International Round Table on Applied Research
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Theoretical and applied problems of the direct conversion of radiochemical energy into electrical energy by the radiation-stimulated SiC*/Si heterostructure

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in cooperation with Rajapov S.A. Institute of Physics and Technology of the Scientific
and Production Association "Physics-Sun" AS RUz

Investigation of the betavoltaic effect in Silicon Carbide doped with C-14

by Combined Methods

1. Optimization of the manufacturing process of SiC*/Si heterostructures micro-doped with C-14 in the CVD reactor → industrial site.

   1.1 Phase analysis. depending on the concentration, it can form the phase in Silicon Carbide molecules, but it may not if subcritical.

   1.2 Studies of the relationship between the of electron-hole density at 1 ÷ 5 microns depth and with electron energy less than 100 keV and the efficiency of photobetavoltaic elements or radiation-stimulated semiconductor heterostructures. Proton and heavy ion beams test possibilities.

   1.3 Radiochemical laboratory of the 1st or 2nd class.

2. DFT Calculations of the efficiency and physical parameters of the betaconverter, taking into account the structural features of the studied processes → the software product.

   Providing access to a supercomputer for calculations.

3. Substantiation of the effects of contact formation and metallization, studies of the band structure of the semiconductor, defects, dislocations, the position of the levels, the work function, the manufacture of contacts for betavoltaic materials.
   Scanning tunneling microscope. Encapsulation and packaging of chipsets.

4. Study of the betaconverters 1x1mm +supercapacitors Ø2mm for increasing the operating time of small-volume solid-state energy storage devices with microcontrollers.

   Probe installation, certification.

FORMATION AND EVOLUTION OF DEFECTS OF RADIATION DOPED SiC */Si HETEROSTRUCTURE

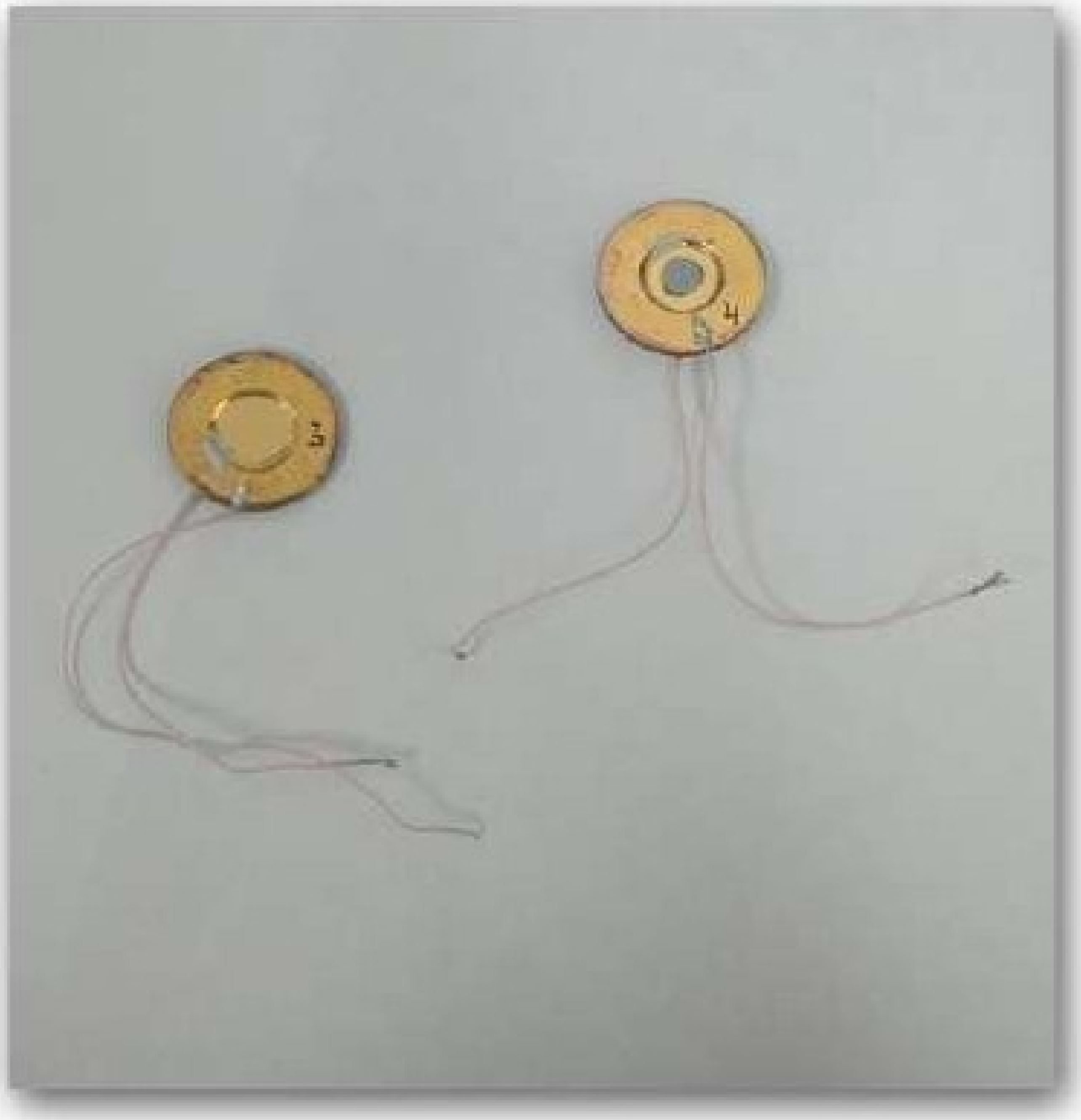
References:

Gurskaya A.V., Dolgopolov M.V., Chepurnov V.I. C-14 beta converter // Physics of Particles and Nuclei 2017. — Vol. 48. Issue 6. — P. 941-944

Alimov L.E., Anufriev A.V., Gurskaya A.V. etc. Silicon Carbide 3C-SiC phase band structures calculation in DFT // Journal of Physics: Conference Series. — 2020. — Vol. 1686. Issue 1.

Chepurnov V., Puzyrnaya G., Gurskaya A., et al. Experimental investigation of semiconductor structures of the power source based on carbon-14 // Physics of Wave Processes and Radio Systems. - 2019. - Vol. 22. - N. 3. - P. 55-67.

RU patents 2020г.: 2 733 616, 2 714 783, 2 714 690, 2 653 398 (2018г.). 2009г. 2 370 851.



Partial Support by the Ministry of Industry and Trade

Introduction

Motivation for the study of betavoltaic energy converters

> Increase of lifetime

> Uninterrupted operation

> Miniaturization

> Reduced power consumption

> Offline work m remote access locations

Betavoltaic battery or beta-converter is a device for transforming beta-decay energy in DC.

HighLights

Direct energy convertion of radiochemical transformations through semiconductor structures with optimal parameters:

the geometry of the structure,

the thickness of the deposition of the radioisotope layer,

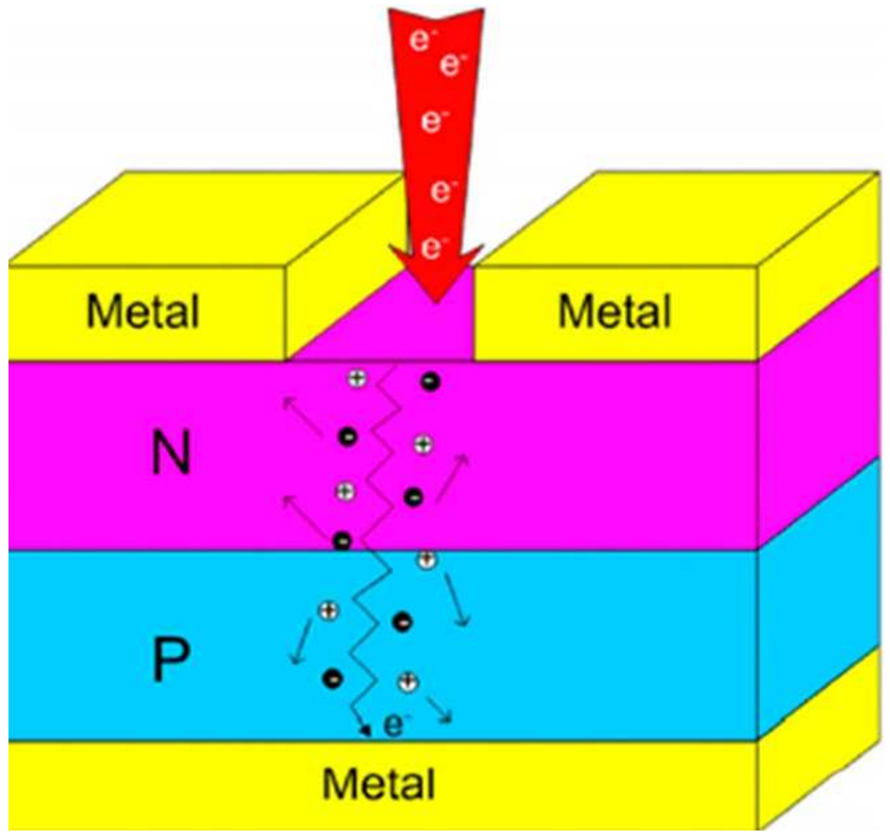
the depth and the width of the p-n junction

Influence factors on energy conversion optimal technology process of growth, self-diffusion, radioactive Carbon isotope phase, the mobility of the radionuclide.

Theoretical modeling of beta converters.

Dark currents from 16 to 90 nA were observed in the external circuit. Idling voltage was amounted to 1.6 mV (results of probe measurements). The thickness of the activated n-SiC film in the heterostructure is 1 - 5 µm.

PROBLEMS OF CONTACTS FORMATION AND EFFICIENCY DETERMINATION FOR SiC*/Si MICROSTRUCTURES



[1] Ehrenberg W,, Lang C.-S., West R. The Electron Voltaic Effect. Proceedings of the Physical Society A. 1951. V.64. p.424

[2] Moseley, H.G.J., Hailing, J. The attainment of higii potentials by the use of radium. Proc. R. Soc. A. 1913. V.88 p.471.

[3] Rappaport P.L, Loferski J. J., bindery E.G. A study program of possible uses new principle. Nucleonics. 1957. V.15. p.99.

