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THE INFLUENCE OF HOLE STATES ON THE ELECTRONIC AND ELECTROSTATIC PROPERTIES OF 2D LAYERS BASED ON THE SILICON-GERMANIUM-SILICON HETEROSTRUCTURE

K. V. Obrazcov[1,2]✉, *A. N. Chibisov*[2], *M. V. Mamonova*[3]

[1] Pacific National University, Khabarovsk, Russia;

[2] Computing Center of the Far Eastern Branch of the RAS, Khabarovsk, Russia;

[3] Omsk State University named after Dostoevsky, Omsk, Russia

✉ 2018102293@pnu.edu.ru

Abstract The performance of a hole qubit in the Si/Ge/Si heterostructure is considered in this work. For this purpose, a quantum mechanical study using density functional theory and the pseudopotential method has been carried out. The zone structure and density of electronic states were constructed for the elementary structure. It was found that the bulk of these states are localized in the energy range from −2 to −4 eV. For the constructed supercell the yield work was calculated and the contribution of electron hole to the electrostatic potential of the system was evaluated. The analysis of the obtained results showed that the change of the yield work in the system is associated with the shift of the energy vacuum level.

Keywords: silicon, germanium, density functional theory, two-dimensional layer, work function, heterostructure

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ВЛИЯНИЕ ДЫРОЧНЫХ СОСТОЯНИЙ НА ЭЛЕКТРОННЫЕ И ЭЛЕКТРОСТАТИЧЕСКИЕ СВОЙСТВА ДВУХМЕРНЫХ СЛОЕВ НА ОСНОВЕ ГЕТЕРОСТРУКТУРЫ КРЕМНИЙ-ГЕРМАНИЙ-КРЕМНИЙ

К. В. Образцов[1,2]✉, *А. Н. Чибисов*[2], *М. В. Мамонова*[3]

[1] Тихоокеанский государственный университет, г. Хабаровск, Россия;

[2] Вычислительный центр Дальневосточного отделения РАН, г. Хабаровск, Россия;

[3] Омский государственный университет имени Ф. М. Достоевского, г. Омск, Россия

✉ 2018102293@pnu.edu.ru

Аннотация. В работе рассматривается поведение дырочного кубита в гетероструктуре Si/Ge/Si. С этой целью проведено квантовомеханическое исследование с применением теории функционала плотности и метода псевдопотенциала. Для элементарной структуры была построена зонная структура и плотность электронных состояний. Установлено, что основная часть этих состояний локализована в диапазоне энергий от −2 до −4 эВ. Для построенной суперъячейки была рассчитана работа выхода и выполнена оценка вклада электронной дырки в электростатический потенциал системы. Анализ полученных результатов показал, что изменение работы выхода в системе связано со смещением уровня энергетического вакуума.

Ключевые слова: кремний, германий, теория функционала плотности, двухмерный слой, работа выхода, гетероструктура

Финансирование: Исследования атомной и электронной структуры выполнены в соответствии с Государственным заданием Министерства науки и высшего образования Российской Федерации (проект FEME-2024-0005). Расчеты работы выхода и электростатического потенциала были выполнены в рамках проекта Российского научного фонда № 24-13-20024.

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Introduction

Creating a quantum computer is a crucial challenge for modern microelectronics. Quantum computers are devices based on the principles of quantum mechanics using quantum bits (or qubits) to process information. Unlike classical bits in classical computers, capable of representing only one of two states (0 or 1), qubits can be in a superposition of several states simultaneously [1, 2], which allows quantum computers to perform calculations faster and more efficiently by orders of magnitude. They can be used to solve complex mathematical problems, in cryptography, optimization, simulation of molecular and chemical processes, artificial intelligence research and in many other fields. The creation of quantum computers promises to transform the way information is processed, opening up new opportunities for innovation and scientific discovery [3–5]. Today, there are many implementations of quantum processors. Photon-based qubits and superconducting qubits are the most popular.

