### **Isotopic nanostructures**

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**Abstract.** This article is devoted to the searching for new materials that can improve the operating speed of electronic and optoelectronic devices in order to increase the speed of transmitting and processing information in computing and telecommunication systems. Creation of a new material is proposed, based on the superstructure model using the isotope effect in solids. It is proposed to obtain isotopic nanostructures by exposing the sample to thermal neutron flux.

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### Introduction

Constant growth of the amount of information to be processed and transmitted by computers and telecommunication systems makes scientists face the task of increasing capacity of communication channels and information processing speed. This requires increasing the operating speed of electronic and optoelectronic devices, namely, operating frequency of transistors, microprocessors, optical modulators and other devices. As it is known, operating speed of technical devices depends on the size of the element base, electronic properties of materials and manufacturing techniques. Therefore, in recent years, transition to semiconductor nanostructures and nanotechnologies has been observed. Speed of information transmission and processing can be significantly increased by using new materials. As evidence thereof, one can take the latest scientific achievements in the field of (carbon nanostructures nanotubes. fullerenes graphene) [1-3]. Designing new materials based on the model of the superstructure should be considered one of the most promising areas in the task [4-8].

### Main part

### Superstructure model

Superstructure is a multi-layered periodic structure formed by alternating mono-layers of two types of semiconductors (Fig. 1) with closely spaced values of the crystalline grid constant [2, 5, 8]. The superstructure concept, first proposed by Leo Esaki in the late 60s and widely used, e.g., for manufacturing motherboards for microprocessors [6-8], has now become the basic model for designing new artificial materials [1]. The superstructure reminds a structure that consists of a set of quantum wells, but with thinner spacer layers, which makes it possible for charge carriers (electrons) to tunnel from one well to another. As a result, band splitting occurs which modifies optoelectronic characteristics of the original semiconductor materials. Mini-areas and mini-gaps are formed (Fig. 2) [5], which can be used for creating, e.g., photodiodes that absorb photons in ultra long infrared light [5]. Furthermore, by increasing the number of monolayers, superstructures can be obtained, that will have "quasi-straight" optical transitions in the band gap, even in case of using indirect-gap semiconductors. [5]



Fig.1. Model of the isotopic superstructure

## Difficulties in creating new materials

For manufacturing high-quality superstructures it is necessary to solve certain problems. The first problem is the searching for the raw materials with the lowest possible discrepancy in the value of the crystal grid constant, and with sufficient difference in electronic characteristics (band gap width). The difference between semiconductors crystal grid constants in the superstructure may be few tenths of a nanometer. But even this value can lead to mechanical stresses between the substrate and layers that appear as distortions of mini-bands and mini-slots in the superstructure. Taking into account the fact that thickness of superstructure layers is very small (approximately few atomic layers), mechanical stress will surely occur. This will certainly affect formation of energy bands and quality of the new material.

Another important task in obtaining superstructures is creating technologies for ensuring precision in manufacturing nanostructures less than 1  $\mathcal{NM}$  thick. It is clear that if layer thickness is approximately few nanometers, precision of manufacturing should be one order less. Otherwise, fluctuations of geometrical size will greatly affect characteristics of superstructures (wave function of change carriers, energy-level splitting). Modern nanotechnologies, e.g., various types of epitaxy, including molecular-beam epitaxy, can ensure accuracy of manufacturing to approximately 10 nm [1, 2]. Hence, the task of achieving the required quality of nanostructures manufacturing is especially vital.

# Ways of solving problems

To overcome difficulties in creating quality superstructures, it is proposed to use isotopes of initial chemical element as superstructure material (Fig. 1). As it is known, isotopes are similar in chemical composition (the same electron shell) and the values of the crystal grid constant, but differ in physical characteristics (band gap width, nuclear spins, refraction index, absorption, etc.). These differences are related to features of isotope effect. The isotope effect is caused by changes in the number of neutrons in the nucleus with constant number of protons [9, 10]. In case of isotopic substitution, not only the phonon spectrum, but also the electron-phonon interaction changes as well. Within the recent decades, detailed studies of the isotope effect have been performed on a large number of semiconductors and dielectrics [9-16].

