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Silicon detectors: from radiation hard devices operating beyond LHC conditions to characterisation of primary fourfold coordinated vacancy defects

(Work in the frame of CERN RD-50 Collaboration)

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Abstract: The physics potential at future hadron colliders as LHC and its upgrades in energy and luminosity Super-LHC and Very-LHC respectively, as well as the requirements for detectors in the conditions of possible scenarios for radiation environments are discussed in this contribution.Silicon detectors will be used extensively in experiments at these new facilities where they will be exposed to high fluences of fast hadrons. The principal obstacle to long-time operation arises from bulk displacement damage in silicon, which acts as an irreversible process in the in the material and conduces to the increase of the leakage current of the detector, decreases the satisfactory Signal/Noise ratio, and increases the effective carrier concentration. These effects must be considered in the design of semiconductor detectors for high energy physics.A major difficulty in the prediction of these effects arises from the fact that there exists a good or reasonable agreement between theoretical models and data for the time evolution of the leakage current and effective carrier concentration after lepton and gamma irradiation, and discrepancies up to 2 orders of magnitude for leakage current and the time interval for inversion after hadron irradiation, and this in conditions where a reasonable accord is obtained between experimental and calculated concentrations of complex defects.In this paper, we argue that the consideration of the existence of the new defect - the fourfold coordinated defect (Si_{FFCD}) could solve these discrepancies and also permits to estimate indirectly the characteristics of the defect.

Key words: high energy physics, TeV energy, LHC, up-grade, silicon detectors, hadrons, leptons, radiation damage, primary defects, kinetics of defects

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1. Introduction

The physics potential at future hadron colliders as LHC and its upgrades in energy and luminosity (Super-LHC and Very-LHC respectively), as well as the requirements for detectors in the conditions of possible scenarios for radiation environments are discussed. Silicon detectors will be used extensively in experiments at these new facilities where they will be exposed to high fluences of fast hadrons. The principal obstacle to long-time operation arises from bulk displacement damage in silicon, which produces primary point defects, and which

produces the degradation of detector parameters. These effects must be considered in the design of semiconductor detectors for high energy physics.

In this paper we argue that the problem related to the different discrepancies between model calculations and experimental data for macroscopic detector characteristics after lepton and hadron irradiation could be solved naturally if the existence, as primary defects, of interstitials, classical vacancies, and of the new pseudo-vacancy defect, theoretically predicted the fourfold coordinated defect (Si_{FFCD}) is considered. Starting from experimental data on the modification of the detector parameters, in the frame of a theoretical model, it was possible to estimate indirectly some characteristics of the Si_{FFCD} defect.

2. Where is now high energy physics?

The current view of the universe is based on a small number of matter constituents acted on by four forces in a four-dimensional space-time. The simple structure of elementary constituents and forces forms the theoretical framework called the "Standard Model", which has been able to predict with very good accuracy the values of many quantities that have been measured by experiments at modern accelerators. But this theory is incomplete because:

- gravity is not included;
- it requires as input a large number of parameters such as the masses of the constituents and the coupling constants of all forces;
- some aspects, as for example the existence of the Higgs particle and the mechanisms of the electroweak symmetry breaking, responsible for the striking asymmetry between the massless photon and the massive W and Z, or the difference by many orders of magnitude between the masses of neutrinos and those of the heavier quarks are not yet understood.

Major steps towards answering these questions would come from developing global theories but invoke energy scales that are far beyond the reach of conceivable accelerators and of obtaining new experimental results at higher energies, or at least observable traces of these theories at accessible energies. Experiments relevant to this quest are in principal to the high energy frontier [1], [2], but it is not restricted; they are also possible at low energy scales.

The Higgs boson is a key element for the Standard Model. Its discovery would be a fundamental confirmation of this model, and the precise measurement of its characteristics would open the way towards a more global theory. One possible extension of the Standard Model is "supersymmetry". It predicts that more than one Higgs boson will ultimately be found, at least one of which is light. It also predicts that each constituent of matter has a supersymmetric partner with zero spin and that each force carrier has partners of spin ½, realising a complete symmetry between forces and matter. Until now searches for these supersymmetric particles at the existing accelerators have been negative. If these particles exist, they should be revealed between about 100 GeV and a few TeV.