In this paper, we consider a hole as a qubit. The main advantage of the hole qubit is its strong spin-orbit interaction and the ability to form superconducting pair correlations. It is these properties of holes that are extremely important for fast control of hole qubits [6, 7]. Possible materials for such a computer are 2D allotropic modifications of silicon (silicene) or germanium (germanene) using a hole qubit [8, 9].

For this purpose, in this paper we decided to consider the Si/Ge/Si interface. This structure has unique electromagnetic properties due to lattice mismatch between silicon and germanium [10]. In this case, due to the low effective mass of the holes [11, 12], it is possible to obtain a qubit with a long coherence time and a convenient way to control its state using an external magnetic field. The structure itself has excellent compatibility with the existing microelectronic components [13] and it is easy to integrate it into existing electronics manufacturing.

The goal of this paper was a quantum mechanical study of the behavior of a hole qubit in a two-dimensional silicon-germanium-silicon (Si/Ge/Si) layer using density functional theory (DFT) within the framework of noncollinear magnetization.

Experimental technique

The characteristics of the structures were calculated using the VASP software package [14–16] based on DFT and the pseudopotential method. Noncollinear calculations were performed taking into account the spin-orbit coupling and additional corrections in the Generalized Gradient Approximation (GGA+U) [17]. To calculate the magnetic and electronic properties, the initial magnetic moment was first found for each atom, then complete relaxation of the system was carried out taking into account the generalized theory of local spin density and the resulting magnetization on the atoms was determined based on the results obtained. A plane-wave basis set with a cut-off energy of 450 eV was used. An 18×18×1 *k*-point grid was used for the unit cells. For the enlarged cell, a 6×6×1 *k*-point grid was used, constructed according to the Monkhorst–Pack scheme [18].

Results and discussion

The first stage in the study of the atomic and electronic structure of 2D Si/Ge/Si interface considered the separate structures of silicene and germanene. At the first stage, we performed complete relaxation of the atomic structures of silicene and germanene to find the minimum forces and total electronic energy for the given systems. Relaxation of the structure was carried out preserving the symmetry of the cell; the procedure was performed for the cell parameters and atomic coordinates.

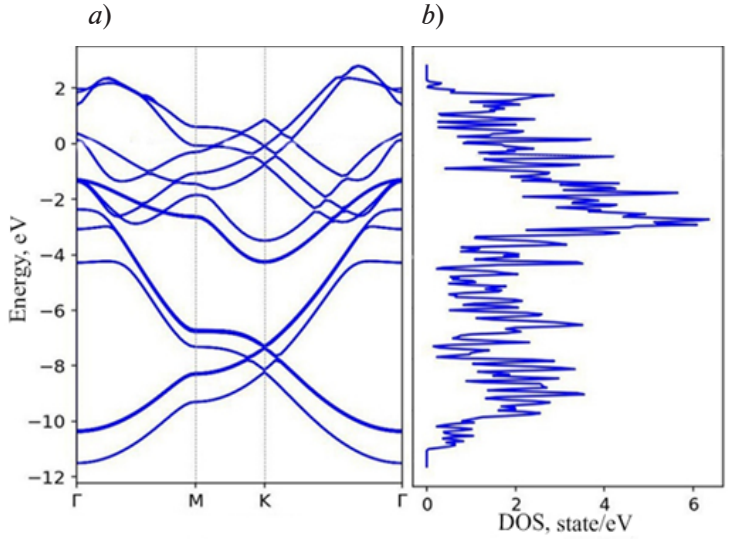

Fig. 1. Band structure (*a*) and density of states (*b*) constructed for Si/Ge/Si interface

At the second stage, we built the atomic structure of 2D Si/Ge/Si interface, a sandwich where the germanene layer was located between two silicene layers. At the third and subsequent stages, complete atomic relaxation of the structure was performed by the same principle as achieved separately for silicene and germanene.

