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Numerical simulation of the effect of gold doping on the resistance to neutron irradiation of silicon diodes

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Abstract: We have carried out a numerical simulation of the effect of gold doping on the electrical characteristics of long silicon diodes exposed to neutron irradiation. The aim is to investigate the effect of gold on the hardness of the irradiated diodes. The reverse current voltage and capacitance voltage characteristics of doped and undoped diodes are calculated for different irradiation doses. The leakage current and the effective doping density are extracted from these two characteristics respectively. The hardness of the diodes is evaluated from the evolution of the leakage current and the effective doping density with irradiation doses. It was found that diodes doped with gold are less sensitive to irradiation than undoped ones. Thus gold appears to stabilise the electrical properties on irradiation. The conduction mechanism is studied by the evolution of the current with temperature. The evaluated activation energy indicates that as the gold doping or irradiation dose increases, the current switches from the basic diffusion to the generation-recombination process, and that it can even become ohmic for very high gold densities or irradiation doses.

Key words: silicon diodes; gold doping; numerical simulation
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1. Introduction

Silicon diodes used as particle detectors such as neutrons are subjected to high doses during their period of use. Irradiation creates several defects activated as traps in the semiconductor gap. They undergo severe degradation in their electrical characteristics. In particular, their charge collection efficiency (CCE) is degraded due to changes in the full depletion voltage. Also their temperature operation is reduced due to the increase in the leakage current[1−3].

Several ways for improving the detector resistance to irradiation, or hardness, are suggested. Among these is doping by so-called life-time killer elements such as gold and platinum[4, 5]. These elements create energy levels in the gap, so their effect is to reduce the minority carrier lifetime and increase the semiconductor resistivity.

In this work, we have used numerical simulation to study the effect of gold addition on the hardness of silicon detectors. The electrical characteristics (current–voltage and capacitance–voltage) are calculated at different irradiation doses for gold-doped and undoped silicon detectors. The full depletion voltage and the leakage current are extracted from the I–V and C–V characteristics and their evolution with irradiation doses is studied.

2. The simulation

The modeling was carried out by numerically solving the basic equations for the semiconductor: continuity and Poisson. For a $P^+N^-N^+$ diode in a one dimensional space coordinate and in the steady-state with no external excitation, these equations are given by:

$$\frac{1}{q}\frac{\partial I_{\mathrm{n}}}{\partial x} - U_{\mathrm{tot}} = 0, \tag{1}$$

$$\frac{1}{q}\frac{\partial I_{\mathrm{p}}}{\partial x} + U_{\mathrm{tot}} = 0, \tag{2}$$

$$\frac{1}{q}\frac{\partial^2 \psi}{\partial x^2} = -\rho(x). \tag{3}$$

J_{n} and J_{p} are the drift–diffusion current for electrons and holes respectively, thus:

$$J_{\mathrm{n}} = q\mu_{\mathrm{n}}\left(\frac{kT}{q}\frac{\partial n}{\partial x} - n\frac{\partial \psi}{\partial x}\right), \tag{4}$$

$$J_{\mathrm{p}} = -q\mu_{\mathrm{p}}\left(\frac{kT}{q}\frac{\partial p}{\partial x} + p\frac{\partial \psi}{\partial x}\right), \tag{5}$$

where $\mu_{\mathrm{n(p)}}$ are the mobilities for electrons and holes respectively.

U_{tot} is the sum of net recombination rates of all energy levels (D: donor and A: acceptor) created by gold (Au) and neutrons (N), thus:

$$U_{\mathrm{tot}} = \sum_i U_{\mathrm{D}i}^{\mathrm{Au}} + \sum_j U_{\mathrm{A}i}^{\mathrm{Au}} + \sum_k U_{\mathrm{D}k}^{\mathrm{N}} + \sum_l U_{\mathrm{A}l}^{\mathrm{N}}. \tag{6}$$

Each one of these rates is given by the well known Shockley-Read-Hall (SRH) expression, which has the general form:

$$U = \frac{pn - n_i^2}{\tau_{\mathrm{on}}(p + p_{\mathrm{t}}) + \tau_{\mathrm{op}}(n + n_{\mathrm{t}})}. \tag{7}$$

