Condensed matter physics

ELASTIC CONDUCTIVITY OF GERMANENE "ARM-CHAIR" NANORIBBONS WITH DONOR IMPURITIES

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In the article, results of theoretical calculations of the piezoresistance characteristics of impurity germanene nanoribbons (NR) of the "arm-chair" type with donor defects with various concentrations uniformly distributed in the crystal lattice of the nanomaterial have been presented and analyzed. Arsenic atoms were used as donor impurities. Investigations of the NR's band structure were carried out in the frameworks of the Hubbard's and Anderson's models. The computation of the main characteristic of the piezoresistance effect, i.e., the longitudinal component of the elastic conductivity tensor was carried out using the Green's function method within the framework of the same theoretical models. An analysis of the dependence of this characteristic on the tensile and compressive strains, the concentration of impurities and the nanoribbon width were carried out.

Keywords: band structure, stress-strain state, piezoresistance effect, elastic conductivity tensor

ЭЛАСТОПРОВОДИМОСТЬ КРЕСЕЛЬНЫХ ГЕРМАНЕНОВЫХ НАНОЛЕНТ С ДОНОРНЫМИ ДЕФЕКТАМИ

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В работе представлены и проанализированы результаты теоретических расчетов пьезорезистивных характеристик примесных германеновых нанолент кресельного типа ("arm-chair") с донорными дефектами разной концентрации, однородно распределенными в кристаллической решетке наноматериала. В качестве донорных примесей использованы атомы мышьяка. Исследование зонной структуры нанолент проведено в рамках моделей Хаббарда и Андерсона. Вычисление основной характеристики пьезорезистивного эффекта — продольной компоненты тензора эластопроводимости выполнено в рамках тех же теоретических моделей с использованием метода функций Грина. Проанализированы зависимости указанной компоненты от относительной деформации растяжения и сжатия, концентрации примесей и ширины наноленты.

Ключевые слова: зонная структура, напряженно-деформированное состояние, пьезорезистивный эффект, тензор эластопроводимости

Introduction

One of the priority problems of condensed matter physics is obtaining of materials with preset properties and a possibility to control them. Since 2004, scientists have been synthesizing and studying carbon based nanomaterials (graphene, graphene nanoribbons) possessing practically important electronic, conductive, optical and mechanical properties which can expand the spectrum of their use [1 − 3].

The electronic properties of graphene nanoribbons are rather diverse and depend on the nature and concentration of impurities, applied external fields, mechanical strain, etc. Since the moment it was synthetized first in 2004, graphene became the object of most promising technologies of nanoelectromechanical systems for the development of nanoelectronic devices. It can replace silicon as a basis for transistors, cantilever for atomic force microscopy, chemical sensors, etc.

Despite its spectrum of unique properties, graphene is still not devoid of some drawbacks in terms of its practical use, e.g. it lacks band gap energy almost completely, which eliminates a possibility to close a graphene-based FET channel [4]. One of the priority solutions of this problem is the search for new non-carbon promising 2D materials with a structure similar graphene, but possessing a sufficient band gap.

In 2013, by means of computer choice among the materials with properties similar to graphene and a 2D-like structure, there were 92 promising analogues identified [5]. Forty of them were never proposed as a compound similar to graphene before, and their properties, including the conductive ones, remain poorly explored. Despite such an abundance of the selected alternatives that are promising in terms of creating a basis for nanoelectronic devices, their application is extremely limited by the problems of synthesis and interaction with the substrate. Therefore, selection of analogues among actually synthesized nanomaterials from the "graphene family" and study of their piezoresistance properties is a relevant task of the first stage of work.

Predicted in 2009 and successfully synthesized in 2014, germanene should be regarded as one of the most promising nanomaterials of the "post-graphene era" [6 − 9].

Band gap and electronic properties of germanene are sensitive to external fields, mechanical strain and chemisorption [10, 11]. According to theoretical studies, the width of the germanene band gap equals approximately 24 meV ($E_g \approx 24$ meV), which by several orders of magnitude exceeds the one known for graphene ($E_g < 0.05$ meV). This expansion of the band gap allows using germanene in devices the work of which is based on field effects, such as transistors. It can be achieved either by applying external impact [12] or by means of intentional doping of a nanomaterial with acceptor and donor impurities of various concentrations. By combining mechanical strain/stress and varying the number of defects, we can create and effective mechanism of controlling the germanene band gap.