For the next two years, the Fermilab Tevatron Collider will be the frontier machine. If the Higgs boson is a light particle, it could be discovered at the Tevatron if its mass is less than about 170 GeV, assuming an integrated luminosity of 30 fb^{-1}, otherwise by experiments at the CERN LHC for masses up to 1 TeV.

The Large Hadron Collider is expected to operate from 2007. The main research goals for the two general experiments, ATLAS and CMS, are the exploration of the electroweak symmetry breaking mechanism, and in particular the discovery of the Higgs particle and the search for physics beyond the Standard Model and in particular supersymmetry. Most probable, around 2010 the results will be conclusive: or the Higgs boson will be firmly experimentally observed as well as the electroweak symmetry breaking via Higgs mechanism, or the theoretical ideas will require a major revision. Similarly, the discovery or rejection of supersymmetry should be possible within the first two years of LHC operation. If the supersymmetry exists, many new particles are expected to be produced and detected at LHC if the masses are of the order of 2 TeV. The partners of the

leptons will mostly be seen in cascade decays and will be difficult to identify above 300 GeV.

3. From LHC to Super-LHC and to Very-LHC

At the present time, despite technological difficulties, significant upgrades in energy and luminosity of the LHC accelerator are considered as Super-LHC and Very-LHC respectively, to respond to these majors physics provocation [3], [4]. The concrete upgrade path will be defined by the results from the initial years of LHC operation. In the conditions in which the final energy programme will attend 240 TeV, the possible physical scenarios include:

- search of supersymmetric particles; if only a few are discovered at lower energies other partners with masses as a few tens of TeV could be discovered,
- search for new heavy fermions,
- search for the existence of heavy neutral Z' and/or charged W' vector bosons,
- search of quark compositeness if traces are observed with a scale of a few tens of TeV,
- possible indications for large extra spatial dimensions confined to distances of the order of femtometers, a scale that can be probed only with collisions energies larger than 100 TeV,
- existence of a new strong W-W interactions.

In this discussion Very-LHC will open a completely new energy regime, which could be probed for new physics.

The main characteristics of LHC and of its possible up-grades are summarised in Table 1.

Table 1. Characteristics of the LHC accelerator and of its possible up-grades

	LHC	SLHC	VLHC (stage 1)	VLHC (stage 2)
$\sqrt{s}$ [TeV]	14	14÷28	40	up to 240
L x10^{34} [$cm^{-2}s^{-1}$]	1	10	1	1-2/**10**
Bunch spacing [ns]	25	**12.5**	**6**, 18	**6**, 18
σ_{pp} inelastic [mb]	≈ 80	≈ 80	≈ 100	≈ 140
N=$\Lambda\sigma_{pp}\Delta t$	20	**100**	20	25-50/**250**
$\langle E \rangle$ charged particles	450 MeV	500 MeV	about 500 MeV	600 MeV

The critical requirements for detectors are specified in the table as bold values.

Actual accelerator principles are able to attend the maximal expected energies and luminosities, but for detectors (in the present paper only silicon detectors are considered) technological aspects are not solved and new research and development studies are necessary to obtain harder radiation materials for expected fields in these environments.

4. Silicon detectors for post LHC era

4.1 The requirements for detectors

At the present time it is possible to discuss only general requirements imposed to detectors. Here we will concentrate on semiconductor options for future experiments.

An important part of the detector design is the shielding necessary to reduce background. A major source of background is the interaction of proton fragments with the beam pipe and other interaction region components. Special shielding design could reduce the background flux by orders of magnitude,

reducing this way the radiation dose to the detector components. These characteristics are important for detector design, in particular for luminosities of $L=10^{35}$ $cm^{-2}s^{-1}$ or higher.

Major challenges for detector operation at such high luminosities are related to the following aspects:

- The detectors must operate at high luminosity that supposes a large number of interactions per crossing. For example, at a luminosity of $10^{34} cm^{-2} s^{-1}$ and beam crossing time of 18.8 ns, the average number of interactions per crossing will be 19 and this number will increase to about 62 for a luminosity of $10^{35} cm^{-2} s^{-1}$ and for a bunch spacing of 12.5 ns.