The VASPKIT software package was used for postprocessing of the obtained data, the density of states and the band structure were calculated for the given interface. Calculations were performed with the number of *k*-points equal to 20. For clarity, the density of states was compared with the band structure of the studied material (Fig. 1).

Analysis of the data in Fig. 1 allows to conclude that the highest-energy states are localized in the range from -2 to -4 eV. The resulting band structure looks very similar to the individual band structures of silicene and

germanene. This indicates the appearance of new energy levels as a result of superposition of two structures, and this in turn causes the formation of interface states at the interfaces between silicon and germanium structures.

For further analysis of the electronic and magnetic properties of the selected system, it was necessary to enlarge the initial system. For this purpose, translation of the initial interface cell was performed with a threefold increase in parameters *a* and *b*. As a result, a supercell with the following structural parameters was formed: a = 11.421 Å, b = 11.421 Å, c = 25.166 Å. The parameter c was chosen equal to 25.166 Å to exclude the influence of interaction between the translated slabs. The Si–Si interatomic distance in the silicene layer was equal to 2.260 Å and the Ge–Ge distance in the germanene layer was 2.486 Å. The distance between the layers was equal to 3.647 Å. The resulting supercell consisted of a total of 54 atoms (Fig. 2).

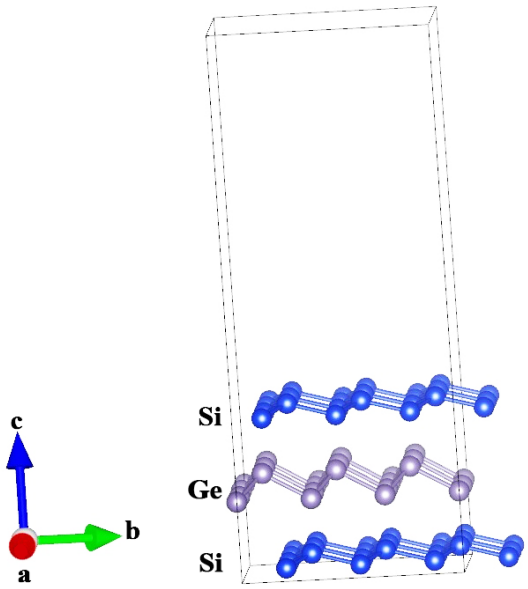

Fig. 2. Structural model of supercell of 2D Si/Ge/Si interface: the structure consists of 54 atoms, 18 of which are germanium atoms and 36 are silicon atoms

Next, a free valence bond (hole) was created in the Si/Ge/Si system and the initial magnetization was set. The hole was created by removing one electron from the system. To illustrate the contribution of the created electron vacancy to the electrostatic potential, we compared the dependences of electrostatic potential of the system on the concentration of holes and the given direction of initial magnetization (Fig. 3).

Evidently, when a hole is added to the system, the electrostatic potential decreases. The graphs are almost identical for the up (Fig. 3,*a*) and down (Fig. 3,*b*) magnetization directions. The only difference is that in the first case the distance between the first peaks is 0.670 eV (Fig. 3,*a*) and in the second case it is 0.642 eV (Fig. 3,*b*). This means that the sign of magnetization practically does not contribute to the distribution of the electrostatic potential in the system, while the larger contribution to the potential value is made by Si atoms.

The electrostatic potential was calculated to subsequently calculate the work function W for each case. The following formula was used for this purpose:

$$W = -e\varphi - E_f,$$

where e is the electron charge, φ is the near-vacuum value of the electrostatic potential, E_F is the Fermi level.