This paper is devoted to a theoretical study (and consequently, to a prediction) of the piezoresistance properties of the impurity germanene nanoribbons (NR): GeNRs.

Model of electronic structure of deformed impurity germanene nanoribbons

Geometric model of GeNRs is chosen based on the view of the two-dimensional hexagonal graphene layer. Fig. 1 shows a deformed unit cell of the germanene crystal lattice, where α denotes the angle between the primitive translation vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, while $\mathbf{\Delta}_i$ is the interatomic spacing vector and a is the constant lattice of the
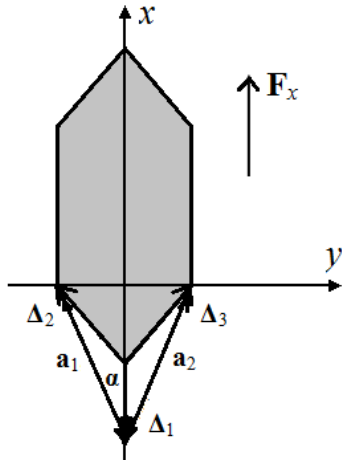
Fig. 1. Fragment of the arm-chair GeNR structure deformed by longitudinal tension of force $\mathbf{F}_x$:
Δ_i ($i = 1, 2, 3$) — interatomic spacing vectors;
$\mathbf{a}_1$, $\mathbf{a}_2$ — primitive translation vectors;
α — angle between vectors $\mathbf{a}_1$ and $\mathbf{a}_2$

deformed GeNR ($a_1 = a_2 = a$). The length and width of the NR are measured along the Ox and Oy axes respectively.

Electronic spectrum of undeformed GeNRs in the frame of the strong coupling method and the nearest neighbors approximation can be presented in the following form [13]:

$$\varepsilon(\mathbf{k}) = \pm t_0 \left\{ 1 + 4\cos\left(\frac{\mathbf{k}(\mathbf{a}_1 + \mathbf{a}_2)}{2}\right) \times \right.$$
$$\times \cos\left(\frac{\mathbf{k}(\mathbf{a}_1 - \mathbf{a}_2)}{2}\right) + \qquad (1)$$
$$\left. + 4\cos^2\left(\frac{\mathbf{k}(\mathbf{a}_1 - \mathbf{a}_2)}{2}\right) \right\}^{1/2},$$

where t_0, eV, is the resonance or hopping integral ($t_0 = 1.47$ eV [6]); $\mathbf{k}$, cm^{-1}, is the wave vector; $\mathbf{a}_1$, $\mathbf{a}_2$, nm, are the primitive translation vectors.

The Fermi level in Eq. (1) is traditionally taken as 0 eV.

The direction of the $(\mathbf{a}_1 + \mathbf{a}_2)$ vector is called "arm-chair", while the $(\mathbf{a}_1 - \mathbf{a}_2)$ vector has a "zig-zag" direction.

The condition of quantizing the wave vector $\mathbf{k}$ along the NR width can be written as follows [13]:

$$3k_x R_0 = \frac{2\pi q}{N_x}, \quad q = 1, 2, ..., N_x \qquad (2)$$

For the arm-chair GeNRs, and

$$\sqrt{3}k_y R_0 = \frac{2\pi q}{N_y}, \quad q = 1, 2, ..., N_y \qquad (3)$$

for the zig-zag NRs.

Here, R_0, nm, is the equilibrium interatomic spacing in the undeformed GeNR; k_x, k_y, cm^{-1}, are wave numbers in the Brillouin zone.

Fig. 1 demonstrates a geometric modification of the arm-chair GeNR lattice hexagon deformed by longitudinal tension of force $\mathbf{F}_x$.

Modeling of band structure of the deformed GeNRs is performed by means of transforming the parameters of the unit cell and the Brillouin zone. This procedure is described in detail in paper [15].