- The radiation fluxes are different than the present situations. U. Bauer et. al. [1] has shown that the total and inelastic cross sections increase only slowly with energy one can extrapolate for energies for future accelerators. Thus, the radiation dose in the central region is a function mostly of the luminosity, not the energy. This conclusion permits to give some predictions for the particle spectra in the central cavity.

These suppositions are not true in the very forward region, where particle momentum scales with beam energy.

- A very good triggering capability is necessary and special fast trigger electronics need to be developed. The trigger system should reduce the initial interaction rate of about 50 MHz to a rate of about 50 Hz for writing events to tape. With a high occupancy of detector elements and a large number of readout channels a typical event size is in multi Mbyte range. This translates to a Gbyte/s tape rate. It is important to select only interesting classes of events at the trigger level and reduce the huge data sample manipulation after events are written to tape.

Semiconductor detectors are mainly used in the central tracking system. Typically this region consists of two sub-detectors: a precision vertex detector and a tracking system for momentum measurement.

Traditionally, silicon sensors have been fabricated using the float zone (FZ) crystal growth technique. For detector applications, the float zone technique ensures high-purity and defect-free silicon. Due to the high resistivity of the material, the detector can be full depleted at relatively low voltage. Naturally the silicon obtained by FZ growth is characterised by low oxygen concentration. A technique to incorporate oxygen in the bulk of the material to improve the radiation hardness of silicon has been developed at BNL [5]. For this material in literature we refer as DOFZ (diffusion oxygenated FZ).

Czochralski growth technology (Cz-Si) is generally characterised by low resistivity. In the last period, silicon with sufficiently high resistivity has been obtained (MCz Magnetic Czochralski), permitting to obtain detectors with low operating voltages.

The main research directions suppose improvement of the behaviour of standard materials in the radiation field, understanding the microscopic phenomena in material (a better identifications of the different defects in material and their kinetics), development of new technologies for detectors (for example epitaxial technology) and new materials (diamond, GaN, SiC, etc.), or new architecture for detectors, as thin detectors or 3D – architecture for example. For details see, e.g. [6].

4.2 Physical phenomena in irradiated silicon and their effects

An incident particle could interact with the electrons or with the nuclei of the semiconductor lattice. In these conditions it loses 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 electrons of the target is ionisation or excitation of the electrons of the target. This phenomenon is used in the detection of the radiation that penetrates into the detector. The effect is reversible.

The nuclear interaction between the incident particle and the lattice nuclei produces bulk defects. As a result of the interaction, depending on the energy and on the nature of the incident particle, one or more light particles are formed, and usually one (or more) heavy recoils. After this interaction process, the recoil nucleus is displaced from lattice position into self-interstitial position, its unoccupied initial position acting as a vacancy. If the recoil energy is large enough, it could 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. This phenomenon could be regarded as a cascade process for production of vacancies and interstitials. We denote by primary displacements all the displacements produced as a result of the primary interactions, without any further rearrangement of the vacancies and interstitials. The physical quantity characterising the process is the concentration of primary defects produced per unit of fluence of the incident particles, CPD, (or related quantities, for example the non ionising energy loss).

Electrically active defects are characterised by energy levels in the band gap and by cross sections for the capture of the majority (minority) carriers. Starting from the microscopic modifications of the characteristics in silicon, consequence of production of defects and of their time evolutions, the leakage current of a reverse biased p-n junction during and after irradiation is due to the generation of electron-hole pairs on the energy levels of defects. The equation for leakage current in the SRH model is:

$$j = q\langle v_{th}\rangle n_i \left[\sum_d N_d \sigma_d \exp\left(-\frac{|E_d - E_i|}{kT} \right) + \sum_a N_{na} \sigma_{na} \exp\left(-\frac{|E_a - E_i|}{kT} \right) \right] \quad (1)$$

The absolute value of the difference between ionised donors and acceptors in the space charge region of the detector, N_{eff} concentration of the device is:

$$N_{eff} = [P] - [VP] + \sum_d \left(\frac{N_C}{N_V} \right) \cdot \left(\frac{\sigma_n}{\sigma_p} \right)_d \cdot \exp\left(-\frac{2|E_d - E_i|}{kT} \right) - \sum_a \left(\frac{N_V}{N_C} \right) \cdot \left(\frac{\sigma_p}{\sigma_n} \right)_a \cdot \exp\left(-\frac{2|E_a - E_i|}{kT} \right) \quad (2)$$

In the two equations, index *"d"* is associated with deep donor defects and *"a"* with deep acceptor defects respectively.