Combination of different isotopes of the same chemical element makes it possible to create space limitations in nanostructures without using other chemical elements. It is known that additives can screen free charge carriers and degrade their optoelectronic characteristics [5]. The "heterojunctions" obtained this way will not cause mechanical stresses in the crystal grid and affect wave functions of free charge carriers. Spatial localization of charge carriers and formation of quantum wells will occur due to the difference band gap width in isotope superstructure layers. If different semiconductors are used, this difference will amount to tenths of eV. For isotope superstructures, for example, of silicon isotope, the difference in the band gap width will be three orders less [1, 4]. However, there exist substances that have a huge difference in band gap width of their own isotopes [10, 12]. This speaks of great possibilities of isotopic nanoengineering [1]. According to the Schrödinger equation, the effect of charge carriers energy quantization in a quantum well exists for any value of the potential barrier [5]. Therefore, properties of superstructures of silicon and germanium isotopes are currently being studied by many researchers [17-20]. Studies of isotope superstructures are conducted in a conventional manner on the basis of Kronig-Penney simulation model [4, 5]. Energy bands in the isotope superstructure have the form similar to that shown in Fig. 2. Only the width of mini-bands and mini-slots will change, which for silicon isotopes is measured in MeV [4].





For parameters:  $V=0.3 \ eV$  (height of energy barrier); m=0.067  $m_0$  (*m* is electron mass,  $m_0$  is electron mass in vacuum), With x=0...10nm; E=0...0.8eV.

# Technology of manufacturing isotope superstructures

Methods of molecular-beam epitaxy (MBE) and neutron transmutation doping (NTD) are the most promising for manufacturing isotope superstructures [1, 2, 21-23].

The method of molecular-beam epitaxy is based on deposition of semiconductor materials films by evaporating the substance in ultra-high vacuum. With that, the deposited substances, such as pure silicon isotopes, are introduced into the working chamber in form of atomic fluxes. These fluxes are formed by material evaporation inside a closed cell with a very small outlet (effusion cells). The fluxes of molecules or atoms generated inside it leave the outlet in ultrahigh vacuum, move without collisions and create collimated beams of particles. Main parts of MBE installation are effusion cells, heated substrate holder and a process monitoring system that uses electron spectroscopy methods [2].

Precision of the manufacturing technology is limited by diffraction effects during samples exposure (to light, electron beams, ions, etc.) used in nanostructures manufacturing. Therefore, resolution of the technology cannot be less than radiation wavelength. From this point of view, the method of manufacturing nanostructures on the basis of the neutron transmutation doping ensures the best quality. This in an industrial method of chip manufacturing implemented with exposing the workpiece to neutron flux. [21]. Wavelength of thermal neutrons with energy 0.02 eV is equal 0.2 nm [24]. Hence, using neutron fluxes, one can obtain isotope superstructures with accuracy less than 1 nm. Thermal neutrons with energies E in the range between 0.025 and 1 eV are of the biggest practical interest for semiconductor materials exposure (Si, Ge, *GaAs*, etc.) [22, 23].

Thermal neutrons enter into an absorption reaction with the target nuclei X as follows:

$$H_{Z}^{A}X + {}_{0}^{1}H \rightarrow {}_{Z}^{A+1}X + \gamma \quad (1),$$

where Z is the atomic number of the substance,

A is mass number

 $\gamma$  is the radiation that carries away the major part of the energy released.

Concentration of isotopes, e.g., silicon, after exposure can be calculated as follows [24]:

$$N_i^1 = N_i \sigma_i \varphi t \,, \quad (2)$$

where  $N_i^1$  is the output of the  $i^{\text{th}}$  isotope after exposure,

 $N_i$  is concentration of the  $i^{\rm th}$  isotope before exposure,

 $\sigma_i$  is cross-section of absorption reaction of the  $i^{\text{th}}$  isotope,

*t* is exposure time.

