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Optimal regime of the double-sided drift of lithium ions into silicon monocrystal

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In this work, we show a new method for obtaining silicon-lithium semiconductor structures using the bilateral drift of lithium particles into silicon mono-crystal in order to create nuclear radiation detectors with a wide bandgap. This method describes the simultaneous distribution of lithium ions on surfaces of cylindrical silicon crystals, which speeds up the process of obtaining the required detector structure. Here in this work, we aimed to identify the most optimal regimes of the electric field applied in the process of bilateral ion drift, as well as to investigate the effect of the thermal factors to create a drift of lithium ions. We can estimate these optimal regimes of voltage and temperature by making theoretical assumptions based on the numerical method for solving the Poisson continuity equation, the calculations of Pell and Louber. At the same time, simplifications were made to neglect the internal interaction of particles. The paper shows the results of modeling the process of bilateral drift under the influence of a stepwise increase in temperature and reverse voltage. This bilateral drift procedure facilitates the fabrication of silicon-lithium nuclear radiation detectors with large diameters and sensitive areas.

Key words: optimal drift mode, Si (Li) nuclear radiation detectors, p-i-n structures, stepped temperature drift mode, stepped reverse voltage mode.
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1 Introduction

Currently, in world practice, silicon detectors, and germanium detectors are mainly used [1, 2] to detect charged particles, also for a long period of time, other detectors have been used including cadmium telluride (CdTe) and gallium arsenide (GaAs-detectors) [3-5], as well as CdZnTe [6,7] for similar purposes.

It is known that Ge detectors possess the highest functional characteristics [2]. However, all detectors (Ge detectors, Si detectors, CdTe detectors, CdZnTe detectors, and GaAs detectors) have a number of disadvantages with regard to their physical, technological, and economic aspects [8-10].

The technology of Si-detectors of various types is quite well developed, however, in order to manufacture Si-detectors with greater sensitivity, it is important to optimize the process of manufacturing such detectors [11]. The processes of diffusion and drift of lithium ions into silicon mono- crystals are the most time-consuming and the most important in all steps of detector fabrication. Therefore, these processes have been attracting the attention of researchers for a long time [12].

Prior to the 1960s, it was very difficult to obtain detectors with a thickness over the sensitive area of more than 2 mm for a p-i-n junction [13], because of the technological shortcomings in obtaining a uniform propagation of charge carriers over the whole structure of the crystal [14]. In the 1960s, Pell proposed lithium drift technology [15], and since that time detector manufacturers have used lithium drift technology to produce lithium donor impurities on separate P-type Si and Ge wafers. This is needed to compensate for acceptor impurities to achieve a balance of carrier concentration and high resistivity. The compensated area has properties similar to those of the inner material, it can be used as a sensitive part of the detector, and its thickness can reach from several mm to more than ten mm [13]. As the current technology for producing high-quality germanium becomes more and more advanced, lithium drift technology is mainly used for silicon lithium drift detectors [14].

Nowadays, high-purity silicon mainly belongs to p-type silicon [15], therefore, donor atoms must be added to the material to achieve equilibrium. Lithium is the only donor impurity that can be doped into silicon in a high enough concentration to compensate for the action of the acceptor. When obtaining a p-i-n structure using this technology, an electric current is applied to a p-type cylindrical piece of the silicon wafer, which has an evenly distributed initial acceptor impurity with a layer of diffused lithium to a depth of about 300 μm, an electric current is applied in a mode of 150 – 300 V and a temperature of 450 °C. With help of applied temperature, and electric field the lithium metal layer penetrates into the silicon crystal from one side. Thus, lithium in silicon is fully ionized into lithium ions. The excited electrons enter the conduction band and act as donors. Lithium ions combine with negative ions, forming neutral ions [16], this significantly reduces the concentration of carriers in this region, thereby significantly increasing the resistance, which is the compensation effect of lithium.