Here $\sigma_n(\sigma_p)$ are the cross sections for the capture of majority (minority) carriers, E_i is the intrinsic level, and $\langle v_t \rangle$ is the average between electron and hole thermal velocities, with q – the electric charge of the electron. N_C and N_V are the effective density of states in the conduction (valence) band.

The principal obstacle to long-time operation arises from bulk displacement damage in silicon, which produces primary point defects, and which, in their turn give rise to stable defects by mutual interaction and by interaction with impurities and defects previously existent in the lattice.

In the prediction of the time evolution of the behaviour of silicon detectors in the radiation environments expected at hadron colliders, a major difficulty arises, because there exists a good or reasonable agreement between theoretical models and data for the time evolution of the leakage current and effective carrier concentration after lepton or gamma irradiation, and discrepancies up to 2 orders of magnitude for leakage current (smaller in model calculation) and the time interval for inversion after hadron irradiation [7], and this in conditions where a reasonable accord is obtained between experimental and calculated concentrations of complex defects.

The cause of this situation is that neither all microscopic defects, nor defect kinetics are completely elucidated.

4.3 Primary defects, new hypothesis and estimated characteristics of the Si_{FFCD} vacancy

The lattice vacancy and self interstitial are, by their nature, the simplest known defects, produced 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 or the existence of impurities or defects destroys the fourfold coordination.

It has been established that the vacancy takes on five different charge states in the silicon band gap: V^{2+}, V^{+}, V^{0}, V^{-}, and V^{2-}. Only relatively recently, in a series of theoretical studies [8] and correlated EPR and DLTS experiments of Watkins and co-workers [9] it has been possible to solve some problems associated with the electrical level structure of the vacancy. 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 are the striking consequence of the fact that the V^{+} charge state is metastable.

For vacancy the structural characteristics are: the bond length in the bulk is 2.35 Å and the bond angle – 109°. The formation energy is 3.01 eV (for p-type silicon), 3.17 eV (intrinsic), 3.14 eV (n-type).

Self-interstitials in silicon could exist in four charge states [10]: I^{-}, I^{0}, I^{+} and I^{2+}, but other authors predict the existence of five charge states [11]. For interstitials, different structural configurations are possible: the hexagonal and the tetrahedheral configurations, the split - <110> configuration or the "caged" one.

In the present paper, using new experimental results [12] combined with some old data [10], we suggest the possible level position assignment for isolated vacancies and interstitials –see Figure 1.

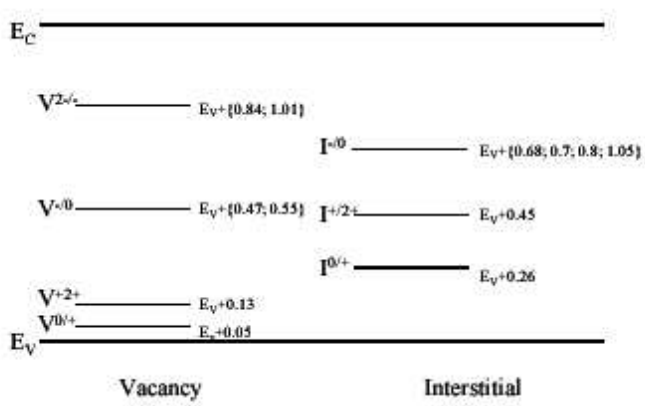

Fig. 1 - Possible levels position assignment for isolated vacancies and interstitials.

