

Zhuravlyova, Lyubov M., Russian University of Transport, Moscow, Russia.

Ivashevsky, Mikhail R., Russian Railways JSC, Moscow, Russia.

Muzafarov, Ildar F., Russian University of Transport, Moscow, Russia.

ABSTRACT

The current problems of increasing the efficiency of optoelectronic devices with the help of new materials are considered in the article. It is noted that the most promising direction of research is the design of semiconductor materials using the own isotopes of chemical elements. Thus, purification from heavy isotopes increases the speed of

optoelectronic devices, quantum efficiency, sensitivity of photodetectors. The greatest effect of isotope purification can be obtained for a nanostructured material (superlattices). This new semiconductor material will create more sensitive instruments for night vision, solar panels, safety systems, medical equipment, ultra-long-range infrared photodetectors.

Keywords: optoelectronics, communication, isotopes, purification, quantum efficiency, superlattices.

Background. Electronics and optoelectronics as its component are the basis of high-tech industries of the world industry. These include production of high-speed telecommunications systems, safety devices, medical diagnostic devices, the elemental base of quantum systems for transmission and processing of information, etc. One of the priorities here is development of semiconductor materials operating on new physical and technological principles and analysis of the possibilities of nanotechnology for production of new-generation nanostructures [1].

Such a promising direction in optoelectronics became the work with isotopic materials. This is a young field of science engaged in the design of semiconductors using own isotopes of chemical elements to obtain new effects and optoelectronic characteristics. An example of an isotopic material can be a variety of graphite – graphene. To use its unique properties in electronics, it is necessary to «open the bandgap» [2, 12]. The desired effect can be obtained by increasing the percentage of heavy isotope. The opposite direction of design is isotopic purification of the initial material from heavy isotopes.

The decrease in concentration of heavy isotopes in the initial chemical element improves the optoelectronic characteristics of the semiconductor material, increasing primarily the speed of the instruments. For this, the technology of gas centrifugation (GCF) is used. The isotopically purified substance is then used to form nanostructures by molecular beam epitaxy (MBE) [1, 4, 5]. Releasing the initial chemical element from heavy isotopes can reduce crystal lattice defects and mechanical stresses between layers [1].

Objective. The objective of the authors is to consider new materials in optoelectronics.

Methods. The authors use general scientific and engineering methods, comparative analysis, mathematical method.

Results.

Estimation of isotopic material

The effectiveness of reducing the concentration of heavy isotopes in semiconductors can be assessed using the example of improving the properties of gallium arsenide when used in a photodetector (PD). These improvements are primarily reflected in the increase in the absorption coefficient α and in the quantum efficiency of the material η .

The isotopic composition of gallium in a crystal GaAs is of the following order: 60, 1 % is attributed to the isotope ^{69}Ga and 39, 9 % – to the heavier isotope ^{71}Ga .

The decrease in the concentration of ^{71}Ga can be interpreted as a reduction in the number of defects in the crystal lattice, which will affect the effective mass of charge carriers, for example, the electron m_{ef} and the band gap E_g . The possible scales of the changes of m_{ef} and E_g can be estimated from the publication [7], which shows the results of studies of the dependence of the effective electron mass and the band gap width on changes in the concentration of doping atoms in gallium arsenide single crystals. Thus, a decrease in the concentration of the heavy isotope ^{71}Ga in a gallium arsenide crystal by two orders of magnitude can reduce: 1) the width E_g – by 0,06 eV; 2) the value of m_{ef} – by two times. This will lead mainly to an increase in the absorption coefficient and quantum efficiency.

It should be noted that the quantum efficiency η has the greatest influence on the optoelectronic characteristics of PD material.

It is known that quantum efficiency is estimated by the formula [8]:

$$\eta = 1 - e^{-\alpha d}, \quad (1)$$

where α – absorption coefficient, d – thickness of a sample.

Absorption coefficient [9]:

$$\alpha = K \sqrt{h\nu - E_g}, \quad (2)$$

where $h\nu$ – photon energy (the product of the Planck constant and the frequency of light). The dependence of the absorption coefficient on the photon energy $\alpha = f(h\nu)$ is directly proportional. From the graph of the dependence $\alpha = f(h\nu)$ for gallium arsenide [9], we can calculate the proportionality coefficient K , starting from the relation

$$0,8 \cdot 10^4 = K \sqrt{1,5 - 1,42}, \left(\frac{1}{\text{cm}} \right). \quad (3)$$

Hence, $K = 2,827 \cdot 10^4 \text{ (cm}^{-1} \text{ eV}^{1/2})$.