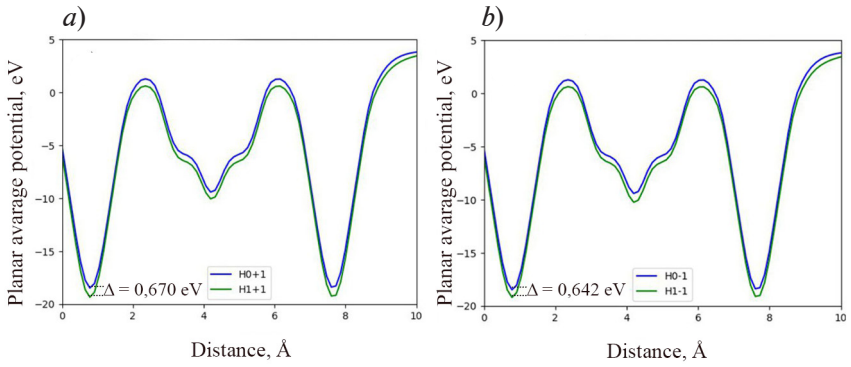

Fig. 3. Comparison of dependences of electrostatic potential of Si/Ge/Si system on concentration of holes with given magnetization directions of the system, +1 (up) and -1 (down): (*a*) and (*b*), respectively

Cases of systems without holes (blue curves) and with one hole (green curves) are compared

The results obtained are given in Table.

It follows from the data in Fig. 3 and Table that the value of the electrostatic potential decreases when a hole is added to the system, and the work function increases. In addition, it can be concluded that in the system with the magnetization direction of -1 (down), the work function in the absence of holes is greater than in a system with the magnetization of +1 (up). In the presence of holes, the work function becomes approximately the same for both cases.

Table

Dependence of work functions for interface on magnetization direction and presence of holes

Magnetization direction	Work function W, eV	
	Absence of hole	Presence of holes
up	4.946	6.460
down	4.970	6.456

Conclusion

We calculated the band structure and density of states for a two-dimensional Si/Ge/Si layer. These calculations indicate that the main part of the electronic states is localized in the energy range from -2 to -4 eV. The changes in the Si/Ge/Si band structure, compared with the individual band structures of germanium and silicon, are due to the formation of interface states, causing new energy bands to appear. If a hole is added to the system, the electrostatic potential decreases due to a shift in the energy vacuum level, while the sign of the given initial magnetization makes an insignificant contribution to the change in the electrostatic potential of the system. We established that the work function is greater in the system with negative initial magnetization than in the system with a positive one, while adding a hole to systems with different magnetization equalizes the values of the work function.

In conclusion, it should be noted that the results obtained can be used to design quantum computers or quantum sensors for next-generation nanoelectronics.

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THE AUTHORS

OBRAZCOV Kirill V.
Pacific National University
136 Tikhookeanskaya St., Khabarovsk, 680035, Russia
2018102293@pnu.edu.ru
ORCID: 0009-0001-6034-7757

CHIBISOV Andery N.
Computing Center of the Far Eastern Branch of the Russian Academy of Sciences
65 Kim Yu Chen St., Khabarovsk, 680000, Russia
andreichibisov@yandex.ru
ORCID: 0000-0002-5410-8661

MAMONOVA Marina V.
Omsk State University Named after Dostoevsky
55-A Mir Ave., Omsk, 644077, Russia
mamonovamv@omsu.ru
ORCID: 0000-0001-7466-086X

СВЕДЕНИЯ ОБ АВТОРАХ

ОБРАЗЦОВ Кирилл Владимирович – *лаборант кафедры физики Тихоокеанского государственного университета.*
680035, Россия, г. Хабаровск, Тихоокеанская ул.,136.
2018102293@pnu.edu.ru
ORCID: 0009-0001-6034-7757

ЧИБИСОВ Андрей Николаевич – *доктор физико-математических наук, ведущий научный сотрудник Вычислительного центра Дальневосточного отделения Российской академии наук.*
680000, Россия, г. Хабаровск, ул. Ким Ю Чена, 65
andreichibisov@yandex.ru
ORCID: 0000-0002-5410-8661

МАМОНОВА Марина Владимировна – *кандидат физико-математических наук, доцент кафедры теоретической физики Омского государственного университета имени Ф. М. Достоевского.*
644077, г. Омск, проспект Мира, д. 55-А
mamonovamv@omsu.ru
ORCID: 0000-0001-7466-086X

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