In the parenthesis are shown all theoretical or experimental values suggested for the considered defect

Goedecker and co-workers [13] predicted the existence of a new type of primary defect (pseudo-vacancy): Si_{FFCD} (**F**our**f**olded **C**oordinated Silicon **D**efect). It is obtained by moving atoms from the initial positions, but this displacement does not break the bonds with the neighbours. The bound lengths are between 2.25÷2.47 Å and angles vary in the 97÷116° range. 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. The authors suggests that this defect has energy levels in the band gap, but the theoretically model used in their prediction is not able to establish the energy gap band and the cross section for capture.

In the paper we introduced the following hypothesis:

a) we supposed that the Si_{FFCD} primary defect is produced simultaneously with the usual vacancy with a concentration that must be determined,

b) it is uniformly introduced in the bulk during irradiation

c) this defect has deep energy level(s) in the gap

d) the defect is stable in time.

In these hypotheses, the reaction of production of primary defects is:

$$Si \xrightarrow{G} V + Si_{FFCD} + I \tag{3}$$

The primary defects are created at a rate G, as a sum of contributions from thermal generation and irradiation; the rate of defect production due to irradiation being calculated as:

$$G_{irradiation} = \int CPD(E) \times Flux(E) dE \tag{4}$$

In the calculation of $G_{irradiation}$, the energy dependencies of CPD produced by different particles in silicon, is used, in agreement with Lindhard's theory and previous authors' papers [14].

The kinetics of defects, treated in the frame of diffusion limited reaction, in accord with the hypothesis of the model developed by authors in successive steps [15], could be summarised by the following processes:

$$I \rightarrow sinks \tag{5a}$$

$$V + V \leftrightarrow V_2 \tag{5b}$$

$$V + P \leftrightarrow VP \tag{5c}$$

$$V + O \leftrightarrow VO \tag{5d}$$

$$I + C_s \leftrightarrow C_i \tag{5e}$$

$$C_i + C_s \leftrightarrow C_i C_s \tag{5f}$$

$$C_i + O_i \leftrightarrow C_i O_i \tag{5g}$$

Defect concentrations for primary and complex defects produced in silicon are solutions of the associated system of simultaneous differential equations. We solved this system numerically.

The results of the modelling must reproduce experimental results both at the microscopic (concentration of the defects) and macroscopic level (leakage current and effective concentration of charge carriers).

The fraction of the vacancies that forms the Si_{FFCD} –defect, the corresponding energy level in the band gap and the cross sections for carrier capture represent the parameters of the model. In these conditions, the characteristics of the new defect are indirectly found.

For concrete calculations, the following experimental results have been used: time evolution of the concentration for VP, VO and interstitial C defects after electron irradiation from Song's paper [16]; time dependence of the leakage current after electron [17], proton [18] and positive and negative pion [19] irradiation; time dependence of the carrier concentration in the space charge region of the detector after proton [18,20], pion [19] and neutron [21] irradiation. Details of this analysis will be published elsewhere [22].

Thus, the Si_{FFCD} defect is produced with a concentration of about 10% from all vacancies per act of interaction, the defect has an energy level in the band gap around E_V+0.47 [eV] and the cross section for capture of majority carriers is around 10^{-16} cm^2.

Considering the contributions of these primary defects to silicon degradation the old discrepancies between data and model calculations are for the first time solved. These results must be confirmed. Probably, exists also some delayed mechanisms to formation of complex defects that not considered in the model and their contributions became observable long time after irradiation.

5. Conclusions

The contributions of primary defects to the leakage current and to the concentration of effective carriers were first time considered.

In the frame of the kinetics model, the time evolution of defects in different silicon material used for detectors can be well reproduced in the hypothesis considered in this paper related to the existence of silicon fourfolded coordinated vacancy.

The existence of this defect explains the modification of macroscopic silicon detector parameters both after hadron and lepton irradiations. In this analysis, the established parameters of new defect are: is produced with a concentration of about 10% from all vacancies per act of interaction; has an energy level in the band gap around E_V+0.47 [eV] and the cross section for capture of majority carriers is around 10^{-16} cm^2.

This defect acts as a "background" signal in the macroscopic characteristics of the detector.

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