Self-organizing mono 3C-SiC endotaxy technology

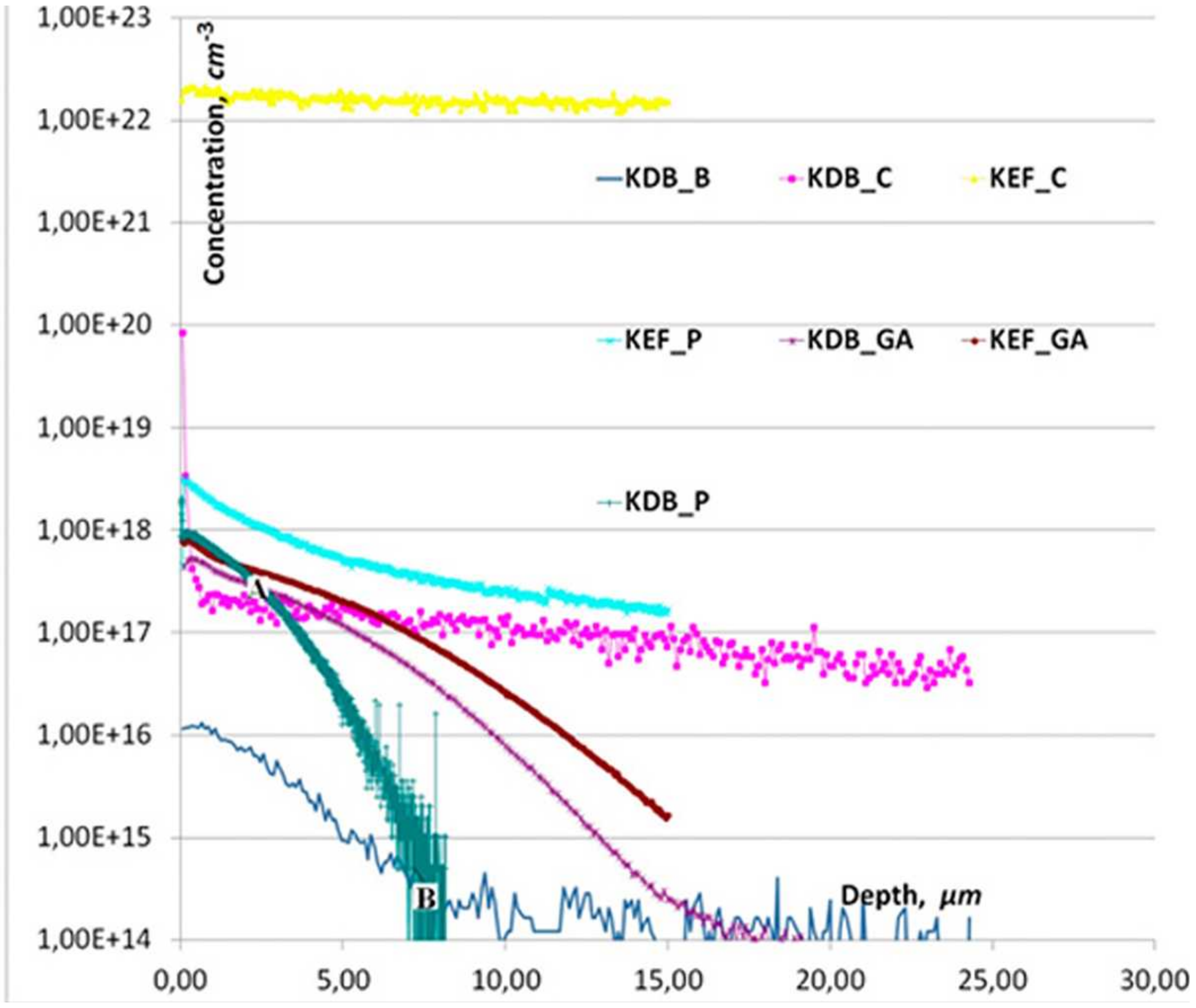
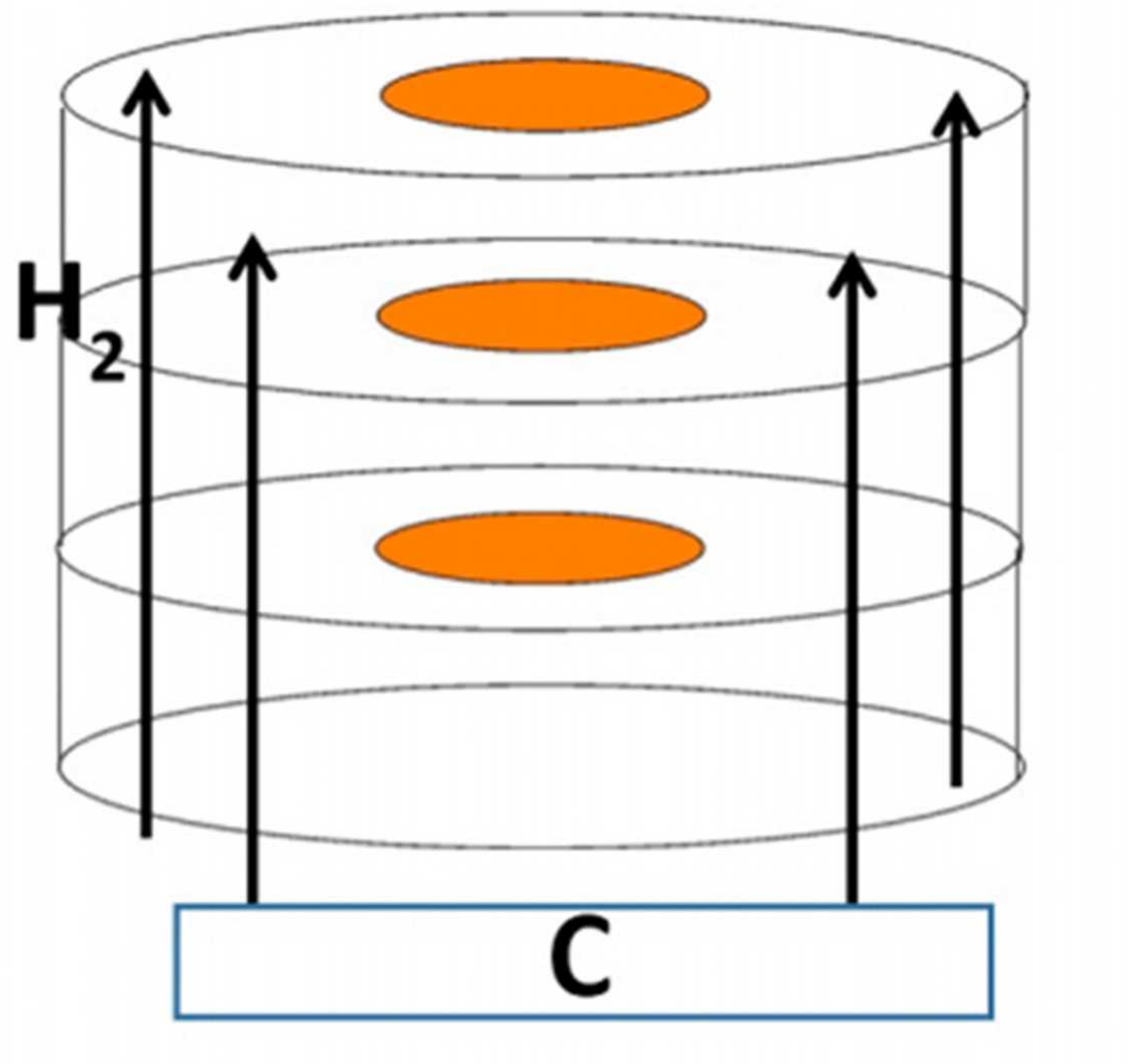
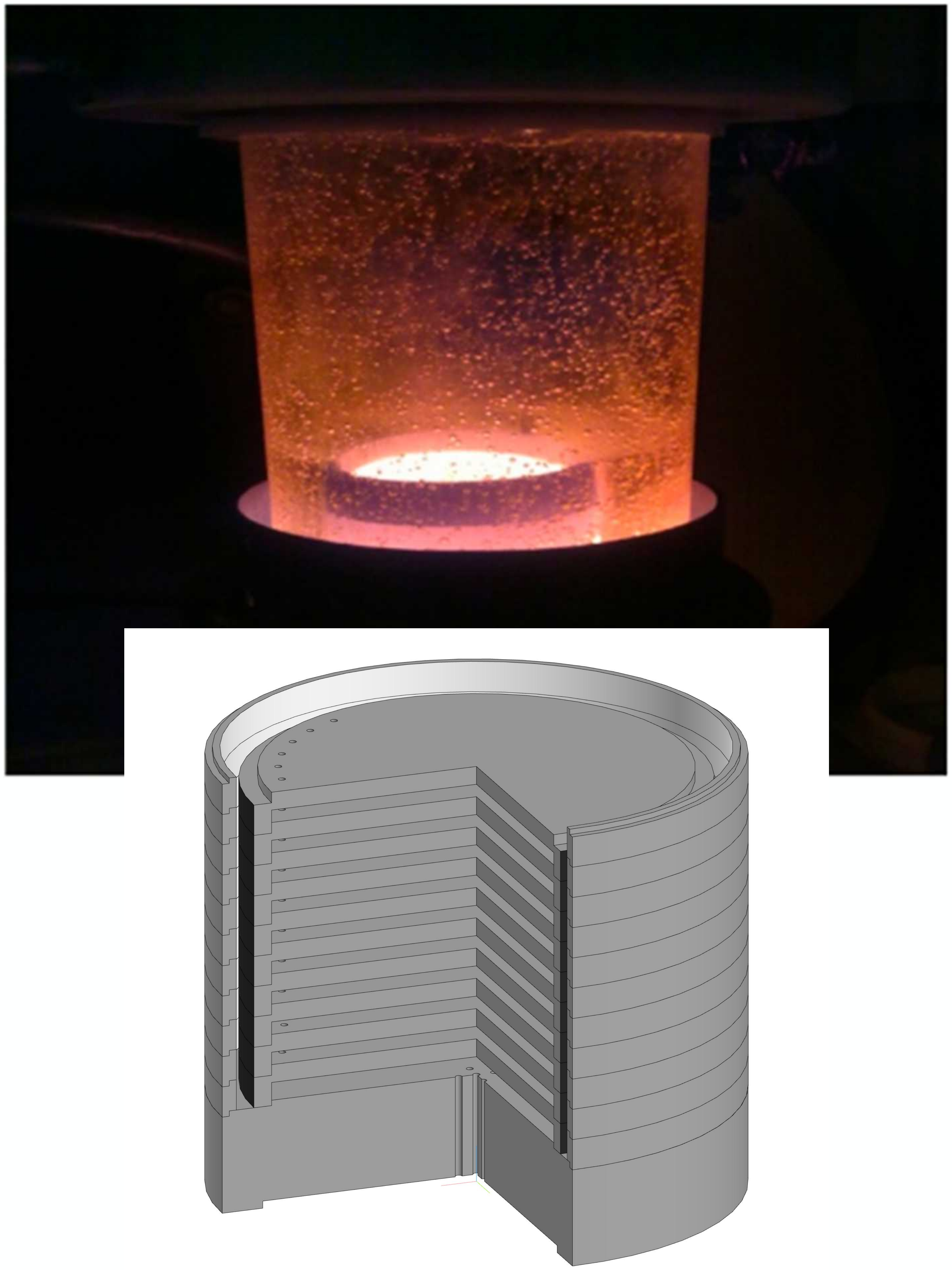


Diagram of concentrations dependencies on depth. The analyzed depth ranges from $5.3 \bullet 10^{-8}$ to $24.3 \bullet 10^{-6}$ m.

The concentration of |C 12 atoms (KDB C curve), depending on the analyzed depth, ranges from $8.4 \bullet 10^{19}$ to $3.2 \bullet 10^{16}$ particles/cm3 .

The microalloying process in the gas chamber



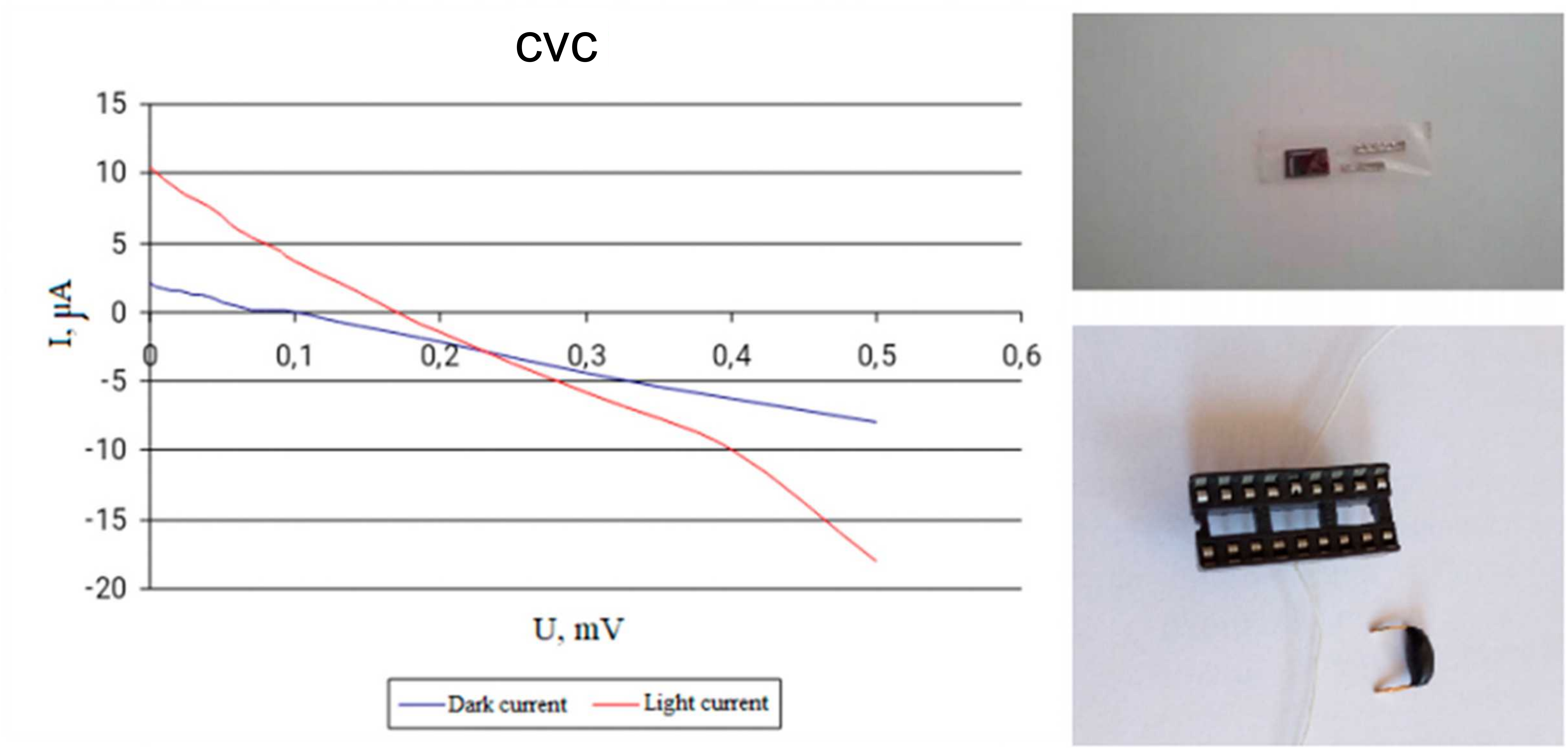


Schematic representation of chemical transport (experimental silicon substrates are indicated in orange); to the right: CVD endotaxy reactor of the SiC / Si family of heterostructures.