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n_i is the intrinsic density, n_t and p_t are the electron and hole densities when the trap level coincides with the Fermi level, they are given by

$$n_t = n_i \exp(-(E_i - E_t)/kT), \tag{8}$$

$$p_t = n_i \exp(-(E_t - E_i)/kT), \tag{9}$$

where E_t is the trap energy level, E_i is the intrinsic Fermi level, and $\tau_{0n(p)}$ is the minority carrier lifetime given by

$$\tau_{on(p)} = \frac{1}{\upsilon_{thn(p)}\sigma_{n(p)}N_t}. \tag{10}$$

where $\upsilon_{thn(p)}$ is the thermal velocity, $\sigma_{n(p)}$ is the capture cross section for electrons and holes respectively, and N_t is the trap density.

$\rho(x)$ is the space charge given by

$$\rho(x) = -\frac{q}{\varepsilon}\left\{ p - n + N_D - N_A + \sum_i \left[\left(1 - f_{Di}^{Au}\right) N_{Di}^{Au}\right] - \sum_j \left[\left(f_{Aj}^{Au}\right) N_{Ai}^{Au}\right] + \sum_k \left[\left(1 - f_{Dk}^{N}\right) N_{Dk}^{N}\right] - \sum_l \left[\left(f_{Al}^{N}\right) N_{Al}^{N}\right]\right\}. \tag{11}$$

f and N_t are the occupancy function and the density of each trap respectively (the subscript and the superscript are the same as those used for the recombination rate).

The occupancy function f of each trap has the general form:

$$f = \frac{\sigma_n n + \sigma_p p}{\sigma_n(n + n_t) + \sigma_p(p + p_t)}. \tag{12}$$

In order to execute a numerical analysis, the structure length d is divided into L points and Equations (1), (2) and (3) are transformed into difference equations in which the fundamental variables: the electrical potential (ψ), the electron density (n) and the hole density (p), are defined at a finite number of division points (M). These difference equations are then linearised by the Taylor expansion in fundamental variables, neglecting higher-order terms[6].

The boundary conditions assume that both ends of the structure are ohmic. Therefore, two conditions apply: the first is that electrical neutrality holds at both electrodes and the second specify the thermal-equilibrium conditions also at both electrodes. These are

$$\rho(0) = \rho(d) = 0, \tag{13}$$

$$n(0) \cdot p(0) = n(d) \cdot p(d) = n_i^2. \tag{14}$$

3. The structure

The simulation was carried out for a silicon $P^+N^-N^+$ structure with 1.04×10^{13} cm^{-3} shallow donors for the active region (N^-). The contacts are P^+ ($N_A = 10^{18}$ cm^{-3}) between 0 and 4.5 μm and N^+ ($N_D = 10^{18}$ cm^{-3}) between 235.5 and 240 μm. This gives a resistivity of 400 Ω·cm. The total length is 240 μm, the area is 1 cm^2 and the temperature 300 K. The electrical characteristics (reverse current– and capacitance–voltage characteristics) are calculated for gold doped and undoped structures, and for different irradiation doses.

Table 1. Traps created by neutron irradiation[7].

Parameter	Acceptor	Acceptor	Donor
E (eV)	$E_C - 0.42$	$E_C - 0.55$	$E_V + 0.36$
σ_n (cm^2)	2.11×10^{-16}	10^{-16}	10^{-15}
σ_p (cm^2)	10^{-14}	10^{-15}	10^{-16}
Introduction rate (cm^{-1})	26	0.08	1

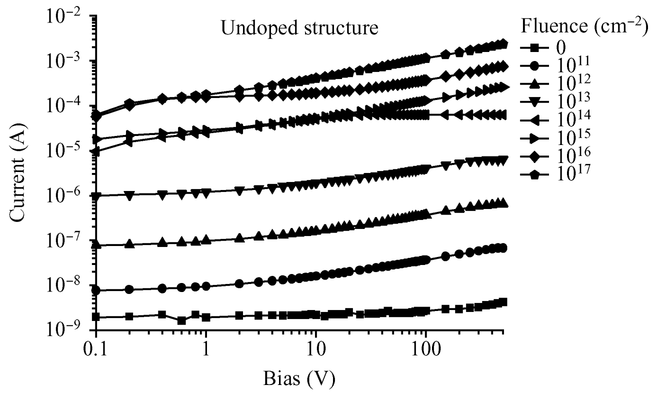

Figure 1. The reverse current–voltage characteristics for the undoped sample at 300 K. The fluence is 0, 10^{10} to 10^{17} cm^{-2} with increasing reverse current at high voltage.