If we present the value of relative strain of the interatomic bond length R as $\delta = \Delta R/R_0$, where ΔR is the change of the equilibrium (Ge-Ge) bond length R_0 ($\Delta R = R - R_0$), then we can obtain the following expressions for the components of the wave vector [15]:

$$\frac{\mathbf{k}_x(\mathbf{a}_1 + \mathbf{a}_2)}{2} =$$
$$= k_x R_0 (1 + \delta)(1 + \cos\alpha),$$

$$\frac{\mathbf{k}_y(\mathbf{a}_1 - \mathbf{a}_2)}{2} = \qquad (4)$$
$$= k_y R_0 (1 + \delta)\sin\alpha = \frac{\pi q}{n},$$
$$q = 1, 2, ..., n$$

for the arm-chair GeNR ($k_x \in$ the Brillouin zone);

$$\frac{\mathbf{k}_x(\mathbf{a}_1 + \mathbf{a}_2)}{2} =$$

$$= k_x R_0 \left[(1+\delta)\cos\alpha + 1 - \delta \right] = \frac{\pi q}{n},$$
$$q = 1, 2, \ldots, n, \tag{5}$$

$$\frac{\mathbf{k}_y(\mathbf{a}_1 - \mathbf{a}_2)}{2} = k_y R_0 (1+\delta)\sin\alpha$$

for the zig-zag type GeNR ($k_y \in$ the Brillouin zone).

Tensile (compression) strain causes changes in the transverse dimensions of the GeNR, and consequently the chiral vector modulus [13] is modified in the following way:

$$C_h = C_{h0}(1 - \nu\delta),$$
$$C_{h0} = a_0 \sqrt{N_x^2 + N_y^2 + N_x N_y}, \tag{6}$$

where a_0, nm, is a constant lattice of the undeformed GeNR, $a_0 = R_0$; N_x, N_y — integers defining the size and the type of the NR ($N_y = 0$ for the arm-chair type and $N_y = N_x$ the zig-zag type); ν is the Poisson's ratio taking values of 0.27 and 0.19 for the arm-chair and zig-zag type GeNRs, respectively.

We can evaluate angle α from relation (6) [15]:

$$\sin\alpha = \left(\frac{1 - \nu\delta}{1 + \delta} \right) \sin\alpha_0,$$

$$\cos\alpha = \sqrt{1 - \sin^2\alpha}$$

for the arm-chair GeNR;

$$\cos\alpha = \frac{1}{(1+\delta)} \times$$
$$\times \left[(1 - \nu\delta)(1 + \cos\alpha_0) - 1 + \delta \right],$$

$$\sin\alpha = \sqrt{1 - \cos^2\alpha}$$

for the zig-zag GeNR.

Finally, the electronic spectrum of the deformed GeNRs takes the form [15]:

$$\varepsilon_a(\mathbf{k}) =$$

$$= \pm\gamma(\delta)\left\{ 1 \pm 4\cos\left(\frac{\pi q}{n} \right) \times \right.$$
$$\times \cos\left[k_x R_0 (1+\delta)(1 + \cos\alpha) \right] + \tag{7}$$
$$\left. + 4\cos^2\left(\frac{\pi q}{n} \right) \right\}^{1/2},$$

$$\varepsilon_z(\mathbf{k}) =$$
$$= \pm\gamma(\delta)\left\{ 1 \pm 4\cos\left[k_y R_0 (1+\delta)\sin\alpha \right] \times \right. \tag{8}$$
$$\left. \times \cos\left(\frac{\pi q}{n} \right) + 4\cos^2\left[k_y R_0 (1+\delta)\sin\alpha \right] \right\}^{1/2},$$

where $\gamma(\delta)$ is the resonance integral of the deformed GeNRs as a function of the relative strain δ; subscripts "a" and "z" denote the spectra of the arm-chair and zig-zag type NRs, the $+/-$ symbols result from the fact that an NR unit cell contains for Ge atoms.

The electronic spectrum of the deformed GeNRs with no impurities, taking into account the Coulomb repulsion at one point, was calculated in the frame of the Hubbard's model [16], which is described in detail in paper [17]:

$$E(\mathbf{k}) = \frac{1}{2}\left[\varepsilon(\mathbf{k}) + \right.$$
$$\left. + U \pm \sqrt{\varepsilon(\mathbf{k})^2 - 2\varepsilon(\mathbf{k})U(1 - 2n_{-\beta}) + U^2} \right], \tag{9}$$

where $\varepsilon(\mathbf{k})$ is the band structure of ideal NRs; U, J, is the energy of the Coulomb interaction at one point that is a semi-empirical method parameter of MNDO quantum chemistry [18], $n_{-\beta}$ is the number of electrons with opposite spin in the zone.

A comparative analysis of the depiction of the band structures $E(\mathbf{k})$ of Eq. (9) and $\varepsilon(\mathbf{k})$ of Eq. (7) for the arm-chair GeNR revealed no significant differences.

