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New aspects of the contribution of primary defects of silicon to long-time degradation of detectors operating in high fields of radiation

S. LAZANU*, I. LAZANU[a]
National Institute for Material Physics, POBox MG-7, Bucharest-Măgurele, Romania
[a]*University of Bucharest, Faculty of Physics, POBox MG-11, Bucharest-Măgurele, Romania*

Silicon detectors will be used in the next generation of experiments in high energy physics and bulk damage is the main limitation in their utilisation. Although silicon is the most studied semiconductor, and the studies of defects in silicon have a long history, until now it is not completely established what are all primary defects in silicon, and what are their properties. In this contribution we investigate the new perspective in understanding fundamental phenomena in silicon and implications for the damage of detector characteristics due to the existence of the new primary fourfold coordinated defect, with a lower value of the formation energy in respect to the "classically" known vacancies and interstitials. The effects of its existence at device level are investigated, and possible consequences for the detectors in the next generation of experiments are discussed.

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1. Introduction

Silicon detectors will represent an important option for the next generation of experiments in high energy physics of accelerated particles and nuclei or astroparticles, where the requirements to work long time in high radiation environments will represent a major problem. After the long-time operation in high radiation fields, these interactions produce bulk displacement damage in the semiconductor material, and manifest at the detector level by the increase of the leakage current and the decrease of the Signal/Noise ratio, increase of the effective carrier concentration and thus of the depletion voltage, decrease of the charge collection efficiency up to unacceptable levels.

Intrinsic point defects in silicon have attracted a great deal of interest because of their technological importance. In Si a paradoxical situation exists: until now it is not completely established what are all primary defects and what are their properties.

In this paper we investigate the fundamental phenomena in silicon and implications for the damage of detector characteristics due to the consideration of the existence of the new primary: fourfold coordinated defect, Si_{FFCD}. Predicted by Goedecker and co-workers [1], its characteristics were indirectly determined in Ref. [2]. The correlation between the intrinsic characteristics of primary defects, their rates of generation, material doping and observable effects is investigated considering silicon of different resistivities and produced by different technologies: FZ and DOFZ, as time, temperature, crystal orientation and fluence dependencies. Due annealing processes, effects in the material and device are dependent on the rate of generation of defects and on the type of irradiation: step by step or continuous. These situations correspond to the expected environments at the next generations of high energy physics experiments.

2. Present status in the knowledge of primary defects in silicon

The lattice vacancy and self interstitial are, by their nature, the simplest known defects, produced by the processes of transfer of energy to the lattice, for example thermally or by irradiation with energetic particles. In thermal equilibrium the concentration of vacancies and self-interstitials is small because their formation energies are several eV.

The stability of crystalline silicon comes from the fact that each silicon atom can accommodate its four valence electrons in four covalent bonds with its four neighbours. The production of primary defects, the existence of impurities or lattice defects destroys the fourfold coordination.

It has been established that the structural characteristics of the "classical" vacancy are: the bond length in the bulk is 2.35 Å and the bond angle – 109°. The formation energy is 3.01 eV (p-type), 3.17 eV (intrinsic), 3.14 eV (n-type).

For interstitials, different structural configurations are possible: a) the hexagonal configuration, a sixfold coordinated defect with bonds of length 2.36 Å, joining it to six neighbours which are fivefold coordinated; b) the tetrahedral interstitial is fourfold coordinated; has bonds of length 2.44 Å joining it to its four neighbours, which are

therefore fivefold coordinated; c) the split - <110> configuration: two atoms forming the defect are fourfold coordinated, and two of the surrounding atoms are fivefold coordinated; d) the 'caged' interstitial contains two normal bonds, of length of 2.32 Å, five longer bonds in the range 2.55÷2.82 Å and three unbounded neighbours at 3.10÷3.35 Å. The calculations [3, 4, 5] showed that the tetrahedral interstitial and caged interstitial are metastable. For interstitials, the lowest formation energies in eV are 2.80 (for p-type material), 2.98 (for n-type) and 3.31 in the intrinsic case respectively.

In silicon the vacancy has five charge states in the band gap: V^{2+}, V^{+}, V^{0}, V^{-}, and V^{2-} and the self-interstitial could exist in four charge states after some authors [6]: I^{-}, I^{0}, I^{+} and I^{2+}, or in five states, after other authors [7].

