Particles-on-surface sensor with potential barriers embedded in a semiconductor target

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Abstract. Recently, we calculated an effect of surface charges on potential barriers embedded inside a Si target. As a result, electrons and holes transport in a semiconductor target could be controlled by ionized atoms or molecules situated inside the surface adsorbate layer. Since GaAs possesses higher electron mobility than Si, in this paper we calculate the potential distribution and charge carriers motion dependences on the GaAs target surface charge value and dopant concentration. Computer simulation was implemented using the software COMSOL Multiphysics. The obtained results can help to improve a design of GaAs radiation detector, particle detector, surface charge detector, biochemical sensor, etc.

1. Introduction
Biomolecular nanomaterials are looking to be relevant to a variety of biomedical, biochemistry, biophysics, electronics, and nano communication applications. A number of electronic elements with embedded biomolecules are diodes, transistors, switches, memory elements. A set of electron devices appear as emerging high efficiency tools, including biochemical sensors, medical biochips, molecular transmitters, nano-batteries, nanoscale energy harvesting systems, nano-memories, nano communication systems and other [1-9]. Due to their low loss and fast switching speeds in GHz-THz frequency band, semiconductor PIN diodes with transit-flight charge carriers are appropriate for radiometric applications as an amplitude modulator, a phase shifter, a limiter, a switch, a sensor.

Recently, new high sensitivity low noise photodetector-integrator based on a dynamical regime PIN diode was developed [10]. That diode is based on embedded potential barrier, produced by gate control depletion region, and trapped charge carriers. Such a device possesses a number of properties required for receiving and de-modulation of an electromagnetic wave in the visible band. Such diodes possess signal-to-noise ratio, SNR > 1, high sensitivity in the wave length range approx. 400-700 nm. An output analog signal is proportional to irradiating light absorbed energy dose.

In previous studies of dynamical Si PIN diode characteristics, dependence was noticed on the presence of external particles on the surface of the substrate [11]. The nature of the appearance of charges on the surface of a semiconductor can be due to various causes: polarization under the action of a static or alternating electric field, including fields of other external charges; physical, chemical and biological reactions occurred on a surface under the influence of external factors; sedimentation of external flows, and others.

Further, the possibility of using the Si PIN diode as a surface charge detector-integrator in a wide frequency range was considered [12]. The charge detection mechanism was given using the theoretical data and the computer modeling. This phenomenon includes surface charge control of potential barrier magnitude, which, in turn, could regulate the charge carrier flow.
Due to higher electron mobility, GaAs elements have some advantages and better performance at GHz-THz frequency ranges when comparing with Si.

In this paper, we present Si and GaAs PIN diodes with embedded potential barriers and mobile charge trapping comparison by means computer simulation. The difference in the potential barriers magnitude for two types of semiconductors in the absence and in the presence of the surface charge is considered.

The obtained results increase possibilities of such Si and GaAs PIN diodes using as a radiation detector, a particle registrar, surface charge sensor, a biochemical sensor, etc.

2. Methods

Dynamical process in PIN diode-triode are described elsewhere [10]. The magnitude of the applied voltage electric fields across the device quickly decrease out of embedded depletion regions. Initially, electrons and holes, trapped by electrostatic potential barriers higher Fermi level, are moving faster near borders of depletion regions. The device is switching on from low zero-field current to high-current state after a certain triggering delay.

In the absence of the external irradiation, the zero-field thermo-generated current \( J_0 \) determines value of self-triggering, or zero-field time,

\[
\tau_m \propto Q_{cr}/J_0(r),
\]

where \( Q_{cr} \) is a critical value of space charge. Typically, \( \tau_m \approx 0.1-10 \) milliseconds.

In presence of the external radiation the triggering time decreases depending on external irradiating intensity \( J_{EMF} \). The high sensitivity of measurements can be provided when decreasing triggering time after irradiation. However, both with the irradiating and without it, the charge carrier motion is controlled by the barriers, in particular, depends on the barrier height [10-11].

The total charge accumulated by the flow of the total thermal generation and photo generation currents can be described by the relation refining formula (1).

The total charge required for the switching is accumulated by the flow of the total thermal generation and photo generation currents and can be expressed using formula (1):

\[
Q(r)\sim \int_0^\tau dt \cdot T^2 \exp\left(\frac{-E_b(t) - E_b(T) - E_{charge}(q)}{kT}\right),
\]

where \( \Delta E_b(\Phi/T) \) is the effective decrease in the height of the barrier due to space charge neutralization by photogenerated carriers (\( \Phi \) is the irradiation dose) [10] and \( E_{charge} \) is the barrier modulation due to the surface charge effect [11-12].

