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Effect of Atomic Substitutions on the Electronic Structure of $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ ($\text{Me} = \text{Ni}, \text{Au}, x = 0.0–1.0$)

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Using zone calculations in the FLAPS (the full-potential linearized augmented-plane-waves) model, information is obtained on the energy, charge and spin characteristics of $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ alloys ($\text{Me} = \text{Ni}, \text{Au}, x = 0.0–1.0$). As established, with an increase in the concentration of nickel or gold atoms the interatomic spatial density of electrons decreases, covalent bonds weaken and the binding energies of atoms in alloys decrease. As found, the dominant contributions to the formation of magnetic moments are made by $3d$ electrons of manganese atoms, and the polarization of electrons at Fermi levels depends on the composition of alloys.

Key words: bandstructure calculations, Heusler alloys, bandstructure, magnetic moments, polarized bandstructure state, spintronic.

За допомогою зонних розрахунків в рамках моделю FLAPS (the full-potential linearized augmented-plane-waves) одержано інформацію про енергетичні, зарядові та спінові характеристики стопів $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ ($\text{Me} = \text{Ni}, \text{Au}, x = 0,0–1,0$). Встановлено, що зі збільшенням концентрації атомів Нікелю або Ауруму зменшується міжатомна просторова густина електронів, послаблюються ковалентні зв'язки і знижуються енергії зв'язку атомів у стопах. Виявлено, що домінують вклади у формування магнетних моментів вносять $3d$ -електрони атомів Мангану, а поляризація електронів на рівнях Фермі залежить від складу стопів.

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

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1. INTRODUCTION

A variety of materials with complex crystal structures that exhibit unusual electronic and magnetic properties have always attracted considerable attention from both theorists and experimenters for the purpose of using these unconventional properties in possible practical applications. One such group of materials which is being actively investigated at the moment are the Heusler compounds. The parent Heusler compounds, the so-called the full-Heusler phases ($L2_1$ -structures), have the general formula X_2YZ , where X and Y are transition metals and Z is an *sp*-valent elements. The half-Heusler phases ($C1_b$ structures) have the same structure, except that one of the sites occupied by the X atom in the parent compound is empty, giving a general formula XYZ [1]. These phases have [2–5] 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.

In 1983 de Groot and co-workers [6] discovered by *ab-initio* calculations that one of the half-Heusler alloys, NiMnSb, is half-metallic, *i.e.*, the minority band have a band gap at the Fermi level. This conclusion is confirmed in a series of other works—see, for example, reviews [7, 8]. $C1_b$ type Heusler compounds have attracted much attention since the discovery of the very large Kerr effect in PtMnSb [9]. This large effect, a maximum of 1.3° at 1.7 eV in the room-temperature Kerr-rotation spectrum, has been attributed to the unusual electronic structure of this material. Long-standing calculations [6] of the zone structure showed that PtMnSb belongs to the class of so-called half-metallic materials, but there is no convincing experimental evidence for this fact in the literature. Moreover, in the calculations [7, 8], the value of 66.5% was obtained for the polarization of valence electrons at the Fermi level in the PtMnSb compound. The addition of gold atoms to the MnSb ‘matrix’ preserves the structural $C1_b$ type of the AuMnSb alloy [10]. The total and partial magnetic moments of the atoms, as well as the equilibrium parameters of the cubic cell of the alloy, are calculated [11] with low accuracy. $MeMnSb$ alloys ($Me = Ni, Pt, Au$) are ferromagnets with Curie temperatures, resistive and magnetic characteristics depending on the type of *Me* atom [10].

An effective way to influence the properties of Geisler phases is the

synthesis of solid solutions based on them. Good model systems of this plan are a series of $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ alloys ($\text{Me} = \text{Ni, Au}$, $x = 0.0\text{--}1.0$) [12, 13]. Here, using x-ray diffraction, the parameters of their cubic lattices were determined, as well as magnetic, magneto-optical characteristics, temperatures Curie and temperature dependence of saturation magnetization were measured.

