A Detailed Microscopic Analysis of Deep Levels in Heavily Irradiated-Medium Resistivity Silicon Detectors

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Abstract—in this work we show a detailed deep levels analysis (an energy resolution of 50 meV was reached) of a set of medium resistivity silicon samples, irradiated up to a fluence of $2.5 \cdot 10^{15}$ n/cm$^2$. In order to discriminate the large number of deep levels which appear to overlap their contributions in TSC and I-DLTS spectra, we adopted an innovative numerical procedure of data analysis which determines a set of deep levels that can account for both TSC and I-DLTS spectra. We finally obtained a consistent and detailed description of deep level population, clearly showing its evolution with fluence. Some results seem to suggest the possibility of quasi-continuous distributions of localized states inside the gap.

Index Terms—Deep levels, I-DLTS, radiation effect, silicon, TSC.

I. INTRODUCTION

It is planned to use Silicon devices as forward tracker detectors both in a Toroidal LHC Apparatus (ATLAS) [1] and compact muon solenoid (CMS) [2] experiments at the large hadron collider (LHC) [3]. The very high radiation levels foreseen in these experiments are expected to seriously worsen the electrical properties of these devices and have motivated the analysis of strongly irradiated silicon detectors [4], [5]. At the same time, during the search for radiation-hard detectors, the interest toward innovative materials has grown tremendously. One of the promising approaches is to use nonstandard silicon, e.g., substrates with medium ($\sim 1 \text{k} \Omega \text{cm}$) and low ($\leq 500 \text{ k} \Omega \text{cm}$) resistivity, as starting materials. Properties of Silicon diodes produced by different technologies and with different resistivities have recently been considered [6]. At the same time, new studies about medium resistivity (down to $1 \text{k} \Omega \text{cm}$) silicon detectors have been presented, concerning both microscopic disorder [7], [8] and bulk properties [9], [9].

Lattice disorder in irradiated silicon detectors is frequently studied by thermally stimulated current (TSC) and current-deep level transient spectroscopy (I-DLTS) techniques, because they are effective even when a large concentration of defects afflicts the samples. It should be noted that these techniques involve current measurements that do not allow the discrimination between electrons and holes emissions [10]. As a consequence, the data analysis results in the activation energy values corresponding to the distance between the trap levels and the nearest band but gives no identification of the band. Such information can be obtained only by comparison of TSC and I-DLTS spectra with results from other analyses, such as electron paramagnetic resonance (EPR).

The data analysis is a major issue. Several deep levels, with overlapped spectral contributions, are always found in irradiated silicon, even at low fluences of irradiation. In this situation the traditional Arrhenius plot method, which allows the extraction of the defect parameters of a single defect level from the relative TSC or I-DLTS spectrum, is not completely reliable, and deconvolution procedures are typically used [11]. In this approach the signatures of the various deep levels are obtained by fitting the spectra with a trial-and-error procedure. The arbitrariness and the intrinsic uncertainty of these methods can be reduced by comparing spectra obtained with different techniques [12]. However, in heavily irradiated samples an extremely large number of different deep levels exists, and the use of a deconvolution procedure may become a very difficult task. In spite of all of these, Arrhenius plots and deconvolutions are still widely adopted, due to their simplicity, in order to gain at least an approximate knowledge about microscopic disorder.

In this work we present a detailed microscopic analysis of medium resistivity silicon ($\rho = 500 \text{ k} \Omega \text{cm}$), heavily irradiated up to the fluence of $2.5 \cdot 10^{15}$ n/cm$^2$. We considered TSC and I-DLTS signals, and we adopted an innovative data-analysis procedure, which allows one to look directly for the deep level set consistent with both TSC and I-DLTS measurements. Such a procedure is outlined in Section IV, while details can be found in [13]. Following this procedure we were able to reveal a complicate deep level fine structure in the energy range of 0.3 to 0.5 eV, as described in Section V.

