

Sensitivity characteristics of germanene

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In this paper, we investigate a sensitivity characteristics of germanene based on the tunneling current in the contact of a germanene with a metal or a superlattice. It is shown, that the sensitivity of the considered system to impurity molecules increases when a constant electric field is applied to it along the germanene plane.

Keywords: germanene, impurities, external electric field.

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1. Introduction

Recently, the problem of impurity detecting is relevant, since it is important for many practical applications (detection of low and high concentrations of toxic and explosive gases, monitoring the quality of air in a car cabin, automation of ventilation and air conditioning systems, etc.). The main point is to control the sensitivity of the system to the impurity. Many papers are devoted to the development of sensors based on graphene [1–3], including functionalized ones [4, 5].

In this paper, we propose germanene as a basic element for a gas sensor [6]. This material is a relative of graphene with similar properties, but has a stronger spin-orbit interaction as a silicene [7]. In [8], the adsorption of such gas molecules as N₂, CO, CO₂, H₂O, NH₃, NO, NO₂ and O₂ on germanene was investigated within the framework of the density functional theory. In this paper, we propose a method for detecting impurities based on the study of a tunneling current-voltage characteristic (CVC) of a contact of germanene with two types of materials (Me) – a metal and a superlattice (SL).

We have already tested it when study the sensory characteristics of graphene nanostructures (flakes, nanorings, and nanoribbons) [9, 10] and polymers [11]. The advantage of this method is the ability to select the contacting material, which can significantly affect the CVC of the system and enhance its response to the presence of impurities. The choice of these two contact materials due to the fact that the metal is the main material used for the manufacture of elements of electrical circuits. As for superlattices, they attract much attention due to optical, electrical and transport properties [12]. A superlattice is a solid-state structure in which an additional potential acts on the electrons, apart from the periodic potential of the crystal lattice, with a period that is several times higher than the lattice constant. This leads to a significant change in the electron energy spectrum of the system. Therefore, the superlattice acquire a number of characteristic properties which are absent in homogeneous materials.

2. A statement problem

The geometry of the problem is shown in Fig. 1. We consider a fragment of germanene with the size of NxM sites.

Here site *A* and site *B* correspond to the different germanene sublattices, *d* is the bending height (distance between two sublattices), *d*₁, *d*₂ are the distance between the *A* and *B* sites in the XOY plane, *E*_z is the constant electric field directed perpendicular to the germanene plane, *E*₀ is the external constant electric field.

In this paper, we must to take into account the spin-orbit interaction, which in germanene is four orders of magnitude higher than in graphene and introduces significant changes in the electronic structure of this material. The Hamiltonian for the germanene according to Ref. [13, 14] has the following form:

$$H = -t \sum_{\langle ij \rangle_s} C_{is}^+ C_{js} + i \frac{\Delta_{SO}}{3\sqrt{3}} \sum_{\langle\langle ij \rangle\rangle_s} s v_{ij} C_{is}^+ C_{js} - \sum_{is} \mu_i \Delta_z C_{is}^+ C_{is}, \quad (1)$$

where *C*_{is}⁺, *C*_{is} are birth/annihilation operators of electron, Δ_{SO} is the spin-orbit interaction, Δ_z = *E*_z*d* is the potential at the one lattice site, ≪ *ij* ≫ means that the summation goes over all the nearest neighbors, *s* = ↑↓