Outside of the cited works, a number of comparative characteristics of the electronic structure of these alloys have not been studied. There was no complete information about their energy characteristics, the spin and charge states of atoms, the nature of interatomic chemical bonds, the structure of valence bands and conduction bands. This paper is devoted to finding answers to these problems.

2. THE METHODOLOGY OF THE CALCULATIONS

The ‘parent’ half-Heusler MeMnSb ($\text{Me} = \text{Ni, Pt, Au}$) alloys crystallize in cubic syngony with the space group $F\bar{4}3m$ (No. 216) [10]. Experimental studies of alloys of mixed atomic composition $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ alloys ($\text{Me} = \text{Ni, Au}$, $x = 0.0\text{--}1.0$) [12, 13] did not reveal a significant rearrangement of the symmetry of their cubic crystal lattices. To simplify the calculation procedure in this paper, the positions of the component—atoms of the $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ alloys ($\text{Me} = \text{Ni, Au}$, $x = 0.0\text{--}1.0$) 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 [14, 15].

Band calculations were performed by the LAPW method [16] with a gradient approximation of the electron density (GGA-generalized gradient approximation) in the form [17]. A spin-polarized version of this method was used to calculate the characteristics of the electronic structure [18]. The parameters a of the cubic lattices of the $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ alloys ($\text{Me} = \text{Ni, Au}$, $x = 0.0\text{--}1.0$) required for the calculations are borrowed from the experimental data, obtained in [12, 13]. The radii (R_{mt}) of the MT (muffin-tin)—atomic spheres were chosen from the consideration of minimizing the size of the inter-sphere region in the NiMnSb alloy, which has the smallest unit cell volume. For all alloys and all the atoms in them, these radii were 2.18 Bohr radius (1 Bohr radius = $5.2918 \cdot 10^{-11}$ m). When calculating the characteristics of the electronic structure of all alloys, 172 points in the irreducible parts of their Brillouin zones were used. APW + lo bases are used to approximate the wave functions of the 3d electrons of all atoms, and LAPW bases are used for the wave functions of the remaining valence electrons. The size of the basis set was determined by setting the product $R_{\text{mt}}K_{\text{max}} = 7.0$ (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 were calculated using $l = 4$.

The binding energies (cohesion energies) were calculated as the differences between the total energies of the atoms forming the unit cells of the alloys themselves, and the sum of the total energies of their constituent atoms, separated from each other by 'infinity'. They were determined in accordance with the recommendations [19].

The degree of polarization (P) of Fermi electrons was determined by the formula [20]:

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

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 the works [14, 15, 21], it was found that the chemical composition and atomic disordering affect the interatomic bond energies, the de-

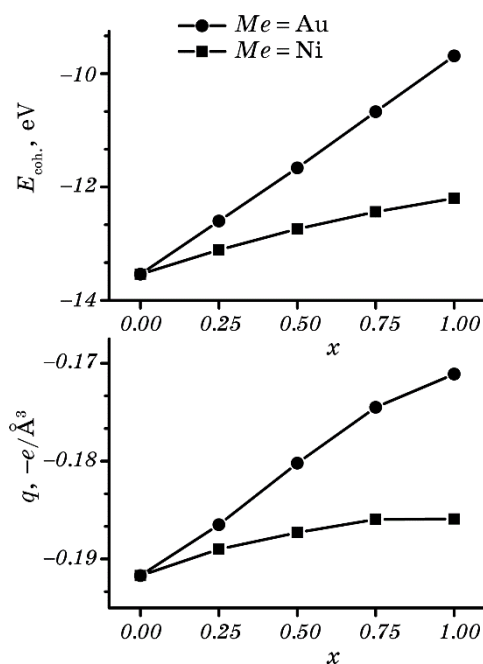


Fig. 1. Concentration dependences of atomic binding energies ($E_{\text{coh.}}$), and spatial electron densities (q , e —electron charge) in the interatomic regions of $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ alloys.