II. PROCEDURES

A. Samples and Experimental Setup

We studied a set of $p^+\text{-}n^+\text{-}n^+$ detectors, produced by boron implantation on phosphorous doped silicon at the Brookhaven National Lab. (Upton, NY). These diodes have a nominal resistivity $\rho = 400$--$500 \text{ k} \Omega \text{cm}$, an active area $A = 0.25 \text{ cm}^2$, and a thickness $W = 200$--$280 \mu\text{m}$. The samples were irradiated at UMass Lowell ($\Phi = 6.4 \cdot 10^{14}$--$7 \cdot 10^{15} \text{ cm}^{-2}$) and at the ATOMKI Institute of Nuclear Research of Debrecen, Hungary ($\Phi = 4.7 \cdot 10^{14}$--$2.5 \cdot 10^{15} \text{ n/cm}^2$). All the fluences have been normalized to 1 MeV neutron. The measurements have been carried...
out eight months after the irradiation at Lowell and two months after the irradiation at ATOMKI. During this time, the samples have been kept at room temperature (RT).

The depletion voltages have been evaluated using both capacitance versus voltage (CV) and transient current technique (TCT) measurements. CV characteristics have been measured at RT, by means of a HP4284A LCR precision meter with a test signal frequency of 1 kHz and a Keithley 237 as the voltage source. The depletion voltage has also been determined from TCT experiments by analysis of current pulse decay, since a step in the current pulse tail arises when the drifting carriers reach the opposite contact at or over the full depletion voltage. An experimental setup for TCT measurements, as well as a description of the data analysis, can be found in [14].

A detailed description of the TSC experimental setup is given in [15]. An optical filling of the traps has been used in the present measurements. The samples were exposed for 30 s to continuous laser light at the temperature $T = 77$ K, and the laser source ($\lambda = 1030$ nm, 25 mW of output power) was coupled to the sample by a one-meter-long optical fiber. We always used a constant heating rate of 0.15 K/s.

In the I-DLTS system, the samples were excited by the same laser diode used for TSC, driven by a pulse generator. The current signal was at first amplified by a broad-band current-voltage converter (Keithley 428) and successively processed by a double boxcar analog correlator (Sula Tech. Spectrometer), in order to extract the DLTS spectrum. The correlator is designed in such a way that the ratio between the transient sampling times $t_1$ and $t_2$ is fixed at $t_2 = 11.5 \times t_1$. The temperature of the sample was continuously increased, by thermal contact with an electrical resistance heater; we used a very slow heating rate, in order to avoid spectrum distortion. The same heating rate ($\beta_T = 0.15$ K/s) was used for TSC experiments. The temperature sensor was a silicon diode (Lake Shore mod. DT-470-CU-11), connected to a temperature controller (Lake Shore model DRC91C), providing the temperature reading.

In the present experiments we always used a reverse bias $V_{\text{rev}} = 5$ V and the following laser pulse parameters: pulse duration 0.2 ms, period 1 ms, peak instantaneous power 8 mW. We always started the measurements from liquid nitrogen temperature and increased it up to 350 K. At higher temperatures, the temperature sensor was a silicon diode (Lake Shore mod. DT-470-CU-11), connected to a temperature controller (Lake Shore model DRC91C), providing the temperature reading. In each experiment the first sampling time was chosen taking into account that a short $t_1$ gives a stronger signal, but also causes the spectrum to shift towards higher temperatures, thus possibly hiding contributions from near mid-gap deep levels. For less irradiated samples, which did not show high temperature peaks, we used a quite short sampling time, i.e., $t_1 = 50 \, \mu$s, but for the three most irradiated diodes the choice $t_1 = 100 \, \mu$s was necessary.

