IODINE IRRADIATION INDUCED DEFECTS IN CRYSTALLINE SILICON

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Abstract–*N-type P-doped silicon single crystals with resistivity higher than 8000 Ωcm were irradiated with $^{127}I^{6+}$ ions of 28 MeV kinetic energy. The penetration of the ions through the target and the processes of energy loss were simulated using the CTRIM Monte Carlo code, and point defect production was calculated in the frame of our diffusion-reaction model. Trapping phenomena were investigated using the method of thermally stimulated currents without applied bias. The modeling of the current-temperature curves takes into consideration both point defects and stress-type trapping centers, produced by the ions stopped into the crystal.*
Keywords: *silicon, ion irradiation, thermally stimulated currents without applied bias, stress induced traps.*

1. INTRODUCTION

One of the hot topics studied nowadays is related to the constituents of the matter which were produced in the early stages of the Universe evolution and which have survived until today due to their stability and to the very low probability of interaction. Hence, they are viable candidates for dark matter [1].

From all dark matter candidates, the weakly interacting massive particles are the most studied, being considered in many particle physics theories. The peculiarity of their interaction with ordinary matter is that they transfer energy to a recoil after, most probably, a singular scattering process produced in the detector [2]. Their detection is a major challenge for the physics today. One of the approaches is cryogenic dark matter search, which uses silicon and germanium crystals [3].

To understand the effects of the local strains induced by a 'big' particle in Si single crystals, we irradiated single crystal Si wafers with ions much heavier than Si.

In the present paper, we report the results of the study of iodine irradiation induced defects in single crystal Si. The study of radiation induced defects in silicon by electrical methods represents a broad area of research, with still open problems [4–7]. The penetration and energy loss of iodine ions in silicon is simulated using the Monte Carlo *Crystal-transport and range of ions in matter* (Crystal TRIM) code [8]. The formation of 'stable' point defects is then modeled. The electrical measurements performed on the irradiated samples are described, and the modeled curves are used to extract the parameters of the traps induced by iodine irradiation.

2. EXPERIMENTAL

N-type float zone Si wafers of 2" from Siltronix, doped with P, with resistivity higher than 8000 Ωcm and thickness of 275 ± 25 μm, oriented along (100) plane and with 3 ± 0.5^{O} off orientation were used. They were irradiated with $^{127}I^{6+}$ ions of 28 MeV kinetic energy, at a fluence of $(5\pm0.5)\times10^{11}$ ions/cm^2, at the Uppsala tandem accelerator [9]. The irradiation was carried out at a temperature of 23^{O}C, using beam currents in the range of 200 pA to 1 nA. The beam spot was about 2-3 mm in diameter and it was scanned across the sample with 64 Hz in the vertical and 517 Hz in the horizontal directions, respectively. A variation in fluence of less than 5% across the wafer was obtained. Sandwich square samples of 1 cm length were prepared from these wafers. Al contacts were deposited by thermal evaporation; thick on the backside, and semitransparent, around 50 nm, on the front side.

The method of thermally stimulated currents without external bias was used to experimentally characterize the damage produced by irradiation. This method allows to evidence traps in materials with different energy gaps (from large to narrow gap semiconductors and nanostructured materials [10−13]. The method consists in two steps:

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firstly, the samples are cooled down to 70 K and are illuminated with monochromatic light of 800 nm wavelength for 20-30 min in order to charge the traps. The chosen wavelength and the illumination time allow for the complete filling of traps. Secondly, after switching-off the light, the sample is heated up at a constant rate of 0.1 K/s, under zero external bias, and the discharge current versus temperature is measured. The relaxation current depends on the frozen-in electric field, which changes during heating due to the sequential discharge of the traps.

3. RESULTS AND DISCUSSION

3.1. Simulations of Ion Penetration and Defect Production

Crystal TRIM is a code based on the binary collision approximation, which takes into account the space arrangement of the atoms in the crystal, as well as the influence of the relative orientation of the ion in respect to the crystalline planes. We simulated the penetration of ^{127}I of 28 MeV in Si, for different relative orientations: along the <100> channeling direction and at different disorientations in respect to it, defined by the angles θ and φ [14]. When the incident ion hits a Si atom placed in its site in the lattice, it interacts with an essentially unscreened Si nucleus. The selfrecoil, of a few MeV kinetic energy, first slows down by ionizing inelastic collisions with the electrons of the lattice atoms. As it continues to slow down, the moving ion begins to lose more and more energy in elastic defect producing collisions with the lattice atoms themselves. The process of partitioning the energy of the recoil nucleus between electrons (ionization) and atomic motion (displacements) is treated in the frame of Lindhard's model [15, 16]. The process of slowing down the recoil nucleus in the lattice leads to an atomic cascade, and continues up to the moment the e-energy imparted to a Si ion is equal to the threshold for displacements [17, 18]. Vacancy-interstitial pairs are generated both along the ion track due to ion–atom collisions, and in its neighborhood initiated by the primary recoils [19].