In the ’80, in a series of theoretical studies [8] and correlated EPR and DLTS experiments of Watkins and co-workers [9], some problems associated with the electrical level structure of the vacancy have been solved. The charge states V^{2+}, V^{+}, V^{0} form the so-called negative U system, caused when the energy gain of a Jahn-Teller distortion is larger than the repulsive energy of the electrons, case in which the (0/+) level is inverted in respect to (+/++) level, which is the striking consequence of the fact that the V^{+} charge state is metastable.

In what regards the energy levels of these defects, only recently, Lukjanitsa [6] identified experimentally levels assigned to vacancies and interstitials. The review of the present knowledge on energy levels in the band gap for isolated vacancies and interstitials is discussed in Ref.[2].

In 2002, Goedecker and co-workers [1] predicted the existence of a new type of primary defect by moving atoms from the initial positions, but this displacement does not break the bonds with the neighbours. It is named and used in the following discussion as: Si_{FFCD} (**F**our**f**olded **C**oordinated **si**licon **D**efect). The bound lengths are between 2.25÷2.47 Å and angles vary in the 97÷116° range. So, bound lengths and angles do not deviate significantly from their bulk values. The formation energy is 2.45 eV (for p-type silicon), 2.42 eV (intrinsic), 2.39 eV (n-type), lower than the energy of formation of both vacancies and interstitials. Al-Mushadani and Needs [10] using *ab initio* density-functional methods investigated the energy of formation of various defects as a function of temperature. They obtained that at low temperatures the Si_{FFCD} is more stable than the vacancy and above 1049 K the stability is interchanged.

Previously, equivalent configurations of Si_{FFCD} have been predicted by different authors in relation with the existence of other possible defects – for an extended discussion see for example Allred and co-workers [11].

In a recent paper [2], the authors considered that this defect is produced more abundantly in irradiation processes at high fluences of particles, supplementary to thermal production, and, using experimental microscopic and macroscopic data established their characteristics. From this analysis, it has been obtained that the Si_{FFCD} defect is produced with a concentration of about 10% from all vacancies per act of interaction and is stable in time. The possibility that new defect to produces complex defects in silicon has not been considered. The defect has an energy level in the band gap between E_c – (0.46 ÷ 0.48) eV, a capture cross section between $(5\div10)\times10^{-15}$ cm^2 and a ratio $\sigma_p/\sigma_n = 1 \div 5$. Despite of its stability and its low energy of formation, the concentration is low in respect to the vacancy because to obtain this new configurational structure it is necessary that two neighbouring atoms in the lattice be excited simultaneously and jump from their usual positions.

The Si_{FFCD} has not yet been detected experimentally. This fact is not unexpected because the search for defects is always guided by theoretical predictions. In principle, this new type of defect could be characteristic for all semiconductors with diamond structure. Moreira, Miwa and Venezuela [12] found that the FFCD exists and is also stable in Ge, and this prediction is in agreement with experimental data [13].

3. Results and discussions

In the investigated bulk degradation of silicon due to irradiation, the formation of complex defects as: V_2, VO, V_2O, VP, C_iC_s, C_iO_i is considered.

The concentration of the primary radiation induced defects per unit particle fluence could be calculated using the explicit formula:

$$CPD(E) = \frac{N}{2E_d} \int \sum_i \left(\frac{d\sigma}{d\Omega} \right)_i L(E_{Ri}) d\Omega$$

where E is the kinetic energy of the incident particle, N is the atomic density of the element, A is the atomic number, E_d - threshold energy for displacements, 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 $(d\sigma/d\Omega)$ - 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. CPD is not proportional to the modifications of material parameters after irradiation, due to the subsequent interactions of primary defects with other defects and impurities in the lattice. So, the primary production of defects depends on crystal orientation in the irradiation field, type of particle and energy.

The anisotropy of the threshold energy for displacements conduces to the anisotropy primary defect production, and consequently influences the radiation damage, especially for low energy particle irradiation. The anisotropy of effective threshold energies (21 eV on <111> and 30 eV on <100>), which affects the concentration of primary defects and further their generation rate is observed in experimental data, and a good agreement of theoretical calculations with these data has been obtained both for FZ and DOFZ silicon with resistivity of the order of 2 kΩcm, – see Figures 1 and 2 respectively.

