Water Clusters in Semiconductor Detectors with Amorphous Carbon/Si Crystalline Hetero-Structures as Capturing or Scattering Centers for Free Charged Particles

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Abstract

In semiconductor type detectors one of the formation mechanisms of the capture or scattering centers (traps) is the diffusion of the water in the silicon's volume, where water molecules endowed with the dipole momentum by blocking in the micro-defects of the Si crystal generate there water clusters which could be considered, for the charged particles, as capture or scattering centers, and for the heavy charged particles - interaction centers. In the present article the features of water cluster formation in micro-defects of Si mono-crystalline as well as the distribution of electrical field potential in the regions of this type of structures are modeled and investigated.

Keywords - *trap, water clusters, micro-defect, Si crystal, semiconductor detector*

I. INTRODUCTION

In experimental nuclear physics in investigations which are realizing with the help of semiconductor detectors the physical parameter characterizing the detectors is particularly important, which is defined as a signal/noise ratio.The solving property of the detector gets substantially worsein the systems, where the electrical field represents a discrete movement of charged particles due to the capturing or scattering of charged particles by traps as it was explained byBorovitskaya&Shur [3], Bedneret.al. [2], Shabuninaet. al. [8].This kind of system can serve the water which associatively penetrats into the microdefects of the Si crystalline net in form of water clusters.

Clarifying structures and specifications of the formation of water clusters, as well as of the distribution of the electrical field potential surrounding them, it can be mentioned that water clusters serve as capturing or scattering centers (traps) for the free charged particles generated as a result of the ionization losses of heavy charged particles in the semicondutcor detector. These clusters have a significant contribution to the formation of the tail section of the amplitude spectrum of heavy-charged particle registration (prolong the quenching duration of amplitude spectrum) referring to Ohanyan [7].

Due to the loss of the charged particles' ionization energy, the generated free charged particles (electrons) in the semiconductor detectors, by interacting with the capturing or scattering centers (traps) existing in the Si crystals, are absorbed by flow absorption constant value λ, as given below:

$$\sum \lambda = \left(1 - e^{-\sigma nd}\right) \quad (1)$$

where,
σ-effective surfase of the scaturing
n - concentration
d -thickness of the crystal.

$$\sum \lambda = \left(1 - e^{-\sigma nd}\right)(1)$$

and correspondingly, are absorbed by the number of occupied charged particles in the traps- $\sum N$:

$$\sum N = N_0\left(1 - e^{-\sigma nd}\right) \quad (2)$$

Some part of the occupied charged particles is re-combining, the other part, by staying in the constant fluctuation process, gains sufficient kinetic energy for being able to get rid of the traps and for being included in the flow of the charged free particles with delay, thereby lengthening the tail part of the charged particles' amplitude spectrum. On the other hand, the start-point of delay time, with a little error, coincides with the movement duration of charged particles occupied in the traps. The lifetime of the charged particles occupied in the traps - τ_{m1}could be described as an empirical dependency, as follows:

$$\tau_{m1} = \frac{1}{\nu_{n(p)}} exp\left(-\frac{E_{m1}}{kT}\right)(3)$$

where,
m_1- type of trap
E_{m1} - energy of trap
$\nu_{n(p)}$ - frequency factor.

In the present work dedicated to the investigation of energetic solvability of the detectors with hetero-structure for heavy charged particles, we have clarified the characteristics of water clusters generation in micro-defects of Si cristalline network

and the distribution of electrical field around that structures.

II. EXPERIMENTAL METHODOLOGY

In the present work we've elaborated the model of Si crystal with the «Hyperchem» computer modeling program and have immersed it into the box full of water, thereafter we've analyzed the mechanism of water clusters' generation by the «Moleculardinamics» calculation method involved in the «Hyperchem» computer modeling program. We've chosen the PM^3 force field, which is, in our case, a common method for calculation of the generated potential fields for all atoms, system energy and molecular dynamics.

In experimental part the semiconductor detector was irradiated by beam of alpha particls and the amplitude spectre was recorded. The form of the tail part of this amplitude spectre was explained by the existence of traps.

III. RESULTS AND DISCUSSION

In Figure 1 the potential fields calculated by PM^3 method are presented for "*line and point*" (1a) and "*stick and boll*" (1b) models. It can be seen that the potential has approximately twice smaller value in green than in violet area and they are localized mainly in the surfaces of crystals.

