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Electronic state of iron atoms doped in germanium

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Received April 28, 2024

Revised July 7, 2024

Accepted July 8, 2024

To study the electronic state of iron atoms doped in germanium, a double film system Fe-Ge was formed under ultrahigh vacuum conditions, obtained by annealing a Fe layer deposited on a Ge film formed on the surface of a Mo(110) crystal. The results obtained using a combination of low-energy ion scattering spectroscopy (LEIS), Auger electron spectroscopy (AES), low-energy electron diffraction (LEED), and Anderson work function measurements indicate that the Fe-Ge double film formed in this way is characterized by a uniform distribution of Fe and Ge atoms over the film bulk. It is shown that a change in the relative content of Fe atoms leads to a significant change in their electronic state. The first measurements of the absolute charge of Fe atoms acquired by them when doped in germanium indicate that as the Fe content increases, the charge value systematically decreases from 0.34e for a single atom to 0.07e for the same Fe and Ge ratio. This is accompanied by a change in the length of the Fe⁺-Ge⁻ interatomic bond within the range from 0.141 nm to 0.118 nm. The latter, being evidence of structural transformations of Ge, characterized by a change in the lengths and angles of the lattice bonds, can be used to identify structural units of doped germanium at different concentrations of the doping component.

Keywords: Thin films, doping, germanium, iron, electronic state, surface analysis methods.

DOI: 10.61011/PSS.2024.09.59223.108

1. Introduction

The germanium doping with metal atoms is one of effective methods of its parameters modification, especially in case of nanoscale structures: geometry of nanocluster, its stability, bond energy, ionization potentials, electron affinity, charge transfer, polarizability etc. [1–11]. These parameters are important for fine adjustment of semiconductor properties and obtaining new materials, in particular, formed due to self-organization of nanoscale clusters, for this the inherent germanium, as a rule, is unacceptable due to some its properties [12,13]. In case of Ge at appropriate selection of the doping metal and its concentration it is possible to form both semiconductor, and metal structures with fine adjustable properties [14]. In this relation the transition metals (TMs) are very attractive due to different effects determined by d ↔ p hybridization of atomic orbitals. For example, Lu an Nagase [15], and Kumar and Kawazoe [16] based on theoretic studies of the nanocluster structures of germanium and silicon doped by the transition metals showed that such hybridization of atomic orbitals leads to energy increasing between the top occupied and bottom unoccupied molecular orbitals (ΔE). As a result, weakening of interaction between the clusters of germanium and increasing of its chemical stability, significantly higher than

in case of Si occurred, this makes Ge nanostructures more attractive for controllable assembly of the nanomaterials. Studies of electronic state of germanium doped by transition metals using the quantum-chemical methods of Hou et al. [2] showed that in case of Cr the hybridization of orbitals occurs as result of charge transfer from Cr to Ge and competitive reverse transfer of charge Cr(d) ← Ge(p). The latter is less effective, as result Cr receives positive charge. Feature of all studied structures of Ge with introduced Cr atoms is that in basic state they have high spin and magnetic moment. As per data of Zhao and Wang [3], same situation is observed also for Fe in Ge. Based on calculation by the cluster density functional method FeGe_n (n = 9–16) they showed that the resulting charge transfer occurs from Fe to Ge, and in spite of that Fe was embedded into cluster Ge_n, its magnetic moment i not change. In this case, the width of the energy band between the top occupied and bottom unoccupied molecular orbitals in the cluster FeGe_n decreases. It is also showed that Fe addition into the lattice of Ge_n increases its stability.

Fundamentally same situation is observed for Cu and Ni atoms embedded in Ge nanoarray, this is confirmed by the results obtained by Wang and Han based on the calculations by density functional method [7,9]. It is shown that for Ge clusters doped by Cu rather strong correlation is

observed between transformation of the molecular orbitals and structure of clusters CuGe_n . Similar to Fe the energy gap between the top occupied and bottom unoccupied molecular orbitals of clusters CuGe_n decreases as compared to the case of undoped clusters Ge_n . It is shown that for all studied systems CuGe_n the charge transfer from Cu to Ge occurs, as well as upon Cu addition there is violation of correlation between polarizability and value ΔE , natural of undoped cluster Ge_n . Unlike Cu, for Ni atoms embedded into the cluster Ge_n , the direction of charge transfer depends on size of cluster NiGe_n . For $n < 7$ the charge is shifted from Ni to Ge, at values $7 < n < 12$ there is reverse charge transfer, and at value $n > 12$ the charge offset again changes its direction from Ni to Ge. At that, irrespectively of the direction of charge transfer, the embedding of Ni atoms in Ge lattice, similar to case FeGe_n , leads to its stability increasing due to increase in averaged interatomic bond energy.