4. Simulation results

4.1. Structures with no gold doping

Irradiation creates deep donors, and deep acceptors. These deep levels can be efficient recombination centres if they are close to mid gap and have comparable capture coefficients for electrons and holes. In our simulation we only consider neutron irradiation since other particles can be treated in the same way. Neutron irradiation of silicon creates two acceptor levels located at E_C – 0.42 eV and E_C – 0.55 eV and a donor level located at E_V + 0.36 eV[7]. These levels have different introduction rates. There may be low concentrations of other levels but they are of less importance in this analysis. This differs from our previous simulation work[8] in which we introduced a generic generation-recombination centre at the mid gap, which remains neutral. The literature gives only parameters for deep donors and acceptors (Table 1).

The simulated current–voltage and capacitance–voltage characteristics have been calculated for different radiation doses. The deep trap density is assumed to be directly proportional to the irradiation dose through the introduction rate of Table 1.

First, the effect of irradiation on the current is shown in Figure 1.

For low radiation doses up to 10^{10} cm^{-2}, the current is the usual diffusion current with saturation. The current then increases almost monophonically as the irradiation dose increases. The type of current also changes, it is no longer saturated. The generation component begins to appear. This is justified for two reasons. First, it is known that the generation current is proportional to the density of the deep level, N_T (and hence to the irradiation dose), and the depletion width, W. That is $I_{GR} \propto N_T W$ and since $W \propto V^{1/2}$, then it is expected that

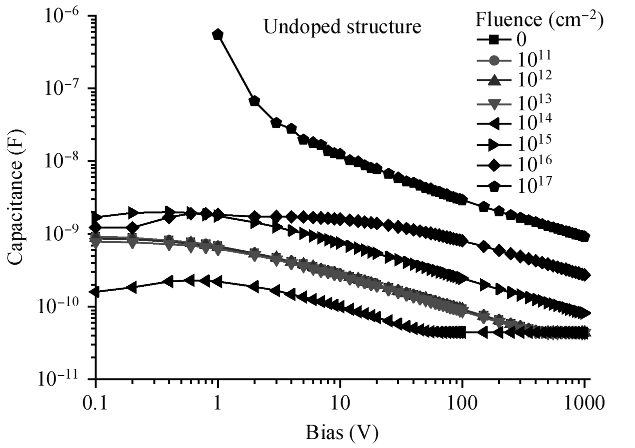

Figure 2. The capacitance–voltage characteristics for the undoped sample at 300 K. The fluence is 0, 10^{10} to 10^{17} cm^{-2} with increasing reverse current at high voltage.

$I_{\rm GR} \propto V^{1/2}$. This is observed in the simulation results for fairly high fluences. Second, the temperature dependence of the I–V characteristics should give more information on the type of current. The activation energy decreases from $\sim$1 eV for low doses to $\sim$0.57 eV for high dose (10^{17} cm^{-2}). These values correspond well with the fact that the current changes from diffusion (for low dose) to generation (for high dose). This indicates that the most effective at high doses is the deep acceptor located at mid gap ($E_{\rm C}$ – 0.55 eV). This trap has the lowest introduction rate hence a very high irradiation dose is required. Experimentally, a value of 0.536 eV is observed after irradiation[9−11]. Values near 0.65 eV have also been reported[12]. In the work on GaAs FETs, the experimental activation energy is also higher than half the band gap of the semiconductor, 0.81 eV in GaAs FET[13].

For the capacitance, the effect of irradiation is shown in Figure 2.

