Theoretical aspects of direct conversion of radio-chemical energy in electric by radiation-stimulated SiC*/Si heterostructure

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Abstract. The authors consider their own CVD technology for the SiC growing on a Si substrate in order to create a beta converter. Since the beta converter contains a heavy C-14 atom, the finished beta converter works as an "inner sun", and the structure has specific mark * in the name: SiC*/Si. Authors focus on the problems of the theoretical description of: 1) the growth of the SiC*/Si film (with C-14 atoms inside) and the position of the p-n junction in the doping process; 2) method of a placement radioisotopes into a semiconductor material; 3) physical properties of radioisotopes; 4) defects formation; 5) generation of secondary electrons in the region of the p-n junction.

1. Introduction
The silicon carbide (SiC) is a well-known semiconductor that is used for various purposes. We are interested in SiC as an energy converter in photovoltaics and betavoltaics. The last direction is rapidly developing nowadays [1]. We can collect all technologies of obtaining this material in four groups. The first group includes the Acheson method [2], and the silicon carbide contains many impurities and defects in this case. So, SiC are used as an abrasive only in the framework of this technologies. The second group [3,4] includes sublimated methods for SiC producing, and they are used for the manufacture of the silicon carbide plates on an industrial scale. All other technologies are aimed at growing SiC film. We have selected chemical methods separately in the third group, and physical methods - in the fourth. The growing of a silicon carbide film was first carried out by Nishino S. [5] for the cubic phase 3C-SiC by chemical approach. Now this method is known as Chemical Vapor Deposition (CVD). Also it has many modification nowadays. As for the physical methods of obtaining SiC film, there are a huge number of technologies [6,7] that we will not be interested in further in the framework of our investigation.

The authors developed one of the modifications of CVD technology for SiC in the betavoltaic direction [8]. It is based on carbon-14 and 3C-SiC structure. And it is an endotaxy process which means a film growth inside initial Si-phase. The process of doping and creating a p-n junction occurs with the carbidization of silicon at the same time. Thus, the silicon carbide is considered as a beta converter in this work. We focus on the problems of the theoretical description of: 1) the growth of the
SiC*/Si film (with C-14 atoms inside) and the position of the p-n junction in the doping process; 2) method of a placement radioisotopes into a semiconductor material; 3) physical properties of radioisotopes; 4) defects formation; 5) generation of secondary electrons in the region of the p-n junction.

2. The placement of p-n junction in SiC*/Si obtained by endotaxy process

Methods for the SiC growing films are being developed as an alternation to sublimated methods. Author’s development is an endotaxy process which means the new phase growth process within another. We are considering now SiC on a Si substrate. To be precise, we mean the cubic phase 3C-SiC. C-14 atom is implemented instead of C-12 in the SiC phase during endotaxy. The carbidization of plates is carried out by the following chemical reactions:

\[ C + 2H_2 \rightleftharpoons CH_4 \]  \hspace{1cm} (1)

\[ CH_4 + Si \rightarrow SiC + 2H_2 \]  \hspace{1cm} (2)

We consider C as the heavy atom C-14. The general scheme of the CVD reactor is shown in Fig. 1 a. The initial reagents (from area 4) containing carbon are transformed to the gas phase by heating to a temperature above 1300\(^\circ\)C. The hydrogen \( H_2 \) in the chamber is used as a transporter of carbon atoms. The transfer takes place by a methane molecule, which is decomposed on the surface of the silicon wafer.

Figure 1. The endotaxy process: a) a distribution scheme of silicon substrates in gas camera (1 - reactor, 2 - a cassette with silicon wafers, 3 temperature area of decomposition of silicon hydrides, 4 - initial reagents area, 5 - area of heating in a high-frequency field); b) photo of the CVD reactor

We should note also that doping to obtain p- or n-types of conductivity is also performed in the CVD reactor. For example, one of the versions of obtaining the p-n junction may include a doping of the Si wafer with P, a carbidization and the doping of SiC with P at the same time, the carbidization and the doping of SiC with B at the same time too. So, it will be the following structure as a result: n-Si(P)/n-SiC(P)/p-SiC(B). Its general scheme is shown in the Fig.2. There is also a variant of metallization of the structure on the scheme.

The process of SiC film growth during endotaxy was mathematically described in the diffusion doping problem [9]. The model allows to calculate the depth of the position of the p-n junction in SiC*/Si structures grown in this reactor. One of the interesting solutions gives us an distribution of electric field inside the structure (Fig. 3). Besides, the p-n junction is located at a depth of 2 \( \mu m \). But
the electric field is distributed within about 5 µm. Thus, if the SiC film is sufficiently thin and locates inside the electric field then it is the most effective in terms of generating secondary charges.

Figure 2. The SiC*/Si structure

Figure 3. Dependence of the electric field strength on the depth. The value of the strength 6 corresponds to the absolute value of the internal electric field $E \sim 10^5$ V/m

3. Selection of radioisotopes
The placement of radioisotopes is carried out either directly on the surface of the structure, or in special channels on the surface of the semiconductor. The author’s technology provides the inclusion of a radioisotope in the chemical composition of a semiconductor. All three cases are shown in the Fig. 4. The choice of the location of the beta particle source is important from the point of view of the converter efficiency.

Figure 4. Various cases for placing a radioisotope inside a semiconductor
The efficiency of the converter on microchannel silicon with Ni-63 was considered in [10]. This corresponds to the picture 4 b. The self-adsorption of radioisotopes in the layer in which ones is placed was considered in the work. The estimation of the half-value layer was carried out by formula (3).

\[ d = \frac{0.095ZE_{\text{max}}^{3/2}}{A}, \]  

where \( Z \) - the charge number of a absorbent, \( A \) - atomic mass of a absorbent, \( E_{\text{max}}^{3/2} \) - maximum beta decay energy of a radioisotope. It was concluded that the output of beta particles of Ni-63 will occur from a depth of no more than 3.8 \( \mu \)m from the surface.