Here, we continue the investigation of the effect of surface charges on the potential distribution and charge carriers motion in such Si and GaAs PIN diodes by means computer simulation using software Comsol Multiphysics (COMSOL).

When modelling the processes in selected diodes using the COMSOL program, the geometry, the impurity concentration, the voltage at the electrodes of the PIN photodiode structure were set. Si and GaAs substrates with different carrier concentrations are considered. The spatial potential distribution along the cutline with different values of surface external charge for two types of semiconductors is calculated. The electron mobility values are \( E_m=1450[\text{cm}^2/(\text{V*}\text{s})] \), \( H_m=500[\text{cm}^2/(\text{V*}\text{s})] \) for Si and \( E_m=8500[\text{cm}^2/(\text{V*}\text{s})], H_m=400[\text{cm}^2/(\text{V*}\text{s})] \) for GaAs. Further, the surface external charged particles were placed on the outer upper surface of the semiconductor substrate. The ionization coefficient \( K_i \) was chosen in the range from 0 to \( 10^3 \), which defined the surface concentration of the atomic charge \( K_iN_i \), where \( N_i \) - Langmuir concentration of the atomic layer is about \( 5\times10^{14} \text{ cm}^2 \).
3. Results
Potential distribution functions along the horizontal cut line with different values of surface charge ionization coefficient $K_i$ for the GaAs substrate are shown at figure 1. Dopant concentration is $10^{12} \text{l/cm}^3$. The surface charge ionization coefficient $K_i$ value varies from 0 up to 0.00125 (approx. 0 - 0.001 C/m2). The following graph (figure 1) shows the barrier magnitude dependence on the surface charge concentration value. Evidently, there are two potential wells separated with barriers (figure 1). Electrons and holes could be accumulated and trapped between anode and cathode barriers.

![Figure 1. Potential distribution along the horizontal cut line with different values of surface charge for the GaAs substrate. The dopant concentration of the bulk is $10^{12} \text{l/cm}^3$. The reference value of the ground (GND) electrode potential equals minus 4.5 eV. The horizontal cut line was set at depth $y=1.5 \mu\text{m}$ inside the GaAs substrate.](image)

The following graph shows potential distribution for two types of semiconductors with different dopant concentration. The dependence of the potential barrier on the surface charge can be approximated by the similar functions but the magnitude of the barrier is higher for the GaAs structure.

According to figure 1, 2, modulating the potential barriers height using surface charges, or changing the bulk dopant concentration as well, the charge carriers flow in the semiconductor can be regulated.

It is seen, that a small surface charge density can change the potential barrier magnitude for value up to $\Delta E_b = 0.05$ eV (at the horizontal cut line, which is situated at depth $y=1.5 \mu\text{m}$ in the substrate), which can affect the charge carrier motion.
Figure 2. The dependence of the barrier magnitude on the surface charge value. The dopant concentrations for Si and GaAs substrates are $10^{12}$, $10^{14}$, $10^{16}$ $1/cm^3$.

Figure 3. Potential distribution along the horizontal cut line for two types of the substrate material (Si and GaAs) with different dopant concentration. Zero surface charge.

According to figures 2, 3, the difference between Si and GaAs substrate is significant at a dopant concentration of $10^{16}$ $1/cm^3$. One can conclude, that in case of GaAs, the cathode potential barrier can be increased which reduces the cathode to anode leakage. Since the cathode leakage is the component of the dark current as well as the thermo generation, the total dark current of the device can be decreased.

4. Discussion and conclusion
The computer simulations and appropriate knowledge obtained in this article can specify the principles of operation and the characteristics of different semiconductor devices (including PIN diodes) and also develop the analytical studies of processes in various semiconductor photodiodes.
The difference in the potential barrier magnitude for two types of semiconductors in the absence and in the presence of the surface charge is presented. Different dopant concentrations were considered. The using of the GaAs possessing higher electron mobility than Si can be perspective in the PIN diode structure and similar devices due to the higher performance of semiconductor elements.

It is shown, that GaAs surface charge sensor with embedded potential barriers and trapped charge carriers could be more effective device in comparison with similar ones based on Si.

The computer simulation results obtained in this article can contribute to the development of a new element base of semiconductor electronics, as well as new equipment and circuit solutions. The simulation data presented in that work are looking useful for the micro- and nanoscale devices development possess analytical features, including nano communications, (bio) molecular sensors and microwave detecting systems.

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