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ELECTRONIC STRUCTURE AND PROPERTIES

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Effect of Atomic Substitutions on Electronic Structure of $Pt_{1-x}Au_xMnSb$ Alloys ($x = 0–1$)

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Using zone calculations in the FLAPW (the full-potential linearized augmented-plane-waves) model, the information on the energy, charge and spin characteristics of $Pt_{1-x}Au_xMnSb$ ($x = 0–1$) alloys is obtained. As established, the interatomic spatial electron density decreases, covalent bonds weaken, and the cohesive energies of the alloys decrease with an increase in the concentration of Au atoms in $Pt_{1-x}Au_xMnSb$ alloys. As found, the dominant contribution to the formation of magnetic moments in $Pt_{1-x}Au_xMnSb$ alloys is made by the $3d$ electrons of manganese atoms. In alloys with $x = 0.25$ and $x = 0.5$, the total polarization of Fermi electrons is registered, which converts these alloys to the half-metallic state.

Key words: band-structure calculations, electronic structure, Heusler alloys, magnetic moments, polarized electron states, spintronics.

За допомогою зонних розрахунків у моделі FLAPW (the full-potential linearized augmented-plane-waves) отримано інформацію про енергетичні, зарядові та спінові характеристики стопів $Pt_{1-x}Au_xMnSb$ ($x = 0–1$). Встановлено, що зі збільшенням концентрації атомів Ауруму в стопах $Pt_{1-x}Au_xMnSb$ зменшується міжатомна просторова густина електронів, послаблюються ковалентні зв'язки і знижуються когезійні енергії стопів. Домінантні вклади у формування магнетних моментів у стопах

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$Pt_{1-x}Au_xMnSb$ вносять $3d$-електрони атомів Манґану. У стопах з $x = 0{,}25$ і $x = 0{,}5$ зареєстровано повну поляризацію фермієвських електронів, що переводить ці стопи в half-metallic стан.

Ключові слова: зонні розрахунки, електронна будова, стопи Гейслера, магнетні моменти, поляризовані електронні стани, спінтроніка.

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1. INTRODUCTION

Intermetallic compounds XYZ with X and Y cations and Z anions in their crystal lattices give rise to a wide series of so-called Heusler alloys (phases). Electropositive elements are most often represented by transition metals or rare earths, while electronegative elements are represented by metalloids or metals of the second half of the periodic table, such as Si, Sn, Sb, Al, Pb, Bi, *etc*. These phases have a complex of magnetic, kinetic, optical, magneto-optical, superconducting, thermoelectric, and other important properties. In the system of compounds under discussion, it is possible to implement topological insulators and the so called half-metallic state of a solid with a completely uncompensated spin density of band electrons at the Fermi level—an important property necessary in technologies for creating materials for spintronics devices. The most common cubic modification among these alloys is most often considered as four face-centred crystal lattices α, β, γ, and δ that penetrate each other [1]. If all the atomic positions are filled, the full-Heusler phases with the atomic composition X_2YZ are realized, and if a vacancy occurs in the position δ with a single probability, the so-called half-Heusler compound alloys of the XYZ are formed.

Due to the wide possibility of using such phases in science and in modern technology, an extensive literature is devoted to the study of their various properties. The state of such studies can be assessed by reading, for example, excellent reviews [2–5]. In them, as in a series of similar publications, the structural, optical, magnetic, magneto-optical, kinetic, and a number of other properties of Heusler phases are most often considered. Moreover, the mentioned studies and discussion of their results mainly concern one of the mentioned types of Heusler phases, for example, half-Heusler compounds [6–11].

There is a series of works devoted to zone calculations of the latter [3, 12–15]. Here discuss the energy band structure, magnetic moments on atoms and in primitive crystal cells, provide evidence that a compound belongs to a series of half-metals, consider the effects of the formation of atomic disorderings on the characteristics of the electronic structure of the compounds. As a comment on these works, we can add that they have not sufficiently clarified the questions about the influence of the atomic composition of compounds on their electronic structure. In particular, no attention is paid to elucidating the role of atomic substitutions in Heusler alloys on the characteristics of their electronic structure. From the point of view of zone calculations, a convenient model system of this plan is a series of alloys with the general formula $Pt_{1-x}Au_xMnSb$ ($x = 0-1$). The crystal structures and magnetic properties of $Pt_{1-x}Au_xMnSb$ compounds are studied using X-ray diffraction and magnetometry in [16]. Here, it is found that the lattice parameters of these compounds increase with increasing Au concentration.