A quantitative evaluation of the energy band gap width of the semiconductor GeNR in case of longitudinal tensile (compression) strain showed its broadening (narrowing). The conduction band, as well as the valence band act in the same

manner. As a result, the density of electronic states in these zones increases (decreases). Such a behavior of the dispersion curves was observed during the study of achiral (arm-chair and zig-zag) carbon nanotubes [15, 17].

The gapless band structure of the conductive arm-chair GeNRs in case of longitudinal tension (compression) is also changed in the above described way. The only exclusion from the identical behavior is the nonoccurrence of band gaps in the spectra of such ribbons as they remain conductive.

Longitudinal tension of the conductive GeNRs also has no essential influence on the qualitative behavior of their band structure, while the band gap is absent at small strain.

Adding impurities in the crystalline structure of the GeNRs under consideration can facilitate the change in their piezoresistance as it is shown on example of graphene nanoribbons in paper [19], which will allow exerting intentional influence on their conductivity.

The calculation of the electronic spectrum of doped GeNRs was conducted using Anderson model [16]. This model consists in separate consideration of collective π-electrons and localized electron, the interaction between which is accounted for by means of introducing hybridization potential. The model is successfully adapted to the studies of the influence point defects (donor and acceptor) have on band structure of graphene nanoribbons [19].

The GeNR electronic spectrum in the frame of Anderson model has the following form [16]:

$$E(\mathbf{k}) = \frac{1}{2}\big[\varepsilon_l + \varepsilon(\mathbf{k}) \pm$$
$$\pm \sqrt{(\varepsilon_l - \varepsilon(\mathbf{k}))^2 + 36|V_{\mathrm{GeD}}(\delta)|^2 \cdot x}\,\big], \qquad (10)$$

where $\varepsilon(\mathbf{k})$, eV, is the band structure of an ideal (undoped) nanoribbon expressed by Eq. (7); ε_l, eV, is electron energy at the defect; $x = N_d/N$ is the concentration of impurities (N is the number of unit cells in the crystal, N_d is the number of defects); $V_{\mathrm{GeD}}(\delta)$, eV, is the hybridization potential which consists in a matrix element of the energy of the crystal/point defect electron interaction

and is the function of the relative strain δ.

This paper considers such donor impurities of arsenic atoms as point defects. The electron energy at the defect can be evaluated as a difference of impurity/crystallite ionizing potential:

$$\varepsilon_l = I_{\mathrm{Ge}} - I_{\mathrm{As}} =$$
$$= (7.88 - 9.81)\ \mathrm{eV} = -1.93\ \mathrm{eV}.$$

The dependencies of the hopping integral $\gamma(\delta)$ and the hybridization potential $V_{\mathrm{GeD}}(\delta)$ on the relative strain were calculated by means of the density functional theory method using the exchange−correlation energy functional B3LYP in the STO-3G basis sets [18]. For quantum chemical calculations, we considered a fragment of germanene surface the size of 6×6 unit cells (UC). Boundary unsaturated bonds were closed with monovalent hydrogen. A defect atom (As) was placed in the center of the constructed cluster to decrease the influence of the boundary atoms. We were modeling the deformation of the structure along the "arm-chair" direction by means of step-by-step freezing of germanium atoms at the opposite boundaries of the fragment. The obtained numerical values of the $\gamma(\delta)$ and $V_{\mathrm{GeD}}(\delta)$ dependencies interpolated by the following analytical expressions:

$$\gamma = \gamma_0 \exp(-1.9523R),$$
$$V_{GeD} = V_0 \exp(-1.9523R),$$
$$R = R_0(1+\delta), \qquad (11)$$
$$\gamma_0 = 171.11\ \mathrm{eV},$$
$$V_0 = 152.37\ \mathrm{eV}.$$

The equilibrium interatomic bond lengths in further calculations were assumed equal to $R_0 = 2.44$ Å; this value was obtained as a result of prior optimization of the geometric structure of the constructed germanene fragment using the above described density functional theory method.

Adding donor impurities of various concentrations to the system of undeformed GeNRs leads to a change in the band structure of the latter. Features of the energy spectrum of low-dimensional structures with donor nitrogen

atoms in the lattice are analyzed on the example of carbon nanotubes in paper [17]. The zone of impurity states in this case is localized in the proximity of the electron energy level at the defect ε_l and contains a local band gap which does not change the crystallite properties as a whole. As the impurity concentration increases, there is a greater change in the band structure of the carbon nanotubes, in particular, there is an increase in the local band gap. The described features of the electronic spectrum of the undeformed carbon nanotubes with impurities are verified by the general Anderson model theory [16].