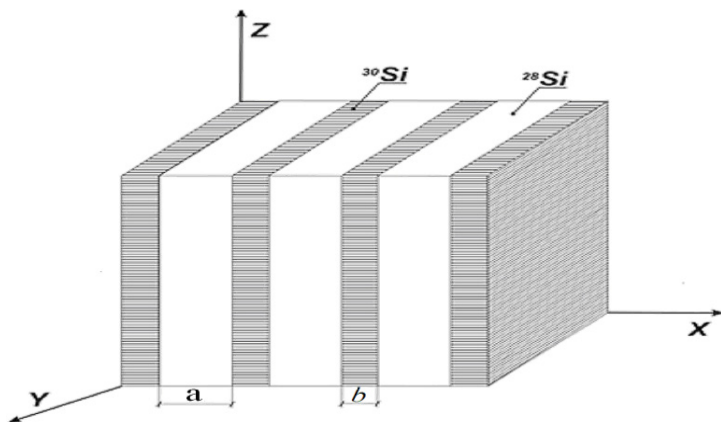
Thus, after isotope purification of gallium from heavy isotopes, the absorption coefficient will be:

$$\alpha = 2,827 \cdot 10^4 \sqrt{1,5 - 1,36} = 1,058 \cdot 10^4, \left(\frac{1}{\text{cm}} \right). \quad (4)$$

The efficiency of isotopic gallium purification is to increase the quantum efficiency by increasing the absorption coefficient. For example, for a bulk crystal of gallium arsenide of thickness $d = 10^{-4} \text{ cm}$ on the basis of formulas (1)–(4), we obtain:

$$\frac{1 - e^{-1,058 \cdot 10^4 \cdot 10^{-4}}}{1 - e^{-0,8 \cdot 10^4 \cdot 10^{-4}}} = 1,23 \text{ times.} \quad (5)$$

That is, the value of η after purification from heavy isotopes increased by 1,23 times.



Pic. 1. Superlattices (MQW) on silicon isotopes (a – quantum well, b – barrier).

It is known that the quantum efficiency η determines the sensitivity, the detectability of PD material and, most importantly, the magnitude of the photocurrent [8]. Hence, the ratio of the signal-to-noise power at the output of PD ρ_{outpd}^2 before and after the isotope purification of the bulk crystal also increases by 1,23 times. This will lead to a decrease in the probability of an error P_{err} and an improvement in the reception quality of optical signals [10].

The most effective material for photodetectors are nanostructures. These are multiple quantum wells (MQW) and superlattices (SL) consisting of alternating layers, for example, gallium arsenide (well) and gallium arsenide aluminate (barriers) or silicon isotopes (Pic. 1) [1]. Differences between MQW and SL in sizes a and b (for SL $a = b < 6$ nm).

For quantum wells, the value of d is of the order of $d = 10^{-6}$ cm (10 nm). Hence formula (1) for calculation of η is transformed into [6]:

$$\eta \approx \alpha_{\text{IQW}} \quad (6)$$

After isotopic purification, we obtain the following changes (increase) in quantum efficiency for gallium arsenide per quantum well:

$$\frac{1,06 \cdot 10^4 \cdot 10^{-6}}{0,8 \cdot 10^4 \cdot 10^{-6}} = 1,325 \text{ times.}$$

Thus, as a result of isotopic purification of the material in the form of MQW, η , the sensitivity of the photoconductivity, the detecting power and the photocurrent, the value of ρ_{outpd}^2 determining the reception quality of PD, will increase by 1,325 times.

Improving the quality of photo reception

Using the result obtained from isotopic purification of PD material on MQW, namely, an increase in the values of the parameter Q^2 and ρ_{outpd}^2 ($\rho_{\text{outpd}}^2 = 4 Q^2$) by more than 1,3 times, we calculate the error probability P_{err} and the anomalous error δ_{an}^2 [8]) respectively according to the formulas (7) and (8):

$$P_{\text{err}} = \frac{2}{\sqrt{2\pi\rho_{\text{outpd}}^2}} \exp\left(-\frac{\rho_{\text{outpd}}^2}{4}\right); \quad (7)$$