The production of Si (Li) detectors with a relatively large sensitive area (diameter of more than 60 mm) is associated with a sequence of difficulties: firstly, during the process of fabrication of Si (Li) detectors, there is a risk of increase of the reverse current and capacitance [17]. Because, as it was mentioned above, obtaining the intrinsic region (i-region) with help of the drift method demands high voltage application up to 450V, and this distorts the nature of the original crystal. Secondly, it takes months of work to fabricate detectors with 4 mm thicknesses and 60 mm in diameter. Additionally, during the formation i-region in the silicon, an inhomogeneous propagation of lithium ions also may occur.

Earlier, in [18-20], in some of our works, it was reported the results of experiments on creating large-sized p-i-n structures using a new approach by providing bilateral diffusion and drift of lithium charge carriers into silicon mono-crystal. Current work describes the results of modeling the process of bilateral drift of lithium charge carriers into silicon mono-crystal to significantly reduce the time of the silicon compensation process at large volumes and to eliminate the negative consequences of long-term holding of the crystal at high temperatures and electrical voltages.

2 Methodology and theory

Regarding Pell's compensation theory [15], here we tried to find the most appropriate modes of bilateral drift of lithium charge carriers into silicon mono-crystal. Accordingly, we modeled the process of bilateral drift of lithium charge carriers into silicon mono-crystal by paying attention to the main physical parameters and setting mathematical equations which are able to describe the process.

As a raw material, we will consider the characteristics of a dislocation-free, p-type, cylindrical silicon mono-crystal refined by the floating zone method (resistivity ρ = 1000–5000 Ohm • cm, diameter 100 mm, the service life of $\tau \geq$ 500 μs and with a thickness 4–5 mm,).

Before the drift process starts it is necessary to provide diffusion of lithium on a pre-determined surface of cylindrical-shaped silicon mono-crystals. The technology of providing bilateral diffusion is as follows: a lithium layer is deposited on the surfaces of a cylindrical crystal to the depth of 300 μm, for t = 3 – 4 minutes, at T = 653–723 K temperature. Here lithium charge carriers inject as donor particles with a concentration of $N_0 = 5 \times 10^{17}$. The lithium distribution is symmetric with respect the center of the two flat crystal surfaces. Due to a larger crystal thickness (more than 4 mm), in theoretical calculations, we can neglect boundary effects which may contribute to the internal interaction of charged particles in a body of a crystal, and the distribution of charge carriers can be assumed as an integral of two independent functions.

As the diffusion process finishes, in order to provide a bilateral drift of lithium charge carriers, i.e. to obtain compensated region, reverse bias voltage with a temperature of 328 – 363 K and voltage 70 V – 300 V is applied. At this moment charged particles of lithium move from the surfaces of the silicon cylinder toward the center until they overlap in the center. The moment of completion of the drift is fixed by an abrupt increase in the reverse current of the detector. It is also important to mention that, technically, the one diffusion part of the detector, which has n – carriers, is ground off to a pre-determined depth regarding its degradation level during the drift process.

According to the widely known diffusion theory, we assume that the distribution of lithium charge carriers mainly depends on a coordinate axis – *x*, where the initial point was set as high-concentration pure lithium. After the diffusion process starts, this lithium will penetrate the silicon due to temperature influence. In order to neglect the effect of thermogenerated carriers we assumed that the applied temperature in the diffusion process must be considered inside the diffusion constant in the expression:

$$N(x,t) = N_s \operatorname{erfc}\left[\frac{x}{2(D_0 t_0)^{\frac{1}{2}}}\right] + N_s \operatorname{erfc}\left[\frac{W-x}{2(D_0 t_0)^{\frac{1}{2}}}\right] \quad (1)$$

where D_0 is the diffusion constant, t_0 is the diffusion time and W is the length of the cylindrical crystal.