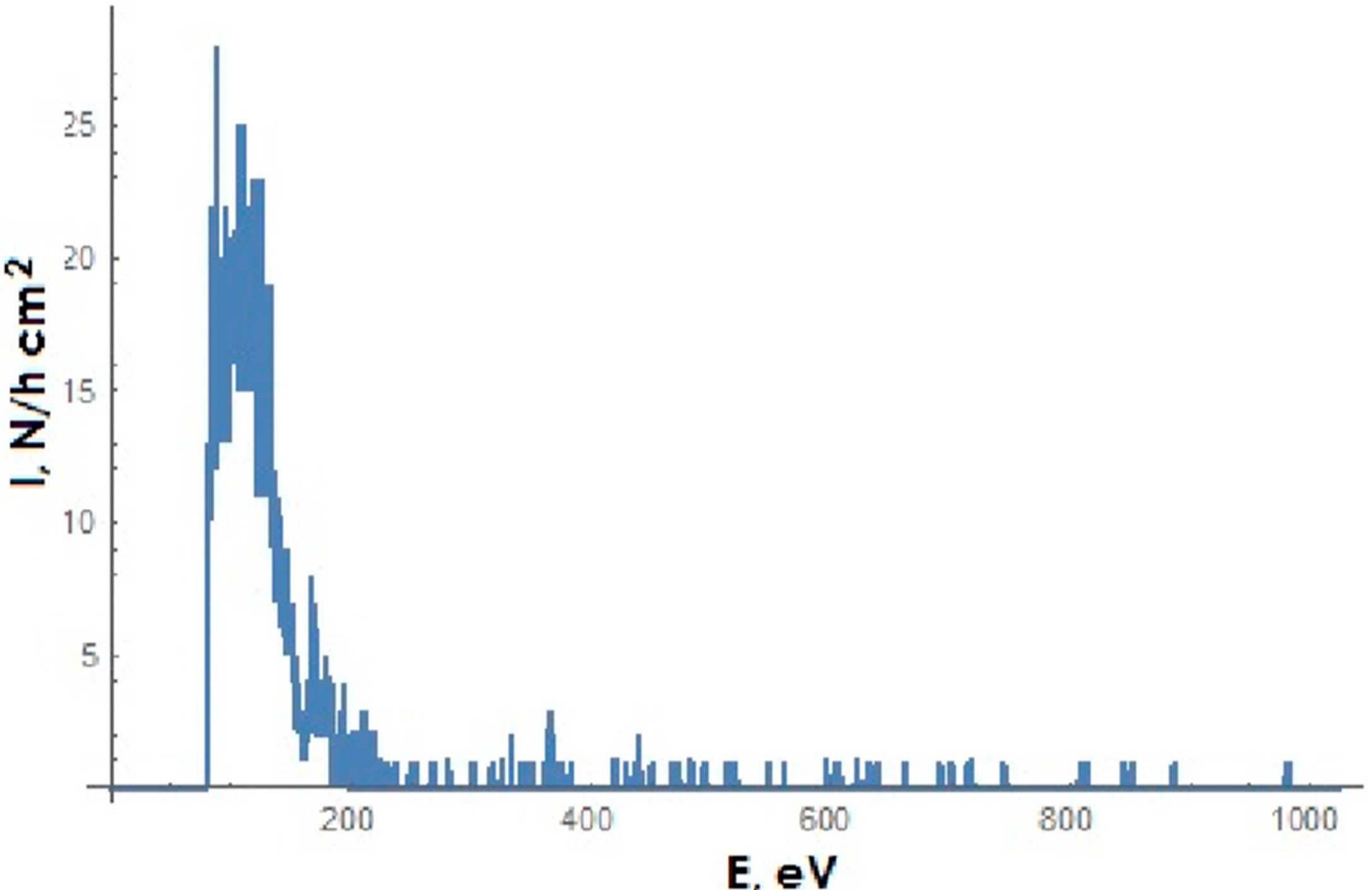
Carbon-14 choice of as the fuel

1. Specific activity of C-14 is different from the Ni-63 about in 10 times per unit volume, due to the huge difference in half-life times.
2. Self-absorption of Ni-63 is larger by approximately three times, which leads to the maximum limit optimal thickness of the layer to 4 microns, and for C-14 this thickness may be up to 60 microns which is better suited. The total quantity of the isotope C-14 may be an order of magnitude greater, therefore, guaranteed more power for the same size of power converters.
3. The specific power of Ni-63 per gram of the substance 5 times (due to more activity) exceeds the power density of C -14. But the maximum and average energies of electrons in the C-14 decay is in 2, and even 3, times more than in the Ni-63 decay.

Current-voltage characteristic and samples

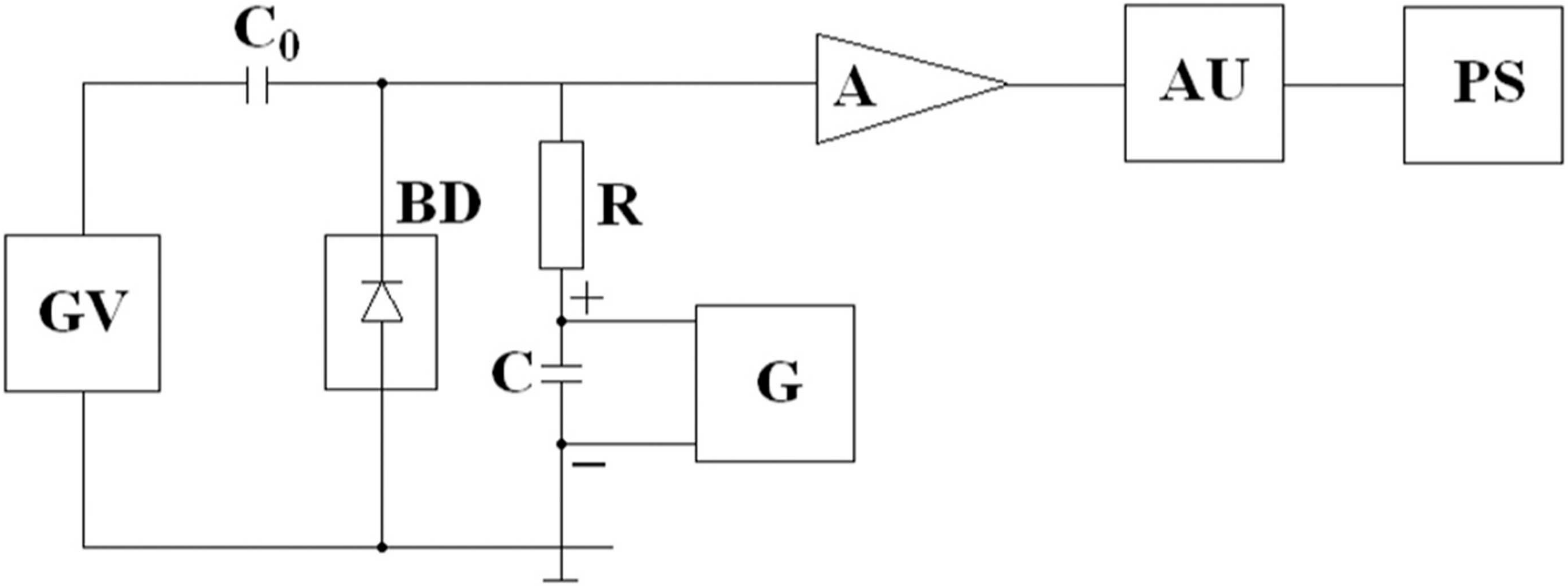


To the left: dark (blue) and light (red) current-voltage characteristics measured on the n-SiC / p-Sic / p-Si structure. To the right: example of the experimental structure with metallization

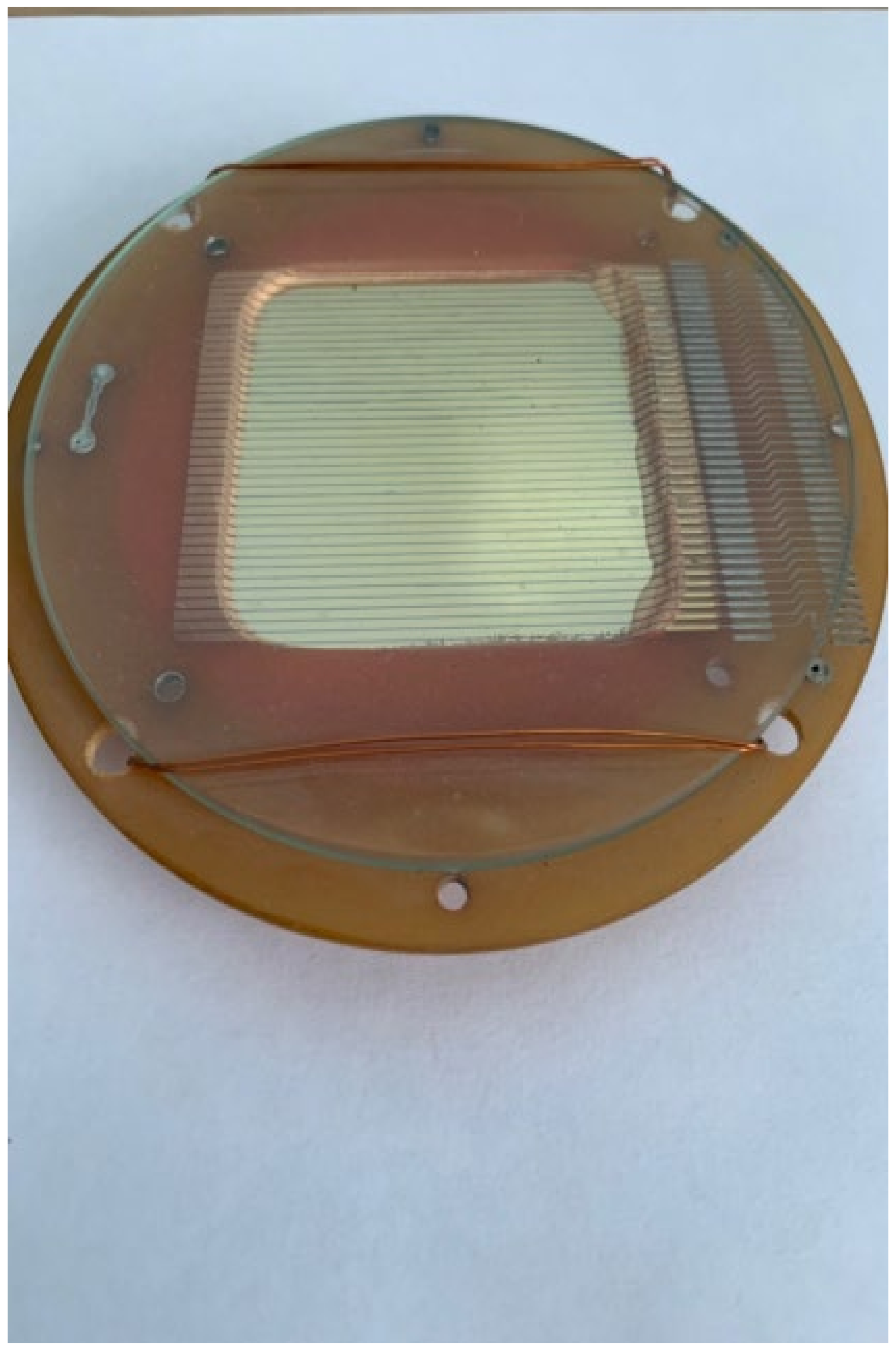


Spectrum of radioactive carbon in SiC structure.

Electrical diagram of the measuring device



BD — detector, AU is the scale Converter, A — charge sensitive amplifier, PS — amplitude analyzer, G — source bias voltage, R - resistor leakage, C is a blocking condenser, GV — generator of voltage pulses, CO — metering capacitor.



Institute of Physics and Technology of NPO "Physics-Sun" of the Academy of Sciences of the Republic of Uzbekistan,

SILICON DETECTORS OF CHARGED PARTICLES WITH SMALL LEAKAGE CURRENTS, MEASUREMENT OF BETA SPECTRA OF TRANSDUCERS

Silicon detectors of charged particles with low leakage currents for nuclear spectroscopy, activation analysis, dosimetry, medicine, biology, high-energy astrophysics, nuclear waste monitoring, archeology, environmental problems, diagnostics of high-temperature plasma, etc. Beta spectrum studies for semiconductor energy converters have been conducted.