Outside of the cited work, a number of comparative characteristics of the electronic structure of the mentioned alloys have not been studied. There is no comprehensive information about their energy characteristics, spin states of atoms, the nature of interatomic chemical bonds, the structure of valence bands and conduction bands. This work is devoted to the search for answers to these problems.

2. THE METHODOLOGY OF THE CALCULATIONS

The 'parent' half-Heusler alloys PtMnSb and AuMnSb crystallize in cubic syngony with the space group *F*-43*m* (No. 216) [7, 17]. Experimental studies of alloys of mixed atomic composition $Pt_{1-x}Au_xMnSb$ [16] did not reveal a significant rearrangement of the symmetry of their crystal lattices. To simplify the calculation procedure in this paper, the positions of the component-atoms of the $Pt_{1-x}Au_xMnSb$ alloys ($x = 0-1$) are set using the symmetry operations of a simple cubic lattice *P*. The correctness of this approach on the example of the study of half-Heusler phases is proved by us in [18, 19].

Band calculations are performed by the LAPW method [20] with a gradient approximation of the electron density (GGA-generalized gradient approximation) in the form [21]. A spin-polarized version of this method is used to calculate the characteristics of the electronic structure [22]. The parameters a of the cubic lattices of the $Pt_{1-x}Au_xMnSb$ alloys ($x = 0-1$) required for the calculations are borrowed from the experimental data, obtained in [16]. The radii (R_{mt}) of the MT (muffin-tin)—atomic spheres are chosen from the consideration of minimizing the size of the inter-sphere region in the PtMnSb alloy, which has the smallest unit cell volume. For all alloys and all the atoms in them, these radii are 2.18 Bohr radius (1 Bohr radius = $5.2918\cdot10^{-11}$ m). When calculating the characteristics of the electronic structure of all alloys, 172 points in the irreducible parts of their Brillouin zones are used. APW+lo bases are used to approximate the wave functions of the 3*d* electrons of all atoms, and LAPW bases are used for the wave functions of the remaining valence electrons. The size of the basis set is determined by setting the product $R_{\mathrm{mt}}K_{\max} = 7.0$ ($K_{\max}$ is the maximum value of the inverse lattice vector). When selecting the maximum orbital quantum number for partial waves inside the MT spheres, the value $l = 10$ is used. The non-muffin-tin matrix elements are calculated using $l = 4$. The convergence parameters for calculating the energies and charges at the final iteration of the calculations are 0.0001 Rydberg and $0.0001e^-$ (electron charge), respectively. These parameters determine the accuracy of determining the energy and charge characteristics of the alloys under study.

The binding energies (cohesion energies) are calculated as the differences between the total energies of the atoms forming the primitive cells of the alloys themselves, and the sum of the total energies of their constituent atoms, separated from each other by 'infinity'. They are determined in accordance with the recommendations [23].

When calculating the average values of the spatial electron densities in the interspheric (interatomic) regions, their volumes in cubic angstroms and the total electron charges localized in them are used. The degree of polarization (P) of Fermi electrons is determined by the formula [24]:

$$P = \frac{D_\uparrow(E_F) - D_\downarrow(E_F)}{D_\uparrow(E_F) + D_\downarrow(E_F)},$$

where $D_\uparrow(E_F)$ and $D_\downarrow(E_F)$ are the total electron state densities at the Fermi level (E_F) with the spin directions up and down, respectively.