After determining the mathematical conditions of the diffusion process it is time to talk about the drift process. Let us make some assumptions about the boundary conditions of the drift process, here we want to consider x region bordering with x = c along the cylinder, where c is the place where donor concentration is equal to acceptors concentration. Correspondingly, from the other surface of the cylinder x = c'. It should be noted that the value of c = c' is much greater than the value of $(D_0\ t_0)^{1/2}$.

$$N_D \approx \frac{(2N_0\,(D_0 t_0)^{\frac{1}{2}}}{x\sqrt{\pi}}[\exp(-x^2/4\,D_0 t_0)\ +\exp(-(L-x)^2/4\,D_0 t_0)]. \quad (2)$$

The intrinsic proportion of the acceptors of the silicon mono-crystal ($N_A \sim 10^{11}$) is equivalent to the concentration of lithium charge carriers in the regions x = c' and x = c. As it is known that the application of voltage from both surfaces of the crystal creates controversial electric fields which facilitate the movement of Li^+ charges along the cylinder. During this process, volumetric charges compensate acceptors, consequently, leading to redistributions of electric fields along the cylindrical crystal. Correspondingly, at this moment, negatively charged carriers start moving toward the surface of the cylinder from their location x = c' and x = c. At a moment when the concentrations of the positive and negative charge carriers are equalized, the internal strength of the electric field inside the cylinder gradually decreases. However, even in this case, lithium carriers continue to move into the n-region because the applied external voltage remains constant. This process leads to the formation of intrinsic regions (i-region) inside the cylindrical crystal.

Also, it should be noted that for the fluent motion of the charge carriers, it is necessary to maintain sufficient temperature regimens during the drift process. The number of mobile charge carriers will be moved from the region where the concentration of the acceptors is equal to the concentration of donors to the whole body of the cylindrical crystal across p-n junctions. Additionally, the applied electric field during the drift should be sufficiently big in order to exceed the diffusion in the silicon crystal structure. If these conditions are satisfied, the lithium charge carriers start to move along the cylinder to compensate for the internal region of the detector.

Distribution of the lithium charge carriers during the drift process can be described by the following expression:

$$\int_0^t E\mu N_A dt = (\int_a^c N_D dx) - (c-a)N_A + (\int_{a'}^{c'} N_D dx) - (c'-a')N_A =$$
$$= (b-c)N_A - (\int_c^b N_D dx) + (b'-c')N_A - -(\int_{c'}^{b'} N_D dx) \quad (3)$$

As it is shown from the expression, integral contains electric field strength and propagation of acceptor concentration by time. This expression can be analytically solved by using the *erfc* function as shown below:

$$\int E\mu N_A dt = cN_0 erfc\left[\frac{c}{2(D_0t_0)^{\frac{1}{2}}}\right] - aN_0 erfc\left[\frac{a}{2(D_0t_0)^{\frac{1}{2}}}\right] +$$

$$+\frac{\left[2N_0(D_0t_0)^{\frac{1}{2}}\right]}{\sqrt{\pi}\left[\exp\left(-\frac{a^2}{4(D_0t_0)^{\frac{1}{2}}}\right)-\exp\left(-\frac{c^2}{4(D_0t_0)^{\frac{1}{2}}}\right)\right]} - (c-a)N_A + c'N_0 erfc\left[\frac{c'}{2(D_0t_0)^{\frac{1}{2}}}\right] +$$

$$+a'N_0 erfc\left[\frac{a'}{2(D_0t_0)^{\frac{1}{2}}}\right] + \frac{\left[2N_0(D_0t_0)^{\frac{1}{2}}\right]}{\sqrt{\pi}\left[\exp\left(-\frac{a'^2}{4(D_0t_0)^{\frac{1}{2}}}\right)-\exp\left(-\frac{c'^2}{4(D_0t_0)^{\frac{1}{2}}}\right)\right]} - (c'-a')N_A \quad (4)$$