Previous study of the betavoltaic device characteristics

There are several methods of calculating a generation rate:

- Via Bethe-Bloch formula

  $$-\left(\frac{dT}{dx}\right) = \frac{2\pi e^4 n_e}{m_e v^2}\left[ln\frac{m_e v^2 T_e}{2I^2(1-\beta^2)} - ln(1-\beta^2) - \beta^2 - \delta - U\right]$$

  (A.A.Gorbacevich et al.//ZHTF, 2016, V.86, no.7, P.94-99.),

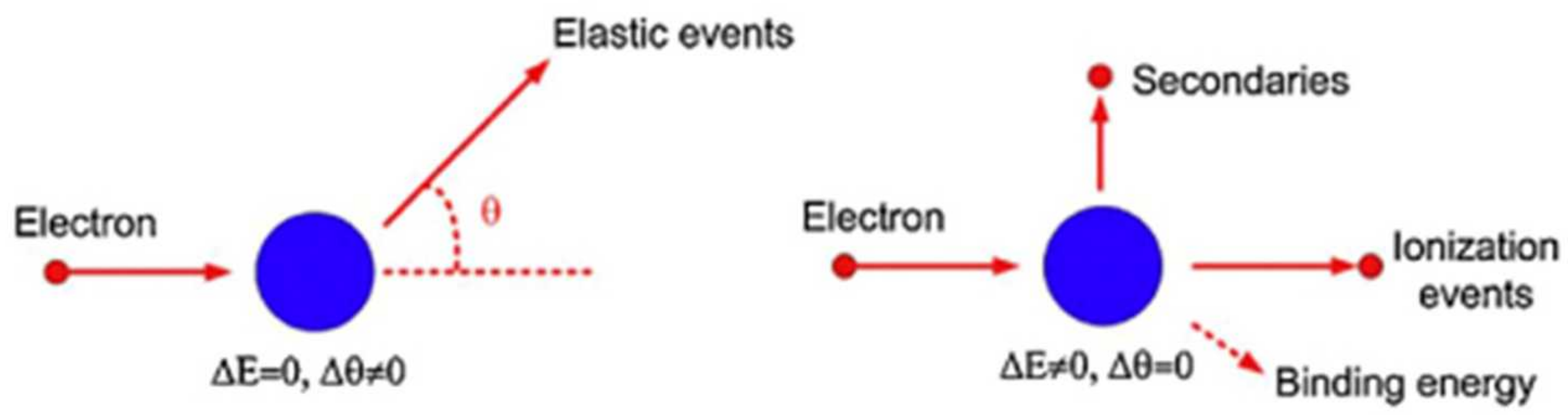
- calculating recombination current density (Bulyarski S. V. et al. /1 Fizika i tekhnika poluprovodnikov. 2017. no.51(l). P.68-74.)

- Mone-Carlo method (S.Theirrattanakul, M.Prelas // Applied Radiation and Isotopes. 2017. no.127. P.41-46.; K.Zhang // Sensors and Actuators A 240 (2016) 131-137)

  etc.

Creating a beta-converter model in GEANT4

► Calculation electron-hole pairs generation rate inside the space charge region of the p-n junction based on secondary electrons from processes

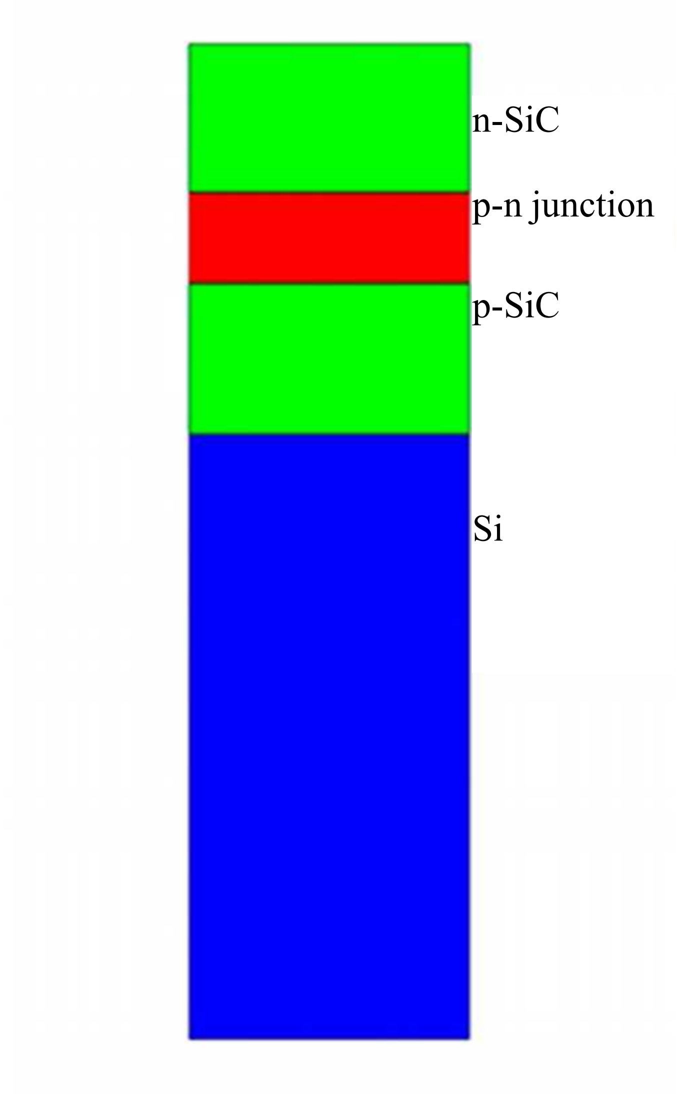


Following Monte-Carlo algorithm:

- Determine primary electron’s initial position, momentum direction and energy based on set probability densities
- Track primary electrons as they fly through the space charge and create electron-hole pairs along the way
- If the electron-hole pair is created inside the space charge region, it is separated by the electrical field of the p-n junction
- Repeat this process many times to achieve good statistical accuracy

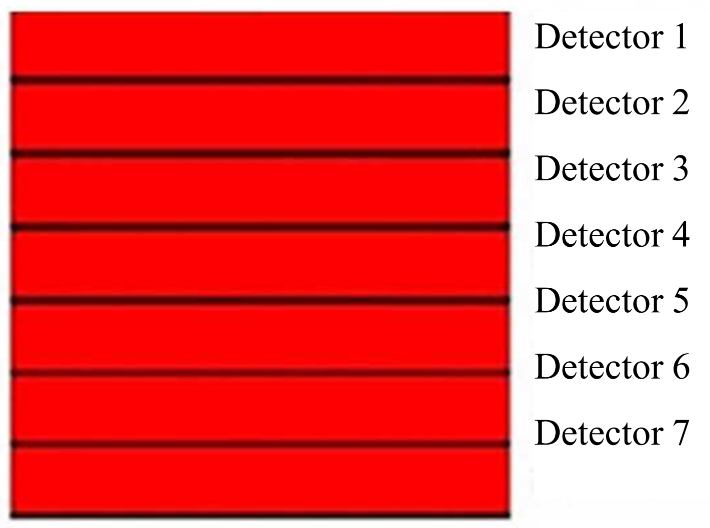
http://cern.ch/geant4

Model in GEANT4



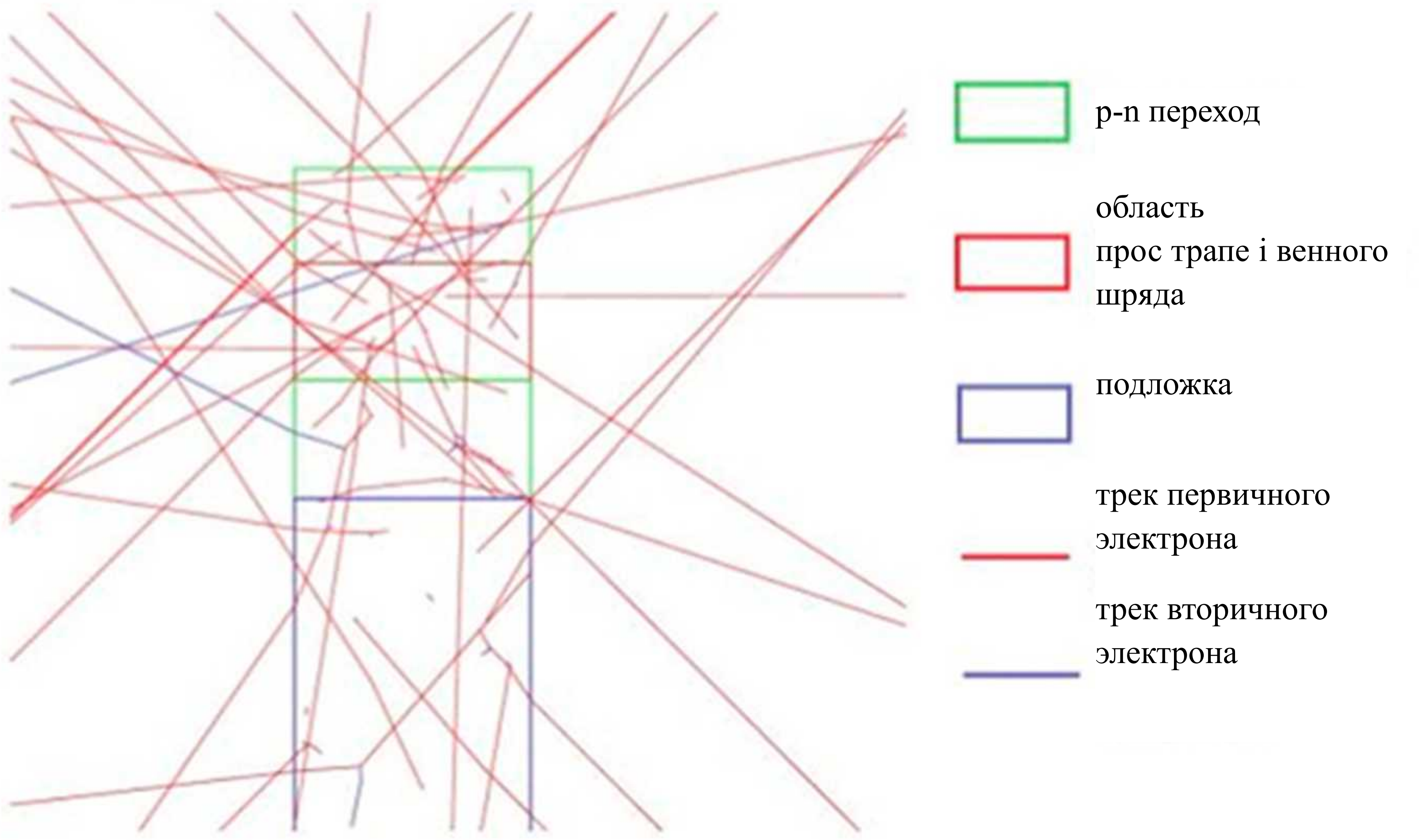
Beta-converter model in GEANT4

Determination of the optimal depth of the p-n junction



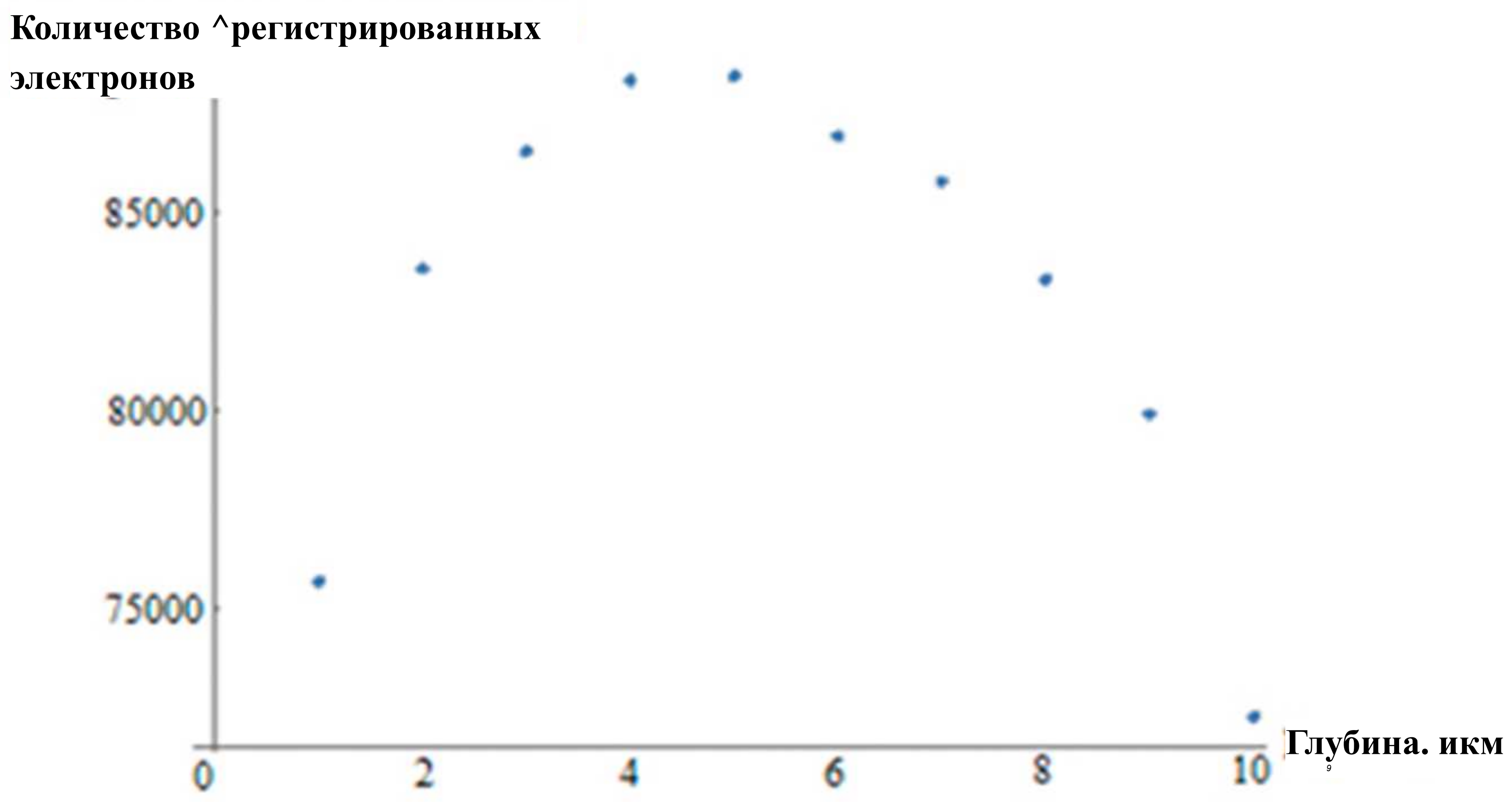
In the upper part there was a layer with the radioisotope C14. Beneath it are layers of detectors each 1 gm thick, which register secondary electrons. The decay process was simulated 10 000 000 times, the results are shown in the table.