Irradiation does not have an immediate effect. Only when its dose overcomes 10^{13} cm^{-2} that it has an effect. This is due to the fact that the shallow doping density is of the order of 10^{13} cm^{-3} so that the charge created by any ionised deep trap less than this value will have no effect. Beyond this dose, the ionised trap density surpasses the shallow density and the capacitance is affected. There is also an apparent type inversion, which will be discussed later. This is indicated by the fact that the capacitance, hence the full depletion voltage, decreases then increases.

4.2. Structures with gold doping

Gold in silicon creates three deep levels[4]. Due to the lack of experimental data capture cross sections[5], the introduction rates in Table 2 are assumed.

We present here the effect that adding gold to silicon has on the I–V and C–V characteristics. In the simulation, the gold density is kept constant at a fairly high value of 10^{16} cm^{-3} and the irradiation fluence is varied from 0 to 10^{17} cm^{-2}.

The current voltage characteristics of irradiated structures are shown in Figure 3.

For relatively low fluences when the dominant irradiation created trap has a smaller density than that of gold, irradiation has no effect. That is, the current does not increase with increasing fluence. However, the current begins to increase with increasing fluence when the trap density created by the latter is comparable in effect to that of gold.

The capacitance voltage characteristics of the doped structure are shown in Figure 4. It is observed that the capacitance is almost unaffected.

Table 2. Traps created by gold doping.

Parameter	Acceptor	Acceptor	Donor
E (eV) [3]	$E_{\rm C} - 0.34$	$E_{\rm C} - 0.55$	$E_{\rm V} + 0.35$
$\sigma_{\rm n}$ (assumed) (cm^2)	10^{-16}	10^{-16}	10^{-14}
$\sigma_{\rm p}$ (assumed) (cm^2)	10^{-14}	10^{-14}	10^{-16}
Introduction rate (assumed) (cm^{-1})	1	1	1

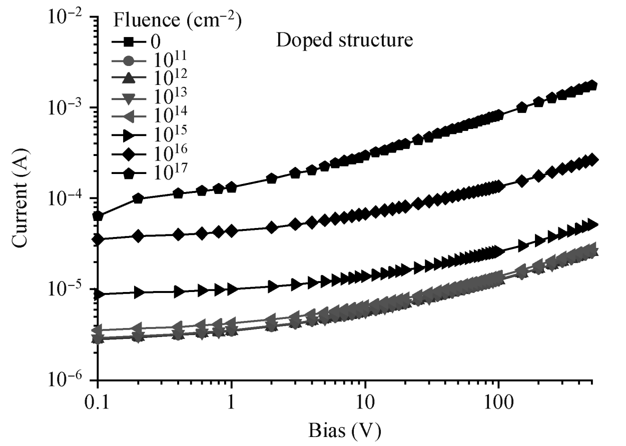

Figure 3. The reverse current–voltage characteristics for the doped sample at 300 K. The fluence is 0, 10^{10} to 10^{17} cm^{-2} with increasing reverse current at high voltage.

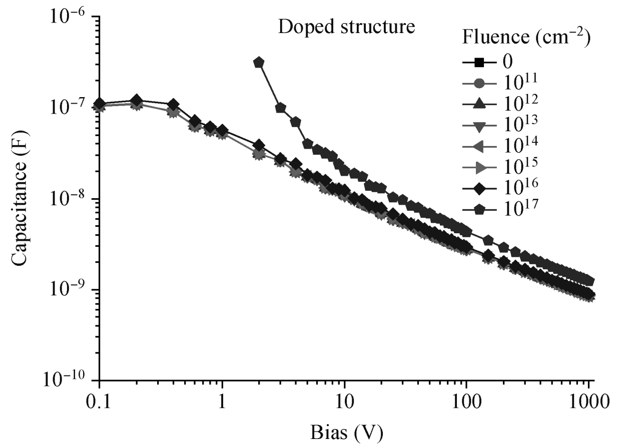

Figure 4. The capacitance–voltage characteristics for the doped sample at 300 K. The fluence is 0, 10^{10} to 10^{17} cm^{-2} with increasing reverse current at high voltage.