Another 3d-metal, vanadium, as doping element of Ge nanocluster, was studied in detail by Deng et al. [5] using methods of anion photoelectron spectroscopy and density functional theory. It is shown that with cluster size increasing from 3 to 12 atoms the cluster structure transforms into sequences exohedral–semi-endohedral scaphoid — distorted structure of hexagonal prism. In all studied cases there is charge offset from Ge to V, at that this offset value decreases with cluster size increasing. The same trend is observed for the magnitude of the magnetic moment. Correlation between structure transformations of cluster VGe_n and features of process of transfer of charge $\text{Ge} \rightarrow \text{V}$ is made.

So, considering the key role of the charge transfer process for properties evolution of the germanium doped by transition metal, it is interesting to determine the absolute magnitude of the transferred charge. Due to this the present paper objective was to determine by experiments the magnitude of the electron charge acquired by Fe atoms in Ge lattice. As follows from the above consideration, the change in the relative ratio of the concentration of atoms of transition metal and germanium in TM-Ge structures leads to the fundamental change in the system parameters. So, it is interesting to track the change of charge magnitude with change in iron concentration starting from case of a single atom in germanium lattice. The latter is rather troublesome problem due to limited sensitivity of the experimental study methods. However, in the present paper it was possible to estimate the absolute magnitude of the charge of the single Fe atom by selecting the method for forming Fe-Ge system and the corresponding adaptation of the analysis methods.

2. Study methods

Studies were performed under controllable conditions of ultrahigh vacuum (pressure of residual gases is $2 \cdot 10^{-10}$ Torr) in surface analysis system VG Escalab MkII

by methods of Auger-electron spectroscopy (AES), low-energy ion scattering spectroscopy (LEIS), low-energy electron diffraction (LEED) and contact difference of potentials un Anderson option for work function measurement. For AES single cascade electron analyzer of cylindrical mirror with coaxial electron gun was used with energy of primary electrons 3 keV and current density 10 mA/cm^2 . The spectra were registered as $dN(E)/dE$, generally assuming „peak-to-peak“ distance as intensity (I) of the appropriate Auger-transition. At that procedure of Auger-signal background correction was not applied. This is quite justified, since the main focus in this paper was on determining not the absolute magnitude of Auger-signal intensity, when background correction is important, but its relative variation during measurements [17]. To obtain averaged information from surface of the studied sample the primary electron beam was defocused with effective size of crossover of about 2 mm.

The atomic structure of surface was studied using LEED with 4 grid electronic optics and coaxial electron gun Varian 981. To optimize the diffraction pattern observed on the luminescent screen located on rear side of the electron gun the energy of primary electrons varied from 60 to 100 eV. This method is sensitive to determination of structure of far atomic order in region with size comparable to wavelength of the primary electrons, this at used electron energy is 10–15 nm [18]. From methodical point of view this electron gun is very often used also to measure the contact difference of potentials in Anderson option to determine the work function (ϕ) [18]. However, there is a drawback associated with the fact that this electron gun does not allow the work function determination with high accuracy, since the electron energy cannot be decreased under control to the energy lower than 10 eV [19]. As a result, in present paper for more accurate work function determination a separate electron gun operating in energy region of primary electrons of 0 to 10 eV, was installed in the vacuum chamber. The delay curves, registered in this case during the system work function measurement, were measured in the entire range of accessible delay potentials of -5 V to $+5 \text{ V}$. Note that the Anderson method does not ensure determination of the absolute magnitude of the work function. It is sensible to change in magnitude of the work function only. To have the possibility to measure the absolute magnitudes of ϕ , a benchmark is required, Mo(110) is selected as such benchmark, its work function is 5.0 eV [19]. LEIS spectra were registered using a standard hemispherical analyzer of Escalab system using ions He^+ with primary energy 1 keV. This method feature is its sensitivity to most top atomic layer of the sample [19].

The germanium doped with Fe atoms was formed *in-situ* under the conditions of ultrahigh vacuum to exclude the uncontrollable effect of foreign admixtures as follows. Initially Ge film of definite thickness was formed by electron-beam sputtering on surface of molybdenum crystal with orientation (110)–Mo(110), supported at temperature 600 K to achieve the equilibrium state. For this