Modeling process



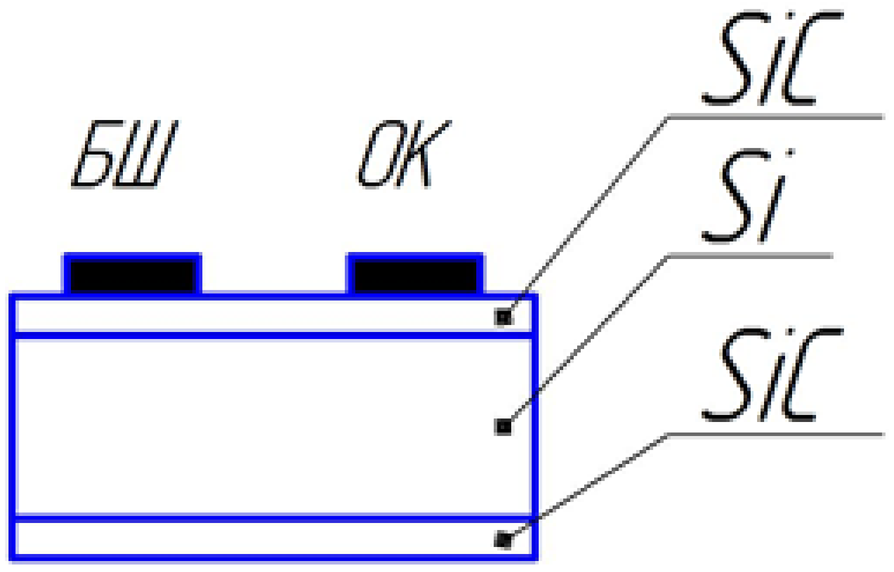
Red trajectories correspond to primary electrons, blue - to secondary electrons (might not be visible due to fast absorption)

Optimal depth determination results

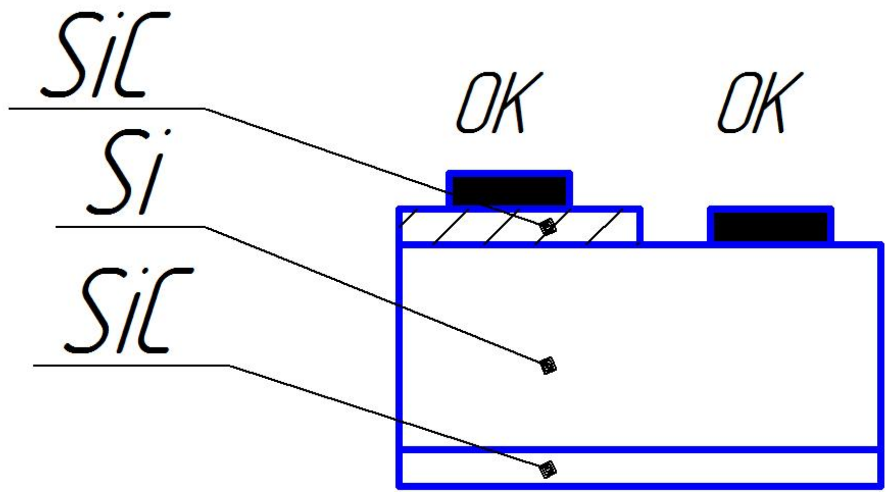


Варианты металлизации

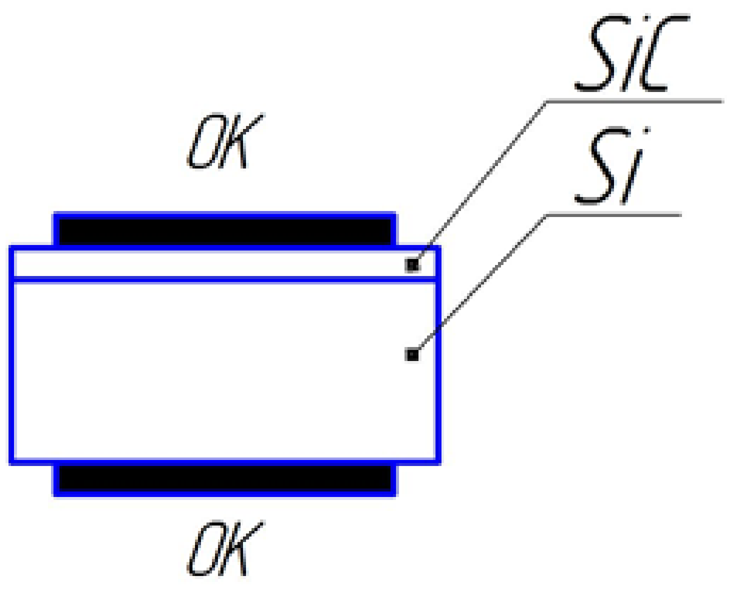
1. Разделение носителей на барьере Шоттки (БШ), второй контакт омический (ОК)

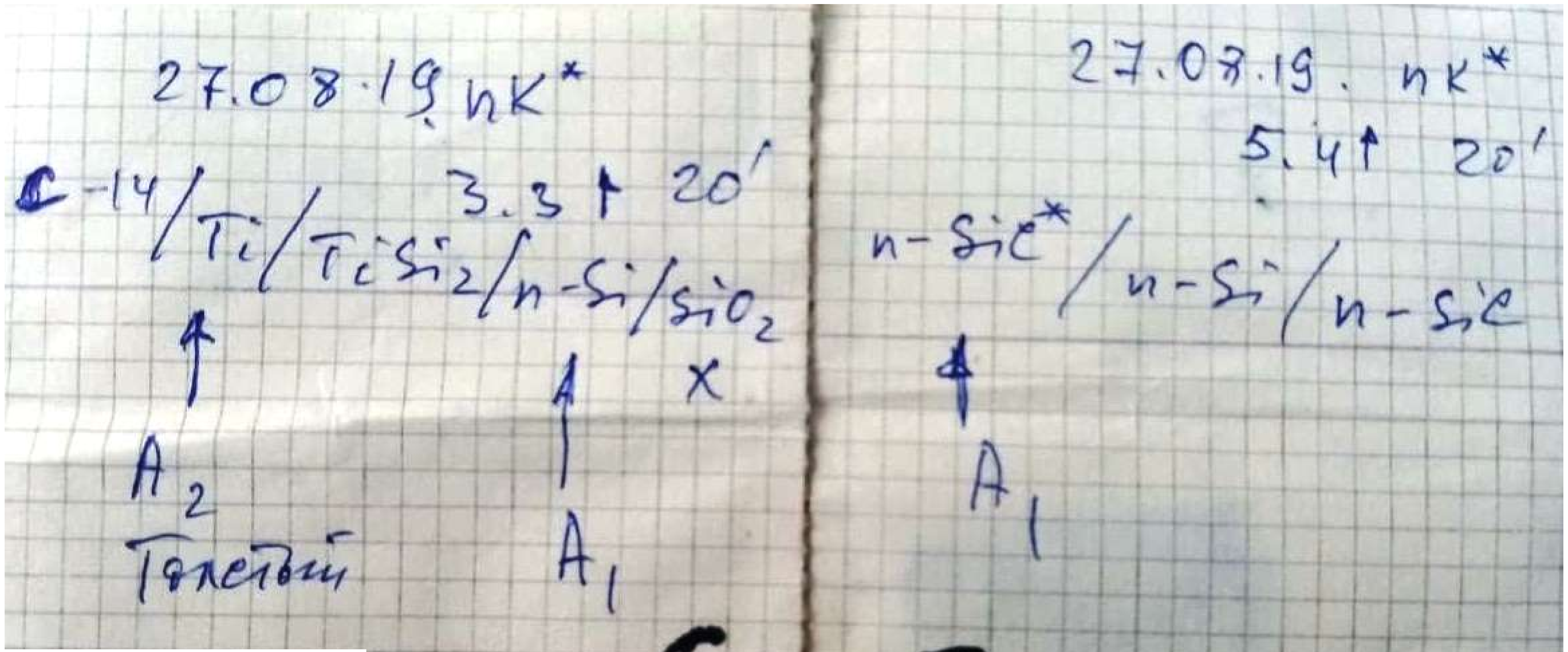


2. Разделение носителей на гетеропереходе SiC/Si, планарное исполнение



3. Разделение носителей на гетеропереходе SiC/Si. Вертикальное исполнение.





27.08.19. nK*

C-14/Ti/TiSi$_2$/n-Si/SiO$_2$ 3.3 ↑ 20'

↑ A$_2$ Толстый

↑ A$_1$

x

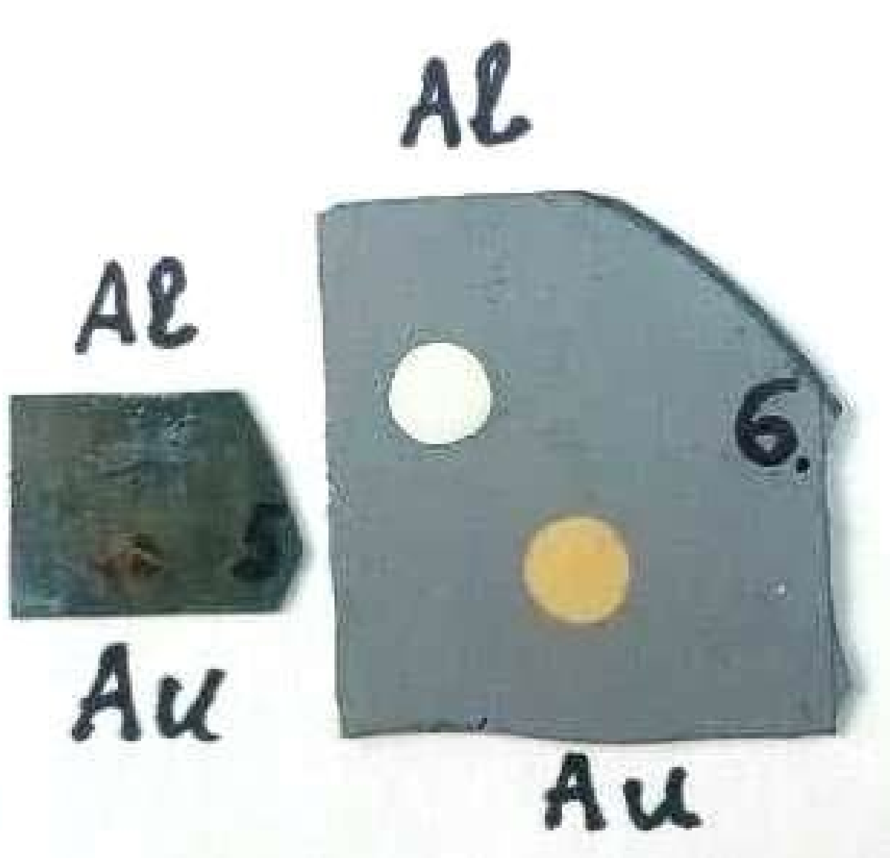
27.08.19. nK*

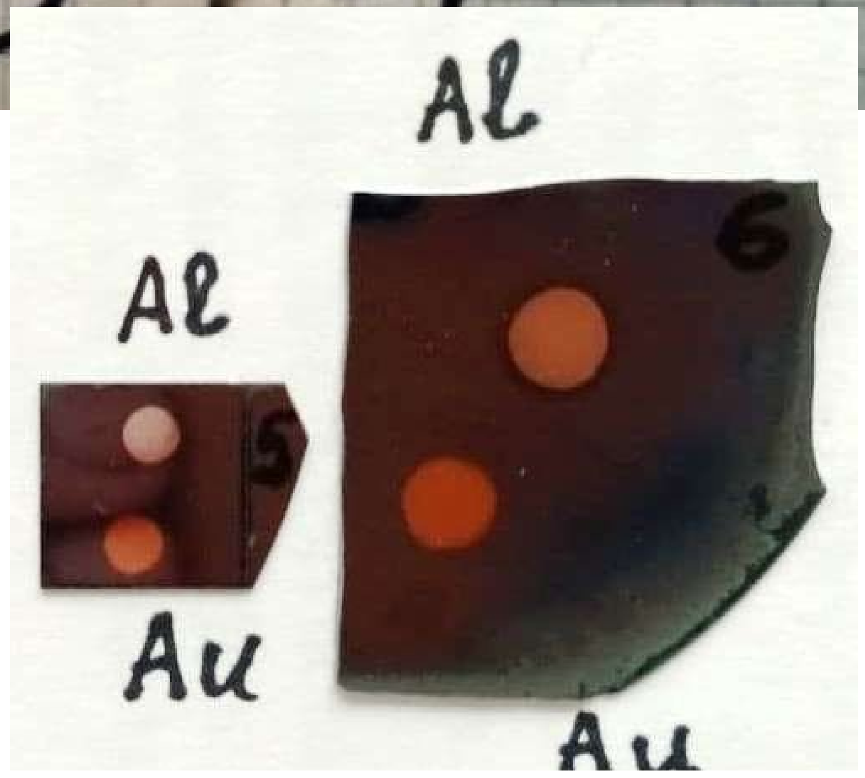
5.4↑ 20'