Elastic conductivity of germanene nanoribbons with acceptor defects

According to the recommendation in book [20], determination of the elastic conductivity tensor of the two-dimensional crystalline structures can be written as

$$\frac{\Delta\sigma_{\xi\rho}}{\langle\sigma\rangle} = M_{\xi\rho\chi\eta}\cdot\delta_{\chi\eta},$$

$$\langle\sigma\rangle = \frac{1}{2}\mathrm{Sp}[\sigma] = \frac{\sigma_{xx}+\sigma_{yy}}{2}, \qquad (12)$$

$$M_{\xi\rho\chi\eta} = M_{\rho\xi\chi\eta} = M_{\rho\xi\eta\chi} = M_{\xi\rho\eta\chi},$$

where $\sigma_{\xi\rho}$ is the conductivity tensor; $\delta_{\chi\eta}$ is the strain tensor; $\xi, \rho, \chi, \eta = x, y$.

For a case of quasi-one-dimensional structures (for example, the arm-chair GeNR), the longitudinal component $M = M_{xxxx}$ of the fourth-rank elastic conductivity tensor can be expressed by the following formula:

$$M = \frac{\Delta\sigma}{\sigma_0}\frac{1}{\delta}, \qquad (13)$$

where $\Delta\sigma$, S/m, is a change of the longitudinal component of the conductivity tensor due to strain; σ_0, S/m, the longitudinal component σ_{xx} of the second-rank conductivity tensor of the un-deformed arm-chair nanoribbons, $\Delta\sigma = \sigma - \sigma_0$ (σ, S/m, is the same component σ_{xx} of the de-formed nanoribbons).

An expression for calculating the longitudinal component σ of the conductivity tensor of the arm-chair GeNRs obtained in the frame of the Green − Kubo theory [21] using Green's fun-ction method and Hubbard model Hamiltonian [18] is presented in works [17, 19]:

$$\sigma = 2\frac{i\pi e^2}{k_{\mathrm{B}}TV}\sum_{\mathbf{k},\beta}\sum_{\mathbf{q},\lambda}v(\mathbf{k})v(\mathbf{q})\langle n_{\mathbf{k}\beta}\rangle\times$$

$$\times\left[\langle n_{\mathbf{q}\lambda}\rangle + \delta_{\mathbf{kq}}\delta_{\beta\lambda}\left(1-\langle n_{\mathbf{k}\beta}\rangle\right)\right], \qquad (14)$$

where V, m³, is the nanoribbon volume; T, K, is the absolute temperature; e, C, is the elementa-ry charge; $\mathbf{k}, \mathbf{q}$ are two-component wave vectors within the Brillouin zone (BZ); β, λ are the spin indices; $v(\mathbf{k})$, m/s, is the longitudinal component of the electron velocity vector in the Brillouin zone; $\langle n_{\mathbf{k}\beta}\rangle$ − is the average number of particles in a quantum state with the wave vector $\mathbf{k}$ and spin β.

The average number of particles $\langle n_{\mathbf{k}\beta}\rangle$ is expressed by the Fermi − Dirac distribution function:

$$\langle n_{\mathbf{k}\beta}\rangle = \left[1+\exp\left(\frac{\varepsilon(\mathbf{k})-\mu}{k_{\mathrm{B}}T}\right)\right]^{-1},$$

where k_{B}, J/K, is the Boltzmann constant; μ, J/mol, is the chemical potential which is found from a condition of distribution function nor-malization by a total number of N_e electrons in the system; this number is expressed as

$$N_e = \sum_{\mathbf{k},\beta}\langle n_{\mathbf{k}\beta}\rangle =$$

$$= \sum_{\mathbf{k},\beta}\left[1+\exp\left(\frac{\varepsilon(\mathbf{k})-\mu}{k_{\mathrm{B}}T}\right)\right]^{-1}.$$

The velocity vector is determined by means of a standard method using the electronic spectrum (10):

$$\mathbf{v}(\mathbf{k}) = \frac{1}{h}\frac{\partial E(\mathbf{k})}{\partial\mathbf{k}}. \qquad (15)$$

Model parameter values used in the calculations

Parameter	Notation	Values
Number of UC along NR length width	N n	10 000 9, 10, 50, 100
Number of defects in NR	N_d	1, 10, 100, 1000
Relative tensile (compression) strain	δ	–0.10; –0.06; –0.04; –0.02; –0.01; 0.01; 0.02; 0.04; 0.06; 0.10
Equlibrium interatomic bond length (Ge-Ge), Å	R_0	2.44
Deformation temperature, K	T	300

N o t e: UC is the unit cell, NR is the nanoribbon.