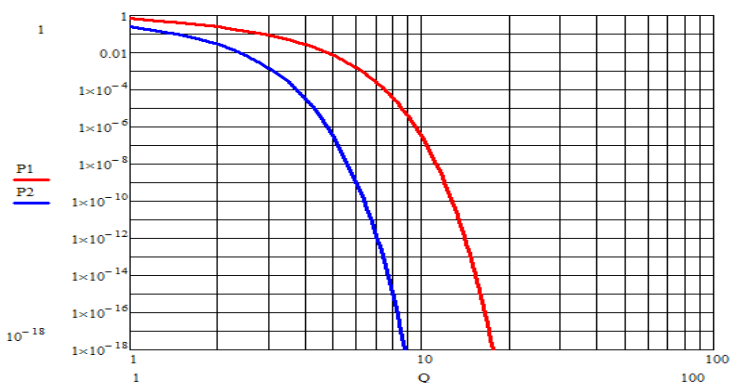
$$\delta_{\text{an}}^2 \approx 12P_{\text{err}} \quad (8)$$

Pic. 2 shows the error probability graphs for PD on a material with a purification $P_{\text{errpur}} = f(Q)$ and without purification $P_{\text{err}} = f(Q)$ from heavy isotopes based on the formula (7).

After isotopic purification of the material, the probability of error P_{errpur} decreases by several orders of magnitude.

The efficiency of purification of the material from heavy isotopes in numerical terms is presented in Table 1. It gives the values of the error probabilities before the isotopic purification of PD material and after it.

Based on the calculated error probability values in Table 1, it is possible to estimate how many times the quality of reception of optical signals will improve by increasing the technical (optoelectronic) characteristics of a semiconductor material (gallium arsenide) after isotopic purification (increasing quantum efficiency, sensitivity, noise reduction). Thus, for a minimum allowable value $\rho_{\text{outpd}}^2 = 50$, which



Pic. 2. Dependence $P_{\text{err}} = f(Q)$ for PD without purification (P_1) and with purification (P_2).

Table 1
Error probability at the output of photodetector before purification P_{err} and after isotopic purification P_{errpur}

ρ_{pd}^2	P_{err}	P_{errpur}
50	$0,142 \cdot 10^{-6}$	$1,54 \cdot 10^{-8}$
100	$1,12 \cdot 10^{-12}$	$1,68 \cdot 10^{-15}$
200	$1,08 \cdot 10^{-23}$	$2,8 \cdot 10^{-29}$

provides the error probability $0,421 \cdot 10^{-6}$ according to the formula (7), purification of the material will reduce the probability of error by 11,51 times. To calculate the possible gain m for improving the quality can be as follows: where $K = 1,325$ – coefficient of increase in the ratio of signal power and noise at the output of the photodetector (6).

The value of the gain m due to purification of the semiconductor material of the photodetector depends on the value of ρ_{outpd}^2 and the coefficient K .

In addition to the quantum efficiency of PD after purification from heavy isotopes of gallium crystals, other characteristics of the material also improve. It is known that purification from heavy silicon isotopes has allowed to increase speed of microprocessors more than twice due to reduction of the effective mass of electrons and increase of mobility of charge carriers [3]. An even greater effect due to more mobile charge carriers in AsGa can be expected from gallium arsenide.

Isotopic superlattices

The most promising material for optoelectronics in various fields of technology, along with MQW, are semiconductor superlattices (SL), which are characterized by splitting of energy levels and formation of conductivity subbands and gaps in quantum wells.

By changing the isotopic composition of the material, for example, gallium arsenide, it is possible to choose the location of energy subbands in the quantum wells and the width of the energy gaps in SL (Pic. 1) for design of new semiconductors. This is due

to changes in the effective mass of the electron m_{ef} and the width of the band gap E_g of the quantum well material.

The width of the slits and the conductivity subbands is determined by the initial material, and also by the width of the barriers and wells. When designing optoelectronic devices, for example, with a photoelectric effect at intersubband transitions, it is important to achieve the required width of the energy gap and the number of subbands in the quantum well. It is difficult to obtain the desired result only with the selection of the parameters a and b of wells for the selected material.

With the help of isotopic nanoengineering, the SL model allows the creation of new materials with predetermined optoelectronic characteristics [1].