In Fig. 1a, experimental (points) and calculated (lines) dependencies of the effective carrier concentration in the space charge region of the detector (N_{eff}) on proton fluence are presented. Continuous lines correspond to calculations where the contribution of Si_{FFCD} is considered, while dashed ones do not take into consideration this defect. As specified before, samples with two orientations have been measured, and two different threshold energies for displacement have been used. Data are from reference [14], while lines are calculations in the present paper.

A good agreement between theoretical calculations and experimental data is obtained when the Si_{FFCD} is introduced in the model. The introduction of the new defect: Si_{FFCD} eliminates all the old known discrepancies between measured degradation of devices, especially after hadron irradiation. Because the concentration of this defect is considered to be a fraction of all produced classical vacancies and interstitials, and it is stable, an accumulation of its concentration appears, with effects observed with the increase of the fluence.

In Fig. 1b, the corresponding concentrations of divacancies are calculated for the same situations and are represented with the same symbols. It could be observed that, as expected, the introduction of the Si_{FFCD} defect reduces the concentration of divacancies, Si_{FFCD} being a competitor of the V_2 defect. Higher displacement energy decreases the CPD and consequently the generation rate and thus lower concentrations of divacancies and lower effective concentration of carriers are obtained.

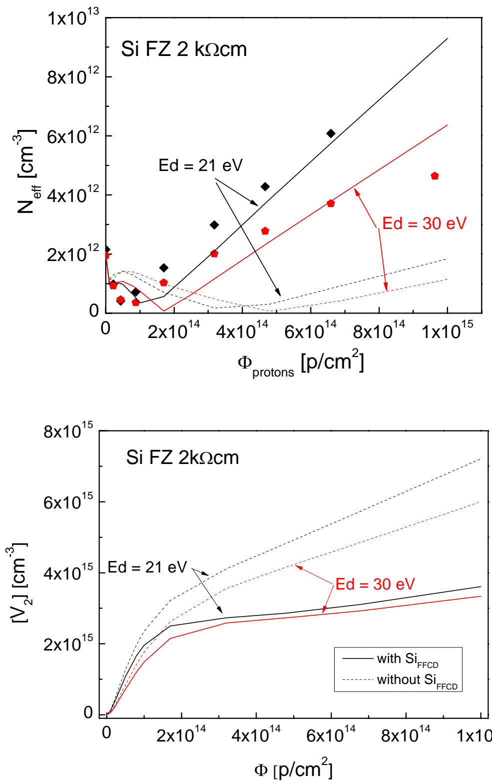

Fig. 1. (a) Dependence of N_{eff} on proton fluence and (b) Concentration of V_2 Vs. proton fluence for FZ silicon. Lines – model calculations; continuous line - with the consideration of the Si_{FFCD} defect and dashed ones - without this contribution, for two values of the threshold energy. Points – data from reference [14].

Figs. 2a and 2b present the same dependencies for DOFZ silicon, the experimental data being also from Reference [14]. In DOFZ Si, oxygen is used as a capture sink for vacancies because the production of the VO defects is favoured. A lower sensitivity of DOFZ silicon in respect to FZ at high energy proton irradiation has been found.

