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**A microscopic explanation for type inversion and the annealing behaviour
of radiation damaged silicon detectors**

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Abstract

A semiconductor device model, DLTS measurements and defect kinetics considerations lead us to propose an explanation for the major changes in the macroscopic properties of silicon detectors caused by neutron irradiation.

Silicon detectors will be widely used in experiments at the CERN Large Hadron Collider where high radiation levels will cause significant bulk damage. In addition to increased leakage currents, changes in the effective doping concentration have been observed which are not fully understood and which represent the limiting factor to long term operation. The principal observations are:

- a) high resistivity n-type detectors apparently invert to p-type after a fluence of around 10^{13} cm^{-2} fast neutrons or high energy protons [1-3].
- b) after irradiation, at room temperature the effective doping density, N_{eff} , initially decreases for some days, then gradually increases over the next few months. This "reverse annealing" can be halted if the detector is cooled below about 5°C [4,5].

Type inversion has been parameterised by hypothesising donor removal, by creation of vacancy-phosphorus complexes, and the generation of shallow acceptors [1]. However, recent Deep Level Transient Spectroscopy (DLTS) measurements have been used to show that the phosphorus removal rate is a factor 30 times lower than required [6]. An alternative hypothesis [6] is that the introduction of deep acceptor levels, close to the centre of the band gap, causes n-type silicon to become effectively p-type *under bias*. A device model which includes a single acceptor in the Poisson equation has been successfully used to describe the observed evolution of N_{eff} with neutron fluence for both p- and n-type detectors. This model has only one free parameter, namely, the introduction rate for the acceptor. Fig. 1 shows the introduction rate required to explain fast neutron data as a function of the acceptor energy level relative to the centre of the bandgap.

Further understanding can be achieved by numerical calculations of the evolution of complex defects formed during irradiation. The elementary defects produced are vacancies (V), interstitials (I) and divacancies (V_2). Divacancies are static until about 600K whereas vacancies and interstitials are very mobile except at very low temperatures and those escaping initial recombination diffuse through the crystal reacting with other defects and impurity atoms, particularly oxygen and carbon. Reaction rates are controlled by the concentration of impurities and defects and their relative capture radii. Davies et al. [7] have explained infra-red absorption spectra of electron irradiated silicon by means of a small number of reactions. A kinetics model, based on this work and suitably extended, has been used to predict the evolution of defects during neutron irradiation [8]. The main reactions, which include those of interstitial and substitutional carbon (C_i and C_s) are listed below:

I Reactions	V reactions	C_i Reactions
<i>Group A</i>		
$I + C_s \rightarrow C_i$	$V + O \rightarrow VO$	$C_i + C_s \rightarrow CC$
$I + V_2 \rightarrow V$	$V + P \rightarrow VP$	$C_i + O \rightarrow CO$
$I + VP \rightarrow P$	$V + VO \rightarrow V_2O$	
$I + V_3O \rightarrow V_2O$	$V + V_2O \rightarrow V_3O$	
	$V + V_2 \rightarrow V_3$	
<i>Group B</i>		
$I + V \rightarrow Si$ (annihilation)	$V + V \rightarrow V_2$	
	$V + V_2 \rightarrow V_3$	

Group A reactions are for vacancies and interstitials diffusing throughout the crystal. The Group B reactions only have a significant chance of occurring during a Primary Knock-on Atom (PKA) cascade. The densities of primary defects in the small volume of the displacement damage region are large compared to impurity atom concentrations in the high resistivity silicon. For this reason the relative introduction rate of V_2 in neutron irradiation is greatly in excess of that in electron irradiation.

For quantitative calculations the oxygen, carbon and phosphorus concentrations ($[O]$, $[C]$, and $[P]$) and introduction rates of I, V and V_2 are required. $[P]$ was determined from electrical measurements as 10^{12} cm^{-3} ; photoluminescence measurements showed that the material was not significantly compensated with boron. $[O]$ and $[C]$ were inferred from DLTS measurements to be $\approx 5 \times 10^{15} \text{ cm}^{-3}$. Introduction rates of I, V and V_2 due to neutron irradiation were calculated from DLTS measurements as 12.8, 3.4 and 4.7 cm^{-1} respectively. These compare with values of 0.167, 0.133 and 0.017 cm^{-1} observed in 2 MeV electron irradiation[9]. Typical uncertainties are $\pm 10\%$. Ratios of capture radii were taken from Davies [7].