This paper presents the results of studying the piezoresistance properties of the arm-chair GeNRs of various width and with different types of conductivity: nArm, where n sets the number of unit cells (UC) along the ribbon width. The values of the parameters used in the calculations are summarized in the Table.

Dependencies of the longitudinal component M of the elastic conductivity tensor on the value of the relative strain δ calculated using Eq. (13), are presented in Figs. 2 and 3. The calculated points in the figures are marked by symbols and connected by lines.

We considered a case of the so-called half-filled band, i. e. each Ge atom gives one electron to the system, while each impurity As atom gives two. Therefore, the total number of electrons was calculated as $N_e = N \cdot n + N_d$.

As it follows from Fig. 2, a, the value of M from the conducting arm-chair 9Arm NR is po-sitive at low concentration of the defects ($N_d = 1$) and negative at all other values of the con-centration. All curves $M(\delta)$ for the conducting 9Arm NR with different concentrations show nonmonotonic decrease while the strain δ rises over the entire range of its values. The case of $N_d = 100$ is an exception, where the coefficient M exhibits monotonic growth in the domain of $\delta > 0$ (tensile strain).

Behavior of function $M(\delta)$ completely correlates with the changes in the band structure of the conducting impurity nanoribbons described above. An increase in the conduction band width leads to a decrease of the states density at the Fermi level with the growth of δ. However, the band gap occurring at the impurity level gets wider as the values N_d and δ grow. Therefore, as a result of the competition between these two effects, the conductivity of the nanoribbon decreases as a whole, which leads to the behavior of the component M described above for the cases of small concentration of impurities ($N_d = 1, 10$).

An increase in the impurities concentration leads to an interesting effect. In general, the numerical value of the coefficient M decreases with the growth of the concentration practically for all the calculated values of the relative strain δ. But at the concentration of $N_d = 100$, the dependence of $M(\delta)$ lies higher than that for the case of $N_d = 100$. Such a behavior of the value M is connected with the fact that due to thermal fluctuations the electrons fill the conduction band of the NR thus facilitating the conductivity growth. The increase of the donor impurities concentration raises the number of charge carriers in the conduction band. All these factors change the conductivity, the contribution to which is made by all filled
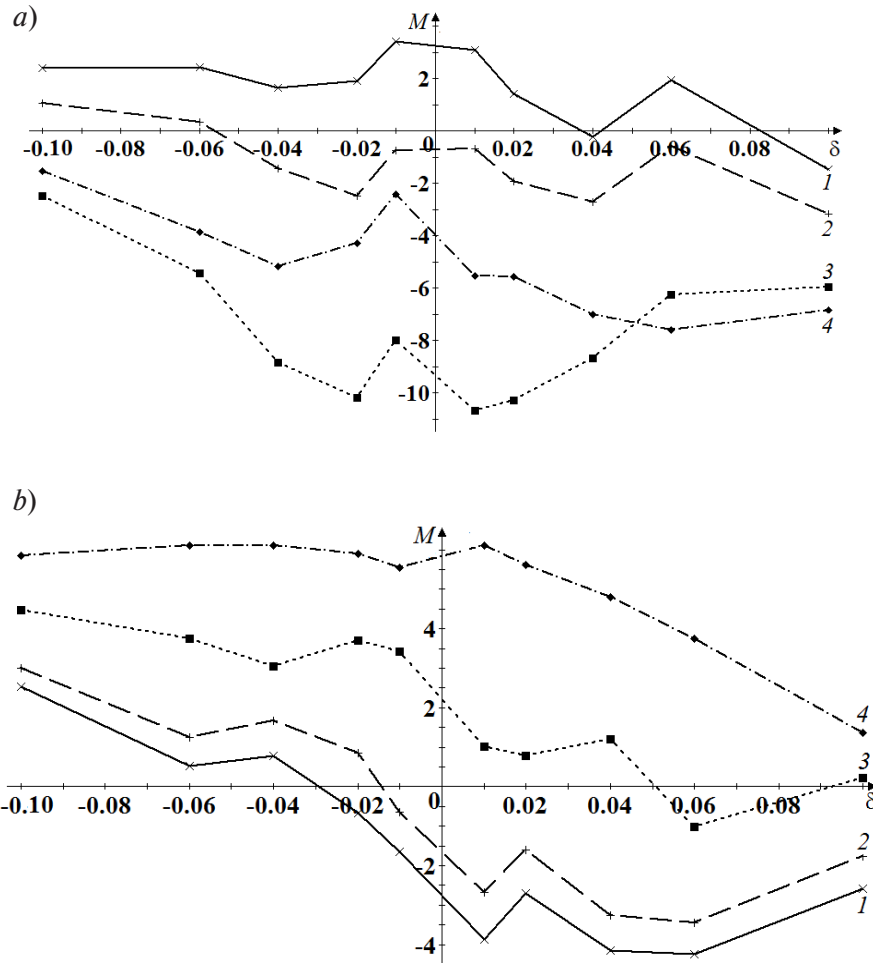
Fig. 2. Dependencies of the longitudinal component *M* of the elastic conductivity tensor
of the arm-chair 9Arm GeNRs (*a*) and 10Arm GeNRs (*b*)
(9 and 10 are the number of the UC along the width) on the value of the relative strain
δ for various donor defect concentrations N_d: 1(*1*), 10 (*2*), 100 (*3*), 1000 (*4*);
The calculated points in the figures are marked by symbols and connected by lines