n-SiC*/n-Si/n-SiC

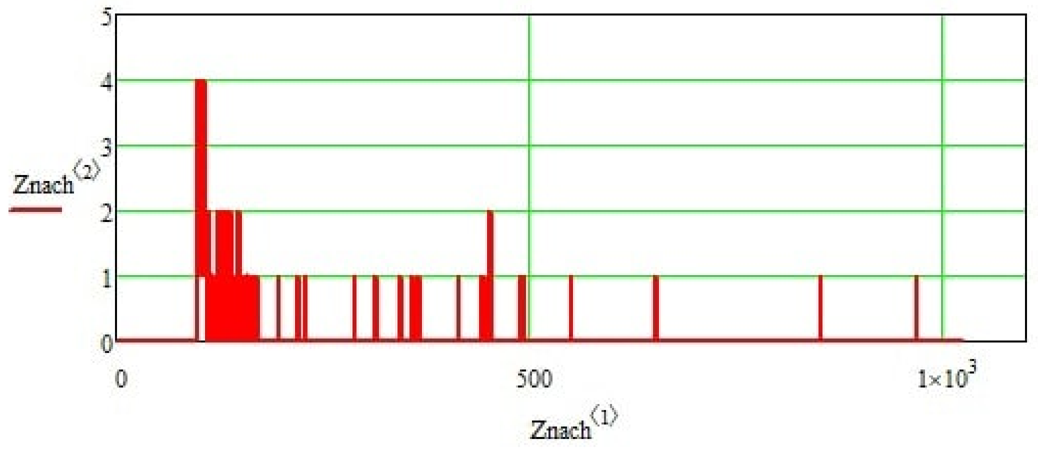
↑ A$_1$

6 5

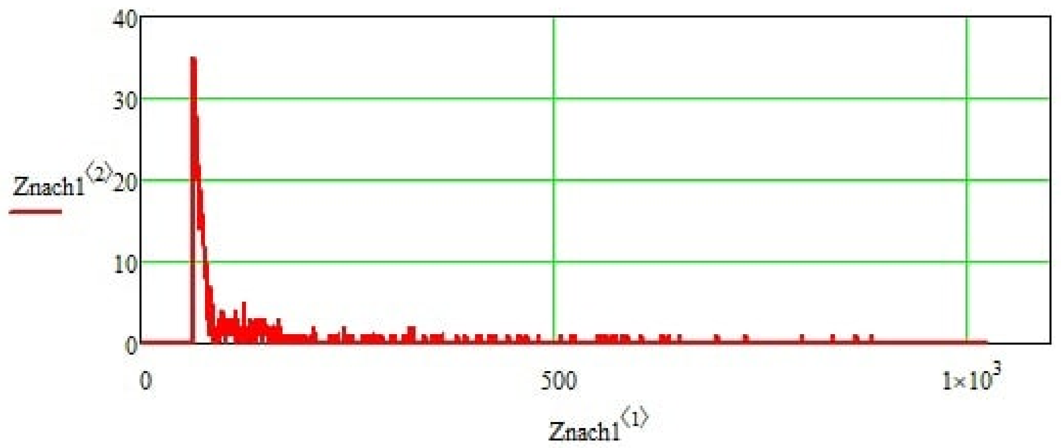


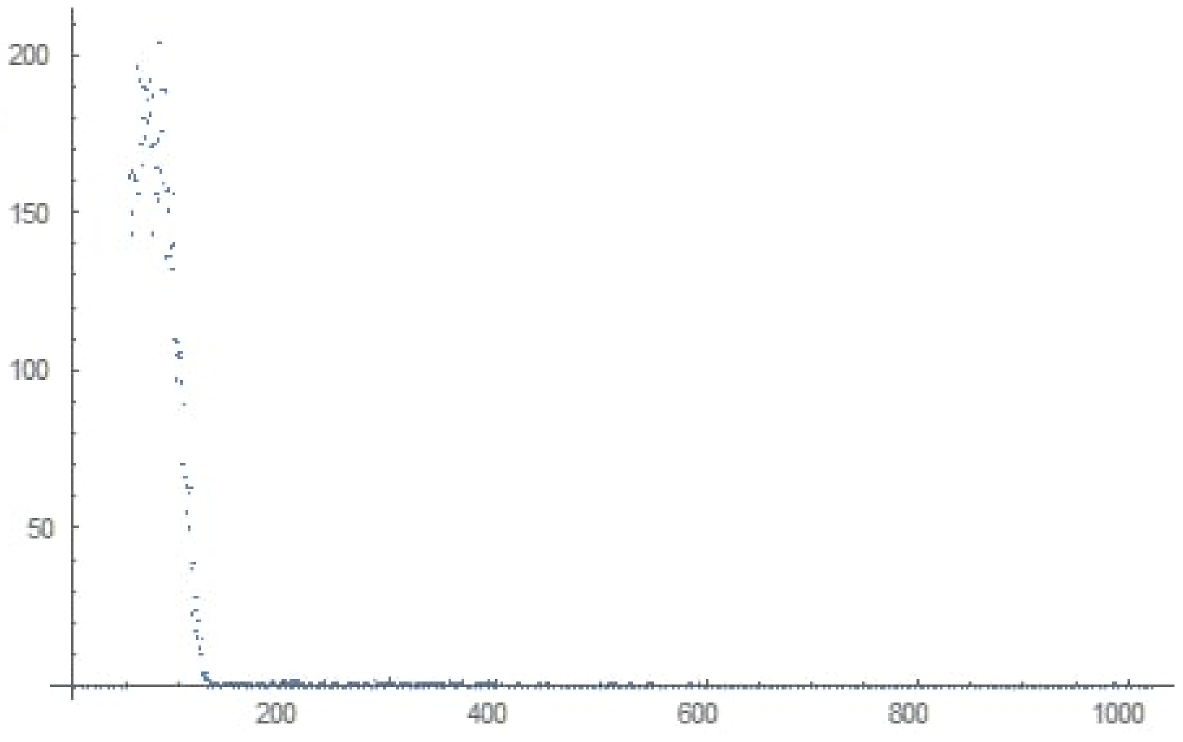


спектр проб №5.2 11_00_18



спектр проб № 6.2 10_13_22





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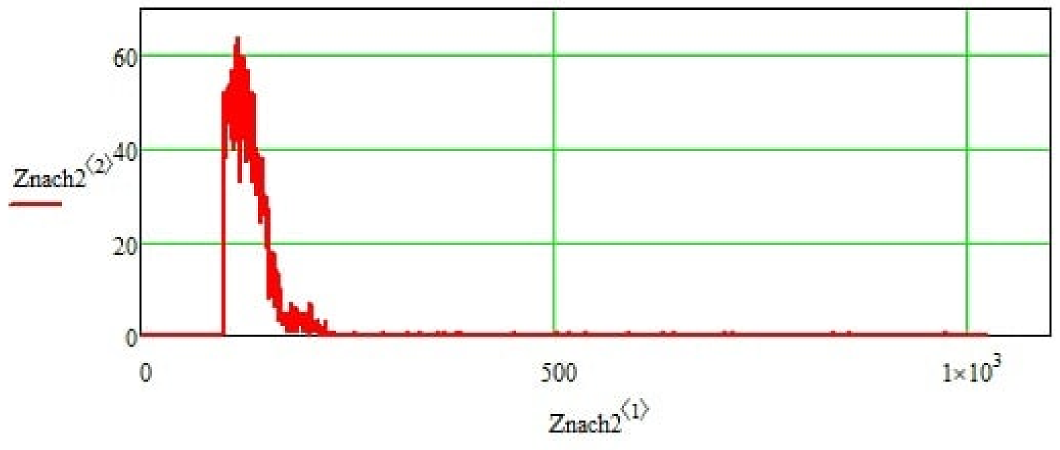
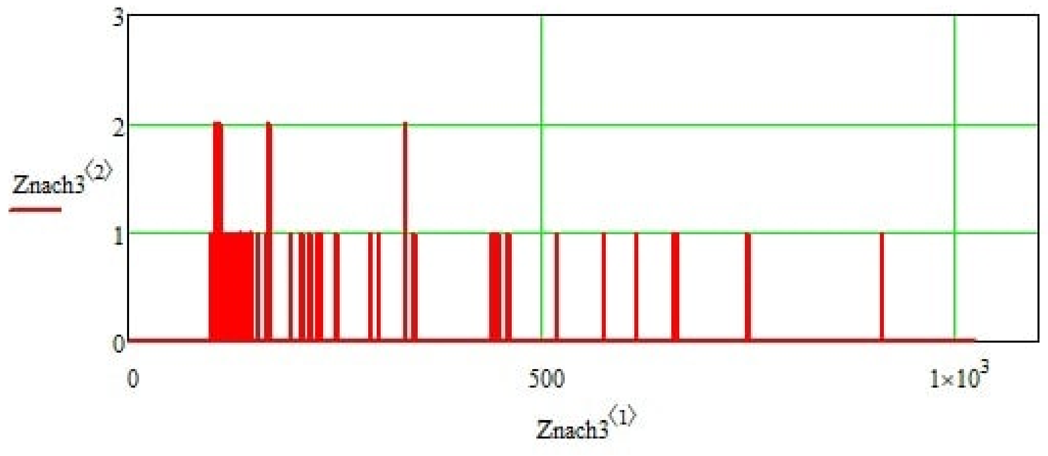


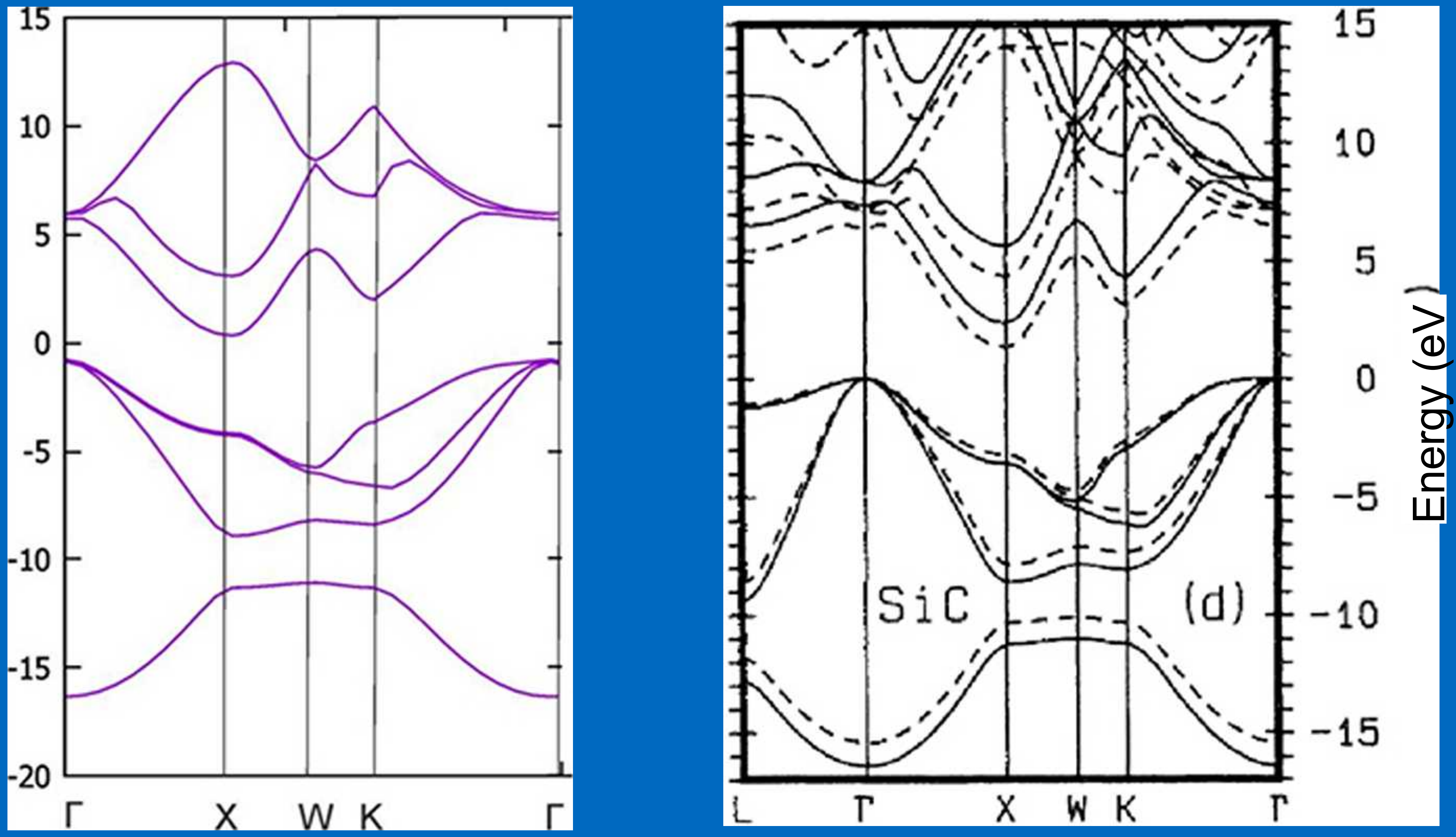
спектр.проб.№5.1 10_36_22



Conclusion

- A beta-converter model was created in GEANT4
- Generation rate of electron-hole pairs was obtained
- Optimal depth of the p-n junction was determined

At temperature $T = 1360 - 1380$ °C and normal pressure $P = 10^5 Pa$, annealing time $t = 60$ minutes, the C^{12} carbon flux density at the boundary $J = 7.98532 \cdot 10^{14}\ particles / cm^2 \cdot s$ and the effective diffusion coefficient of carbon $C^{12}\ D_{e}ff = 0.0495984\ pm^2 / s$ were obtained. The results obtained are in good agreement with the known results. *pTr3.,Ni&i E Edefect* 3C-SiC.

