ cm}^{-3}$ atoms of oxygen, and $5 \times 10^{15} \text{ cm}^{-3}$ atoms of carbon respectively.

In some previous studies, e.g. [29] the following conclusions are drawn for 20°C temperature: 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 CO_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 is 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. 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. 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, [28], [29]. 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, $n, p \ll n_i$ (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 [30]:

$$I = qU = q \langle v_t \rangle n_i \frac{\mathbf{s}_n \mathbf{s}_p N_T}{\mathbf{s}_n \mathbf{g}_n e^{(E_i - E_i)/kT} + \mathbf{s}_p \mathbf{g}_p e^{(E_i - E_i)/kT}} \quad (7)$$

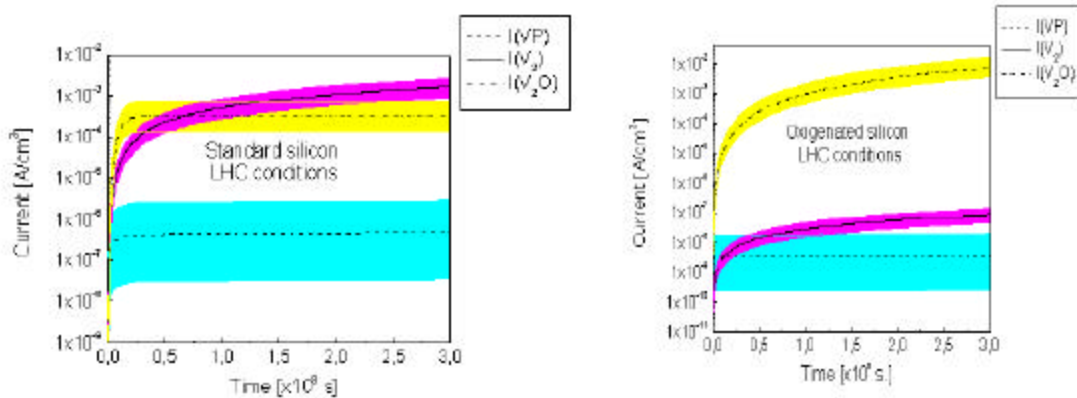
where \mathbf{g}_n and \mathbf{g}_p are degeneration factors, \mathbf{s}_n (\mathbf{s}_p) are the cross sections for majority (minority) carriers of the trap, $E_i = (E_c - E_v)/2$ and $\langle v_t \rangle$ is the average between electron and hole thermal velocities.

In the Shockley-Read-Hall model [31] used for the calculation of the reverse current, each defect was supposed to have 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 physical quantities 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 [15] and [32]), 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. Silicon used in high-energy physics detectors is n-type high resistivity ($1 \div 6 \text{ k}\Omega \cdot \text{cm}$) 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. The present model confirms these conclusions.

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 $5 \times 10^{17} \text{ cm}^{-3}$ is obtained. These materials can be enriched in substitutional carbon up to $1.8 \times 10^{16} \text{ cm}^{-3}$.

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 [28] and [29]. 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 $+20^\circ\text{C}$ (reference temperature), $+10^\circ\text{C}$, 0°C and -20°C with 24 GeV/c protons at a flux of about $5 \times 10^9 \text{ cm}^{-2} \text{ s}^{-1}$, up to the fluence $1.1 \times 10^{14} \text{ cm}^{-2}$ [33] were used to investigate model predictions.

In Figure 3, 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 represent the maximal uncertainties due to the energy position of the defects and to their cross sections.