gree 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 $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ ($\text{Me} = \text{Ni}, \text{Au}, x = 0.0-1.0$) alloys. It can be seen that the drop in the charge density in the interatomic region is accompanied by a decrease in the binding energies of the atoms in the alloys under study. Based on this and the valence theory [22], the following conclusion can be formulated: a decrease in the spatial density of electrons in interatomic regions with an increase in the concentration of nickel or gold atoms in $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ ($\text{Me} = \text{Ni}, \text{Au}, x = 0.0-1.0$) alloys leads to a weakening of covalent chemical interatomic bonds. This fact may indicate a possible loss of thermodynamic stability of $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ ($\text{Me} = \text{Ni}, \text{Au}, x = 0.0-1.0$) alloys with an increase in the concentrations of substitution atoms in them. This instability is most characteristic of alloys with gold, since their binding energies ($E_{\text{coh.}}$) are significantly lower in comparison with those for phases with nickel.

The concentration dependences of the parameters a of the crystal lattices of alloys correlate with the charges of atoms (Fig. 2). The de-

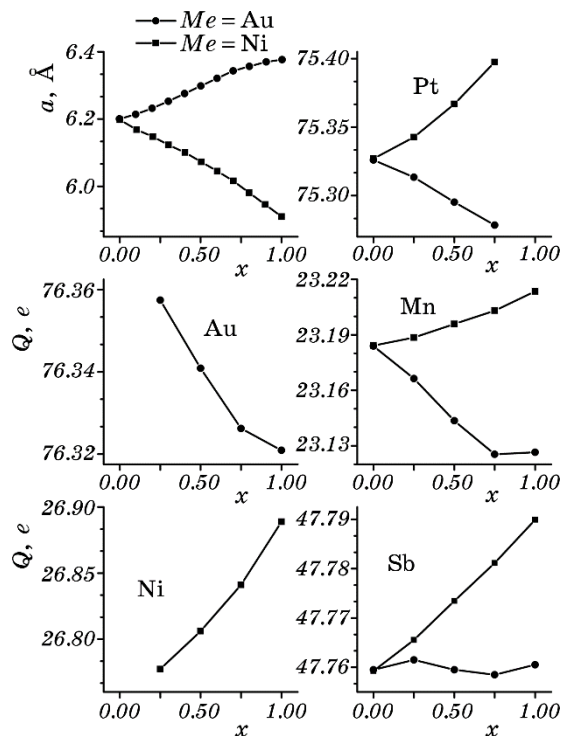


Fig. 2. Concentration dependences of atomic charges (Q , e —electron charge) and parameters (a) [13] of conventional cells of $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$.

clining trend of curve $a(x)$ with an increase in nickel concentrations in $\text{Pt}_{1-x}\text{Ni}_x\text{MnSb}$ alloys ($x = 0.0-1.0$) is due to a reduced atomic radius of nickel 1.24 Å compared to the same for platinum atoms, equal to 1.39 Å [23]. As a consequence of this and the already mentioned 'striving' of alloys for dense atomic packages (F-structures) this inevitably leads to a decrease in the values of parameter a with an increase in the nickel concentration in the alloys. If the atomic radii of the substituting components exceed the size of the platinum atoms, then, according to the above considerations, in a series of solid solutions, the parameter a should increase with increasing concentrations of the embedded atoms. Indeed, such a pattern can be seen for a series of $\text{Pt}_{1-x}\text{Au}_x\text{MnSb}$ alloys (Fig. 2) for which the atomic radius of gold is 1.44 Å [23]. Another confirmation of the above assumptions is the course of the dependence $a(x)$ in $\text{Pt}_{1-x}\text{Cu}_x\text{MnSb}$ series alloys ($x = 0.0-1.0$) [13]: here, at an atomic radius of 1.28 Å copper [23], a decreasing course of the curve $a(x)$ at $x \rightarrow 1.0$ is observed, as in nickel alloys. It should be noted that the current values of $a(x)$ in copper alloys exceed those for nickel alloys [13]. The latter circumstance is explained by the somewhat larger radius of the copper atoms.