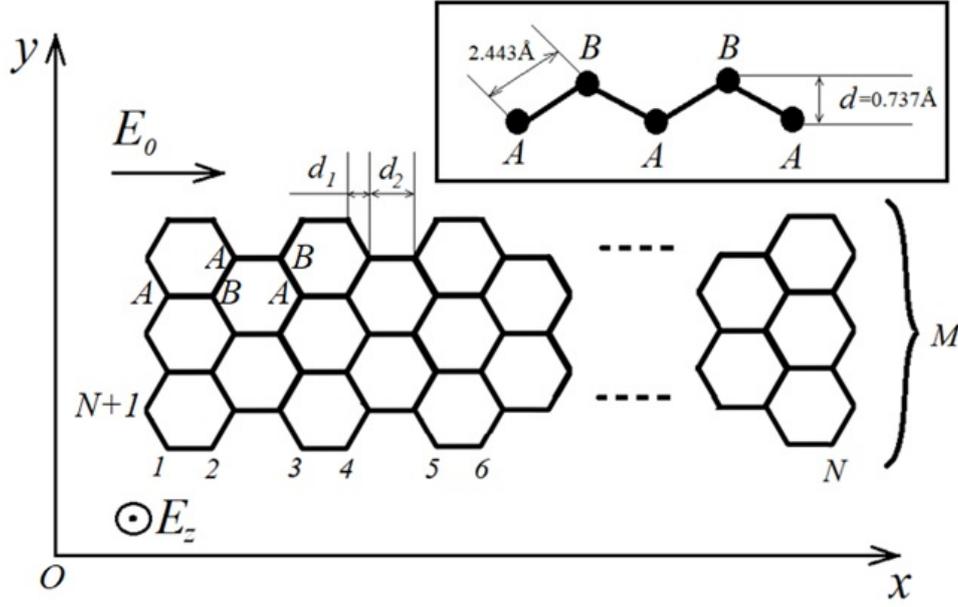


FIG. 1. The geometry of the problem. Side view (parallel to the YOZ plane) is in rectangular area

(if s as an index), $s = \pm$ (if s as a multiplier) [15]. The first term describes the usual electron hopping between the nearest neighboring sites with energy t . The second term is the spin-orbit interaction, where $v_{ij} = +1$ in the case if jumps between neighbors occur counterclockwise, $v_{ij} = -1$ in the case if jumps between neighbors occur clockwise [16]. The third term describes the potential of the chess sublattice with $\mu_i = +1$ (-1) for the sites $A(B)$.

A two-dimensional array of carbon atoms is renumbered for the further calculations into a one-dimensional one. The numbering starts from the bottom and goes to the axis OX, then we go up one level vertically and continue the numbering. Thus, we can obtain the Hamiltonian (1) in the matrix form. For example, we write the Hamiltonian for the germanene fragment 4×3 :

$$H_{up} = \begin{pmatrix} a_{up} & -t & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -t & b_{up} & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a_{up} & -t & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -t & b_{up} & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 \\ -t & 0 & 0 & 0 & a_{up} & 0 & 0 & 0 & -t & 0 & 0 & 0 \\ 0 & -t & 0 & 0 & 0 & b_{up} & -t & 0 & 0 & -t & 0 & 0 \\ 0 & 0 & -t & 0 & 0 & -t & a_{up} & 0 & 0 & 0 & -t & 0 \\ 0 & 0 & 0 & -t & 0 & 0 & 0 & b_{up} & 0 & 0 & 0 & -t \\ 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & a_{up} & -t & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & -t & b_{up} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & a_{up} & -t \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & -t & b_{up} \end{pmatrix}, \quad (2)$$

$$a_{up} = \frac{\Delta_z - \Delta_{SO}}{2}, \quad b_{up} = \frac{-\Delta_z - \Delta_{SO}}{2}.$$

Note, the matrix for the spin “down” looks similar with the replacement: of a_{up} by a_{down} , b_{up} by b_{down} :

$$a_{down} = \frac{\Delta_z + \Delta_{SO}}{2}, \quad b_{down} = \frac{-\Delta_z + \Delta_{SO}}{2}. \quad (3)$$

Also, we take into account the external constant electric field E_0 . It is important because the application of the external field allows us to control the material properties. The electric field has a great influence on the process of electron tunneling at the contact of the germanene with a metal and a superlattice. The Hamiltonian (2) in this

case has the form:

$$H_{up}^E = H_{up} + \begin{pmatrix} \Phi_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \Phi_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Phi_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Phi_4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \Phi_5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \Phi_6 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \Phi_7 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Phi_8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Phi_9 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Phi_{10} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Phi_{11} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Phi_{12} \end{pmatrix}, \quad (4)$$

$$\begin{aligned} \Phi_1 &= \Phi_9 = d_1 E_0; & \Phi_2 &= \Phi_{10} = (d_1 + d_2) E_0; & \Phi_3 &= \Phi_{11} = (3d_1 + 2d_2) E_0; \\ \Phi_4 &= \Phi_{12} = 3(d_1 + d_2) E_0; & \Phi_5 &= 0; & \Phi_6 &= (2d_1 + d_2) E_0; \\ \Phi_7 &= 2(d_1 + d_2) E_0; & \Phi_8 &= (4d_1 + 3d_2) E_0. \end{aligned}$$

where Φ_k describes the potential of the electric field E_0 at the site k .