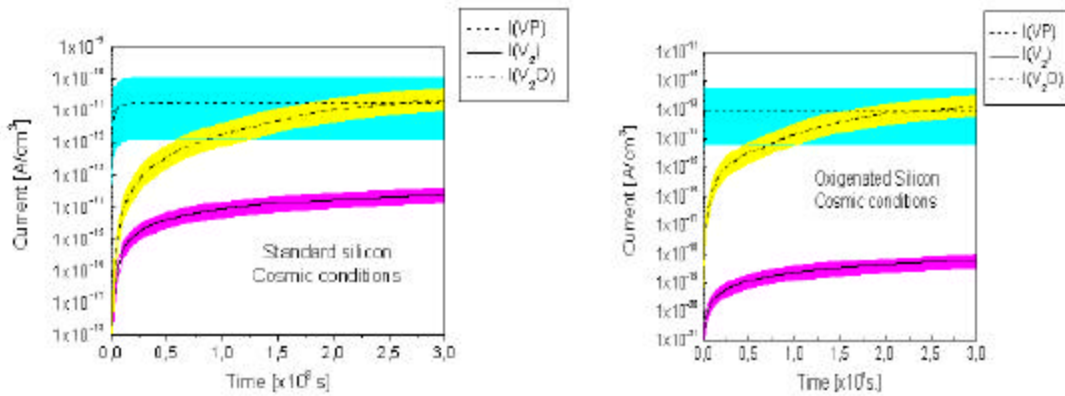
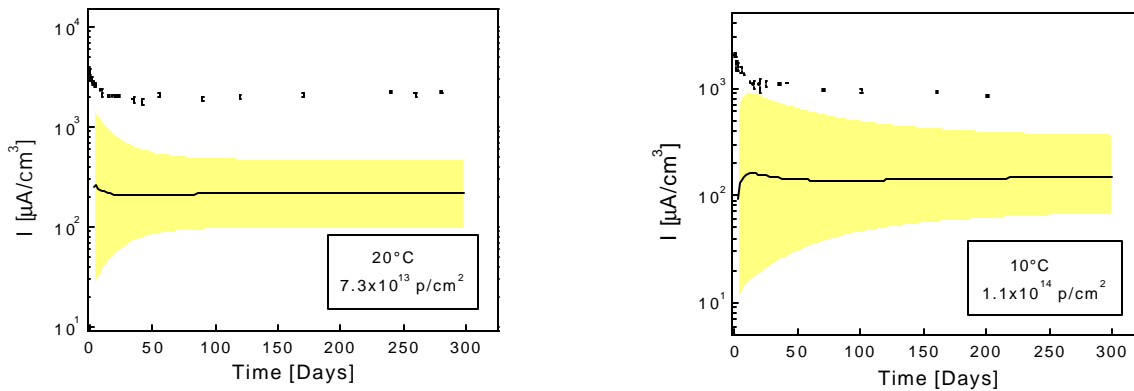


Fig. 3 - Time dependence of the generation current due to divacancy (continuous line), VP (dashed line) and V_2O (dashed dotted line).

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. 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 also maximal uncertainties in leakage current calculations due to the unsatisfactory knowledge of energy positions of the defects and of their cross sections. This comparison puts 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.



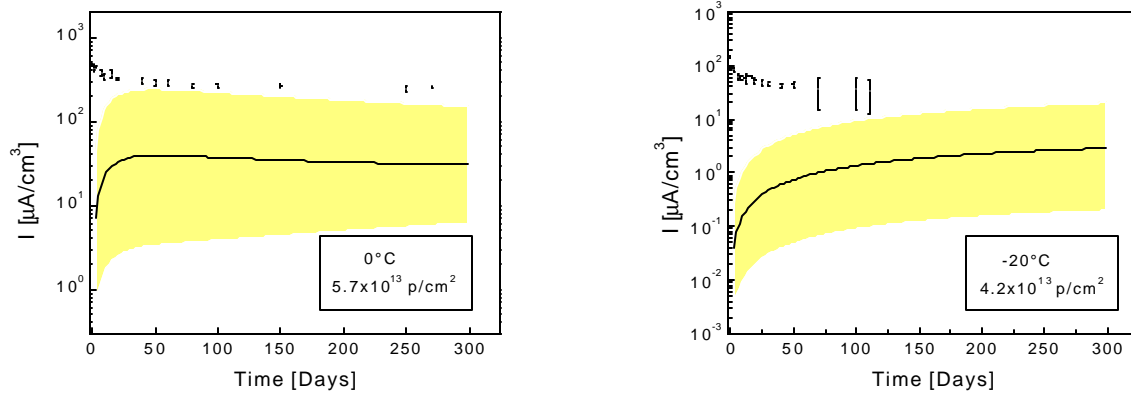


Fig. 4 - Time dependence of the leakage current density induced by 24 GeV/c proton irradiation in silicon detectors at 20°C, 10°C, 0°C and -20°C respectively. Experimental data: points, calculations: line.

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 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 Schottky's affirmation [26] that the independent and interacting energy level cases are indistinguishable if the energy levels are more than a few $k_B T$ apart). At lower temperature, other defects and annealing mechanisms must probably be considered.

SUMMARY

The phenomenological model developed previously to explain defect generation and evolution in silicon has been extended to consider the reactions of decomposition of vacancy - impurity complexes by interstitials, and of interstitial - impurity complexes by vacancies, as well as vacancy migration to sinks. It 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 $0 \pm 20^\circ\text{C}$, 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 has 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 higher oxygen content in silicon becomes visible with the decrease of the generation rate.

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