In Fig. 1 we present the depth dependence of the ionization and nuclear energy loss in Si, for the direction of interest, for the exact <100> direction, and for disorientations in both θ and φ of 15$^{\mathrm{O}}$. As could be seen, the range is considerably higher on the <100> direction, in accordance with the theory of channeling [20, 21].

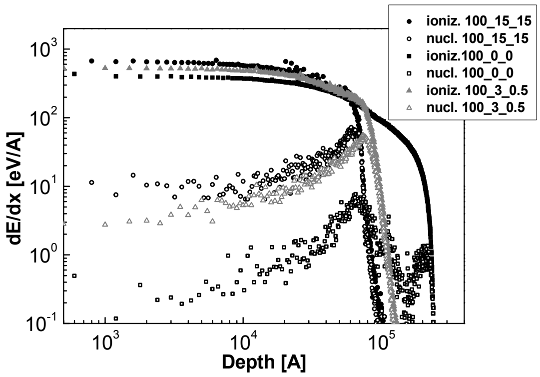

Fig. 1. Depth dependence of the ionization and nuclear energy loss of iodine ions in Si, for different orientations.

The generation of Si selfinterstitials by iodine ions as a function of their penetration depth in Si obtained from the simulation, is presented in Fig. 2.

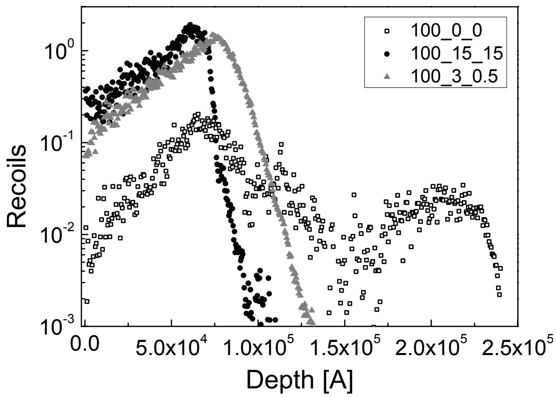

Fig. 2. Depth dependence of recoil production by iodine ions in Si, for different orientations.

In the case of our wafers, the depth corresponding to the generation of maximum vacancy-interstitial pairs due to 28 MeV ^{127}I irradiation is 7.5 – 8 μm.

In Si, both the vacancy and the interstitial are highly mobile, and hence were not detected at room temperature. They annihilate, migrate to sinks and form 'stable' defects with the impurities existent in the wafer. Our samples contain small quantities (~ 5×10^{11} cm^{-3}) of P, and around 10^{15} cm^{-3} O and C, respectively [22]. In this situation, the formation of the following defects is most probable: V_2, VO, C_iC_s, C_iO_i and VP. The relative concentrations of these defects, as well as their depth distribution are illustrated in Fig. 3, as calculated in the frame of our reaction-diffusion model described in Refs. [23, 24]. V_2 and C_iO_i concentrations have a peak at 8 μm, while the other defects are relatively uniformly distributed in the first 10 μm under the surface.

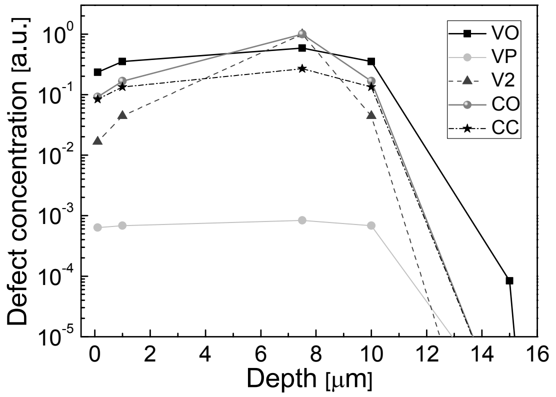

Fig. 3. Depth distribution of point defects produced by the I irradiation of Si.

3.2. Electrical Characterization of Defects

The samples were illuminated with monochromatic light of 800 nm at 70 K for 30 min, than the temperature was raised with 0.1 K/min. The discharge current was recorded, and its temperature dependence is represented in Fig. 4 – the curve drawn with continuous line. The fractionary heating curves were also measured, and they evidence three activation energies of 0.19, 0.23–0.28, 0.41–0.46 eV.

The discharge currents were modeled, starting from the experimental values of the activation energies. The model is detailed in Refs. [12, 25, 26]. The discharge current is due to both the non-equilibrium charge carriers released from the traps during heating, and the equilibrium ones. They move in the frozen-in electric field of the still trapped ones.