The current density can be written as [17]:

$$j_{tun} = 4\pi e |T_{pq}|^2 \int_{-\infty}^{\infty} d\varepsilon \sum_p \delta(\varepsilon + eV - \varepsilon_p^1) \sum_q \delta(\varepsilon - \varepsilon_q^2) (n_f(\varepsilon) - n_f(\varepsilon + eV)), \quad (5)$$

where $\delta(x)$ is the Dirac delta-function, both factors with summation determine the tunneling density of states for each material in contact; $n_f(\varepsilon)$ is the equilibrium number of fermions with the energy ε , V is the voltage applied to material 1, T is the matrix element of the tunneling operator between the states p and q (the germanene plane is perpendicular to the surface of the contact material).

As a material for which we calculate the density of the tunneling current, we choose a metal and a superlattice. Electron spectrum for these substances can be written in the form (6):

$$\begin{aligned} Me : \varepsilon_p^1 &= \frac{p^2}{2m}, \\ SL : \varepsilon_p^1 &= \varepsilon_0 - \Delta \cdot \cos(p) \end{aligned}, \quad (6)$$

here, p is the momentum, m is the effective electron mass, ε_0 is the energy of quantum well electrons, Δ is the overlap integral, which is determined by the overlapping of the electron wave functions in the neighboring “wells” of the superlattice.

3. Results and discussion

The dependence of tunneling current (contact with a metal and a superlattice) on the voltage for the germanene fragment 26×7 with the impurity molecule and without it is shown in Fig. 2.

As can be seen from Fig. 2, the most preferable contact is the germanene with a superlattice. In this case, our method is suitable for detecting impurities. Moreover, the more impurity molecules are adsorbed on the surface of the germanene, the greater the response of the system:

$$\Delta R = \frac{R_1 - R_0}{R_0}, \quad (7)$$

here, R_0 is the resistance value without impurity, R_1 is the resistance value with impurity. According to the right Fig. 2, we can conclude that the response decreases with increasing impurity concentration. This result is consistent with the data on the effect of the impurity concentration for graphene obtained, for example, in Ref. [18].

The influence of an external constant electric field E_0 on the tunneling current is shown in Figs. 3, 4.

According to Fig. 3, the introduction of an external constant electric field increases the magnitude of the response (7) and makes it easier to detect an impurity adsorbed on germanene. The applying of an external electric field most significantly affects the shape of the CVC for the contact with a superlattice. Which again speaks in favor of choosing as the second material in the contact of a SL.

The greater the external electric field applied to the system, the more sensitive it is to the presence of impurities.

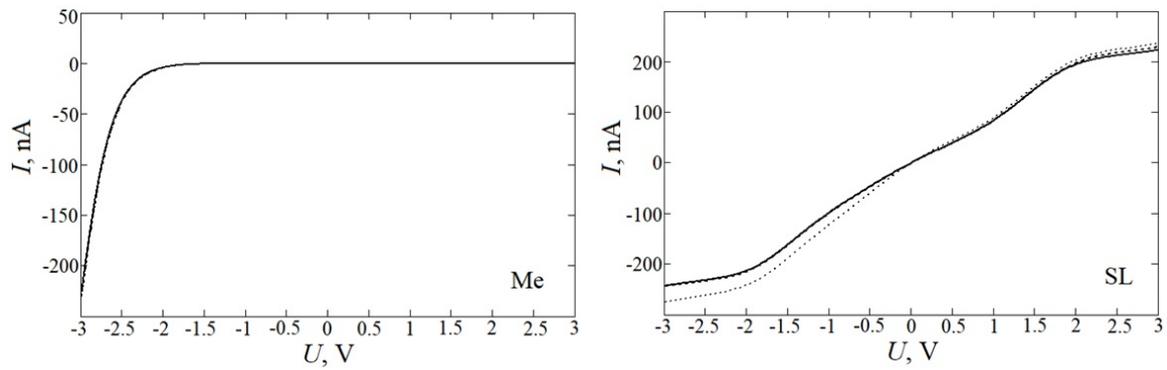


FIG. 2. CVC in the absence of an external field E_0 : on the left – contact with a metal; on the right is the contact with a superlattice. The solid line corresponds to the case without impurities, the dotted line – to 1 impurity molecule, the dashed line – to two impurity molecules