Because of its concentration and capture radius, oxygen is the dominant capture site for vacancies; carbon behaves similarly as a sink for interstitials. The effectiveness of vacancy capture at oxygen and related defects prevents significant VP production, despite the relatively large capture radius of phosphorus, and the model supports the experimentally measured low phosphorus removal rate. It also indicates possible candidates for the deep level acceptor(s) responsible for type inversion. The introduction rates calculated from the kinetics model for defects (excluding known

donors) are indicated in fig. 1; the energy level of each defect has been taken from ref. [10]. The strongest candidate is the V_2O centre; V_3O may also contribute.

To complete the picture the model should also explain the annealing behaviour of the detectors, which has so far been unexplained. For detectors irradiated past type inversion, a simple expression between deep acceptor concentration and effective carrier lifetime in the depletion region has been analytically derived. The same lifetime controls the detector leakage current. As a result one can write that

$$\frac{N_{eff}}{\Phi} \approx constant \times \sqrt{\frac{N_{deep}}{\Phi} \left(\frac{\alpha}{n_i} \right)}$$

where N_{Deep} is the concentration of deep acceptors, Φ is the fluence, α is the leakage current damage constant (volume current density per unit fluence) and n_i is the intrinsic carrier concentration. Only a small fraction of the deep acceptors are filled. Higher leakage currents result in more acceptors being filled which increases N_{eff} . The RD2 collaboration [11] have carefully measured both N_{eff} and α as a function of time from 1 hour to 200 days for detectors at temperatures of 20°, 10°, 0° and -20°C. The initial annealing of N_{eff} is proportional to $\sqrt{\alpha}$, fig. 2. In other words, in the early phase after irradiation, the density of deep acceptors is approximately constant but fewer remain filled as the leakage current reduces during annealing.

N_{eff} starts to exhibit reverse annealing (become more p-type) at room temperature once the leakage current reduction has ceased. This implies that N_{Deep} is increasing. The reason for this can be inferred from the DLTS spectrum shown in fig. 3. The electron trap at 226K consists of the divacancy and an unknown defect with a similar energy; the contribution of VP centres to this peak is negligible [6]. This defect disappears slowly at room temperature and is completely removed by an anneal at 350K. This is the same threshold temperature found in elevated annealing experiments [12]. Moreover, simultaneously the VO peak at 90K roughly doubles in size which must therefore be a consequence of vacancy release and capture by oxygen. This new source of vacancies then generates more deep acceptors which causes N_{eff} to increase. This successfully explains the observed features of reverse annealing, namely the strong temperature dependence and eventual saturation of the effective doping concentration. The identification of the V_2O centre as the most likely candidate for the deep acceptor is also consistent with this picture; the “delayed” vacancies react with VO centres to form more V_2O defects.

We hypothesise that the unidentified defect is the tri-vacancy (V_3) which is unstable at room temperature and breaks up releasing a vacancy. The origin of a significant V_3 concentration can be explained only by production in PKA cascades during irradiation. This is consistent with the enhanced V_2 production observed in neutron irradiation and is expected from the defect reaction picture where mobile vacancies combine with each other and static V_2 in the cascade volume. At present a numerical estimate of the V_3 concentration has not been derived.

In conclusion, although it may not be possible to prevent damage to silicon detectors by irradiation, the explanation given in this paper gives some hope that process modifications might lead to harder detectors. Clearly it is desirable to prevent formation of the V_2O defect. Modification of the carbon and oxygen

concentrations appears to be one approach which is being studied using the kinetics model. Alternatively, the addition of vacancy capture sites, e.g. Ge [13], with a concentration that leads to an average spacing which is less than the typical dimensions of a PKA cascade would suppress V_2 and V_3 production.

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Figure captions.

1. The introduction rate for a deep level acceptor required to be consistent with a rate of change of $N_{\text{eff}} = 0.016\text{cm}^{-1}$, as a function of the acceptor level within the band gap. Different assumptions for the ratio of hole and electron capture cross-sections (σ_h/σ_e) have been used; the most likely case is $\sigma_h/\sigma_e = 1$. On the figure are plotted as symbols the identified candidates for such a state.
2. The relationship between the leakage current damage constant (α) and the effective doping density (N_{eff}) for diodes irradiated at different temperatures to similar fluences. The data plotted are points generated using the parameterisation by the authors of ref [11].
3. DLTS electron trap spectrum of neutron irradiated diode before (open circle) and after (solid) isochronal annealing to 440K. The VO peak at 90K increases in magnitude while the other peak decreases by a similar amount.

Fig. 1

Fig. 2

Fig. 3