### III. Experimental Results

The depletion voltages ($V_{\text{dep}}$) have been determined by measuring the $C$–$V$ characteristics and the TCT signals for all the investigated samples. It is worthwhile to mention that the TCT analysis performed on the samples irradiated with a fluence of $4.7 \times 10^{14}$ n/cm$^2$ or higher, showed the double junction effect, widely discussed in recent years (see, e.g., [16]). The $V_{\text{dep}}$ values evaluated by the two methods are in good agreement, the differences lying within the experimental uncertainty. From the $V_{\text{dep}}$ values we calculated the effective space charge concentrations ($N_{\text{eff}}$) as a function of the fluence $\Phi$. Fig. 1 shows $N_{\text{eff}}(\Phi)$ for all the investigated samples. In agreement with literature [17], the data has been fitted using the following law:

$$N_{\text{eff}}(\Phi) = \left| N_{\text{eff}}(0)e^{-\alpha\Phi} - \beta\Phi \right|$$  \hspace{1cm} (1)

where $\alpha$ is the removal coefficient and $\beta$ is the introduction rate of the deep acceptors. The initial decrease of $N_{\text{eff}}(\Phi)$ is related to the radiation-induced shallow donor removal. This effect has been verified directly by means of TSC measurements in the low temperature region (8–20 K) on the same set of samples [18]. At higher fluences, $N_{\text{eff}}$ increases due to the introduction of deep acceptor levels. As indicated in [17], $\beta$ depends on the time after irradiation and on the temperature at which the samples have been stored during this time. In our case, generation rates of stable defects $\beta \approx 0.04$ cm$^{-2}$ and $\beta \approx 0.02$ cm$^{-2}$ have been found for the samples irradiated up to $7 \times 10^{23}$ n/cm$^2$ and for the heavily irradiated samples ($4.7 \times 10^{14}$ n/cm$^2$ and $9.3 \times 10^{14}$ n/cm$^2$), respectively. The best fit suggests a value of the removal coefficient $\alpha = 9.10^{-15}$ cm$^2$. The inversion fluence was observed at $1 \times 10^{14}$ n/cm$^2$; this value is in agreement with other measurements recently performed on medium and low resistivity silicon detectors [8].

Fig. 2 shows TSC measurements performed on five samples with irradiation doses ranging from $3.5 \times 10^{23}$ n/cm$^2$ up to $2.3 \times 10^{25}$ n/cm$^2$. During the measurements the samples were biased with a reverse voltage of 100 V. All the spectra present the same “low temperature” contributions near 145 K, but in the most irradiated samples new “high temperature” contributions arise between 155 and 195 K. All these peaks appear to be quite “broad” in comparison with the single-level theoretical line-shape, thus revealing the presence of a multitude of traps induced by irradiation in the lattice.
Fig. 2: TSC spectra of all the samples (after background suppression); $\beta_T = 0.15$ K/s; the optical filling occurred at $T = 77$ K.

Figs. 3 and 4 show I-DLTS spectra obtained on the same samples. Similarly to what was observed in the TSC case, the samples irradiated up to $4.8 \times 10^{13}$ n/cm$^2$ generate only one main component (at about 260 K), while at higher fluences a second contribution is observed near 320 K. It must be mentioned that a minor peak, not shown here, appears in I-DLTS spectra around $T = 100$ K, but has not been considered in our analysis. With the present experimental conditions, the corresponding peak is not clearly distinguishable in TSC spectra, and the detailed analysis according to the procedure described in Section IV is not possible. The observation of this peak in medium resistivity silicon samples has been reported in [5] too, together with a tentative discussion of its origin and possible identifications. The signal increase near 350 K is due to the pulse response of the samples, whose amplitude increases with temperature. This current increase, which could possibly hide small contributions from levels extremely close to the midgap, has not been considered during data analysis.

