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DEFECT ENGINEERING RADIATION TOLERANT SILICON DETECTORS

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Abstract

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Abstract. It is planned to use silicon detectors for many applications at the CERN Large Hadron Collider, where they will be exposed to unprecedented particle fluences. After hadronic irradiation, such detectors exhibit macroscopic changes in their electrical characteristics which lead to a degradation in performance. It is shown that these changes can be explained at the microscopic level using a combination of defect kinetics, defect characterisation of irradiated devices and device models. New results include evidence for inter-centre charge transfer between clustered defects and indications of multi-interstitial and multi-vacancy related defects. Finally, the work of the ROSE Collaboration (CERN RD48), whose aim is to defect engineer more radiation tolerant detectors, is described.

1. Introduction

The electrical characteristics of silicon detectors used in space and at accelerator-based research laboratories degrade during irradiation due to the introduction of defects. The detectors used in particle physics are basically diodes, which consist of p-type strips ion-implanted on a high resistivity n-type float-zone (Fz) substrate. Radiation damage effects in silicon devices have been studied for over 40 years, driven mainly by the nuclear reactor and weapons industries. However, the silicon for such devices is normally low resistivity material grown by either the Czochralski (Cz) or epitaxial methods. Consequently, radiation damage effects in high resistivity Fz substrates were poorly understood.

Due to its importance for experiments at CERN's Large Hadron Collider (LHC), work on this material has been intensive over the last five years or so. The LHC will commence operation around the year 2005, although the choice of material for inner detector layers will have to be made several years prior to this date. About 200 m² of silicon will be used by the LHC experiments. The radiation environment at the LHC will be particularly harsh. The detectors will have to withstand an ionising dose of ~10 Mrad and a hadron fluence equivalent to a few×10¹⁴ cm⁻² 1 MeV neutrons over a 10 year period [1].

2. Irradiation effects in detectors

Particle detectors are usually processed on n-type Fz material with a resistivity of 5-10 k Ω .cm and a depth of 300 μ m. The observed effects of hadronic irradiation fall into two categories; changes in leakage current and changes in effective doping concentration.

Significant charge trapping is also seen for particle fluences greater than ~ 10^{14} cm⁻², although this will not be discussed here. In addition to the primary changes which take place during irradiation itself, annealing effects have also been observed which are often more important in determining device operability. The changes in diode characteristics are found to scale linearly with Non-Ionising Energy Loss (NIEL). Examples of NIEL calculations may be found in [2]. These calculations can be used to relate the damage caused by particles of different types and energies, which is vital for predicting the damage in a particle physics environment where the received fluence may have many components. The various effects observed are described below.

2.1 Leakage current changes

Detector leakage currents increase significantly during irradiation. The current is described in terms of J_v , which is the leakage current per unit volume. It is well established that the increase in J_v is directly proportional to particle fluence:

$$\Delta J_v = \alpha \Phi \tag{1}$$

The proportionality constant, α , is known as the "damage" constant and has the value (5-10)×10⁻¹⁷ A.cm⁻¹ immediately after irradiation [3].

The leakage current is observed to anneal exponentially after the end of irradiation with a series of time constants, all of which are temperature dependent. At room temperature the current anneals by ~50% over a period of about 14 days.

2.2 Effective doping changes

In an unirradiated device, the space-charge results from shallow dopants in the silicon, usually phosphorus and boron. Photoluminescence studies indicate that the level of compensation by boron contamination is very low. Irradiation results in an accumulation of negative space-charge in the depletion region due to the introduction of deep levels. N-type detectors therefore become progressively less n-type with increasing hadron fluence until they invert to effectively p-type at around 2×10^{13} n.cm⁻² and then continue to become more p-type beyond this point, apparently without limit [4,5]. Typical results are shown in Fig. 1. In practice, the detectors still work beyond the inversion fluence because the junction moves from the p⁺ strips to the n⁺ back-plane contact.