From Figure 2 it can be seen that with increasing nickel concentration in $\text{Pb}_{1-x}\text{Ni}_x\text{MnSb}$ alloys, the number of electrons in atomic spheres increases monotonically. Note that the transition to alloys with a maximum nickel concentration is accompanied by an increase in the number of electrons on the Pt, Sb, Ni and Mn atoms by 0.09, 0.06, 0.41 and 0.12 percent, respectively. A different situation is observed for alloys with gold. Here, with an increase in the concentration of gold in $\text{Pb}_{1-x}\text{Au}_x\text{MnSb}$ alloys, the number of electrons in the atomic spheres of metals monotonically decreases (for manganese atoms up to $x = 0.75$), although the expected situation should be the opposite. Indeed, in each act of replacing platinum with gold, one electron is added to the electronic subsystem from each gold 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 volumes of crystal cells of alloys that the spatial density of electrons decreases, providing the observed concentration dependence of 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 0.048, 0.064, and 0.246 percent, respectively. The charges of antimony atoms undergo a more complex and less noticeable (third decimal place) concentration evolution.

As can be seen, the changes in Q values for Sb, Pt and Au atoms are insignificant, whereas for 3d metal atoms the Q variations turn out to be significantly higher. A possible reason for such variations in Q is an increase in the degree of delocalization of valence electrons in a num-

ber of atoms Au, Pt, Sb, and Ni, Mn—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 nickel and manganese atoms provides an increased dynamics of the formation of their chemical bonds with the surrounding atoms and, as a result, leads to large changes in the Q values.

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 in the form of curves representing the electron state densities are shown in Fig. 3.

The total densities and total atomic densities of the electronic states of the studied phases for both spin orientations are complex structures that vary depending on the atomic composition of the alloys. It can be seen from the discussed figure that the influence of the atomic composition of alloys manifests itself in a change in the shape and energy localization of the densities of electronic states.