3. RESULTS AND DISCUSSION

In our works [18, 19, 25], it is found that the chemical composition and atomic disorderings correlationally affect the interatomic bond energies, the degree of their covalence, and the parameters of the unit cells in half-Heusler alloys. Similar dependences, as indicated in Fig. 1, are also characteristic of $Pt_{1-x}Au_xMnSb$ ($x = 0$–1) alloys. It can be seen, that the increase in the parameters of the elementary cells is accompanied by a similar, monotonous, decrease in the binding energies and the spatial density of the negative electron charge in the interatomic region of the alloys. Based on this and the theory of valences [26], the following conclusion can be formulated: a decrease in the spatial density of electrons in interatomic regions with an increase in the concentration of Au atoms in $Pt_{1-x}Au_xMnSb$ alloys leads to the loosening of chemical interatomic bonds, which leads to an increase in the parameter a of their crystal lattices. By-turn, this same reason leads to a concomitant decrease in the cohesive energies in these alloys. The latter fact may indicate a loss of thermodynamic stability of $Pt_{1-x}Au_xMnSb$ alloys with an increase in gold concentrations in them.

The concentration dependence of the parameters a of the crystal lattices correlates with the charges of the atoms in the alloys. The quantitative values of these charges and their dependences on the concentrations of Au atoms in the alloys are shown in Fig. 2. It can be seen that with an increase in the concentration of gold in $Pt_{1-x}Au_xMnSb$ alloys, the number of electrons in the atomic spheres of metals monotonically decreases (for manganese atoms to $x = 0.75$), although the expected situation should be the opposite.

Indeed, in each act of replacing platinum with Au, one electron is added to the electronic subsystem from each Au atom, and with an increase in the gold concentrations in the alloys, one would expect an increase in the Q values. But this does not happen, and this can be explained by the fact that an increase in the parameter a leads to such an increase in the volume of crystal cells of alloys that the spatial density of electrons decreases with increasing gold concentrations, providing the observed concentration dependence Q. Note that the transition to alloys with a maximum concentration of gold is accompanied by a decrease in the number of electrons on the Au, Pt, and Mn atoms by

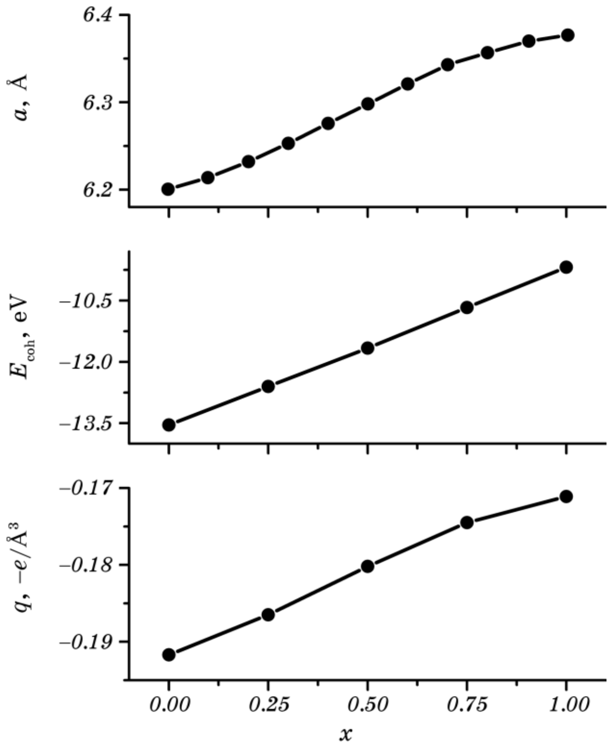

Fig. 1. Concentration dependences of lattice parameters (a) [16], atomic binding energies (E_{coh}), and spatial electron densities (q, where e—electron charge) in the interatomic regions of $Pt_{1-x}Au_xMnSb$ alloys ($x = 0{-}1$).

0.048, 0.064, and 0.246 percent, respectively. The reason for such variations in Q is an increase in the degree of delocalization of valence electrons in a series of Au, Pt, and Mn atoms—a reaction to a sequential decrease in the charges of the nuclei of these elements. In particular, the increased delocalization of the valence electrons of manganese atoms provides an increased dynamics of the formation of its chemical bonds with the surrounding atoms and, as a result, leads to large changes in the Q values. The charges of antimony atoms undergo a more complex and less noticeable (third decimal place) concentration evolution. It can be assumed that such small changes in the charge states of antimony atoms should not affect the characteristics of chemical bonds in the alloys under study. However, we note the correlation of the positions of the inflection points (x = 0–0.2 and x = 0.6–0.8) on the curve $a(x)$ (see Fig. 1) with the position of $Q(x)$ values close to $x = 0.25$ and $x = 0.75$ for Sb atoms (Fig. 2).