The effective doping concentration, N_{eff} , can be inferred from the voltage required to obtain full depletion, V_{depl} :

$$N_{eff} = \frac{2\varepsilon_0 \varepsilon_{Si}}{ed^2} V_{depl}$$
(2)

where *d* is the diode thickness. At high fluences, N_{eff} can be such that the depletion voltage exceeds the breakdown voltage of the device and efficient operation is no longer possible. This effect represents the limiting factor for long-term operation at the LHC.



Fig. 1. Evolution of N_{eff} with neutron fluence for high resistivity n-type detectors from two manufacturers.

In the period after irradiation, the annealing behaviour of N_{eff} displays two distinct phases. There is an initial reduction in negative space-charge, which is later dominated by a slower, but much larger, increase in acceptor concentration. This second phase is known as "reverse annealing". The data were originally believed to be consistent with a "secondorder" model, in which two electrically inactive defects combine to form an electrically active acceptor state. However, recent careful measurements indicate that a simple firstorder dissociative process is a more likely explanation [6]. The rate at which reverse annealing proceeds is highly temperature dependent; the changes can take tens of years at 0°C but are accelerated to a matter of hours at 100°C. On account of these effects it is anticipated that detectors at the LHC will have to be operated considerably below room temperature, which is clearly problematic.

3. Defect kinetics modelling

A detailed understanding of radiation effects can be achieved by numerical calculations of the evolution of complex defects formed during irradiation. A 1 MeV neutron can transfer up to 130 keV to the primary knock-on atom (PKA). An atom with this energy can produce a cascade of many interactions, some of which produce energetic secondary recoils. Each of these terminates in a damage cluster which contains a high density of self-interstitial (I) and vacancy (V) pairs. At the centre of the cluster, where the initial concentration of defects is very high, I-V recombination is the dominant process and most (> 90%) of the primary radiation-induced defects are annihilated in a very short time. Some vacancies combine to form divacancies (V₂), and possibly larger multi-vacancy complexes (see Section 4).

Those interstitials and vacancies which escape initial recombination diffuse through the crystal and react with other defects and impurity atoms, particularly oxygen and carbon. Interstitial oxygen is the dominant sink for vacancies while substitutional carbon is the dominant sink for interstitials. Reaction rates are controlled by the concentrations of defects and impurities and their relative capture radii. Davies et al. [7] have explained optical absorption data after irradiation with 2 MeV electrons by means of a small number

of defect reactions. A kinetics model, based on this work but suitably modified, has been used to predict the evolution of defects during neutron irradiation [8,9]. The list of reactions is shown in Table 1. Note that the carbon interstitial, C_i , which is produced by the Watkins displacement reaction I + $C_s \rightarrow C_i$ + Si, is mobile and can complex with other impurities.

List A - primary reactions (in the PKA cluster)

I reactions	V reactions	C _i reactions
$I + V \rightarrow Si$	$V + V \rightarrow V_2$	

List B - diffusion reactions	(outside the cluster)
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I reactions	V reactions	C _i reactions
$I + C_s \rightarrow C_i$	$V + V \rightarrow V_2$	$C_i + C_s \rightarrow CC$
	$V + V_2 \rightarrow V_3$	$C_i + O \rightarrow CO$
$1 + CC \rightarrow CCI$	$V + O \rightarrow VO$	
$I + CCI \rightarrow CCII$	$V + VO \rightarrow V_2O$	
$I + CO \rightarrow COI$ $I + COI \rightarrow COII$	$V + P \rightarrow VP$	
$I + VO \rightarrow O$		
$I + V_2 \rightarrow V$		
$I + VP \rightarrow P$		

Table 1. Kinetics model reaction scheme [8].

The reactions in list A only have a significant chance of occurring during a PKA cascade. The densities of primary defects in the small volume of the damage cluster are large compared to the concentrations of impurity atoms in the high resistivity material. Consequently the relative introduction rate of divacancies during neutron irradiation is greatly in excess of that during electron irradiation. The reactions in the PKA cluster occur over ~100 ps, whereas the diffusion reactions (list B) take place over a much longer period.