We can continue these estimates by extending them to the three most used isotopes in betavoltaics: H-3, Ni-63, C-14. Note that the formula for the half-value layer is applicable only for pure substances. Therefore, if we consider the adsorption of isotopes in a semiconductor, in addition to self-adsorption, then we cannot make a calculation for SiC. Instead, we use Si. A comparative table of isotopes characteristics is presented in Table 1.

| Isotop   | \( T_{1/2,\text{year}} \) | \( E_{\text{max}} \) | Activity (pure), \( Ci \) | Adsorbent | \( d, \text{mg/cm}^2 \) |
|----------|----------------|----------------|----------------|----------|----------------|
| Ni-63    | 100.1          | 0.067          | 56.67          | Si       | 0.82          |
|          |                 |                |                | Ni-63    | 0.73          |
| C-14     | 5730           | 0.156          | 4.45           | Si       | 2.93          |
|          |                 |                |                | C-14     | 2.51          |
| H-3      | 12.3           | 0.019          | 9700           | Si       | 0.12          |
|          |                 |                |                | H-3      | 0.08          |

The worst values for the half-value layer are for C-14. We can conclude that the layer of this isotope should be thinner than the layer with Ni-63 for an effective operation. But this conclusion takes place only for models in Fig. 4 a and 4 b.

As for the Activity of radioisotopes, this parameter is several orders of magnitude lower than in the reality due to the inability to obtain absolutely pure substances. Note also that Ni-63 does not exist in nature. Special work on nickel enrichment is necessary to obtain final one. In contrast, C-14 and H-3 are more available, and are waste at nuclear power stations. The other two parameters (the half-life \( T_{1/2} \) and the maximum beta decay energy \( E_{\text{max}} \) are stable, and are also important in the estimation the efficiency of energy conversion inside a semiconductor. The \( T_{1/2} \) gives us an information of the stable properties saving of the beta converter throughout an operation life. From this point of view, a tritium battery will noticeably weaken its functional properties over time.

4. Defects formation
Defect formation occurs both during the growth of the film and during the decay of radioisotopes.

The problem of a pure material growth is a technical task that requires separate consideration. From the point of view of the theoretical description of the problem, today we have powerful computer tools for modeling the structure. Due to the developing capacities of computer powers and methods of quantum chemistry, we have attracted of DFT [11,12] to our research. The problem of the effect of doping on the semiconductor band structure was considered [13]. As for the defect formation, we were able to theoretically confirm the movement of atoms in vacancies. Other defects were not considered.

So, the 3C-SiC phase was investigated by DFT with doping atoms: P, Ga, and N. The main purpose was estimation the value of the band gap width as a function of the number of doped atom in the 3C-
SiC cell. A more important result of the binding energy calculation has shown the ability of doped atoms to leave the lattice composition. The full investigation is presented in [13].

5. Secondary electrons generation

The task of the secondary electrons generating was considered in the framework of the Monte Carlo method in the GEANT package [14, 15]. This program was specially developed for modeling the processes of interaction particles with matter. The code allowed us to define the ”Inner Sun” point of C-14 beta radiation source randomly. And this point was located in a layer of silicon carbide.

The direction of the momentum of the primary beta electron and its initial energy are determined randomly too. The secondary electrons generation was take place when beta particles reached p-n junction with electric field which is modulated above (with depth $5 \mu m$). The trajectories of all secondary electrons was tracked. The program allowed us to put the so-called ”detectors” of secondary electrons at various depths. 6039018 electron-hole pairs were separated by a p-n junction from $10^7$ primary beta-electrons. This value is linearly scaled with radioisotope activity. We used value $Act_{C-14} = 5.203 \times 10^{18}$ Bq in model.

Note that $10^7$ primary electrons can create about one million electron-hole pairs at each 1 µm depth. An increasing the width of the p–n junction by 1 µm will lead to additional generation of million electron-hole pairs. Thus, 1 µm of the width of the p-n junction gives an average 10% increase in efficiency.

6. Conclusion

We can summarize our results in several positions:

- according to the mathematical model of SiC/Si endotaxy, the position of the p-n junction is located at a depth of 2 µm, and the electric field is distributed along thickness of just over 5 µm in the region of the p-n junction;
- there are three approaches to the implantation of radioisotopes into the structure: in the form of a planar layer, in the prepared microchannels and in the form of embedded atoms in the chemical structure of a semiconductor;
- it makes sense to consider the self-absorption of a radioisotope when the isotopes are located as a layer only (not inside chemical structure);
- the activity of the radioisotope depends on the method of obtaining the radioisotope (specific activity);
- the formation of defects in the structure is energetically advantageous according to the vacancy mechanism;
- the model of generation of electron-hole pairs with Activity $C-14 = 5.203 \cdot 10^{18}$ Bq gives an approximate estimate of the number of secondary electrons ( 6039018 electron-hole pairs out of 10000000 primary electrons).

Finally, we would like to highlight the obvious advantages of our beta converter. We can grow the SiC film inside the Si substrate in such a way that its thickness will be as effective as possible from the point of view of the distribution of the electric field. The placing the isotope inside the structure as part of the chemical structure helps us to avoid self-absorption one. The choice of C-14 is explained from the benefits of using CVD technology, as well as the advantages of this isotope concerning the parameters $T_{1/2}$ and $E_{max}$. Despite the uniqueness of the technology, there are difficulties in describing various processes. Especially, it is necessary to consider in more details at the structural level the behavior of isotopes and their interaction with a semiconductor.
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