The maximum contributions to the densities of states from antimo-

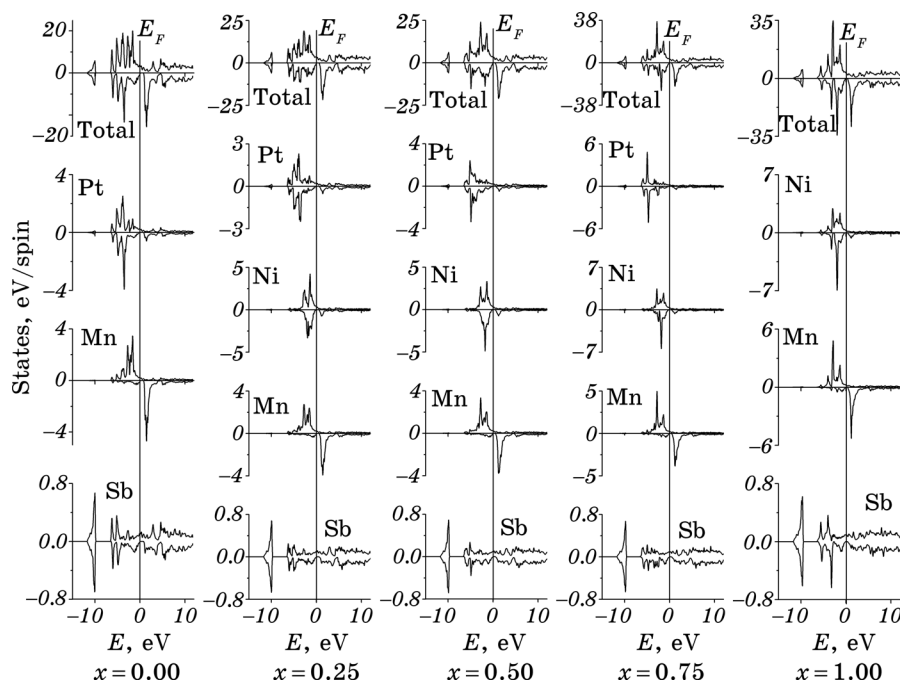


Fig. 3. Total electron densities (top panel) and total atomic electron densities of $\text{Pt}_{1-x}\text{Ni}_x\text{MnSb}$ alloys ($x = 0.0-1.0$). Densities with positive and negative values correspond to the spin-up and spin-down orientations of the electrons respectively. E_F is the position of the Fermi level.

ny atoms in all alloys are concentrated in the region of deep lying (~ -10 eV) quasi-core states genetically associated with Sb 5s electrons. In general, these contributions are insignificant. The states of antimony atoms in the region of valence electron localization ($-5-0$ 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 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 [22]: in the absence of spatial symmetry constraints, the degree 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 Figure 3, these characteristics of the electronic states of metal atoms depend on the atomic composition of the alloys. In the PtMnSb alloy, the states of metal atoms occupy close energy positions, hybridize well and split energetically. These facts indicate a high degree of covalence of Pt–Mn chemical bonds, which provides high values of the binding energy of the PtMnSb alloy (Fig. 1).

A consistent increase in the nickel concentration in $\text{Pb}_{1-x}\text{Ni}_x\text{MnSb}$ alloys ($x = 0.0-1.0$) is accompanied by a decrease in the degree of hybridization of the electronic states of platinum atoms. In the limiting case ($x = 0.75$), the electronic states of platinum turn out to be localized in a narrow energy region remote from those similar for nickel and manganese atoms. The latter remain split and hybridized when the nickel concentration changes, thereby providing covalent Mn–Ni interactions. Based on these arguments, we can understand the fact that the decrease in the binding energy (Fig. 1) of $\text{Pb}_{1-x}\text{Ni}_x\text{MnSb}$ alloys ($x = 0.0-1.0$) alloys is probably due to a decrease in covalent interactions of platinum atoms with surrounding atoms.

It also follows from Figure 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.

A similar analysis of the distribution of electron densities of alloys with gold led to the following conclusions. It is established here that antimony atoms in the lattices of $\text{Pt}_{1-x}\text{Au}_x\text{MnSb}$ alloys are held by ionic bonds, whereas metal atoms in the studied alloys are bound to each other 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 binding energy of the PtMnSb alloy. Sequential replacement of gold atoms with platinum atoms increases the binding energies of $\text{Pt}_{1-x}\text{Au}_x\text{MnSb}$ alloys ($x = 1.0-0.0$) by increasing the covalence of interactions of Pt–Mn atoms.

There was also a discrepancy between the shapes and values of electron densities corresponding to different spin directions, which indicates the polarization of electronic states. As in nickel alloys, this effect was most pronounced for the electronic states of manganese atoms.

Polarization effects lead to the appearance of magnetic moments on 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 corresponding data are shown in Fig. 4. It can be seen that the determining contribution to the formation of magnetic moments in alloys is associated with the $3d$ electrons of manganese atoms. The contribution of Mn s , p electrons is insignificant. This can be completely attributed to the electrons of all symmetries of atoms of other metals and antimony in all types of al-