electronic states in the conduction band.

The dependence of $M(\delta)$ for the number of defects $N_d = 1000$ retains the general behavior trend of the NR 9Arm longitudinal component. The competition between two factor, in particular, the broadening of the band gap in the proximity of the impurity level due to defect concentration growth and the relative strain, and the increase in the number of free carriers, leads to a reduction of $M(\delta)$ in the domain of δ < 0 (compression strain) and its rise in the domain of δ > 0 (tensile strain).

In case of the semiconductor arm-chair GeNRs (10Arm, 50Arm, 100Arm), the behavior of the longitudinal component of the elastic con-

ductivity tensor M depends on the width of the nanoribbon studied. Thus, function $M(\delta)$ GeNR 10Arm monotonically decreases with the growth of the relative strain over the entire range of value δ (Fig. 2,*b*) for various values of the defects concentration ($N_d = 1, 10, 100, 1000$). Starting from δ = −0.1, the value of *M* is positive for all values of N_d. The positive value is due to crystallite conductivity increasing along with the compression strain (δ < 0) as a result of band gap narrowing and the number of the conduction band free carriers rising.

Then, for the case of small concentrations of the defects ($N_d = 1, 10$), the curves go into the negative value domain. As in the case of ideal
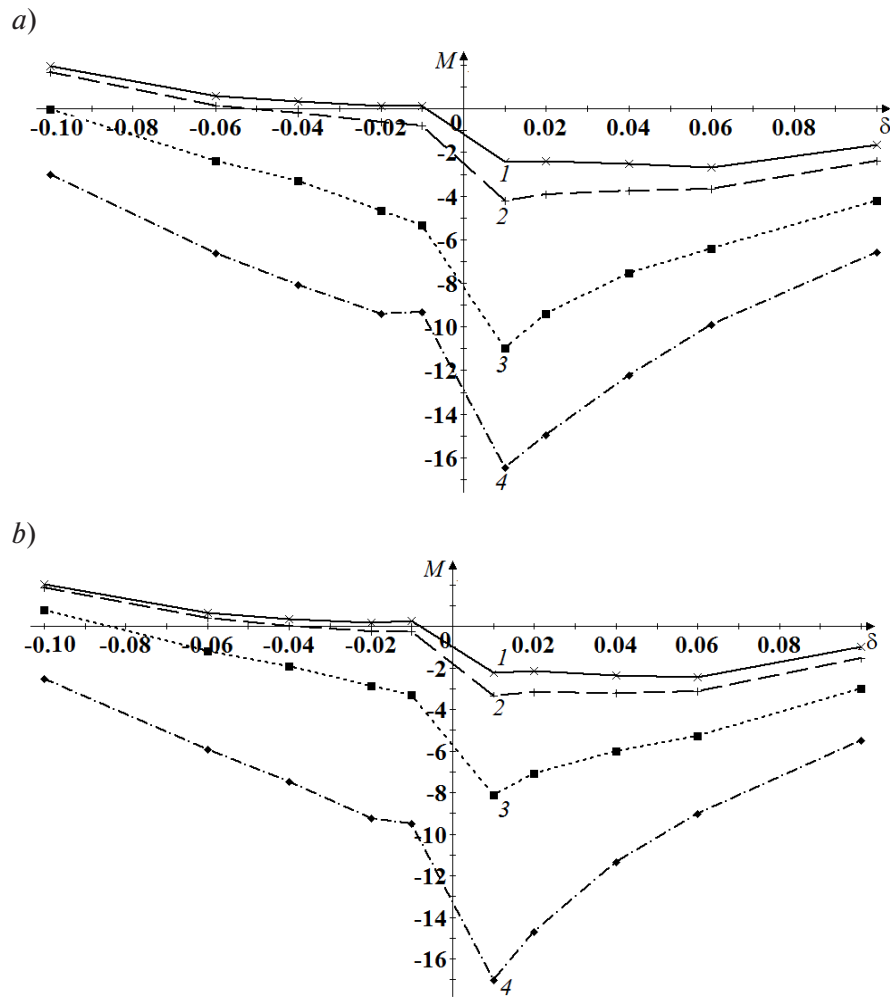
a)