undoped (inherent) Ge with purity 99.998% was used. The advantage of choosing the thin film of germanium on the metal surface compared to bulk Ge is due to the fact that in the latter case the so-called „charging effect“ may occur, when the use of electron and ion spectroscopy methods can lead to uncontrolled charge accumulation in the sample, distorting the measurement results [19]. In case of thin film on surface of the metal sample the excessive charge occurred on the surface as result of action of primary electron ion beams is minimized by tunneling into conductive substrate. The film sputtering rate and amount of deposited Ge atoms were determined using the quartz resonator installed in the ultrahigh vacuum chamber axial-symmetrically to the studied sample, and were monitored by registration of intensity decreasing of Auger-signal of the substrate, Mo MNV (188 eV) in submonolayer region. The accuracy of measuring the surface concentration of atoms, provided by the quartz resonator, is 15%. Considering the atom radii of Mo (0.145 nm) and Ge (0.125 nm), and supposing dense packing of two-dimensional lattice of Ge on surface of Mo(110), the amount of deposited Ge atoms, and, hence, film thickness or coating (θ), for convenience can be expressed in monoatomic layers (monolayers, ML). Considering that surface concentration of atoms of Mo(110) face is $1.45 \cdot 10^{15} \text{ cm}^{-2}$ [20], the amount of Ge atoms corresponding to one monolayer, is $1.68 \cdot 10^{15} \text{ cm}^{-2}$ ($\theta = 1 \text{ ML}$). The amount of Ge atoms deposited per square centimeter of Mo(110) surface, and measured using the quartz resonator is $5.08 \cdot 10^{16}$, this corresponds to the film thickness about 7.5 nm or coating $\theta = 30 \text{ ML}$.

To the formed in such way surface of Ge film the Fe atoms were deposited by thermal sputtering from Knudsen cell. At that the substrate temperature corresponds to the room temperature. Fe film thickness and its coating were determined by method similar to the above method for Ge, considering appropriate value of atom radius of Fe (0.140 nm). Four systems were formed and studied, they differ by amount of Fe atoms deposited on Ge film (30 ML), corresponding to coating 30 ML, 21 ML, 12 ML and 6 ML, this corresponds to the following values of ratio of Fe atoms concentration to concentration of Ge atoms (n^*): 1.0, 0.7, 0.4 and 0.2 accordingly. To form mixed system Fe/Ge, the double film system Fe-Ge was heat treated, resulting in interdiffusion of Fe and Ge atoms. To clarify the nature of the mutual mixing of iron and germanium layers, the distribution of Fe and Ge atoms through the depth of the double layer was recorded. For this ion etching of layer by Ar^+ ions with energy 5 keV was performed in direction perpendicular to surface plane. Before implementation of procedure of Ge and Fe films formation the substrate Mo(110) was subjected to *in-situ* cleaning for foreign admixtures removal. For this a standard annealing procedure was implemented for Mo(110) at temperature of 1600 K was in oxygen atmosphere injected into the ultrahigh vacuum chamber up to partial pressure 10^{-6} Torr,

and further high temperature annealing of („flashing“) at temperature of 3000 K and pressure of $2 \cdot 10^{-10}$ Torr [19].

3. Results and discussion

At initial stage of formation of double system Fe-Ge the germanium film 7.5 nm ($\theta = 30 \text{ ML}$) thick was deposited to surface Mo(110) kept at 600 K to reach equilibrium state. At that it is important to know the mechanism of Ge film growth, its morphology and atomic structure, as properties of Fe film deposited on its surface fundamentally depend on these parameters.

One of the most effective methods studying the film growth mechanism, in particular, in the submonolayer region, is LEIS due to its high sensitivity to the external atomic layer of the sample [19,21]. LEIS spectra transformation during coating growth of Ge film on Mo(110) surface in the submonolayer region is shown in Figure 1. It is obvious that intensity of the most high energy line, corresponding to scattering of He^+ ions from Mo atoms, decreases, at the same time the intensity of low energy line, corresponding to Ge, increases, with stabilization at coating $\theta = 1 \text{ ML}$. The fact that at such coating there is no line, corresponding to Mo, states that continuous multilayer film Ge is formed on Mo(110) surface. Dependence of line Mo intensity on coating of Ge atoms in submonolayer region can be approximated by the straight line, see Figure 2. Such dependence states that with rise of surface concentration of Ge atoms there is growth of two-dimensional film, completely covering the substrate surface at coating $\theta = 1 \text{ ML}$. Such behavior agrees also with measurement results of concentration dependence of work function (θ) with growth of Ge film on Mo(110) surface, see Figure 3. The characteristic feature of this dependence is that the value of the work function stabilizes at level of 4.6 eV at coating close to monolayer. If there is formation of three-dimensional clusters of Ge in submonolayer region, the work function would stabilize at significantly higher values of coating, when merging of these three-dimensional islands occurs resulting in complete coating of the substrate surface. Another sequence of this dependence $\phi(\theta)$, additionally to behavior of spectra LEIS (Figure 1), is that Ge atoms upon adsorption on Mo(110) surface do not diffuse into the substrate. This indicates the formation of well visible interface Ge/Mo(110), which agrees, in particular, with results of Ageev et al. [22]. Close agreement of lattice parameters of Mo and Ge, as well as increased substrate temperature, stimulating the surface migration of Ge atoms, facilitates the formation of equilibrium atomic structure of film, corresponding to Ge(111). According to LEED results such structure is formed starting from coating 2 ML and keeps till $\theta = 30 \text{ ML}$. The corresponding LEED pattern, see Figure 1, *a*, is close to that obtained by Osiecki and Uhrberg for bulk crystal Ge(111) [23]. Figure 1, *a* shows that for film 30 ML thick there is diffraction background and band between reflexes $(00) \leftrightarrow (11)$, this confirms the