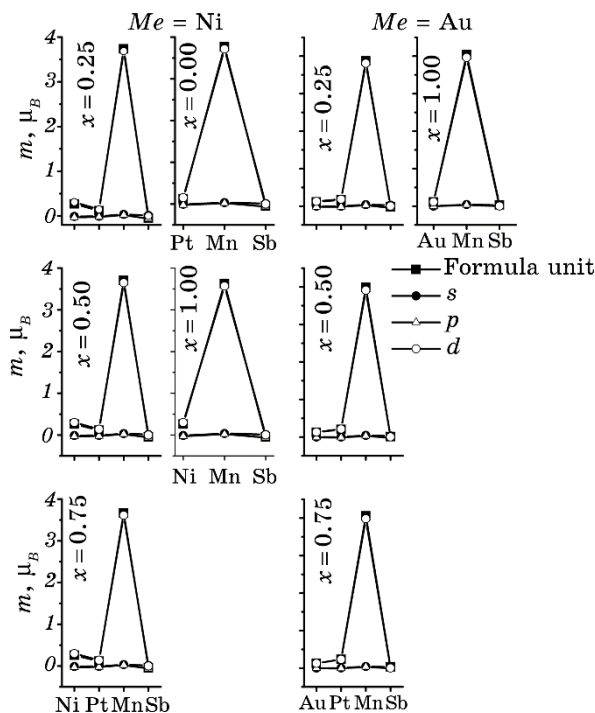


Fig. 4. Partial contribution of electronic states to the formation of magnetic moments (m, μ_B —Boron magneton) on atoms in $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ alloys ($x = 0.0-1.0$).

loys.

Figure 5 shows the concentration dependences of magnetic moments and electron polarizabilities in $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ alloys ($x = 0.0-1.0$). In the experimental work [12] it was noted that the values of these magnetic moments essentially remain constant over the entire range of nickel concentrations in alloys. In Figure 5, this is indicated by a horizontal line, which, according to the authors, is the result of averaging experimental data. These data at the qualitative level coincide with those obtained in this work. Indeed, the calculated values of the magnetic moments practically do not depend on the concentration of nickel atoms in the studied alloys. Recall that the 'outliers' of the values of experimentally measured magnetic moments at the content of nickel atoms $x = 0.25$ in alloys are associated [12] with the presence of other phases with concentrations reaching 15%. In general, the samples studied here also contained other phases in concentrations up to 5%. Perhaps these reasons led to systematic differences between the experimental and calculated values of magnetic moments. Note that these differences for most alloys ($x \geq 0.25$) were $\sim 1.5\%$. As for the initial

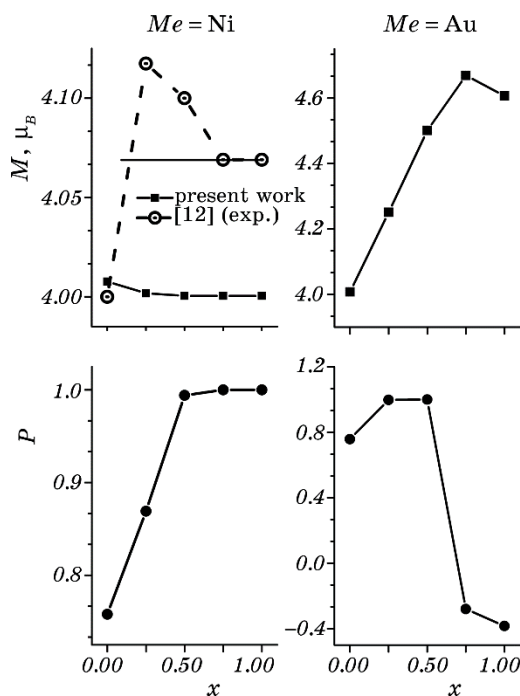


Fig. 5. Magnetic moments (M) per formula unit of $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ alloys ($x = 0.0-1.0$). The horizontal solid line in the experimental part of the figure is the result of averaging the measurements [12]. P —electron polarization at the Fermi level in $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ alloys.

composition of PtMnSb, the experimental and calculated values of the magnetic moments actually coincided.

Substituting nickel atoms change the polarization P of electrons at the Fermi level (Fig. 5). The transition from the PtMnSb metal alloy with a relatively high ($P = 0.76$) electron polarization to alloys with $x \geq 0.5$ is accompanied by full polarization of Fermi electrons ($P = 1.0$) and converts these alloys to half-metallic state.