In order to make quantitative calculations, the oxygen, carbon and phosphorus concentrations ([O], [C_s] and [P]) and introduction rates of I, V and V₂ are required. It is now well established that [O] and [C_s] in detector material are typically a few×10¹⁵ cm⁻³. Electrical measurements yield [P] $\cong 10^{12}$ cm⁻³. Introduction rates of I, V and V₂ have been calculated from DLTS measurements. These are of the order of 1 cm⁻¹, although there is some controversy between the various groups working in this field as to the exact values. For comparison, the values of $\eta_{\rm L}$, $\eta_{\rm V}$ and $\eta_{\rm V2}$ for 2 MeV electron irradiation are 0.167, 0.133 and 0.017 cm⁻¹ respectively [10].

Fig. 2 shows how various defect species evolve as a function of 1 MeV neutron fluence. The uncertainties in the predicted concentrations are difficult to estimate, arising mainly from errors on primary introduction rates, the concentrations of oxygen and carbon and uncertainties in the ratios of capture radii. The effectiveness of vacancy capture at oxygen prevents significant VP (E centre) production in high resistivity material. This process is not, therefore, a major factor in the observed doping changes.



Fig. 2. Kinetics model predictions for various defect concentrations as a function of 1 MeV neutron fluence.

With a knowledge of defect introduction rates and energy levels, it is reasonably straightforward to assess their influence on N_{eff} using Shockley-Read-Hall (SRH) theory. The lines on Fig. 3 show the introduction rate of a deep acceptor level required to describe the experimental N_{eff} vs. fluence data as a function of acceptor position relative to midgap [11]. The points superposed upon Fig. 3 are the predictions of the kinetics model for the introduction rates of the known acceptor complexes. The strongest candidate is the divacancy-oxygen (V₂O) complex [12,13]. There is now experimental evidence for the production in detector material of a defect believed to be V₂O [14], but at a lower introduction rate than predicted by the kinetics model (0.03 cm⁻¹ as opposed to ~1 cm⁻¹). The ratio of the hole and electron capture cross-sections of this defect is, unfortunately, still unknown. However, the situation is more complicated than it would appear on the basis of Fig. 3 because it is now known that the occupancies of some defects which occur in the terminal damage clusters, including the divacancy, are significantly higher than would be expected from SRH statistics (see Section 4).

Nevertheless, in principle, a significant improvement in detector tolerance should be achievable by decreasing the introduction rate of V₂O. The surface plot in Fig. 4 shows the model predictions for η_{V2O} as a function of the initial oxygen and carbon concentrations. It is apparent that an **increase** in the initial oxygen concentration leads to a substantial reduction in V₂O production. This is because the oxygen impurity getters the vacancies produced during irradiation and suppresses the channel V + VO \rightarrow V₂O. These results have prompted the ROSE Collaboration to investigate oxygenated material as a solution to the problem of radiation hardness (Section 6). This is defect engineering in its truest sense; the deliberate addition of impurities to a semiconductor to affect the formation of electrically active defect centres and thus control macroscopic device parameters.



Fig. 3. The lines ascending to the right show the introduction rate for an acceptor state at a given energy level required to explain the experimental N_{eff} data for different assumptions of electron and hole cross-sections [11]. The markers show known acceptor state introduction rates from the kinetics model.



Fig. 4. Model predictions for dependence of η_{V2O} on initial values of [O] and [C_s]. Note the sensitivity to the oxygen concentration.

4. Inter-centre charge transfer

It is possible to calculate the leakage current in an irradiated detector from the defect concentrations predicted by the kinetics model. Such calculations provide compelling evidence that the generation lifetime in devices irradiated with heavy particles is considerably shorter than expected on the basis of standard Shockley-Read-Hall theory [15]. This discrepancy can be explained by inter-centre charge transfer between neighbouring divacancies and other defects in the terminal clusters. Simple calculations indicate that the local V₂ density within a typical cluster is ~10²⁰ cm⁻³. Since the extent of the bonding distortion caused by a single divacancy in the lattice is ~10 Å, direct carrier transitions between some of the defects are clearly possible.