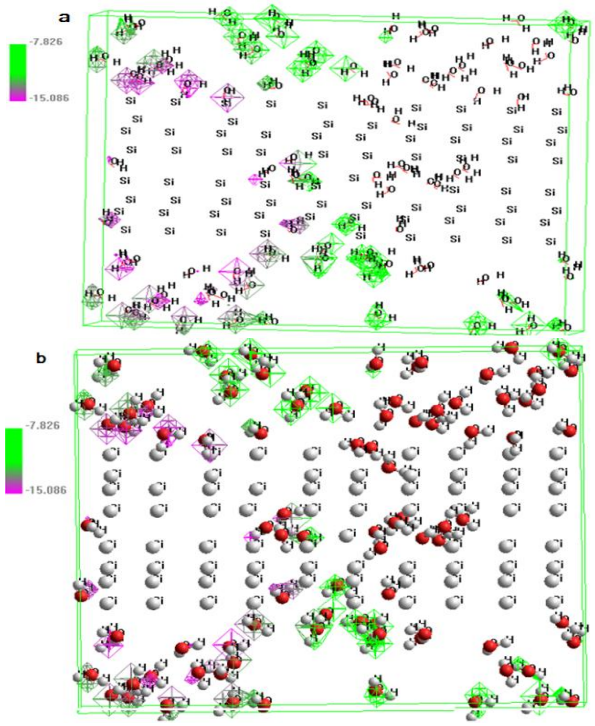

Fig 1: The distribution of the equipotential surfaces of electric field in the Si crystal pores in (a) -"line and point" and (b) - "stick and ball" rendering (2D view)

As a result of computer modeling it was revealed that regardless to the amount of water in the "box", the structure of water clusters in micro-defects depends on the sizes of the defects, rather than the quantity of water in the surroundings. If the average diameter of a defect is less than $5A^0$, then the minimum amount of water molecules in clusters is 3. Otherwise the penetration of water into the hollow of the micro-defect is not beneficial from the point of view of the energy minimum. The amount of the water molecules (N) hydrating the Si atoms is determined by the equation (4):

$$N = 4\pi\rho \int_0^{2\pi} G(r)r^2 dr \quad (4)$$

where,

ρ - water density

$G(r)$ - radial distribution

r - radius vector.

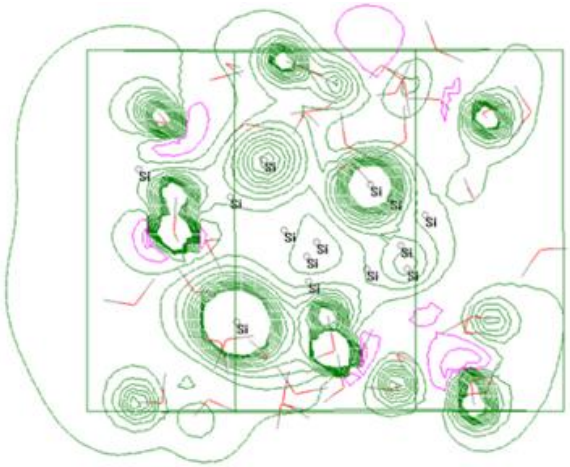

Fig 2: shows the distribution of electrical potentials for the cases of small sized defects ($\sim 5A^0$)

Based on the energetic results of the radial distribution, it was obtained that water penetrates into the micro-defects in the associated form, which is beneficial from the point of view of the energy saving. Referring to Kolesnikovet. al. [6],Badalyanand Grigoryan 2006[1] and Carrascoet. al. [4]in this case at least 3 water molecules are necessary to be arranged in such a way, and the dipole momentum of the associate will be decreased providing its minimum energy state.

However, in the literature[5], [9], [10] there exists the information that the unique (independent) molecule of water could penetrate into the 0.5 nm micro-defect of beryllium crystalline. This would mean that the deployment of the beryllium network by the water molecule occurs, which is not energetically beneficial (for the beryllium the network constants are a=2,286 Å; c=3,584 Å).

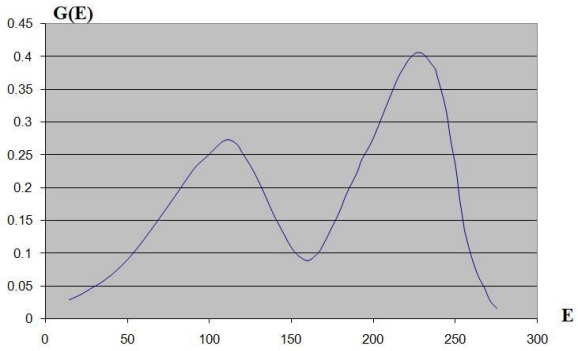

Fig 3: The dependence of the radial distribution on energy

Along with the increase of the defect sizes the amount of water molecules increases not constantly, but partially, by generating five-pointed pentagonal structures, where the energy of interaction is greater than in the hexagonal case. The Figure 3 shows the dependency of radial distribution on the energy.

As a consequence the energetic levels of water molecules are denser, and the potential values of the surroundings are higher that for the water's fee phase, and because of the small sizes of the micro-defects the negative electric field tension in the edges of micro-defects became 10^7 – 10^9V/m, which could act as a scattering or capturing centers for alpha particles and electrons. The Figure 4 shows the levels of the water molecules hydrating the Si defects surface near the edge of micro-defects.