Additional information about the nature of chemical bonds in the studied alloys can be obtained by considering the energy structure of their valence bands and zones of vacant states. The corresponding data

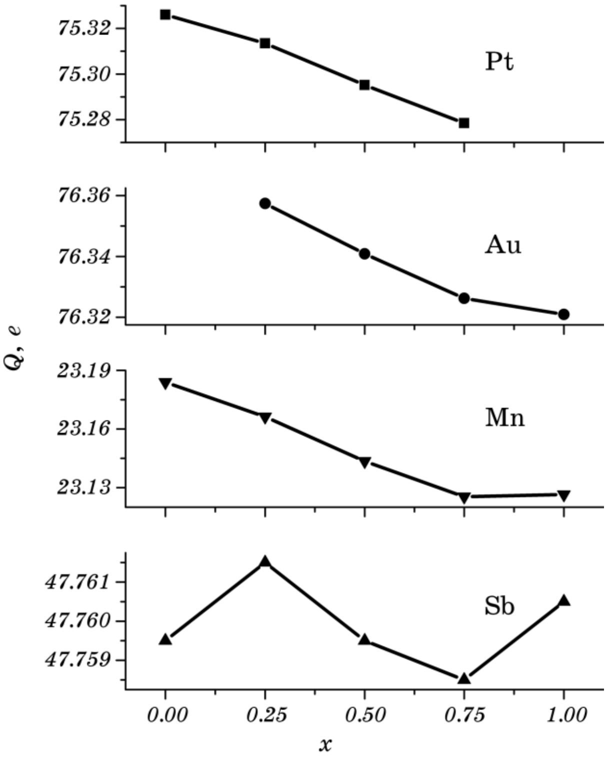

Fig. 2. Atomic charges (Q) in units of electron charge (e) in alloys $Pt_{1-x}Au_xMnSb$ alloys (x = 0–1).

in the form of curves representing the electron state densities are shown in Fig. 3. The total atomic densities of the electronic states of the studied phases for both spin orientations are complex structures that change with the atomic composition of the alloys. These changes affect the shape and energy localization of atomic valence states.

The maximum contributions to the densities of states from antimony atoms in all alloys are concentrated in the region of deep-lying (~ −10 eV) quasi-core states genetically associated with Sb5*s*-electrons. In general, these contributions are insignificant. The states of antimony atoms in the region of valence electron localization (0–−5 eV) have even smaller contributions. This indicates that the antimony atoms in the crystal lattices of the alloys are mainly held by ionic bonds.

The localization of the electronic states of metal atoms in this energy region and their hybridization (mixing) indicate that the metal atoms in the alloys are bound together mainly by covalent interaction. Their further analysis is based on the basic principles of quantum chemistry [26]: in the absence of spatial symmetry constraints, the de-