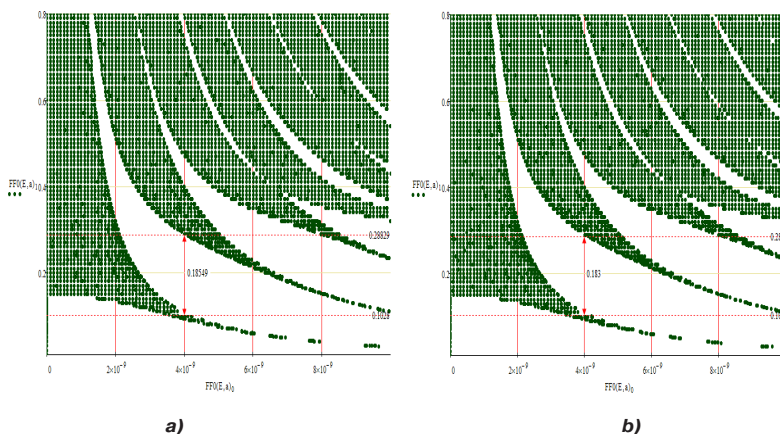
As already noted, heavy isotopes can be regarded as crystal lattice defects that significantly affect the electrical, optical and mechanical properties of the material.

The mechanism of influence of crystal lattice defects on mobility of electrons can be estimated according to the classical theory of electrical conductivity. Thus, the uniformly accelerated motion of an electron in a crystal under the action of an electric field terminates in a collision with a crystal lattice defect [11]. In this case, the acquired velocity in the direction of the electric field drops practically to zero, then the acceleration of the electron again begins. The «acceleration – scattering» cycle is repeated again and again many times. The average distance traveled by an electron from a collision to a collision is called the mean free run. For silicon crystals, it is known that after purification from heavy isotopes ^{28}Si , ^{30}Si , which constitute about 8 % of all atoms, the mobility of electrons has doubled [3].

For natural gallium, which consists of two isotopes (^{69}Ga – 60,1 %; ^{71}Ga – 39,9 %), purification of the crystal from the isotope ^{71}Ga can increase the electron mobility by more than two times. Taking into account the fact that gallium is lighter than silicon (the ratio of effective mass m_{ef} for Si and Ga is 2,84), we can expect a greater effect from isotopic purification. In

$$m = \frac{2}{\sqrt{K \rho_{outpd}^2} 2\pi} \exp\left(-\frac{\rho_{outpd}^2 K}{4 \cdot 2}\right) / \frac{2}{\sqrt{\rho_{outpd}^2} 2\pi} \exp\left(-\frac{\rho_{outpd}^2 K}{4 \cdot 2}\right), \quad (9)$$

$$m = (\sqrt{K}) \cdot \exp\left(\frac{\rho_{outpd}^2 (K - 1)}{4 \cdot 2}\right) = \sqrt{1,325} \exp\left(\frac{50 \cdot 0,325}{4 \cdot 2}\right) = 11,51 \text{ times},$$



Pic. 3. Dependences of the energy levels of SL before and after purification of gallium from heavy isotopes.

addition, the number of «acceleration – scattering» cycles for gallium will be greater in comparison with silicon, and consequently, purification will be more effective. In the case of silicon, collisions with a heavy isotope occur on average every nine atoms, for gallium, approximately every two.

Estimation of the effect of purification from heavy isotopes of gallium crystals for superlattices can be obtained by mathematical modeling of the dependence of the energy levels on the width of the well. Thus, the value of the effective mass as a result of purification from heavy isotopes of gallium can be reduced by two times, i. e. to make the value $0,067/(2m_0)$. The value of the band gap after purification can be reduced by $0,06$ eV, i. e. become $1,424-0,06 = 1,364$ eV [7].

Pic. 3 presents the results of mathematical modeling of distribution of energy bands for SL from gallium arsenide and gallium arsenide aluminate without purification of gallium from heavy isotopes (Pic. 3a) and with purification (Pic. 3b).

Calculating the width of the energy gap in the quantum well for the parameters $a = b = 4$ nm has shown that purification reduces the width of the first energy gap by 3 meV, and this can be a significant factor for achieving a certain long-wavelength photoeffect boundary, for example, in safety systems, devices for detection of hazardous substances, product quality assessment, etc.

Thus, on the basis of mathematical modeling, changes in the optoelectronic characteristics (distribution of energy bands in SL structure) after purification of the material from heavy isotopes of gallium have been proved. With the help of isotopic SL, it is possible to design new semiconductor materials for ultra-long-range infrared photodetectors (an atmospheric window with a wavelength of light up to 20 μm) that cannot be created in the usual way.

Conclusions. A change in the isotopic composition of the initial semiconductor affects the optoelectronic characteristics of the material (mobility of charge carriers, width of the band gap, quantum efficiency, etc.).