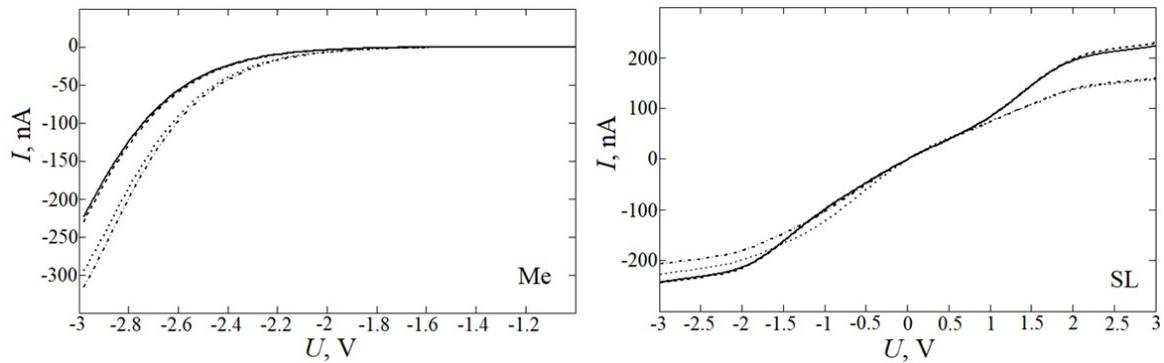


FIG. 3. CVC: on the left – contact with a metal; on the right is the contact with a superlattice. The solid line corresponds to the case without field and impurity, the dashed line – with field and without impurity, the dotted line – without field and with impurity, the dashed point line – with field and impurity

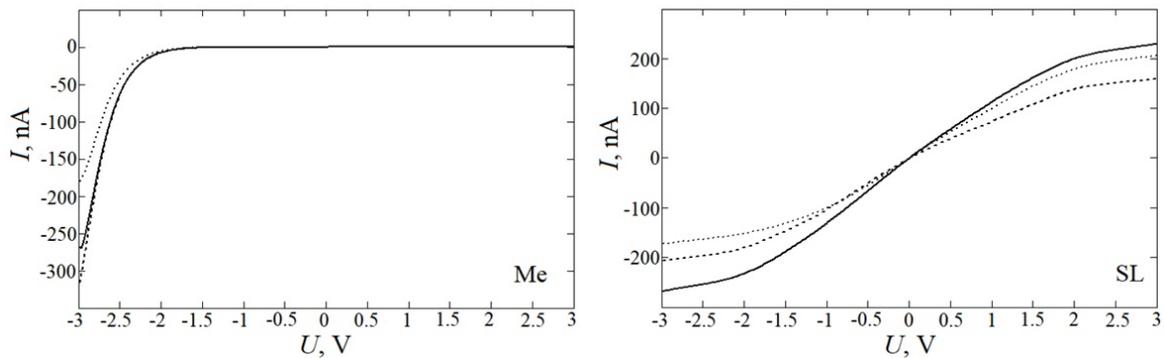


FIG. 4. CVC in the presence of an external field E_0 : on the left – contact with a metal; on the right is the contact with a superlattice. The electric field strength: a) $E_0 = 0.5 \cdot 10^7$ V/m; b) $E_0 = 1.0 \cdot 10^7$ V/m; c) $E_0 = 5.0 \cdot 10^7$ V/m

4. Conclusions

In conclusion, we formulate the main outcomes:

1. The method is proposed for calculating the tunneling density of states for the contact of an impurity germanene with a metal and a superlattice with consideration of a strong spin-orbit interaction.
2. The simulation of the interaction of an external electric field with a contact is made.
3. It is shown, that the introduction of an external field increases the response of the system, which makes it more sensitive to the detection of impurities.

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