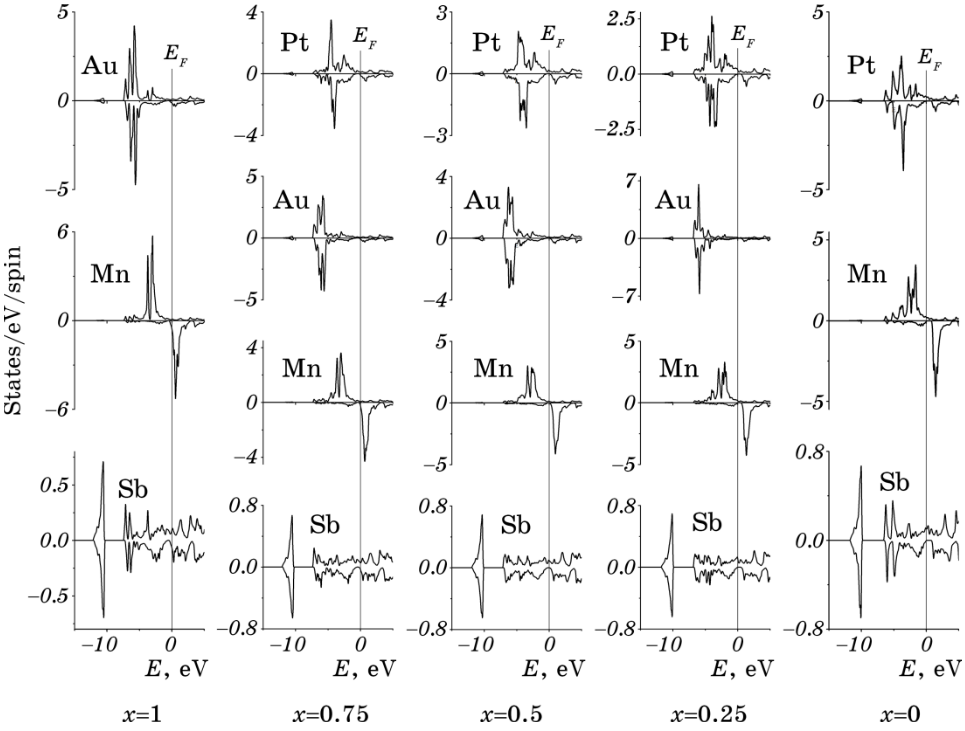

Fig. 3. Total atomic electron densities of $Pt_{1-x}Au_xMnSb$ alloys (x = 1–0). Densities with positive and negative values correspond to the spin-up and spin-down orientations of the electrons respectively. E_F is the position of the Fermi level.

gree of interactions of the electrons entering into chemical bonds depends on the proximity of their energies and manifests itself in the energy splitting of the final states and the degree of their hybridization.

As can be seen from Fig. 3, the hybridization of the electronic states of metal atoms depends on the atomic composition of the alloys. This is most clearly seen in the ‘boundary alloys’ of AuMnSb and PtMnSb. In an alloy with gold, the distributions of the valence electronic states of metals are separated on the energy scale and have a substantially localized character. Low-intensity components in the spectra of the electronic state distributions of Au and Mn atoms indicate a small mutual hybridization of their valence electrons. These facts indicate that in the alloy with gold, the covalent interactions of the metal atoms are weakened. For the PtMnSb alloy, a different picture is observed—the states of metal atoms occupy the same energy positions, hybridize well and split energetically. These facts indicate a high degree of covalence of the Pt–Mn chemical bonds, which provides high values of the cohesion energy of the PtMnSb alloy (Fig. 1).

The weakening of the covalent chemical bonds of Au atoms with platinum and manganese atoms in alloys of intermediate compositions ($x = 0.75–0.25$) is manifested in a decrease in the hybridization of the states of Au atoms, their energy localization and actual atomization during the sequential transition to the $Pt_{0.75}Au_{0.25}MnSb$ alloy. These facts, in turn, indicate the concomitant dominance of the ionic component in the chemical bonds of Au with the surrounding atoms. Opposite effects are observed in the state distributions of the valence electrons of manganese and platinum atoms in alloys of mixed atomic composition. Here, with decreasing gold concentrations, the mutual splitting of the energy and intensity of the components in the state spectra of the Pt and Mn atoms increases.

These effects are the result of concentration changes in the mutual energy positions of the valence state spectra of metal atoms. From the figure under consideration, it can be seen that a decrease in the concentrations of Au atoms in alloys is accompanied by a shift in the valence states of metal atoms to the Fermi level. The greatest displacement (~1.0 eV) is experienced by the states of manganese atoms during the transition from AuMnSb to PtMnSb. The states of the platinum atoms shift by a smaller amount, and the energy positions of the state spectra of the Au atoms practically do not change. These displacements are caused by the localization of electrons in the spheres of metal atoms (Fig. 2), which stimulates a decrease in the binding energies of their valence electrons due to intraatomic electron shielding. The greatest effect is achieved for the manganese atoms, which take on higher electron charges. In their ‘aspiration’ to the Fermi level, the valence states of manganese atoms shift to the energy region of the states of platinum atoms, and in the limiting case of PtMnSb, this process leads to the highest hybridization of the states of metal atoms. After such explanations, it can be argued that the successive substitution of Au atoms with platinum atoms increases the cohesive energy (Fig. 1) alloys of $Pt_{1-x}Au_xMnSb$ ($x = 1 \rightarrow 0$) mainly due to an increase in the covalence of the interactions of Pt–Mn atoms.