When creating isotopic materials, it is possible to increase or decrease the percentage of heavy isotopes in a substance. Thus, purification of gallium from heavy isotopes (gallium arsenide material of the photodetector) increases the signal-to-noise power ratio at the output of PD and reduces by several orders of magnitude the probability of error.

The most promising direction is creation of isotopic superlattices (new-generation nanostructures). On the basis of ISL, new semiconductor materials can be obtained for effective night vision devices (thermal imagers), solar batteries that capture dark photons, safety systems, medical equipment, etc.

In addition, isotopic purification of the original chemical element from heavy isotopes will allow creating more sensitive pixels of cameras and higher-quality (effective) video surveillance systems, photodetectors of ultra-long infrared range.

The studies have proved once again the effect of purification on the optoelectronic characteristics of a bulk functional material and, correspondingly, on the width of energy gaps in quantum structures (SL).

REFERENCES

1. Zhuravleva, L. M., Plekhanov, V. G. Perspectives of the application of isotopic nanoengineering in telecommunication systems. In: Successes of nanoengineering: electronics, materials, structures [Perspektivy primeneniya izotopicheskoy nanoinzhenerii v telekommunikatsionnykh sistemah // Uspehi nanoinzhenerii: elektronika, materialy, struktury]. Ed. by J. Davis, M. Thompson. Moscow, Technosphaera publ., 2011, pp. 478–491.
2. Plekhanov, V. G., Zhuravleva, L. M. Isotopic creation of semiconductor graphene [Izotopicheskoe sozdanie poluprovodnikovogo grafena]. *Nanotehnika*, 2012, Iss. 3, pp. 34–38.
3. Press Release (2001) of Isonics Corporation, Golden, Colorado.
4. Zhuravleva, L. M., Malykh, A. N. Nanomaterials and Optoelectronics in High-Speed Communication Systems. *World of Transport and Transportation*, Vol. 14, 2016, Iss. 2, pp. 74–80.
5. Collins, A. T., Lawson, S. C., Davis, G., Kanda, H. Indirect energy gap of ^{13}C diamond. *Phys. Rev. Lett.* Published 13 August 1990.
6. Separation of isotopes [Razdelenie izotopov]. [Electronic resource]: http://ru.wikipedia.org/w/index.php?title=Разделение_изотопов&oldid=62541612. Last accessed 05.04.2018.
7. Bogdanova, V. A., Davletkildееv, N. A., Semikolenova, N. A., Sidorov, E. N. Effective mass of electrons in heavily doped gallium arsenide in the ordering of impurity complexes [Effektivnaya massa elektronov v sil'no legirovannom arsenide galliya pri upravlenii primesnykh kompleksov] // Physics and Technology of Semiconductors. 2002, Vol. 36, pp. 407–411.
8. Rosencher, E., Vinter, B. Optoelectronics [Optoelektronika]. Moscow, Technosphaera publ., 2006, 588 p.
9. Martinez-Duart, J. M. Nanotechnology for micro- and optoelectronics [Nanotehnologii dlya mikro- i optoelektroniki]. Moscow, Technosphaera publ., 2007, 368 p.
10. Zhuravleva, L. M., Ivashevsky, M. R. [et al]. Evaluation of the quality of signal transmission of intelligent video surveillance systems [Ocenka kachestva peredachi signalov sistem intellektual'nogo videonabljudeniya]. *Proektirovanie i tekhnologiya elektronnykh sredstv*, 2017, Iss. 3, pp. 10–15.
11. Vereshchagin, I. K., Kokin, S. M., Nikitenko, V. A. [et al]. Physics of the solid body [Fizika tverdogo tela]. Moscow, Vysshaya shkola publ., 2001, 236 p.
12. Zhuravleva, L. M., Nikulina, Yu. A., Lebedeva, A. K. Prospects of Graphene Nanoelectronics. *World of Transport and Transportation*, Vol. 14, 2016, Iss. 1, pp. 72–78. ●

Information about the authors:

Zhuravlyova, Lyubov M. – D.Sc. (Eng), professor of Russian University of Transport, Moscow, Russia, zhlubov@mail.ru.

Ivashevsky, Mikhail R. – leading engineer of Moscow-Ryazan Regional Communication Center of Moscow Communications Directorate of Russian Railways JSC, Moscow, Russia, misha_13@mail.ru.

Muzafarov, Ildar F. – student of Russian University of Transport, Moscow, Russia, muz.il@yandex.ru.

Article received 12.03.2018, revised 15.04.2018, accepted 22.04.2018.