IV. DATA ANALYSIS

When a large number of different deep levels, possibly continuously distributed, affects the sample, it is convenient to describe them by introducing a deep level density $G(E)$ and an energy dependent cross section $\sigma(E)$. In this case $G(E)$ and $\sigma(E)$ can be connected to TSC and IDLTS spectra by

$$S_{TSC}(T) = \int_0^{E_{gap}/2} K_{TSC}(T, E, \sigma(E)) G(E) dE$$  \hspace{1cm} (2a)

$$S_{IDL}(T) = \int_0^{E_{gap}/2} K_{IDL}(T, E, \sigma(E)) G(E) dE.$$  \hspace{1cm} (2b)

If all the deep levels are discrete, $G(E)$ goes clearly into a sum of Dirac deltas. This system of two nonlinear integral equations must be solved to get the common unknown functions $G(E)$ and $\sigma(E)$. The expression of the $K$-functions is

$$K_{TSC} = \frac{q}{2} \frac{\beta_T}{c(T, E)} \exp \left[ -\frac{1}{\beta_T} \int_{T_0}^{T} c(T, E) d\tau \right]$$  \hspace{1cm} (3)

$$K_{IDL} = \frac{q}{2} \frac{E}{c(T, E)} \left[ \exp(c(T, E)t_1) - \exp(c(T, E)t_2) \right]$$  \hspace{1cm} (4)

where $c(T, E) = \gamma \sigma(E) T^2 \exp(-E/kT)$ is the emission coefficient, $x_d$ is the depletion depth, and $\gamma$ is a characteristic constant depending on the crystal structure; $q$ is the electron charge. We have calculated the depletion depth from the depletion voltage as $x_d = W_{d} / \sqrt{V_{dc}/V_{th}}$. If $\sigma$ is fixed to a constant value, then (2a) and (2b) reduce to linear integral equations (Fredholm equations of first kind), which can be solved independently using an iterative procedure. By repeating this procedure with properly chosen, different values of $\sigma$, and comparing the TSC and I-DLTS results, it is possible to infer the correct signature of each deep level, thus giving a deep level distribution $G(E)$ consistent with both TSC and I-DLTS measurements.

If an equal trap filling is not guaranteed in TSC and I-DLTS experiments, this fact must also be taken into account. We adopted a filling time such that a longer excitation did not result in a higher TSC signal, and we assumed that this time corresponded to the saturation of the deep levels. Moreover, by comparing TSC and I-DLTS spectra amplitudes, it was clear to us that only a fraction of the population of traps emits carriers during the I-DLTS experiment. Consequently, a proper scaling factor has been considered while dealing with (2b). This is because TSC and I-DLTS
Fig. 5. Activation energies and concentrations of the deep levels found in the various samples. Their depletion depth $x_d$ at $V_{rev} = 5$ V ranges from 25 to 45 $\mu$m. Inside (e), which contains all the deep levels visible in the others figures, the cross sections, normalized to $10^{-15}$ cm$^{-2}$, are reported.

experiments require different filling procedures: in TSC the sample is exposed for a long time to continuous light at constant temperature; on the contrary, during I-DLTS measurements the sample is periodically lighted by short flashes, while changing its temperature. The details of carriers capture processes may change with temperature, and level-level interactions depending on their occupancy may possibly complicate this picture.

Note that the constant $\gamma$ has different values for electrons and holes traps. In silicon $\gamma_e = 6.387 \cdot 10^{23}$ (Kms)$^{-2}$, while $\gamma_h = 3.31 \gamma_e$. In the following analysis, however, we will always use $\gamma = \gamma_e$ for the sake of simplicity. Thus if a deep level is known to be a hole trap its cross section should be scaled by a factor 3.31.

V. DISCUSSION

The results of data analysis are depicted in Fig. 5(a)–(e), where the concentration of deep levels found in five samples is plotted as a function of the activation energy; the main features of the deep level population are summarized in Table I too. In Fig. 5(e), which corresponds to the most irradiated sample, the cross sections are reported normalized to $10^{-15}$ cm$^{-2}$. It can be observed that the energy levels concentrate around
Fig. 5. (Continued.) Activation energies and concentrations of the deep levels found in the various samples. Their depletion depth $x_d$ at $V_{NC} = 5$ V ranges from 25 to 45 µm. Inside (e), which contains all the deep levels visible in the others figures, the cross sections, normalized to $10^{-15}$ cm$^2$, are reported.