It also follows from Fig. 3 that the states of the conductivity bands of the alloys are mainly formed by the electrons of the manganese atoms with a spin-down orientation. Attention is drawn to the discrepancy between the shapes and values of the electron densities corresponding to different spin directions, which indicates the polarization of the electronic states. This effect is most pronounced in manganese.

Polarization effects lead to the appearance of magnetic moments on the atoms. It is useful to consider the question to what extent certain electronic states are involved in the formation of magnetic moments on the atoms of the alloys under discussion? The relevant data are shown in Fig. 4. It can be seen that the determining contributions to the formation of magnetic moments in alloys are assigned to the 3*d* electrons of manganese atoms. It can be seen that the dominant role in this proc-

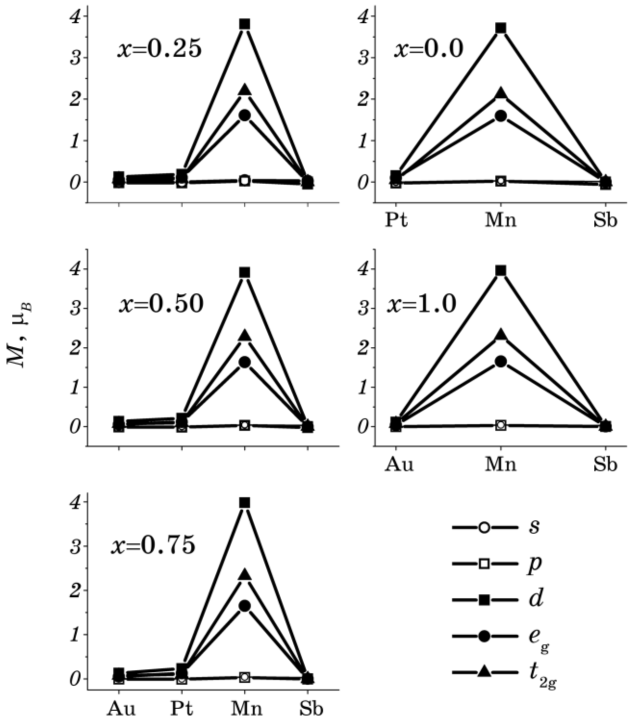

Fig. 4. Partial contribution of electronic states to the formation of magnetic moments (M, μ_B—Boron magneton) on atoms in $Pt_{1-x}Au_xMnSb$ alloys ($x = 0$–1).

ess is played by the electrons of its t_{2g}- and to a lesser extent e_g-orbitals. The contributions of Mn*s*, *p*-electrons are negligible. This can be fully attributed to the electrons of all the symmetries of other metal atoms and antimony in all types of alloys.

Figure 5 shows the concentration dependences of the magnetic moments localized on the t_{2g}- and e_g-orbitals of the manganese atoms. It can be seen that the increase in the concentrations of Au atoms in the $Pt_{1-x}Au_xMnSb$ alloys increases the magnetic moments on manganese up to the values of $x = 0.75$. Then there is a summary decline in the values of the magnetic moments. The same decrease in the magnetic moments on the manganese atoms is recorded in the experiment [16] at gold concentrations in alloys with $x > 0.6$. As defined here, the magnetic moment per Mn atom in these compounds has a maximum value of $4.30\mu_B$ at $x = 0.6$. In our work, the maximum magnetic moment on the manganese atoms is fixed for the $Pt_{0.25}Au_{0.75}MnSb$ alloy and is $4.06\mu_B$, which is close to the experimental value. Note that within the framework of the accepted model (see the methodology of the calculations), the