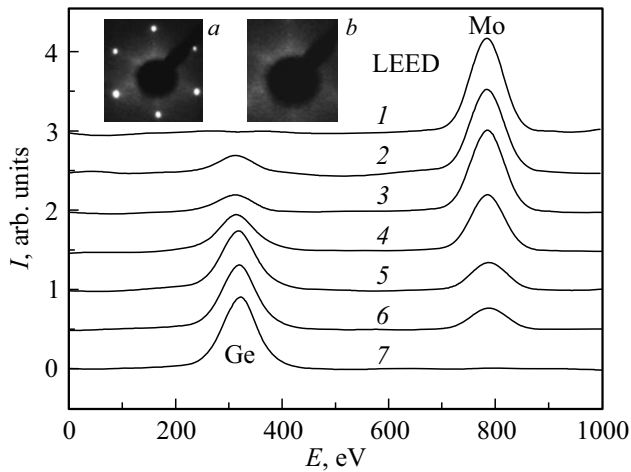


Figure 1. LEIS spectra upon increasing the coating of Ge atoms on Mo(110) surface maintained at temperature 600 K. Coating Ge, ML: 1–0; 2–0.2; 3–0.3; 4–0.5; 5–0.7; 6–0.75; 7–1.0. LEED patterns corresponding to Ge film at coating 30 ML (a) and mixed double film Fe/Ge (b).

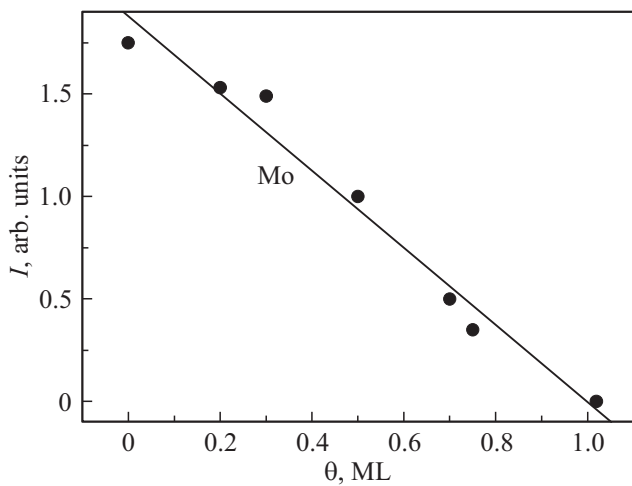


Figure 2. LEIS signal intensity of Mo vs. coating of Ge atoms in submonolayer region.

surface reconstruction attributed to the formation of structure with (2×8) [23].

Fe atoms were deposited *in-situ* by thermal sputtering from Knudsen cell on surface of the formed film Ge(111) 30 ML thick, maintained at room temperature. Like in case of Ge, LEIS results indicate the two-dimensional growth of Fe film in submonolayer region. This is confirmed by concentration dependence of work function inherent to this situation — regular decrease accompanied by stabilization of the value ϕ at coating close to monolayer (Figure 4). Unlike ordered growth of Ge film on Mo(110) surface, the LEED pattern, corresponding to Fe film (Figure 1, b), shows only the diffusion background without obvious diffraction reflexes. This indicates absence of atomic ordering of Fe film on Ge(111) surface.

To study systems characterized by different ratio of atoms concentrations of Fe and Ge (n^*), four systems Fe/Ge(111) were formed, they were characterized by different coating of Fe atoms on surface 30 of monolayer film Ge(111), namely: $\theta_{Fe} = 6, 12, 21, 30$ ML, this corresponds to value n^* , equal to 0.2, 0.4, 0.7 and 1.0, respectively. To determine nature of interaction and mutual diffusion of layers Fe and Ge, the Auger-signals were registered during heat treatment of the initially formed double films. Figure 5 shows dependence of intensities of Auger-lines of Fe and Ge on temperature of heat treatment for case $n^* = 1.0$. The annealing time at each temperature is 3 min, most likely sufficient to reach the equilibrium state for systems of discussed type. It is obvious that in temperature region 300–450°C the intensive mixing of Fe and Ge starts, it stabilizes at temperature about 550°C. To determine