Figure 5 also shows that an increase in the concentration of gold atoms in $\text{Pb}_{1-x}\text{Au}_x\text{MnSb}$ alloys increases their magnetic moments up to concentrations $x = 0.75$. Then there is a decrease in the values of magnetic moments. The same decrease in magnetic moments was recorded in the experiment [13] 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 manganese atoms was fixed for the $\text{Pt}_{0.25}\text{Au}_{0.75}\text{MnSb}$ alloy and amounted to $4.06\mu_B$, which is close to the experimental value. Note that within the framework of the accepted model (see calculation methodology), the $\text{Pt}_{0.4}\text{Au}_{0.6}\text{MnSb}$ alloy could not be calculated.

Substituting gold atoms change the polarization of P electrons at the Fermi level (Fig. 5). The transition from the PtMnSb metal alloy with a relatively high degree of electron polarization to alloys with $x = 0.25$ and $x = 0.50$ is accompanied by complete polarization of Fermi electrons ($P = 1.0$) and converts these alloys to a half-metallic state. A further increase in the content of gold atoms in alloys with $x = 0.75$ and $x = 1.0$ translates them into a state of metallic conductivity.

4. CONCLUSIONS

1. With an increase in the concentration of nickel or gold atoms in $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ ($x = 0.0-1.0$) alloys, the interatomic spatial density of electrons decreases, which leads to a weakening of interatomic covalent bonds and, as a consequence, to a decrease in the binding energies of the alloys. These energies for alloys with gold are significantly lower compared to those for phases with nickel.
2. The course of the concentration dependences of the parameters $a(x)$ of cubic crystal lattices of $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ solid solutions ($\text{Me} = \text{Ni}, \text{Cu}, \text{Au}, x = 0.0-1.0$) is determined by the ratio of the radii of the substitution atoms and platinum. If this ratio is less than one ($\text{Me} = \text{Ni}, \text{Cu}$), then the dependence $a(x)$ ($x \rightarrow 1.0$) has a descending and in the opposite case ($\text{Me} = \text{Au}$) an increasing character.
3. The densities of the electronic states of $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ ($x = 0.0-1.0$) alloys are complex structures that vary in shape, energy position and localization. The zones of valence electrons ($-5-0$ eV) of alloys are dominated by hybridized states of metals, while the vacant states are

formed mainly by Mn electrons with spins oriented downwards.

4. Antimony atoms in the crystal lattices of $\text{Pt}_{1-x}\text{Me}_x\text{MnSb}$ ($x = 0.0-1.0$) alloys are mainly held by ionic bonds, whereas metal atoms are mainly covalently bound to each other. Covalent interactions are maximal in PtMnSb and with an increase in the concentration of nickel or gold in alloys, they weaken due to a decrease in the role of platinum valence electrons in the formation of chemical bonds.

5. The densities of electronic states with different spin orientations do not correspond to each other, which indicates the polarization of electrons in alloys. Polarization effects lead to the appearance of magnetic moments on the atoms. The determining contributions to the formation of magnetic moments in alloys are associated with the 3d electrons of manganese atoms. The values of the magnetic moments practically do not depend on the concentration of nickel atoms in the studied alloys. An increase in the concentration of gold atoms in $\text{Pb}_{1-x}\text{Au}_x\text{MnSb}$ alloys leads to an increase in their magnetic moments up to concentrations with $x = 0.75$, then there is a decrease in the values of magnetic moments.

6. Substituting nickel or gold atoms change the polarization of P electrons at the level of Fermi alloys. The transition from the PtMnSb metal alloy with a relatively high ($P = 0.76$) electron polarization to alloys with a nickel concentration of $x = 0.5$ is accompanied by complete polarization ($P = 1.0$) of Fermi electrons and converts these alloys to a half-metallic state. $\text{Pt}_{1-x}\text{Au}_x\text{MnSb}$ alloys with $x = 0.25$ and $x = 0.50$ are also half-metals, and beyond these concentrations alloys are metals.

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