The divacancy has 4 charge states which give rise to 3 energy levels in the forbidden gap: a donor (+/0) at E_v +0.20 eV; a first acceptor (0/-) at E_c -0.41 eV; and a second acceptor (-/=) at E_c -0.23 eV. By writing general expressions for the rates of emission and capture between any two of these states it is possible to solve for the occupancy of each state as a function of local divacancy density in the cluster (the full calculation is described in [15]). It is found that the occupancy of the first acceptor, denoted f_2 , is significantly enhanced over the value predicted by the SRH calculation due to the charge exchange reaction $V_2^0V_2^0 \rightarrow V_2^+V_2^-$. Results are shown in Fig. 5. The divacancy can therefore make a rather larger contribution to N_{eff} than one would expect from Fig. 3. Due to the high emission rates of the states closest to the band edges, the charge exchange process also results in a large enhancement in the leakage current, the predicted value being in good agreement with experimental data [15].



Fig. 5. Enhancement of V_2 first acceptor occupancy over SRH prediction due to inter-centre charge transfer [15].

Further evidence for inter-centre charge transfer has been provided by phenomena associated with two defects, denoted E70 and E170, which are believed to be formed in the terminal clusters [16]. The names of these defects are derived from the fact that they anneal out at 70°C and 170°C respectively. The annealing of each of these centres is correlated with a large reduction in detector leakage current. Both defects are too far from mid-gap to explain the magnitude of the changes in the current unless inter-centre charge

transfer is occurring [16]. The annealing behaviour of defect E170 suggests that it is probably the four-vacancy (V₄). This defect has been observed by EPR after MeV ion implantation [17] and is believed to anneal into the five-vacancy (V₅) at around 170°C.

5. Reverse annealing

Although reverse annealing is an important problem for long-term detector operation, until very recently little progress had been made in understanding its microscopic origins. In the last few months, however, the changes in N_{eff} have been correlated with two experimental observations. The first of these is a growth in the concentration of a bistable acceptor at E_v +0.32 eV [18]. The second is the appearance of the photoluminescence 'W' line [9]. The plot in Fig. 6 shows the intensity of this line in 5 samples which were originally irradiated to the same neutron fluence but were then stored at different temperatures for nearly 3 years. The samples have therefore undergone different amounts of reverse annealing. It is clear that the intensity of the line is broadly correlated with the magnitude of the reverse annealing, ΔN_{eff} .



Fig. 6. Correlation between strength of the W line and reverse annealing amplitude [9].

The W centre is, in many ways, an intriguing defect. Information may be found in [19]. It does not appear to be associated with any impurity but its production does saturate with increasing dose. It is normally seen after a heavy neutron fluence ($\sim 10^{16}$ cm⁻²) followed by a 250°C anneal for 30 minutes. The stress response of the line suggests that interstitials, rather than vacancies, are involved. It therefore seems most likely that the W is an intrinsic centre involving interstitials somehow trapped at a cluster of damage. This new result shows that the W centre can form at room temperature, albeit with a very long time constant.

At present, it is not clear whether the bistable acceptor identified in [18] and the W are the same defect, or, indeed, if they are actually responsible for the changes in N_{eff} . However, some inferences may be drawn. Reverse annealing sets in at ~170°C during elevated temperature studies [6]. This is the temperature at which V₄ anneals into V₅ (see above), and hence, by implication, the temperature at which the defect clusters undergo substantial re-ordering. Such a re-ordering would provide a natural mechanism for the

creation of the W centre. DLTS studies have consistently found that a large number of the interstitials created during irradiation of detector material are 'missing', i.e. unaccounted for by the observed defect complexes (see, for example, [20]). It is not, therefore, surprising that the rearrangement of the damage region results in the appearance of an interstitial-related complex.