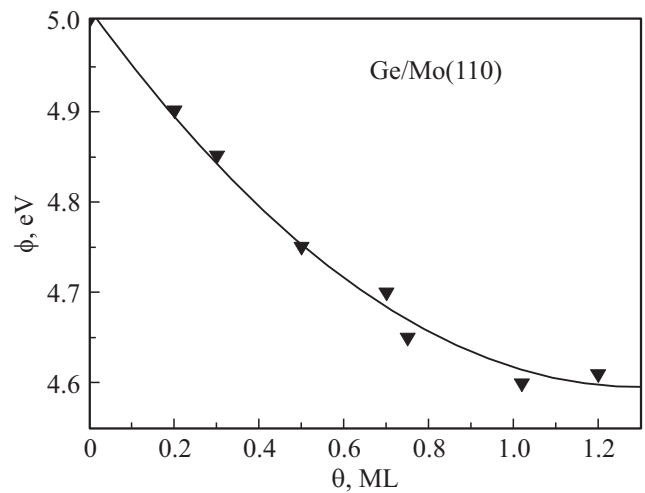


Figure 3. Work function (ϕ) vs. coating of Ge atoms on Mo(110) surfaces maintained at temperature 600 K.

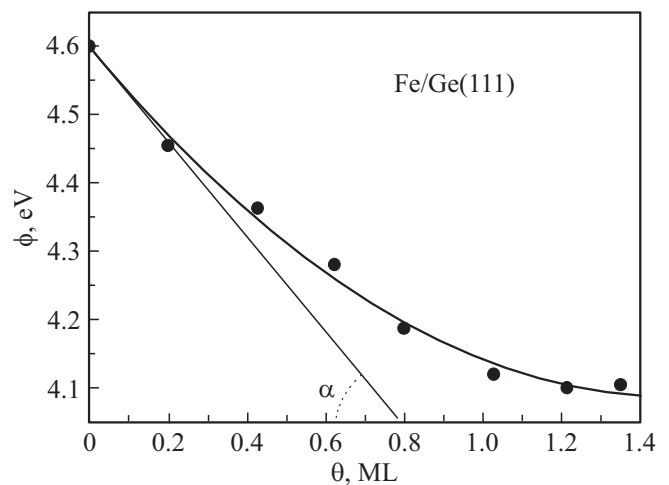


Figure 4. Work function (ϕ) vs. coating of Fe atoms on surface of Ge(111) film at temperature 300 K. Inclination angle (α) determines the value of dipole moment of chemisorption bond Fe-Ge in appropriate point.

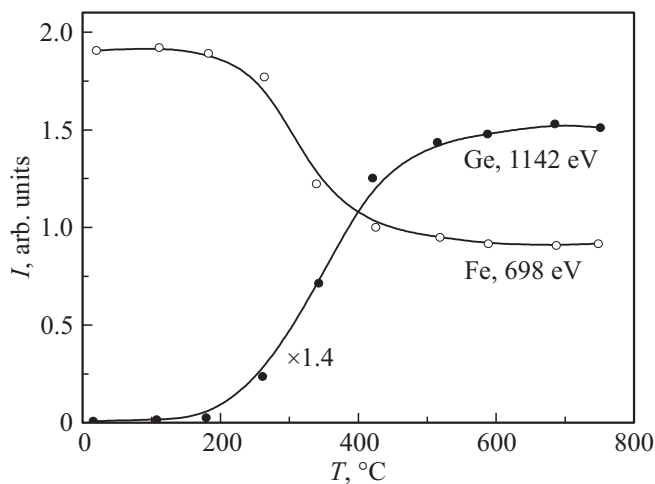


Figure 5. Intensity of Auger-signals of Fe and Ge vs. annealing temperature of initially formed double film at coating of films Fe and Ge equal to 30 ML. The annealing duration at each temperature is 3 min. The spectra were registered at temperature close to room temperature.

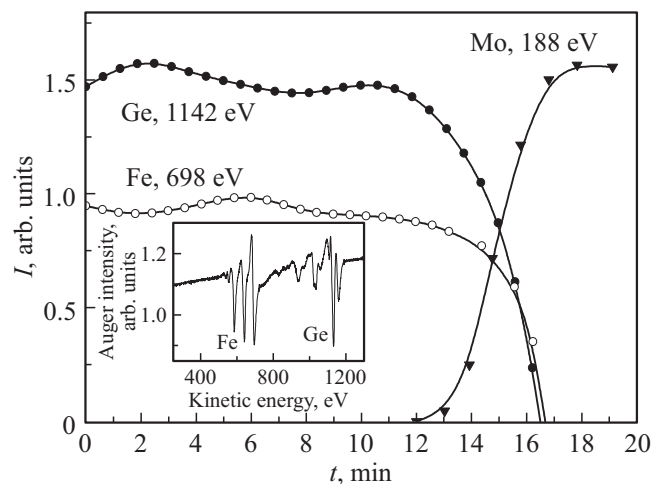


Figure 6. Intensities of Auger-signals of Fe, Ge, Mo vs. time of Ar^+ -ion etching of double system Fe(30 ML)-Ge(30 ML). Energy of ions Ar^+ is 5 keV. The insert shows the Auger-spectrum obtained after 7 min. of ion etching and corresponding to middle of mixed double film Fe/Ge.