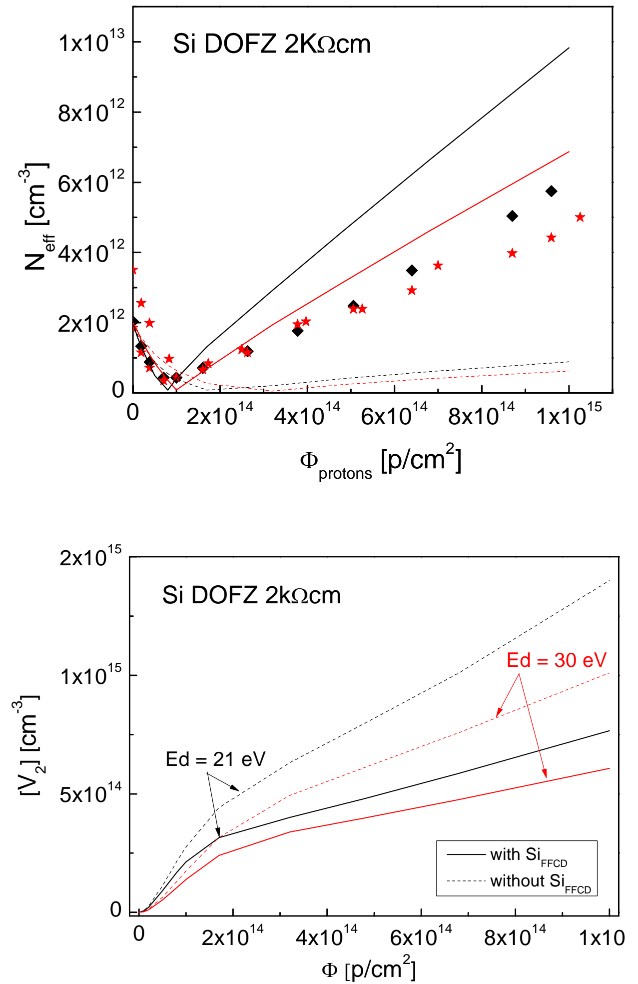

Fig. 2. Same as in Fig. 1 for DOFZ silicon.

Because all considered processes are thermally excited, the utilisation of detectors at lower temperature has beneficial results from the point of view of the degradation. This aspect is very clearly observed in the Figs. 3 – 5.

In Fig. 3, the dependence of the alpha degradation constant of the leakage current after proton irradiation on the time after irradiation at 20, 10 and 0 °C is presented. Experimental points are from reference [15], and lines are present calculations. Detectors at 20 °C have been irradiated at 7.5 10^{13} p/cm^2, at 10 °C - 1.12 10^{14} p/cm^2, and at 0 °C - 5.7 10^{13} p/cm^2 respectively. Continuous lines represent model calculations with Si_{FFCD}, while dashed ones are without this defect.

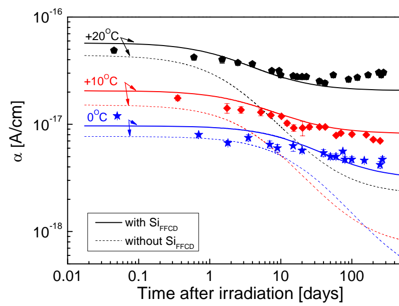

Fig. 3. Time dependence of the degradation constant of the leakage current at 20, 10 and 0°C. Points - experimental data from [15]; lines - model calculations: with (continuous) and without (dashed) Si_{FFCD}.

The dependence of N_{eff} on the time after irradiation is represented in Fig. 4 for the same detectors – data from Ref. [15], for 20 and 0 °C, with and without Si_{FFCD}.

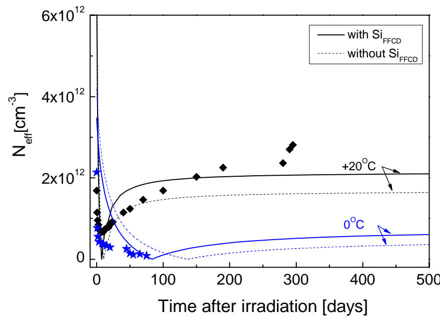

Fig. 4. N_{eff} Vs. the time after irradiation at 20 and 0 °C. Points - experimental data from [15]; lines - model calculations: with (continuous) and without (dashed) Si_{FFCD}.

From all defects, the divacancy is most affected by the presence/ absence of the Si_{FFCD}. In Fig. 5, the dependence of its concentration on the time after irradiation is represented.

If Si_{FFCD} is a defect stable in time, thus, in conditions of continuous irradiation, as will be the case of the next experiments in HEP, the accumulation of this defect will produce a strong degradation of the parameters of devices. Consequently, the silicon materials, technologies and temperature of operation must be carefully selected, to diminish production of Si_{FFCD}.

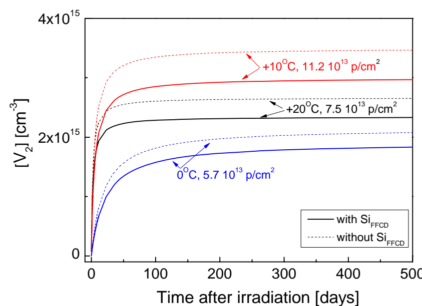

Fig. 5. $[V_2]$ Vs. the time after irradiation at 20, 10 and 0 °C: model calculations: with (continuous line) and without (dashed line) Si_{FFCD}.

4. Summary

In this contribution we investigated the role of primary defects, in particular of the Si_{FFCD}, in the processes of degradation of silicon induced by irradiation. Because radiation field is an important source of production of defects, the correlation between different conditions of irradiation and effects in detector characteristics has been investigated. The conclusions obtained represent a useful tool to obtain materials and devices with harder radiation properties.

Acknowledgments

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*Corresponding author: lazanu@infim.ro