0.37 eV, between 0.4 and 0.45 eV, and above 0.47 eV (close to the midgap). Many of these levels are closely spaced in energy, have similar cross sections, and their concentrations grow together as the fluence is increased; thus they may belong to quasi-continuous distributions of localized states. Unfortunately, the accuracy of our analysis does not allow, at present, to discriminate levels with energy separations lower than 50 meV. This uncertainty can be ascribed to: 1) the noise which affects measured spectra and 2) the fact that many similar levels distributions may determine spectra which are indistinguishable from the practical point of view. Fit errors can be made considerably small by refining $G(E)$ and $\sigma(E)$, but it has no meaning to reach a resolution higher than the uncertainty. All the deep level distributions shown in Fig. 5 generate fits which are in very good agreement with experimental data; however it should be noted that:

1) In the case of isolated levels it can be assumed an uncertainty of 50 meV for the energy and 50% for the cross section.
2) When many levels group together forming a continuous, or quasi-continuous, distribution, the greater information is given by their envelope in $N(E)$ plots. In general, many distributions with the same envelope, the same total concentration and similar cross sections may generate indistinguishable spectra.

A main component is found in all the samples at $E_t = 0.37$ eV, $\sigma = 7 \cdot 10^{-16}$ cm$^2$, with concentration increasing with the fluence from $3.5 \cdot 10^{12}$ cm$^{-3}$ up to $5 \cdot 10^{13}$ cm$^{-3}$. This level is probably a donor one, related to the carbon complex $C_7O_5$, placed in the lower part of the silicon gap [19]. It was found to be the main defect level responsible for the high resistivity saturation, which was observed in silicon bulk samples irradiated with very high fluxes [20].

The large set of deep levels observed in the region between 0.4 and 0.44 eV, with $\sigma = 10^{-14}$–$10^{-16}$ cm$^2$ and concentrations increasing from $10^{13}$ cm$^{-3}$ up to $10^{14}$ cm$^{-3}$, may be related to the double vacancy (VV)$. In fact an energy level at $E_v = 0.4$ eV is related to the transition $VV^0 \leftrightarrow VV^-$ [21]. A similar issue has been discussed in [22], where a continuous distribution of deep levels has been proposed to explain the broadening of some I-DLTS peaks in highly irradiated sample spectra. This phenomenon was attributed to the level degeneracy coming from divacancies grouping into large damaged regions, or clusters. The total concentration of levels in the energy range of 0.4–0.45 eV increases with irradiation up to approximately $9.5 \cdot 10^{12}$ cm$^{-3}$ for the highest fluence studied here.

The spectrum portions at the highest temperature are produced by emissions from a set of levels with energies in the range from 0.45 to 0.5 eV. The number of levels and the concentrations increase with the irradiation up to approximately $15.5 \times 10^{12}$ cm$^{-3}$ for the highest fluence. A donor level at 0.5 eV has also been observed in the past by other I-DLTS investigations [4] and by TCT analysis [23] on neutron irradiated silicon. It has been related to a vacancy complex, probably $V_2O$. This complex was observed by EPR analysis reported in [24].

Recently, a model with two dominant deep levels was proposed in literature [9]. This two-level model can reasonably describe many observations about irradiated silicon, such as space charge sign inversion (SCSI), the quasi-intrinsic ($\pi$) type neutral bulk, the double junction effect (DEJ) observed in TCT experiments, and the shift of the Fermi level position. Typically a donor level placed at $E_A = E_C = 0.46$ eV is invoked. The results reported in this work confirm that the main defects in the irradiated silicon give rise to deep levels at energies around 0.36 eV and above 0.41 eV. The former ones may be related to the $C_7O_5$ (which is a donor-like), while the latter may be reasonably considered as cluster levels related to double vacancies; they may include $VV^-$ (which is an acceptor) and $V_2O$ (an electron trap).