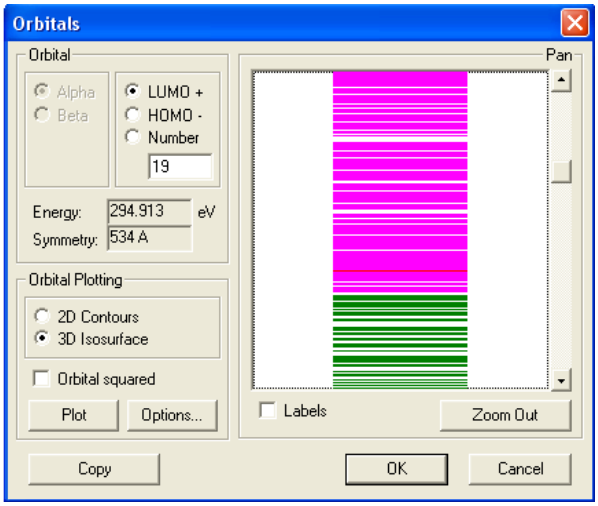

Fig 4: The energetic levels of the electrons in water touching the micro-defect of Si

In case of large defects water clusters are generated in the form of several layers of pentagonal structures. The following layers have more dilapidated, fragile structures rather than previous layers which are directly interacting with the atoms of *Si*. It can be seen in Figures 5 and 6 that there exist 2 small distribution peaks also, the half-width of each of them islongerthan the previous one. It means that the third and subsequent layers have worse arrangement, i.e. the orientation of water molecules in it is not a strict certain and the dipole moments of water molecules are weakly regulated, and finally the last layers become not arranged. We are sure in it when we're taking the option of the molecular dynamic considering the radial distributions of Si, oxygen and hydrogen atoms. This can be mentioned in the radial distribution corves of silicon, oxygen and hydrogen.

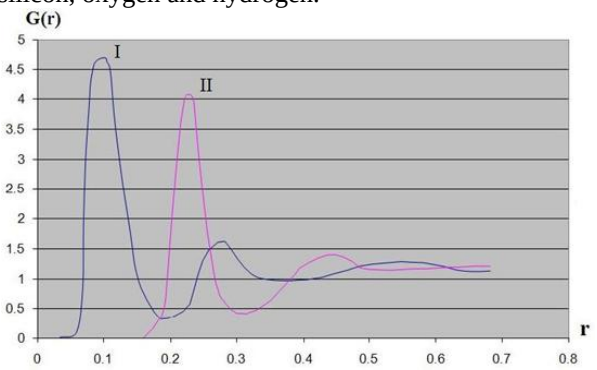

Fig5. The radial distribution curves for oxygen (I) and hydrogen (II)

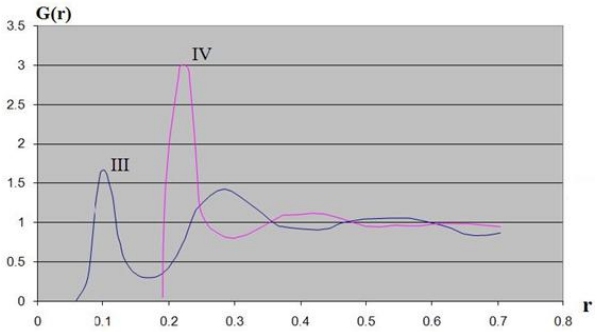

Fig6. The radial distribution curves for Si (III) and hydrogen (IV)

This leads to the fact that in the edges of the defects the energetic field potential becomes greater because of the smaller radius. Consequently, the tension of the electric field in the defects increases from 10^5 to 10^7 V/m. So, it turns out that there exist effective sizes of the defect for the occupation of positive particles, in which case the tension of the electric field is 10^7V/m.

Free charges occupied by the water clusters with pentagonal structures in the volume of Si generate local centers, which lead to the re-distribution of the electrons. As a result in the monocrystalline of Si the electric field becomes inhomogeneous according to the $E = E(x)$ function, and a great electric field tension is generated in the traps, where the water energetic levels reach up to 294 eV, which corresponds to the gamma domain's electronic transitions, where the general as well as the tunnel crossings of the proton are possible.

The big tension of the electric field in the traps is a favorable condition for the tunnel crossing for protons and it is recovered as a hydrogen atom within the volume of Si due to free electrons, existing in the volume of Si charged particles. In Kolesnikovet. al.[6]work it was indicated as a tunnel crossing of hydrogen, however in our case it is a tunnel crossing of proton, which is more supposedly in our opinion.

IV. CONCLUSIONS

The amplitude spectrum investigations of the registered alpha particles show that such kind of associates have a great contribution into the formation of tail part of the amplitude specters for the charged particles, which is due to the ability to release of the electrons from the traps and to participate into the free charged particles flow process with the delay. As a result of the process the lengthening quenching time of the particles registration signal is occurred. The above mentioned process was observed during the experimental study of the alpha particles spectrum registration signal.

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