Here we need to pay attension than *a* and *a'* is the lithium charge carriers spreading lenth along the crystal, b and b' is the regions in the center of the crystal. b and b' becomes wider when compensation of i-region complete:

$$\int_0^t E\mu N_A dt \cong \frac{(c-a)^2}{2L} + \frac{(c-a)^3}{6L^2} + \frac{(c'-a')^2}{2L} +$$

$$+\frac{(c'-a')^3}{6L^2} \approx \frac{(b-c)^2}{2L} + \frac{(b-c)^3}{6L^2} +$$

$$+\frac{(b'-c')^2}{2L} + \frac{(b'-c')^3}{6L^2} \quad (5)$$

Bilaterial drift depth can be easyly derived from the expression 5. If we consider here halfe thikness of the crystal as W and W' and make appropriate assumption for the expression 5 we can see that the approximate solotion for the integral can be written in the following way:

$$\int E\mu N_A dt \approx \frac{W^2}{8L} + \frac{W'^2}{8L} \quad (6)$$

Here L is the whole lenth of the crystal. We know that in bilateral drift L = W + W', so considering this we can come up with final solution of the expression 6 as:

$$\int E\mu N_A dt \approx \frac{W^2}{4L} \quad (7)$$

From the expression 7 we can see that the electric filed propagation in the crystal and the gradient of the charge carriers are proportional to the lenth of the cylindrical crystal. Since the lenth is halved according to bilaterial drift process, we can assume that the time for drift process is also decreased several times.

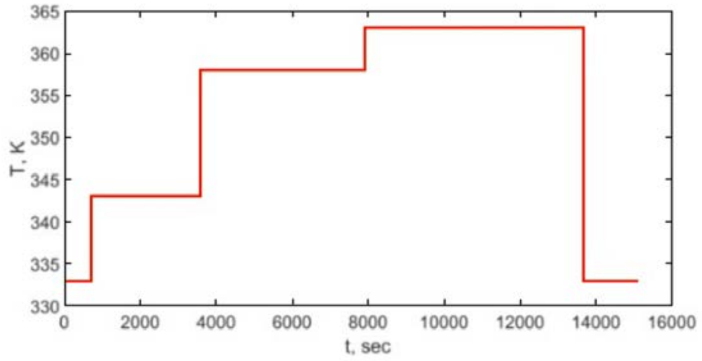
Thus, the proposed method makes it possible to quadruple the semiconductor compensation time and, therefore, it is obvious that the quality of the compensated region is significantly improved by suppressing the influence of free carriers generated at the bilateral drift thermal regimes, as well as due to the absence of blurring of the lithium front.

When the compensation process completes, i.e. when two opposing fronts of lithium drift are closed, one of the diffusion n + – regions is ground to a depth determined by its blurring during the drift. Then the entire crystal is subjected to chemical processing. Metal contacts are applied to the finished structure.

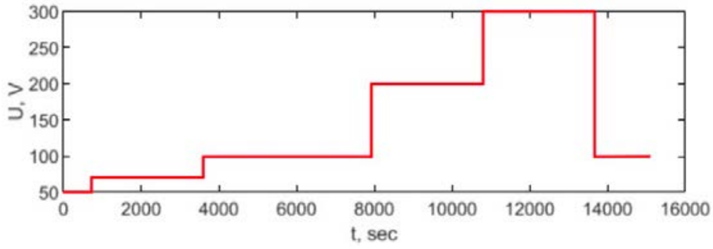
In the final step of the readiness of the detector structure, a specially developed technology of extra bilateral leveling drift is provided to the detector. This ensures the highest quality of the compensated area.

3 Results and Discussion

Detectors with a large volume of the sensitive area are usually used in nuclear physics research involving high-energy and long-range charged particles. The main difficulty in the manufacture of such detectors is associated with ensuring the uniformly propagation of the electric field lines in their sensitive region; on which, as is known, the spectrometric properties significantly depend. To maintain a uniform propagation of lithium charge carriers in a cylindrical silicon body, it is necessary to choose the correct drift mode; since the drift process is the most basic, long-term and energy-consuming process in the manufacture of Si (Li) detectors [19].



a)



b)

Figure 1 – Temperature – time regime (a) and voltage supply regime (b) during the drift of lithium charge carriers in Si

Figure 1 has been obtained by mathematical modeling and shows the temperature-change regime and the regime of voltage supply during the process of two-sided drift. One can see that the supply of temperature and voltage occurs in a stepwise mode with the passage of time.