<table>
<thead>
<tr>
<th>Energy [eV]</th>
<th>$\sigma \times 10^{12}$ [cm$^2$]</th>
<th>Concentrations $\times 10^{13}$ [cm$^{-3}$]</th>
<th>(Relative Concentrations [%])</th>
<th>Probable nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.33-0.4</td>
<td>4.0-0.5</td>
<td>-</td>
<td>0.64(1) 1.4(1) 1.7(1)</td>
<td>Not Clear</td>
</tr>
<tr>
<td>0.36-0.38</td>
<td>0.25-1.2</td>
<td>4.2(5) 5.5(2) 5.5(2) 7.2(5) 7.2(5)</td>
<td>Peaked Band</td>
<td></td>
</tr>
<tr>
<td>0.40-0.44</td>
<td>1-10</td>
<td>3(40) 3(20) 3(15) 4(14) 4(13)</td>
<td>Broad Band</td>
<td></td>
</tr>
<tr>
<td>0.41</td>
<td>0.5</td>
<td>-</td>
<td>1(5) 1.3(5) 1.6(5)</td>
<td>Single Level</td>
</tr>
<tr>
<td>0.43</td>
<td>2.5</td>
<td>0.8(8) 1(5) 1.3(5) 1.5(4)</td>
<td>Single Level</td>
<td></td>
</tr>
<tr>
<td>0.45</td>
<td>5</td>
<td>0.1(1) 0.2(2) 1(5) 1.2(5) 1.4(4)</td>
<td>Single Level</td>
<td></td>
</tr>
<tr>
<td>0.47-0.49</td>
<td>6.5-10</td>
<td>0.2(3) 0.5(5) 4.5(21) 6(21) 7.5(25)</td>
<td>Broad Band</td>
<td></td>
</tr>
<tr>
<td>0.49</td>
<td>2.5</td>
<td>-</td>
<td>0.3(3) 3(8) 19(19) 6(21) 8(25)</td>
<td>Single Peak</td>
</tr>
</tbody>
</table>

TABLE I SUMMARY OF DATA ANALYSIS. LEVELS WHICH SEEMS TO BE STRONGLY CORRELATED HAVE BEEN COLLECTED TOGETHER AND Labeled AS PART OF A BAND IN THE LAST COLUMN. FOR EACH OF THE SAMPLES AND FOR ANY GROUP OF DEFECTS ARE GIVEN: 1) THE TOTAL ABSOLUTE CONCENTRATION AND 2) THE RELATIVE VALUE OF THE TOTAL DEEP LEVELS CONCENTRATION IN THAT SAMPLE.
Thus our results may be considered to give experimental support to the two-level model if all the double vacancy-related levels were taken as an "equivalent one," introduced to describe, in a simple way, the connection between the complex traps population and the macroscopic parameters.

VI. CONCLUSION

We performed a deep levels analysis on a set of medium resistivity silicon samples, neutron irradiated up to the fluence of $2.5 \times 10^{15}$ n/cm$^2$. TSC and I-DLTS experiments reveal the existence of a large number of deep levels overlapping their spectral contributions. In order to distinguish the overlapping deep levels, we adopted an innovative numerical procedure of data analysis, which finds out a set of deep levels that are able to account for both TSC and I-DLTS spectra. Finally, we obtained a consistent description of deep level population and its evolution with fluence.

According to our present energy resolution, which is about 50 meV, we found that quite a number of levels, up to 21 in the most irradiated sample, are needed to fit both TSC and I-DLTS spectra. Moreover, we noted that deep levels tend to concentrate in some regions of the energy gap, possibly forming quasi-continuous distributions. This result is in agreement with recent findings of other authors. A possible explanation, in terms of continuous distributions, is in agreement with recent findings of other authors. A possible explanation, in terms of continuous distributions, is proposed.

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