b)

Fig. 3. Dependencies similar to the ones indicated in Fig. 2, but for 50Arm GeNRs (*a*)
and 100Arm GeNRs (*b*) and the same concentration of donor defects N_d

GeNRs [12], it stems from the reduction of the conductivity along with the growth of strain δ. We can explain this effect with the broadening of the band gap E_g of the semiconductor NRs, which decreases the number of the filled electronic states in the conduction band.

The growth in the donor defects concentration (N_d = 1, 10, 100, 1000) in general does not change the behavior trend of the M value only increasing its numerical value.

The character of the functional dependence $M(δ)$ changes for wide NRs of 50Arm and 100Arm. In the negative domain of δ (compression), we can observe the value of M GeNR 50Arm decreasing for all defects concentrations (Fig. 3,*a*). During the transition to the positive

strain (tensile) domain for the case of N_d = 1 the longitudinal component of the elastic conductivity tensor faces practically no changes until δ = = 0.1 ("plateau" domain), in the latter case we observe we see its growth. Further growth of the defects concentration (N_d = 10, 100, 1000) leads to dramatic rise of the M value in the tensile strain domain. Producing a wider ribbon (100Arm) results in a "plateau" for the case of N_d = 10 (Fig. 3,*b*) as well. Such an effect corresponds to the behavior of the band structure of the deformed semiconductor NRs. There is a competition between two factors. The first one is connected with the growth of the NR conductivity thanks to the increase in the number of free carriers in the conduction band cause by the donor

defects. The second factor consists in the blocked conductivity of the ribbon due to an increase of E_g along with the growth of δ.

In general, wider GeNR leads to a reduction of the band gap $E_g \sim 1/H$, where $H -$ is the ribbon width. In turn, this increases the crystallite conductivity and, consequently, the numerical value of the coefficient M (Fig. 3,*b*).

The approach described above and the analytical algorithm were applied to the study of the piezoresistance properties of graphene nanoribbons with donor and acceptor impurities [19]. The comparison of the trends in the dependencies behavior $M(\delta)$ presented in this paper along with the literature data on piezoresistance properties of graphene nanoribbons showed a qualitative agreement of the obtained results. We should expect that the described properties are characteristic of the other graphene family structures as well.

Conclusion

A theoretical study of the piezoresistance of germanene nanoribbons of the "armchair" type with donor defects with different types of conductivity doped with point substitutional defects showed a number of features of a qualitative and quantitative change of the longitudinal component of the elastic conductivity tensor M.

A study of the behavior and value of the constant M depending on the concentration of donor impurities, the geometric parameters of the nanoribbon (in particular, its width), the extent of the strain, demonstrates a complete picture of the change in the longitudinal conductivity of nanoribbons caused by mechanical tension and compression.

The sensitivity of the elastic conductivity tensor to the listed factors proves the possibility of effective control over the conductivity of germanene.

The obtained theoretical data can be proposed for quantitative calibration of nanoelectromechanical devices that function on the basis of the piezoresistance effect and have germanene nanoribbons as their primary structural material.

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