the nature of distribution of Fe and Ge atoms through depth of the double film, it was *in-situ* etched by argon ions with synchronized registration of intensities of Auger-signals of Fe and Ge. The appropriate dependence is shown in Figure 6. Neglecting the minor modulation of intensities of Auger-signals, we can conclude that there is rather uniform distribution of elements through depth of the double layer. This is also confirmed by the Auger-spectrum shown in the insert, which corresponds to the middle of the double layer and is characterized by rather intense lines of both Fe and Ge. Formation of layer with uniform distribution of elements through its depth

is typical for all studied values n^* . The formation of such homogeneous double layers Fe/Ge is confirmed by the results of Ottaviano [6], Shabanova et al. [8] and Schleberger [10] indicating high solubility of atoms of Fe and other 3d-metals in germanium.

Considering the nature of work function change upon deposition of Fe atoms on Ge(111) film surface in the submonolayer region (Figure 4), we can suppose that in this case the polarization of charge of valence shell of Fe towards the substrate occurs. As a result the surface dipole layer is formed, it is oriented with positive pole towards vacuum, which according to general point of view [19,24] leads to the observed decrease in work function. Value of formed dipole moment (μ) can be determined from Helmholtz equation $\phi = 4\pi\theta\mu e$ [19]. Considering that value μ for definite coating of surface with Fe atoms is characterized by the inclination angle (α) of curve $\phi(\theta)$ at appropriate value θ . Value μ at $\theta \rightarrow 0$ corresponds to value of dipole moment of single atom Fe, adsorbed on Ge(111) surface, and is 0.5D. With increase in surface concentration the value of the dipole moment decreases reaching negligible value at coating close to monolayer. This is associated with redistribution of charge from chemisorption bonds on the lateral bonds between atoms Fe with their concentration increasing.

Additionally to value of the dipole moment the important parameter determining the variety of physical and chemical properties is value of absolute charge acquired by atoms of doping component. In view of experimental approach to this issue solution, the set of methods ensuring such measurements is rather limited, especially in case of ultra low concentrations of the doping component, especially for a single atom. AES is one of the methods implementing this, at least in specific cases. In particular, for 3d-metals the ratio of intensities of components of LMM-triplet (R) depends as follows on value of the valence charge of metal atom (q) [25]:

$$R = I(L_{23}M_{45}M_{45})/I(L_{23}M_{23}M_{23}) = Cq(q-1), \quad (1)$$

where $I(L_{23}M_{45}M_{45})$ and $I(L_{23}M_{23}M_{23})$ are intensities of appropriate lines, q value of charge (number of electrons) on valence level of atom, C — constant. Value C , determined from ratio (1) for free atom Fe, is 0.03. This approach was used previously to determine the absolute values of the charges of a number of 3d-metals acquired by them during chemisorption on Mo(110) surface [26,27]. Considering that for the above mentioned four types of samples characterized by different value of ratio of Fe and Ge concentrations ($n^* = 0.2, 0.4, 0.7$ and 1.0) the Auger-spectra of Fe were registered in region of LMM transitions (Figure 7). These spectra correspond to central in depth portion of mixed double film Fe/Ge, that became reachable after the ion etching. Dependence of ratio of intensities of Auger-lines $R = I(L_{23}M_{45}M_{45})/I(L_{23}M_{23}M_{23})$ on value n^* is shown in Figure 8. This dependence states that the lower the content of Fe atoms in Ge is the lower electronic charge is on its