5. Discussion

The effect of gold doping can be illustrated by plotting the current at a fixed bias and the effective density as a function of the irradiation created deep level density. These are shown in

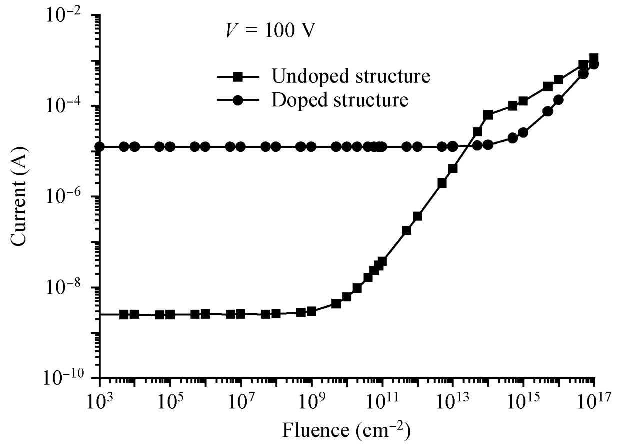

Figure 5. The reverse current versus radiation dose at 100 V.

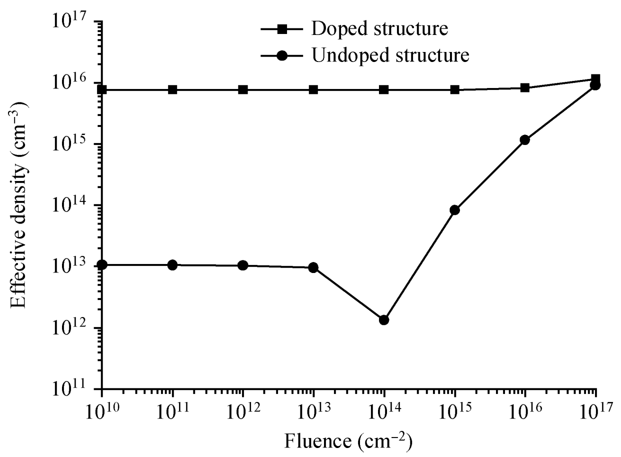

Figure 6. The effective density versus radiation dose at 100 V.

Figures 5 and 6 respectively.

It can be seen that the undoped diodes start with just the diffusion current but a generation current develops as the defect concentration increases. The gold doped diode has a constant generation current until the irradiation damage current dominates the generation process.

We discussed above that the fact that the activation energy of the diode current is not found in our model is a clear indication of the dominant internal process.

The other significant experimental observation is that if the sample is irradiated after gold doping, it appears to produce less of an (incremental) effect in the current. The increase in current with fluence is seen to be nearly linear, but it is only small for the gold doped sample. For the undoped diode, the increase is large but sublinear.

A possible explanation for this may be because the irradiation has moved the state of the sample near to that where the current increase has saturated on approach to full ohmic relaxation behaviour. The current increase may then be dominated by the increase in the ohmic region.

It is possible that there is an interaction between the gold and irradiation defects when both are present together. Another explanation is that in real samples, there is a contribution made by gold levels other than the dominant mid gap acceptor, which acts as a g–r centre.

This study has provided information on the behaviour of particle detector diodes. It is also applicable to the general topic of lifetime killers in fast diodes. Irradiation can help with the limited solubility of gold in silicon and also to remove this element from the processing environment. It can also help in the production of isolation between elements of integrated circuits. Similar behaviour should be expected from other impurities, such as platinum[14].

6. Conclusion

A numerical simulation has been carried out to study the effect of neutron irradiation of long silicon diodes doped with gold. The reverse current–voltage and capacitance–voltage electrical characteristics were measured for different neutron irradiations and gold dopings. The aim is to investigate the effect of gold on the hardness of the irradiated diodes. The leakage current and the effective doping density are then extracted. The leakage current and the effective doping density with irradiation doses characterise the hardness of the diodes. It was found that diodes doped with gold are less sensitive to irradiation than undoped ones with gold. It is concluded that gold may stabilise the electrical properties against irradiation. The conduction mechanism is studied by the evolution of the current with temperature. The evaluated activation energy indicates that as gold doping or the irradiation dose increases, the current switches from basic diffusion to the generation-recombination process and can even become ohmic for very high gold densities or irradiation doses.

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