The irradiation produces point defects, as a consequence of the interaction of primary vacancies and interstitials between themselves and with the impurities present in the Si wafer (P, O and C). On the other side, iodine ions, which are much bigger and heavier than Si, are stopped in the sample, producing a local deformation in the crystal, and a local electric field. This way, they could be assimilated to a stress-type trap, in the sense discussed in Refs. [27–29]. The modeled curve is also presented in Fig. 4 as a dashed line.

By modeling, the cross sections were determined, and the experimental activation energies were corrected. The fitting parameters of the curve are given in Table 1. The trapping centers were assigned to defects considering the results from the literature.

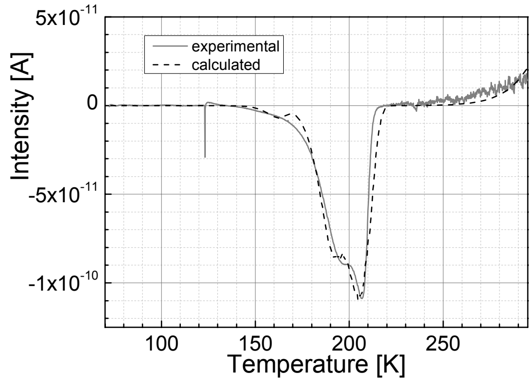

Fig. 4. Experimental current (continuous line) and model calculation (dashed line).

Table 1. Parameters of the trapping levels

Trap signature		Type	Origin
E (eV)	σ (x10^{-15} cm^2)		
0.17	1	p	C_iC_s
0.29	1	n	V_2
0.41	3	n	V_2
0.43	0.1	n	
0.455	0.05	n	VP
0.5	$10^{-5}\exp\left(-\frac{(T-360)^2}{50}\right)$	p	Iodine induced stress

The deepest trapping level in the Si band gap is related to the stress induced by the stopping of iodine ions, which is permanent, compared with the type of stress investigated in Ref. [27]. Its cross section is a Gaussian function in temperature, with a rather large half width (5°C).

Although the wafer is of n-type due to the P doping, the much higher C concentration makes plausible to attribute the trap with activation energy of 0.17 eV to C_iC_s.

4. SUMMARY AND CONCLUSIONS

In this paper we evidenced for the first time the trapping levels of defects induced by the irradiation with iodine ions. As they are heavier than Si, and are stopped in the Si target, we consider that the irradiation produces stress-induced traps besides normal trapping centers.

The simulation of the nuclear energy loss and of primary defect production shows that the nuclear energy loss has a peak at about 8 – 10 μm depth, and the concentration of primary defects as well. Modeling of the point defect production in the frame of diffusion-reaction theory shows that concentrations of V_2 and C_iC_s have a distribution with a peak around 8 μm, while the VO, C_iO_i and VP are uniformly distributed up to 10 μm from the surface.

From the modeling of discharge currents it results 5 normal traps, with activation energies of: 0.17, 0.29, 0.41, 0.43, 0.455 eV, one p-type and 4 n-type, all correlated with normal traps associated with point defects. The sixth activation energy, i.e. the deepest one (0.5 eV), is associated with a stress-induced trap, produced by the stopping of the ions in Si.

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References

[1] J.L. Feng, "Dark matter candidates from particle physics and methods of detection", *Annu. Rev. Astron. Astrophys*, **48**, pp. 495–545, 2010.

[2] I. Lazanu, S. Lazanu, "Interactions of exotic particles with ordinary matter", *Nucl. Instr. Meth. Phys. Res. B* **278**, pp. 70–77, 2012.

[3] E. Previtali, "20 years of cryogenic particle detectors: past, present and future", *Nucl. Phys. B, Proc. Supplement* **150**, pp. 3–8, 2006.

[4] "Proceedings of the 1st Conference on Radiation Effects in Semiconductors", *J. Appl. Phys.*, **30**, 1959.

[5] D.V. Lang, "Deep level transient spectroscopy: A new method to characterize traps in semiconductors", *J. Appl. Phys.*, **45**(**7**), pp. 3023–3032, 1974.

[6] M. Bruzzi, "Radiation Damage in Silicon Detectors for High-Energy Physics Experiments", *IEEE TNS* **48**(4) pp. 960–970, 2001.

[7] J.H. Bleka, H. Malmbekk, E.V. Monakhov, B.G. Svensson, and B.S. Avset, "Annealing dynamics of irradiation-induced defects in high-purity silicon in the presence of hydrogen", *Phys. Rev. B*, **85**(8), pp. 085210, 2012.

[8] Crystal-TRIM (04/1D -last revision May 2004), developed by Matthias Posselt 1991-2005, Forschungszentrum Rossendorf, Dresden, Germany.