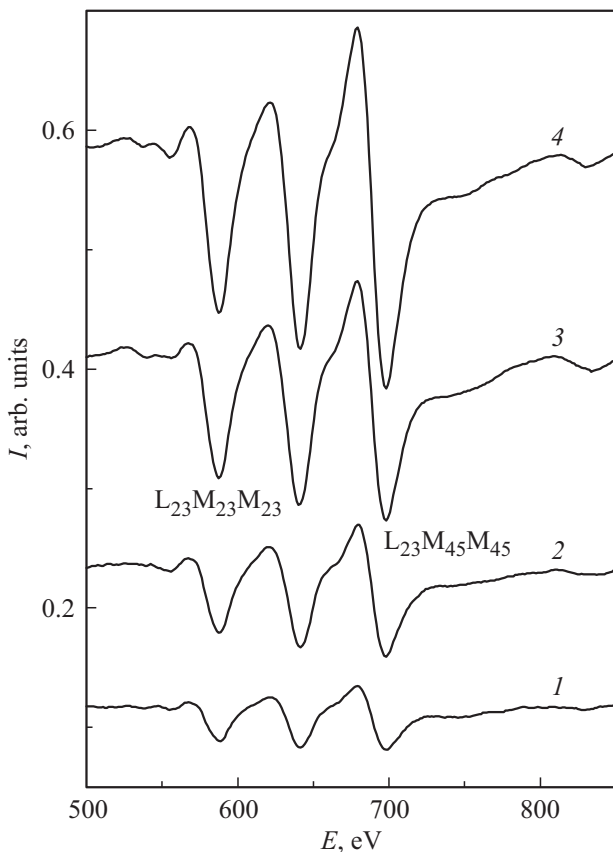


Figure 7. Fe LMM Auger-spectra corresponding to middle of double mixed film Fe/Ge for values n^* : 1–0.2; 2–0.4; 3–0.7; 4–1.0.

valence level, obviously due to its transfer to Ge. In this case ratio (1) will be written as follows

$$R = I(L_{23}M_{45}M_{45})/I(L_{23}M_{23}M_{23}) \\ = C(q - \Delta q)(q - \Delta q - 1), \quad (2)$$

where Δq is value of absolute charge transferred from Fe to Ge. Considering this the dependence in Figure 8, replotted in coordinates Δq and n^* is shown in Figure 9. It characterizes what is charge transferred from Fe to Ge depending on relative content of Fe atoms in Ge. This dependence extrapolation to $n^* \rightarrow 0$ ensures evaluation of charge of single atom Fe in germanium, which, see Figure 9, is $+0.34 \pm 0.06$ (in units of electron charge. Trend of charge transfer in the system 3d-metal–Ge is demonstrated by some theoretical studies, according to which d-orbitals of various symmetry are polarized towards the hybridized 4s4p orbitals of Ge [1,2,5]. Figure 9 shows that with increase in relative content of Fe in Ge the value of charge of Fe atom decreases from $+0.34e$ at $n^* = 0$ to $+0.07e$ at $n^* = 1$. Such significant change in value Δq indicates that nature of bond between atoms Fe and Ge significantly depends on the relative concentration of the doping component (Fe).

Comparing results shown in Figure 9 and Figure 4 we can suppose that with change in relative concentration of Fe there is change not only in value of charge of atom Fe, but also in length of bond Fe \leftrightarrow Ge (arm of dipole L). Value L , determined as $L = \mu/\Delta q$, vs. relative concentration of atoms Fe (n^*) is shown in Figure 10. Change in charge polarization degree length of bond with change in value n^* , probably, is responsible for structural transformations in lattice Ge with increase in concentration of the doping atoms Fe. In spite of that the results of LEED method sensitive to far atomic order do not demonstrate occurrence of ultrastructural reflexes (Figure 1, b), we can not exclude the formation of ordered structures in nanoscale blocks of doped germanium with size lower the coherence length of LEED. Such situation is observed, e.g.,

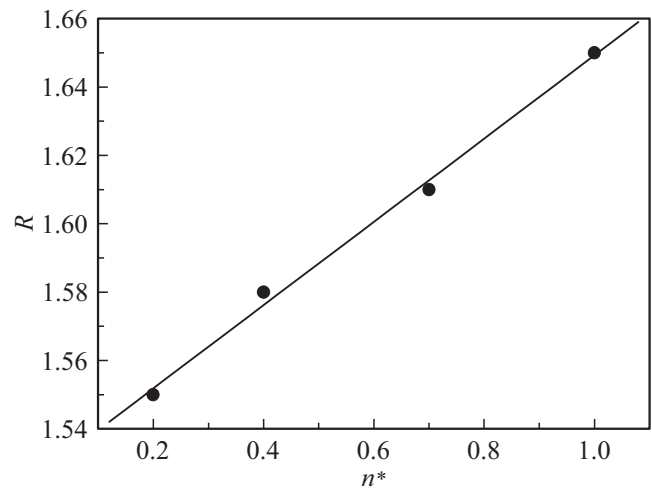


Figure 8. Ratio (R) of intensities of Auger-transitions of Fe $I(L_{23}M_{45}M_{45})/I(L_{23}M_{23}M_{23})$ vs. value n^* — ratio of concentrations of atoms Fe and Ge.