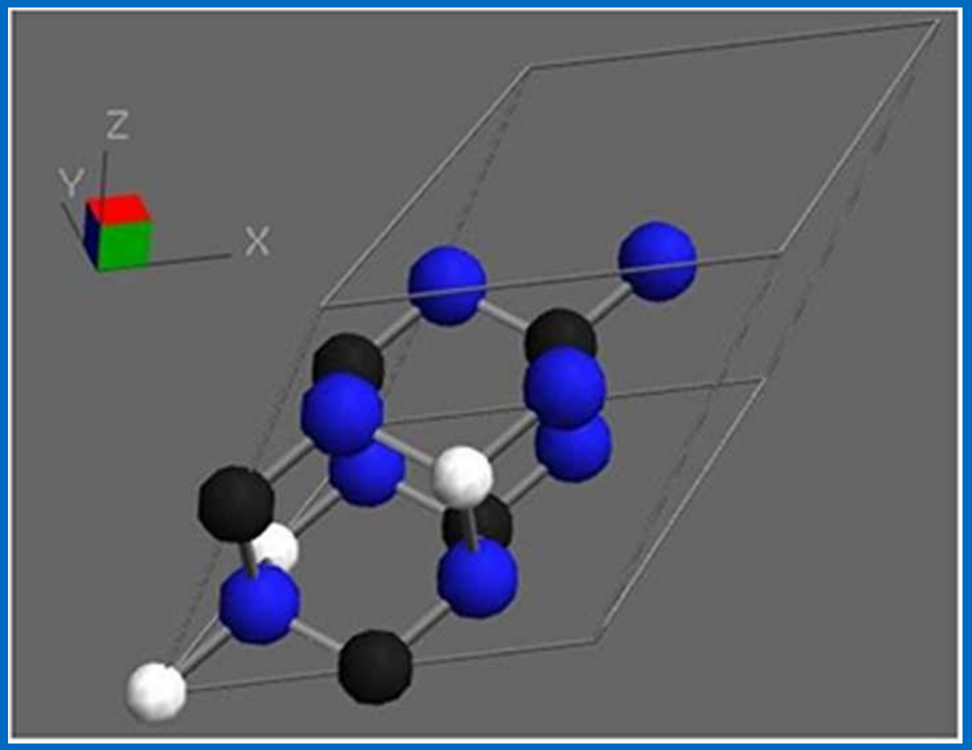


Сравнение DFT-расчетов зонной структуры 3C-SiC:
а) собственные расчеты в VASP;
б) Phys Rev B Condens Matter. 1993 Dec 15,48(24): 17791 - 17805

Тип легирования:

n-SiC (+P), p-SiC (+Ga),

C^{14}-SiC (+N): C^{14} N^{14} + e- + u_e



Вид структуры SiC, допированой тремя атомами(белый цвет)

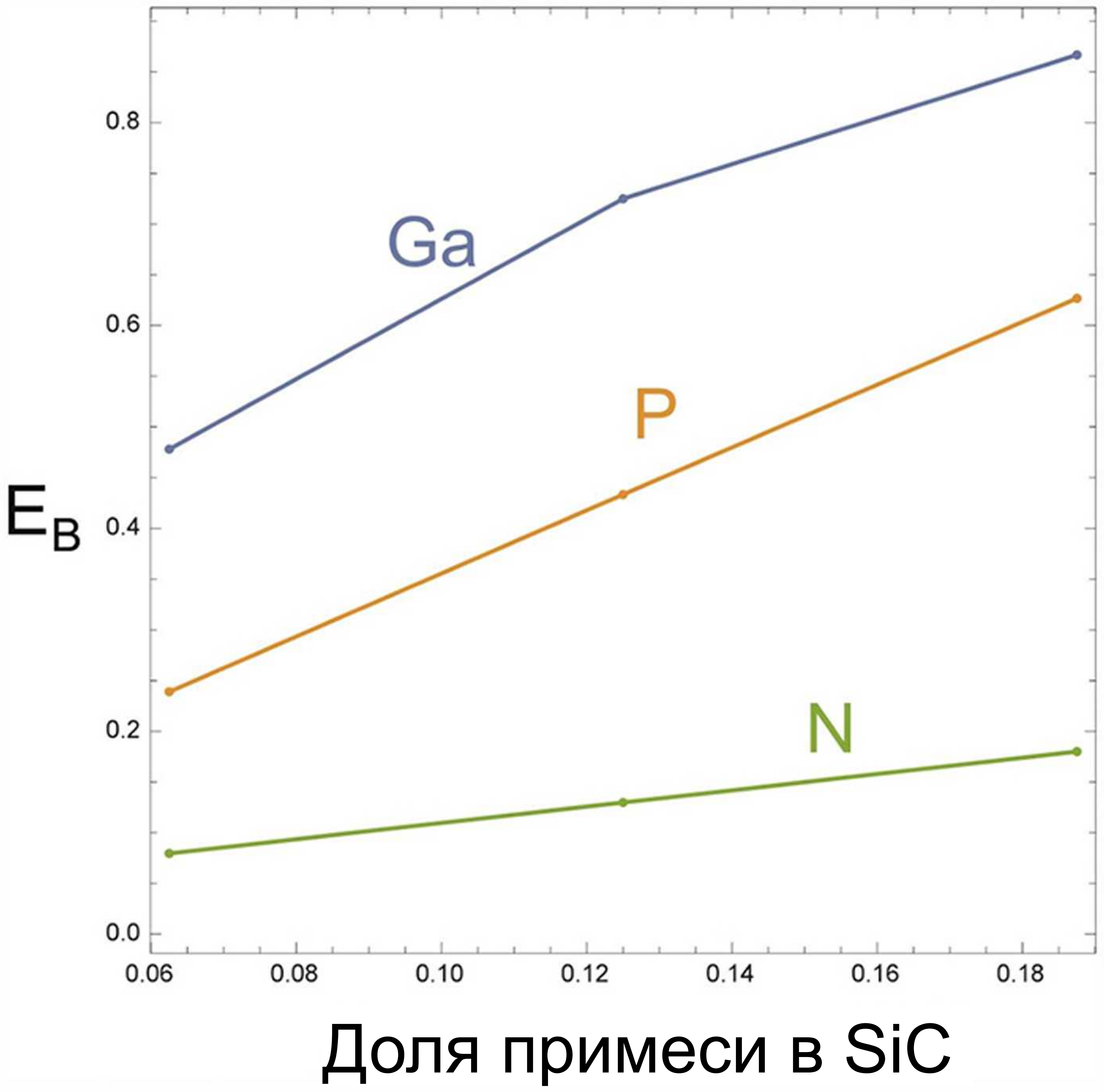
Энергия растворения

$$E_B = \frac{E_m - E_{\mathrm{d}} \cdot N_{\mathrm{d}} - E_{SiC} \cdot N_{SiC}}{N_{\mathrm{d}} + N_{SiC}},$$

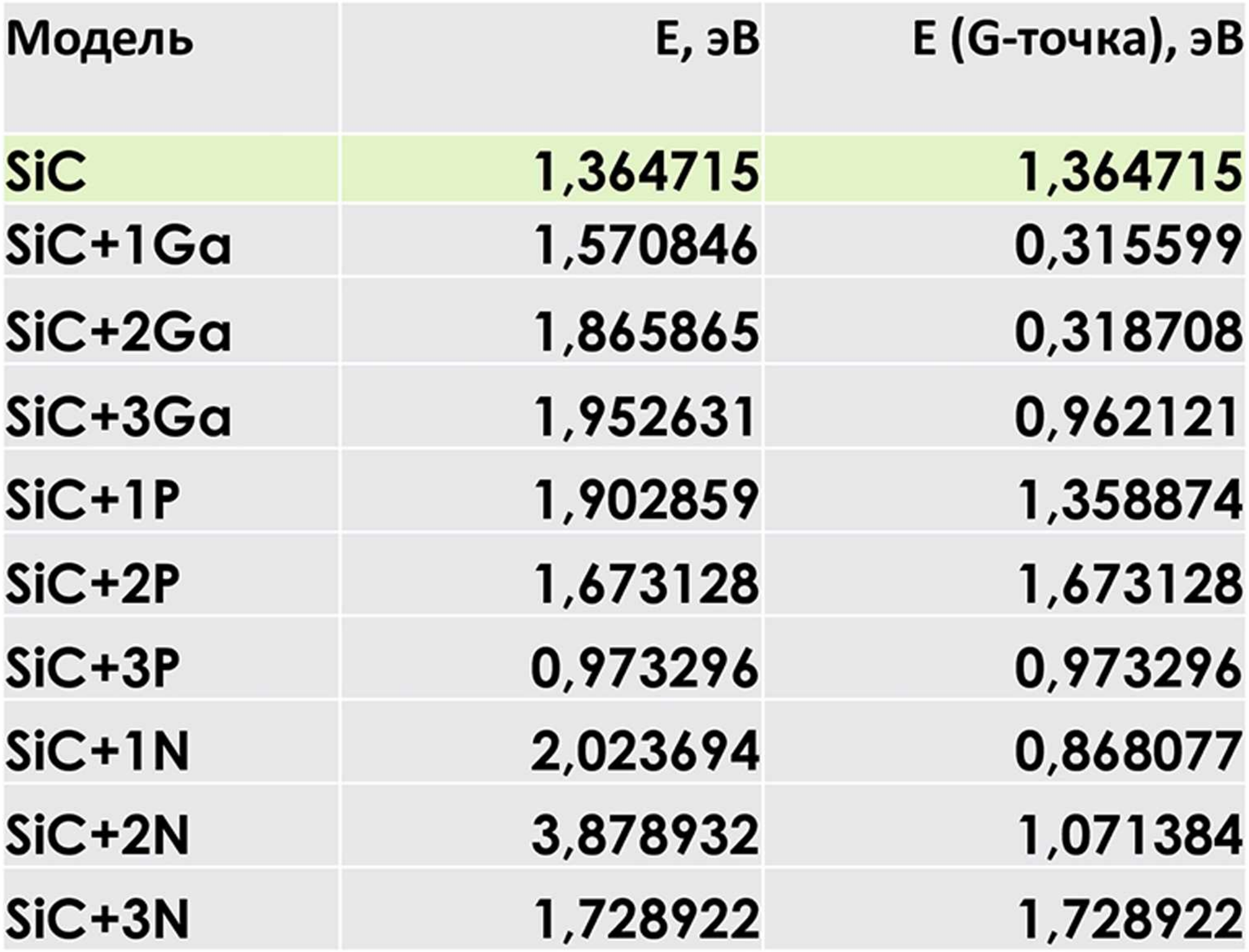
где E_T *- полная энергия молельной структуры,*
N_d, N_{sjc} *- число атомов в эл. ячейке чистых веществ,*
E_d, E_{sjc} *- энергии чистых веществ.*

- Vienna Ab Initio Simulation Package *(Phys. Rev. B 54, 11169 (1996))*

- функционал Перлью-Бурке-Эрзенхова (PBE) (Phys. Rev. Lett. 78, 1396 (1997))



Ширина запрещенной зоны



Модель	E, эВ	E (G-точка), эВ
SiC	1,364715	1,364715
SiC+1Ga	1,570846	0,315599
SiC+2Ga	1,865865	0,318708
SiC+3Ga	1,952631	0,962121
SiC+1P	1,902859	1,358874
SiC+2P	1,673128	1,673128
SiC+3P	0,973296	0,973296
SiC+1N	2,023694	0,868077
SiC+2N	3,878932	1,071384
SiC+3N	1,728922	1,728922

Заключение

- Произведен расчет величин E_T, E_{sjc}, E_d с помощью пакета VASP.