In respect to silicon isotopes, for example, output of  $^{29}$  Si from isotope  $^{28}Si$  after the nuclear reaction may be:

$$N_i^1 = 10^{-3} N_i$$

where  $N_i = 0.9218$  is concentration of <sup>28</sup> S<sub>i</sub> isotene of silicon in natural state

the  ${}^{28}Si$  isotope of silicon in natural state.

After substituting the latter expression into the formula (2) we obtain the value of integral exposure, namely,  $\varphi t$ 

$$\varphi t = 10^{-3} / \sigma_i$$
, (3)

For thermal neutron energy E = 0.025 eVand  $Si^{28}$  we have:  $\sigma_i = 0.08$  barn [24],  $\varphi t = 12.5 \cdot 10^{21} n / cm^2 = [23].$ 

With the average value of neutron flux intensity  $\varphi = 10^{17} n/cm^2 \text{sec}$ , time of exposure will reach 34.72 *hours*. These figures speak of feasibility of manufacturing isotope superstructures using neutron irradiation.



Fig. 3. Scheme of work piece thermal neutron irradiation

The possibility to shape inside homogeneous work piece the volumes of different isotopes for obtaining nanostructures is explained by high permeability of neutrons and by reactions of neutron absorption by the nuclei of the material exposed to radiation [24]. So, figure 3 shows a diagram of a work piece irradiation with a neutron flux [22,23]. "Denser" structure elements (superstructure layers) are created by neutron irradiation of corresponding areas, for example, in order to increase concentrations of silicon isotopes  $Si^{29}$  and  $Si^{30}$  compared to natural content in other parts of the work piece. By modifying irradiation pattern, one can form not only quantum wells, but quantum wires and quantum points as well [1, 22].

This method will make it possible to create new material with high precision, without defects and "roughness" in "heterojunctions".

### Areas of using isotope superstructures

New materials based on isotope superstructures will be used in telecommunication devices (lasers, photo detectors, optical modulators) and computation systems (microprocessors), energyefficient technologies (solar batteries), security tools (scanning devices), medicine (diagnostic equipment, high-precision thermal cameras) [4].

Promising direction of using isotope nanostructures could be creating computational gates for quantum computers on their basis [1, 25]. It is known that the most difficult problem in implementation of a quantum processor is ensuring coherence of quantum objects for execution of computational operations [1, 25-27]. For quantum wells with excited electrons (excitons), this means maximizing the "lifetime" of the quantum object. Any collision of an object (exciton) with a defect in the quantum well leads to disturbance of coherence and well destruction. Isotope quantum wells can ensure maximum possible "lifetime" of excitons by means of purity of initial material (absence of additives). Besides, influence of local phonons in isotopic quantum wells will also be reduced due to absence of mechanical stresses in "heterojunctions" made of different isotopes of the same chemical element [1, 5].

### Conclusion

Development of telecommunication and computer systems is related to improvement of the element base of electronic and optoelectronic devices. The main direction in this work is the searching for new materials [1]. In order to create new materials, various models may be used (carbon nanotubes, fullerenes, planar nanostructures, etc.). The most promising one is the development of new materials basing on superstructure model [2, 4, 8]. This model makes it possible to design new materials with preset characteristics. Initial materials should be substances with similar crystal grid constants. Most suitable for this purpose are isotopes of the chemical element used, which have the same crystal grid constants. The possibilities of "doping" the material with its own isotopes are explained by peculiarities of the isotope effect [9-16]. Absence of additional chemical elements in superstructure layers will reduce the number of charge carrier scattering channels and optical loss of light in isotope nanostructures. This will ensure maximum speed of electrons, as well as operating speed of electronic and optoelectronic devices.

### Conclusions

1. Increasing operating speed of electronics and optoelectronic devices is related to improving element base, and mainly search for new materials.

2. A promising direction of development of new materials is the model of superstructure.

3. The isotope effect can be the base for creating new materials for electronic and optoelectronic devices.

4. For manufacturing isotope nanostructures it is appropriate to use the method of irradiation with thermal neutrons, which have high penetrating power and short wavelength.

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5/20/2014

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