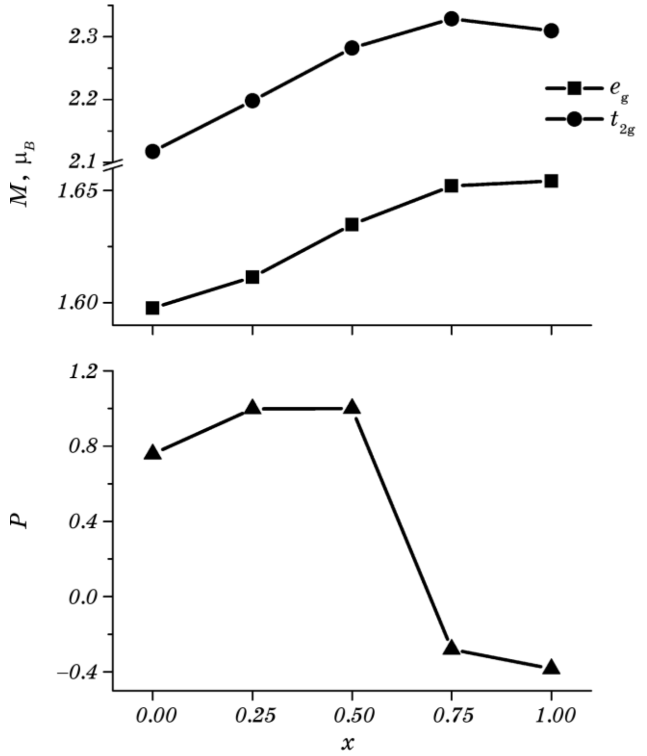

Fig. 5. Concentration dependences of magnetic moments (*M*), localized on the t_{2g}- and e_g-orbitals of manganese atoms, and polarizations (*P*) of electrons at the Fermi level of $Pt_{1-x}Au_xMnSb$ alloys ($x = 0–1$).

$Pt_{0.4}Au_{0.6}MnSb$ alloy could not be calculated.

The substituting Au atoms change the polarization of the P electrons at the Fermi level (Fig. 5). The transition from the PtMnSb metal alloy with a relatively high degree of electron polarization to the alloys with $x = 0.25$ and $x = 0.50$ is accompanied by a complete polarization of the Fermi electrons ($P = 1$) and transfers these alloys to the half-metallic state. A further increase in the content of Au atoms in alloys with $x = 0.75$ and $x = 1$ transforms them into a state of metallic conductivity with negative P.

4. CONCLUSIONS

1. With an increase in the concentration of Au atoms in $Pt_{1-x}Au_xMnSb$ alloys, the interatomic spatial density of electrons decreases, which leads to a weakening of interatomic covalent bonds and, as a result, to a decrease in the cohesive energies of the alloys and an increase in the parameters $\boldsymbol{a}$ of their crystal lattices.
2. The antimony atoms in the lattices of the $Pt_{1-x}Au_xMnSb$ alloys are held by ionic bonds, whereas the metal atoms in the alloys under study are bound together mainly by covalent interactions. In the AuMnSb alloy, the covalent interactions of metal atoms are weakened, whereas in the platinum alloy, the degree of covalence of Pt–Mn bonds is maximal, which provides abnormally high values of the cohesion energy of the PtMnSb alloy. The sequential substitution of Au atoms with platinum atoms increases the cohesion energy of $Pt_{1-x}Au_xMnSb$ alloys ($x = 1 \rightarrow 0$) by increasing the covalence of the interactions of Pt–Mn atoms.
3. The main contribution to the formation of magnetic moments in $Pt_{1-x}Au_xMnSb$ alloys is made by 3d electrons of manganese atoms. The dominant role in this process is played by the electrons of its t_{2g}- and to a lesser extent e_g-orbitals. The contributions of Mns,p-electrons are insignificant, and the contributions of electrons of other metals and antimony in all types of alloys are also small. An increase in the concentration of Au atoms in the $Pt_{1-x}Au_xMnSb$ alloys leads to an increase in the magnetic moments on the t_{2g}- and e_g-orbitals of manganese to the values of $x = 0.75$, then there is a total decrease in the values of the magnetic moments.
4. Substitution of platinum atoms with Au in $Pt_{1-x}Au_xMnSb$ alloys changes the electron polarization at the Fermi level. The transition from the PtMnSb alloy with a relatively high degree of electron polarization to the alloys with $x = 0.25$ and $x = 0.5$ is accompanied by full polarization of the Fermi electrons and converts these alloys to the half-metallic state. A further increase in the content of Au atoms in alloys with $x = 0.75$ and $x = 1$ transforms them into a state of metallic conductivity with negative values of electron polarization.

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