- Рассчитана энергия растворения, и проведено сравнение ее значения для всех модельных структур методом выпуклой оболочки.

- Рассчитаны ширины запрещенных зон для допированного карбида кремния, наибольшая в зонной структуре и прослежено изменение в разнице энергий в G-точке

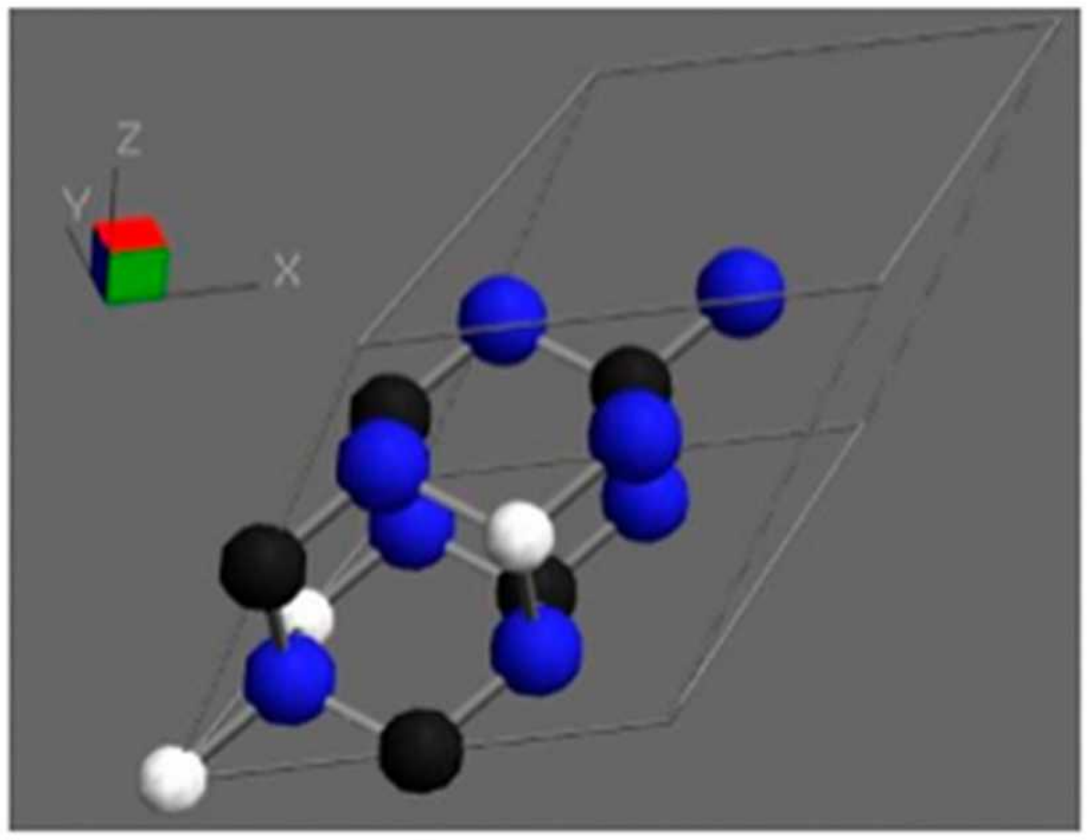
The energy of dissolution of the doping atoms

The 3C-SiC structure includes a C-14 molecule that decays:

$$C^{14} \longrightarrow N^{14} + e^{-} + \upsilon_{e}$$

We have three types of atoms to doping the structure:

n-SiC (+P), *p-SiC (+Ga),* *C^{14}-SiC (+N):*



3C-S/C *includes:*

White - atom doping

Black - C-atom

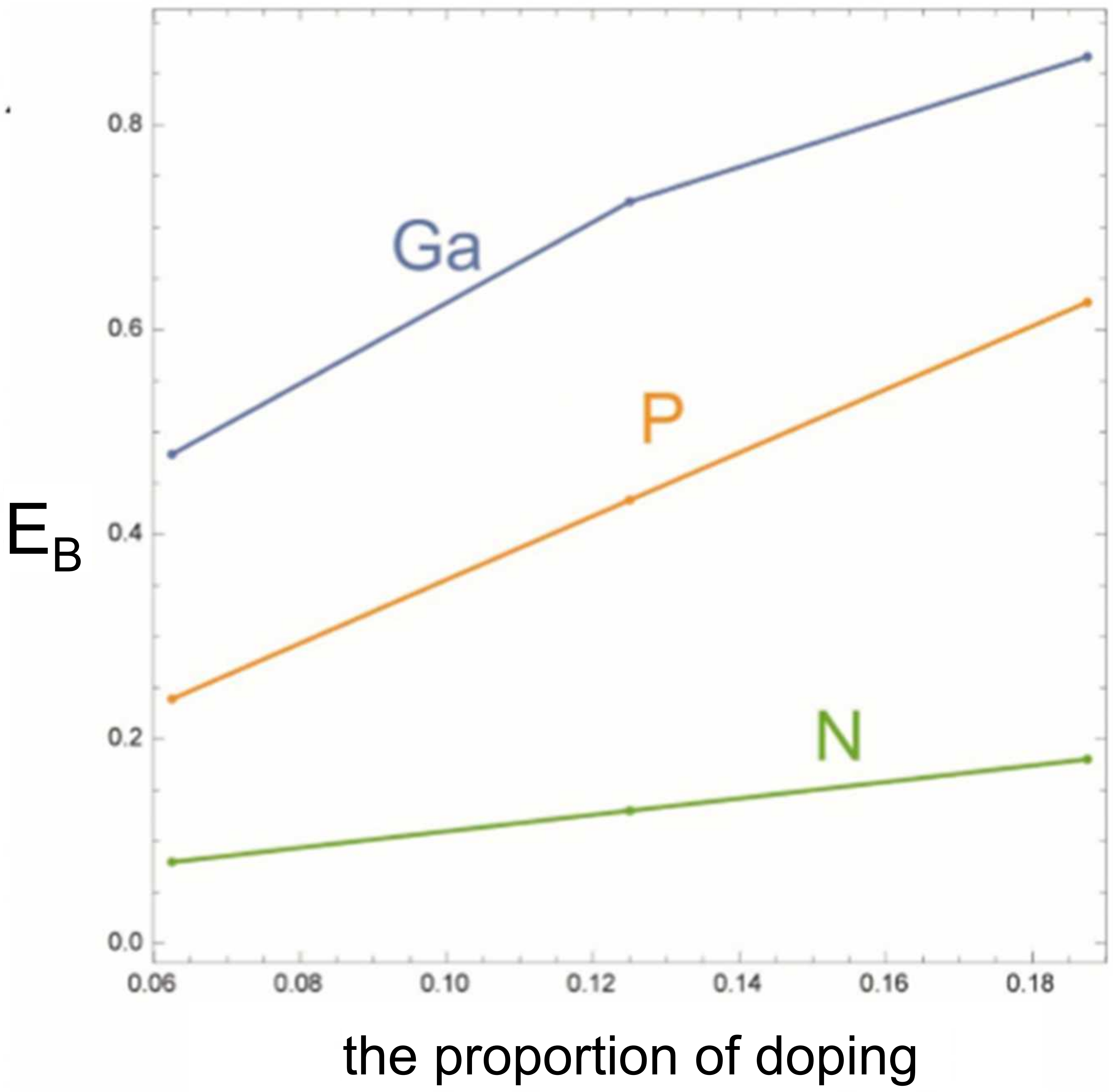
Blue - Si-atom

The energy of dissolution of the doping atoms

$$E_B = \frac{E_m - E_{\mathrm{d}} \cdot N_{\mathrm{d}} - E_{SiC} \cdot N_{SiC}}{N_{\mathrm{d}} + N_{SiC}}$$

where E_m - total energy of system mogel,
N_d, N_{SiC} - number of atoms inside unit cells of pure substance,
E_d, E_{SiC} - energy of pure substance.

- Vienna Ab Initio Simulation *Package (Phys. Rev. B 54, 11169 (1996))*



The energy of dissolution of the doping atoms

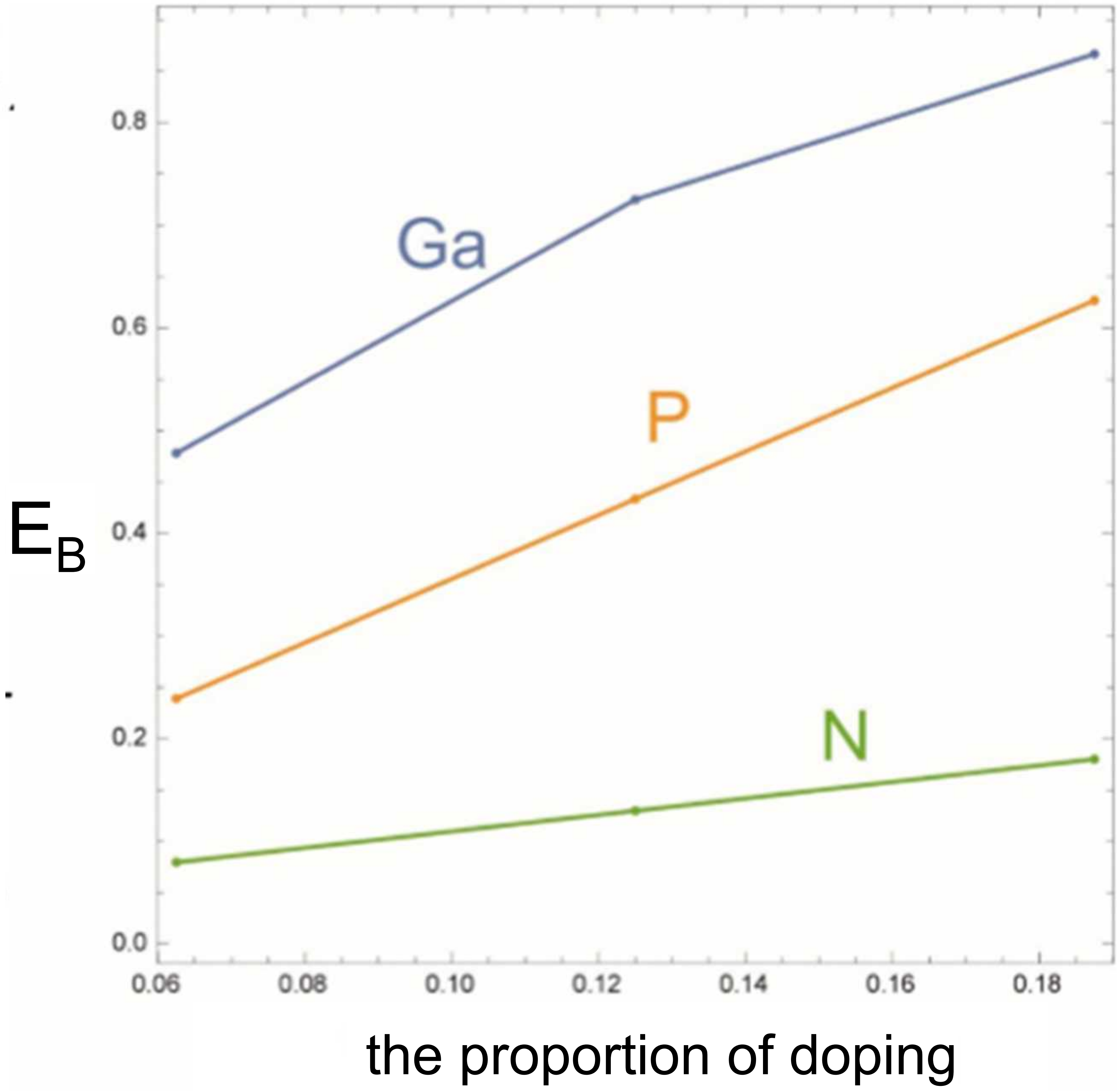
$$E_B = \frac{E_m - E_{\mathrm{d}} \cdot N_{\mathrm{d}} - E_{SiC} \cdot N_{SiC}}{N_{\mathrm{d}} + N_{SiC}}$$

resume:

- From a physical point of view, E_B is expected to be negative. A positive value indicates that there are no bonds between the atom and the lattice

- Immediately after the beta decay of C-14, a new N-14 atom leaves the lattice

- The N-atom has an energy lower than other dopants that this atom is predisposed to be a structural defect to a greater extent



Актуальность

Что влияет на эффективность бета-преобразования?

- избирательное поглощение излучения полупроводником

- технология легирования и положение р-п-перехода (глубина его залегания)

- процессы дефектообразования в структуре

- диффузионная длина пробега собственных генерированных вторичных электрон-дырочных пар носителей

- геометрические особенности готовых образцов и металлизации

- самопоглощение радиоизотопа и его активность, а также период полураспада

- способ внедрения радиоизотопа в материал полупроводника