It is evident that careful studies of the defects produced during reverse annealing, and of the dynamics of cluster re-ordering, are vital if a thorough understanding of the origins of the changes in N_{eff} is to be achieved.

6. The ROSE Collaboration

The ROSE Collaboration is a CERN R&D project which consists mainly of international groups working on detectors for particle physics experiments at the LHC. In addition, the Collaboration benefits from the very valuable input of solid state physicists and the expertise of silicon manufacturers, without whose cooperation progress in this field would be virtually impossible. To date, the impurity levels in standard material have been understood, epitaxial material is being studied and more exotic variants are being manufactured. The current status of the work is summarised in Table 2.

Material	Manufacturer	Made	Tested
Epitaxial	MACOM	Yes	Yes
	ITME	Yes	In progress
Fz + O	Polovodice	Yes	Yes
Fz + C	Polovodice	No	No
Fz + N	Polovodice	Yes	Yes
Fz + O + C	Polovodice	No	No
Fz + 0.1% Ge	Topsil	Yes	Yes
Fz + Sn	Topsil	Yes	No

Table 2. Status of materials under investigation by the ROSE Collaboration.

Very promising results have been obtained from diodes fabricated on reasonably high resistivity epitaxial material [21]. These devices consist of a 100 μ m, n-type, 900 Ω .cm epitaxial layer grown on a Cz substrate. SIMS measurements indicate that oxygen and carbon levels in the epitaxial layer are considerably higher than in Fz material. This is because these impurities out-diffuse from the Cz substrate during growth. Typical results are shown in Fig. 7. It is apparent that doping changes in the epitaxial material are substantially suppressed. At present, however, it is not clear whether this is due to suppression of V₂O production on account of the high oxygen concentration (Fig. 4) or some other, unidentified, effect. Whatever the cause, epitaxial material is an ideal solution for pixel layers at the LHC since these detectors do not require a 300 μ m layer for good signal-to-noise performance.



Fig. 7. Comparison between evolution of V_{depl} with proton fluence for epitaxial material (results normalised to 300 µm thickness) [21] and Fz material of the same initial resistivity (Fz results are simulated using an established parameterisation for the evolution of N_{eff} with fluence [22]).

Although a high oxygen concentration should be beneficial, other avenues of investigation are equally important. Current evidence suggests that, if divacancy production could be suppressed, the material would be extremely radiation hard both from the point of view of the leakage current and the changes in N_{eff} . This requires very high impurity concentrations to ensure that gettering centres are distributed on a similar scale to the PKA cascade. Isoelectronic elements such as germanium (Ge) and tin (Sn) appear to be suitable candidates. However, Fz devices with Ge levels of ~0.1% are no more radiation tolerant than standard detectors [22]. It is possible that a higher impurity fraction of germanium is required. Doping with tin is known to suppress V₂ production in Cz material [23]. Unfortunately, there are technological problems associated with processing such material and no working devices have yet been produced.

7. Outlook

This tour of current ideas and recent results demonstrates that our understanding of the underlying physics of radiation-induced bulk damage in Fz material has greatly advanced in the last three years. Recent results on epitaxial material provide the first experimental evidence that the defect engineering of radiation tolerant detectors is possible. The other types of silicon currently being evaluated will undoubtedly provide new insights into our models of defect formation and the influence of these defects on device parameters.

Particular areas of interest are the origins of reverse annealing and the phenomenon of inter-centre charge transfer. It is now a priority to obtain direct experimental evidence for the latter using EPR and related techniques. The community now has both the theoretical framework (defect kinetics and device models) and sophisticated characterisation techniques (DLTS, PL, IR, EPR etc.) to understand completely the observed effects. Although the proposed schedule is challenging, it is hoped that it will be possible to demonstrate truly radiation hard detectors for inclusion in the LHC experiments within the time remaining.

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