During the drift of lithium charge carriers into silicon monocrystal, the choice of the drift mode is a particularly important factor. If the drift temperature is too high, close to 200 ^{0}C, thermal donors can be generated in the whole length of the crystal; and this can significantly slow down the drift process or even lead to thermal destruction of the structure. However, if the thermal mode is not appropriately chosen, then in this case the drift process may not give the desired result due to the shortage of mobility of charge carriers.

Table 1 shows drift modes. One can see that closer to the end of the process, when two counter streams of lithium ions meet and form an i-layer, the drift voltage drops sharply. This shows full compensation and readiness of the structure.

Table 1 – Temperature-time mode and voltage supply mode in the process of double-sided drift

t * 10^3, seconds	**U, V**	**T, K**
0-0.72	45-50	334
0.72-3.6	65-70	344
3.6-7.92	95-100	359
7.92-10.8	195-200	364
10.8-13.68	295- 300	362
13.68-15.12	95- 100	332

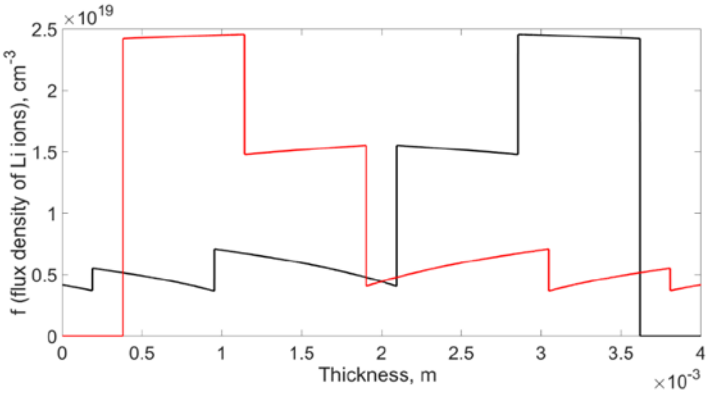


Figure 2 – Profile of the distribution density of counter fluxes of lithium ions in monocrystalline silicon

Figure 2 shows the profile of the density of counter fluxes of lithium ions in monocrystalline silicon with bilaterial drift and symmetrical distribution of lithium charge carriers along applied external electric field. It can be noted that in the begininnig of drift process the flux of lithium charge carriers sharply increases due to a strong electric field close the surface of the cylindrical crystal, then with the weakening of the electric field, the flux of moving charges also dropped down and finally, two fronts are met in the middle side of the cylindrical crystal to form an i-region.

Finally, regarding all conditions that were mentioned in this paper, our research group managed to successfully develop and test Si (Li) p-i-n structured detectors. Our detector had the following characteristics: the thickness of sensitive area – W = (4 – 5) mm; diameter (105 – 110) mm. Also, it should be noted that the thickness of the sensitive area of the detector was determined by standard capacitive measurements and applying chemical staining. The obtained model using mathematical modeling is in good agreement with the experiment.

Thus, the drift of lithium charge carriers into silicon, with high content and inhomogeneous distribution of impurities, has significant features associated with the developing of dipole structures at the sites of inhomogeneities of the acceptor impurity content; as well as the possibility of heating of crystals during the drift modes of stepwise two sided drift of lithium ions.

4 Conclusions

Physical processes were studied during the new method of bilateral drift of lithium into silicon mono-crystal. The application of a bilateral electric field from both sides of the silicon crystal accelerates the process of fabrication of a silicon detector of nuclear radiation by several times. The model of the bilateral drift process was based on numerical solving of continuity equation with simplification of interactions of particles in crystal. The proposed model shows the distribution of flux density of lithium charge carriers in silicon mono-crystal under an optimal regime and reflects the physical process of compensation. The bilateral drift of lithium charge carriers into a silicon mono-crystal is carried out by the method of synchronous stepwise rise in temperature range: 328 K – 363 K; and a reverse bias voltage range: 70V – 150V. In general, the simulation results show that the detectors obtained by this method have better electrophysical characteristics, a higher detecting ability and require less time to fabricate. This drift mode is the most optimal for detectors of nuclear radiation.

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