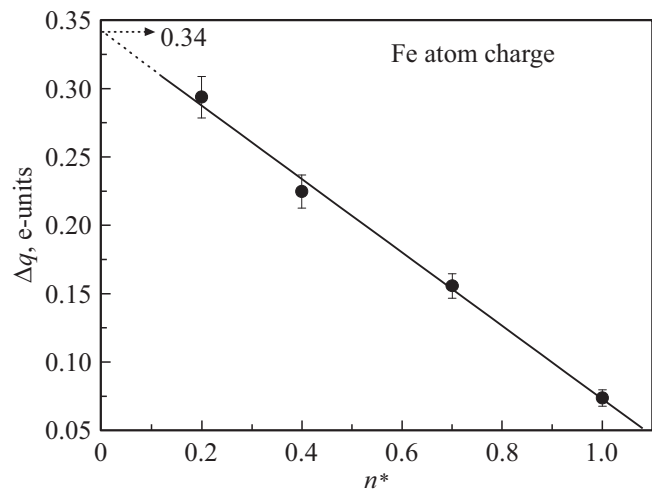


Figure 9. Absolute value of charge (Δq) of Fe atom in Ge vs. value n^* . This dependence extrapolation to $n^* \rightarrow 0$ ensures evaluation of charge of single atom Fe doped in germanium, which is $+0.34e \pm 0.06e$ (in units of electron charge).

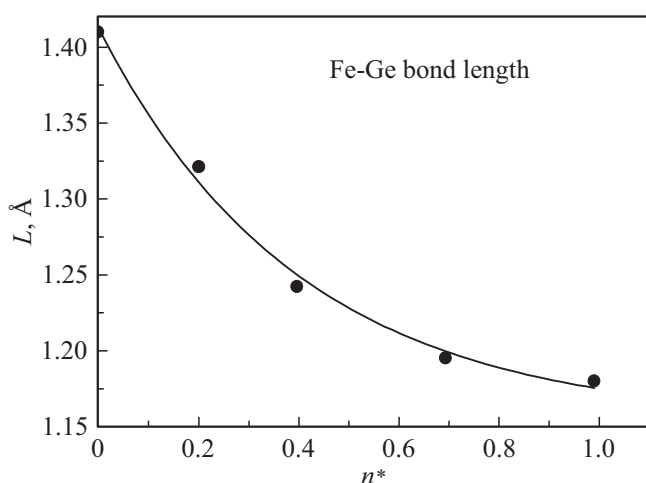


Figure 10. Length of bond Fe \leftrightarrow Ge in double mixed film vs. ratio of concentrations of atoms Fe and Ge.

during germanium doping with atoms of other 3d-metals — Cr, Ni, Cu [2,7,9]. In all these cases there is direct correlation between value of charge transfer in system TM-Ge and some structural transformations of appropriate nanoclusters occurred even at significant (within units of percent) change in relative concentration of metal atoms. In present case, see Figure 10, the length of bond Fe-Ge, which is maximum at $n^* = 0$ and is equal to 0.141 nm, with increase in relative concentration of Fe consistently decreases to permanent value 0.118 nm at same content of Fe and Ge. This circumstance is evidence of structural transformations of Ge, characterized by change in the lengths and angles of bonds, with change in the relative content of Fe. This allows the measured values of L to be used for possible identification of structural units of doped germanium at different concentrations of the doping component.

4. Conclusion

As result of study of germanium films doped with iron atoms in wide range of relative concentrations Fe/Ge, *in-situ* formed in ultrahigh vacuum we demonstrate the formation of interatomic bond Fe \rightarrow Ge polarized towards Ge. Based on analysis of the thin structure of Fe LMM of Auger-triplet in studied range of relative concentrations Fe/Ge we for the first time evaluate the absolute value of charge of Fe atom as parameter determining variety of properties of doped Ge. With increase in iron concentration the charge of Fe atom consistently decreases from values $+0.34e$ for single atom to value $+0.07e$ for the case of same concentration of Fe and Ge atoms. The result of electronic state transformation of Fe atoms in Ge is change in length of interatomic bond Fe $^+$ -Ge $^-$, which in same concentration region varies in rather wide range of 0.141 nm to 0.118 nm. The obtained values may be of interest for establishing and adjusting the electronic,

magnetic and structural properties of iron-doped germanium as the object of modern technologies of the corresponding profile.

Acknowledgments

The study was carried out within the framework of the scientific part of NOSU State Assignment of the Ministry of Education and Science of the Russian Federation (scientific topic code FEFN-2024-0002). The authors express their gratitude to the staff of NOSU laboratory of physics of adsorption phenomena, working under the State Assignment, for their assistance in study execution.

Conflict of interest

The authors declare that they have no conflict of interest.

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Translated by I.Mazurov