[9] G. Possnert, "AMS with the Uppsala en tandem accelerator", *Nucl. Instr. Meth. Phys. Res. B*, **5**(2), pp. 159–161, 1984.

[10] D. Petre, I. Pintilie, M.L. Ciurea, T. Botila, "Interface trapping states in MISIM structures, with ZnS:Mn", *Thin Solid Films*, **260**(1), pp. 54–57, 1995.

[11] M. Draghici, M. Miu, V. Iancu, A. Nassiopoulou, I. Kleps, A. Angelescu, M.L. Ciurea, "Oxidation-induced modifications of traps parameters in nanocrystalline porous silicon", *Phys. Stat. Sol.* (a), **182**(1), pp. 239–243, 2000.

[12] V. Ioannou-Sougleridis, A.G. Nassiopoulou, M.L. Ciurea, F. Bassani, F. Arnaud d' Avitaya, "Trapping levels in nc-Si/CaF_2 multi-quantum-wells", *Mater. Sci. Eng. C*, **15**(1-2), pp. 45–47, 2001.

[13] V. Iancu, M.L. Ciurea, M. Draghici. "Modeling of optical charging spectroscopy investigation of trapping phenomena in nanocrystalline porous silicon", *J. Appl. Phys.*, **94**(1), pp. 216–223, 2003.

[14] M. Posselt, "Crystal-TRIM and its application to investigations on channeling effects in ion implantation", *Radiat. Eff. Defects Solids*, **130/131**, pp. 87–119, 1994.

[15] J. Lindhard, V. Nielsen, M. Schraff, P.V. Thomsen, "Integral equations governing radiation effects",*Mat. Fys. Medd. Dan. Vid. Selsk,*. **33**(10), pp. 1–42, 1963.

[16] P. Sigmund, Stopping of Heavy Ions – A Theoretical Approach, Springer, 2004.

[17] S. Lazanu, I. Lazanu, "Analytical approximations of the Lindhard equations describing radiation effects", *Nucl. Instr. Meth. Phys. Res. A*, **462**(3), pp. 530–535, 2001.

[18] I. Lazanu, S. Lazanu, U. Biggeri, E. Borchi, M. Bruzzi, "Non-ionising energy loss of pions in thin silicon samples", *Nucl. Instr. Meth. Phys. Res. A* 388(**3**), pp. 370-374, 1997.

[19] S. Lazanu, I. Lazanu, "New aspects of the contribution of primary defects of silicon to long-time degradation of detectors operating in high fields of radiation", J.Optoel.Adv.Mat., **9**(6), pp. 1839–1842, 2007.

[20] M.A. Kumakhov, "The theory of channeling at small depths", *Radiat. eff.*, **26**(1-2), pp. 43–48, 1975.

[21] J. Lindhard, M. Scharff, H.E. Shiøtt, "Range concepts and heavy ion ranges", *Mat. Fys. Medd. Dan. Vid. Selsk.*, **33**(14), pp. 1–42, 1963.

[22] Landolt Börnstein, Group III, **22**, Semiconductors, Subvolume b, Impurities and defects in group IV elements and III-V compounds.

[23] S. Lazanu, I. Lazanu, M. Bruzzi, "Microscopic modelling of defects production and their annealing after irradiation in silicon for HEP particle detectors", *Nucl. Instr. Meth. Phys. Res. A*, **514**(1-3), pp. 9–17, 2003.

[24] I. Lazanu, S. Lazanu, "The role of primary point defects in the degradation of silicon detectors due to hadron and lepton irradiation", *Phys. Scripta*, **74**(2), pp. 201–207, 2006.

[25] M.L. Ciurea, V. Iancu, M.R. Mitroi, "Trapping phenomena in silicon-based nanocrystalline semiconductors", *Solid State Electron*., **51**(10), pp. 1328–1337, 2007.

[26] M.L. Ciurea, "Trapping Phenomena in Nanocrystalline Semiconductors", *Nanoelectronics and Photonics*, Springer, New York, 2008.

[27] M.L. Ciurea, S. Lazanu, I. Stavarache, A.M. Lepadatu, *et al.*, "Stress induced traps in multilayered structures", *J. Appl. Phys.*, **109**(1), pp. 013717, 2011.

[28] A.M. Lepadatu, I. Stavarache, S. Lazanu, V. Iancu, M.R. Mitroi, R.R. Nigmatulin, M.L. Ciurea, "Temperature dependence of capture coefficients in trapping phenomena", *CAS 2010 Proc. IEEE CN CFP10CAS-PRT*, **1**, pp. 371–374, 2010.

[29] M.L. Ciurea, "Trapping aspects in silicon-based nanostructures", *P. Romanian Acad. A*, **12**(4), pp. 315–323, 2011.