COMPOSITION AND ELECTRONIC PROPERTIES OF FILM CoSiO BY ION IMPLANTATION

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Abstract. The morphology, composition and electronic properties of the CoSiO film obtained on the $CoSi_2$/Si (111) surface by implantation of O_2^+ ions in combination with annealing were studied. Parameters of energy zones are determined and information about the density of the state of electrons of the valence zone and conductivity zone is obtained. In particular, it is shown that the band gap width of this film is ~ 2.4 eV. It was ascertained that the CoSiO/Si/$CoSi_2$ heterosystem is very promising for creating efficient solar energy devices.

Keywords: Surface, annealing, nanoscale system, ion implantation, nanocrystalline phase, energy zone, band gap width, solar energy.

1.Introduction.

Nano-dimensional structures and films with different band gap widths based on Si can be used to construct various structures such as metal-dielectric-semiconductor and semiconductor-dialectical-semiconductor, ultra-high frequency transistors and diodes, solar energy modules, etc. In particular, to increase the efficiency of solar cells it is necessary to create structures that intensively absorb light radiation in the energy range from 0.3 - 0.4 eV to 3.5 - 4 eV. The width of the forbidden $CoSi_2$ zone is 0.5 - 0.7 eV, silicon - 1.1 eV, silicon oxides ≈ 8.5 eV, and silicon nitride - 4.5 eV. By changing the chemical composition of metal silicides it is possible to reduce the width of the prohibited zone to 0.4 - 0.5 eV. Si films provide high efficiency in the energy range from 1.1 to 2 eV. Therefore there are problems of creation of nanostructures with the band gap width ~ 2 - 2.5 eV.

It is shown in [1-5] that conducting solid-phase epitaxy of Co on the Si(100)2x1 oxidized surface contributes to the formation of more advanced epitaxial $CoSi_2$ films. The mechanism of the ongoing processes is disclosed in [6-8], which found that when applying cobalt atoms on the surface of Si(100)2x1, oxidized in situ, the metal atoms penetrate under the oxide layer at room temperature. The result of this effect is the formation of a three-component interface phase Co - Si - O at the interface between the oxide layer and silicon and the subsequent formation of a layer of Co - Si solid solution under it.

However, to date, studies aimed at obtaining Co - Si - O type nanofilms have not been conducted; therefore, their stoichiometric composition, crystal and electronic structure have not been studied.

In the works shown earlier [8-10] that low-energy ion implantation makes it possible to obtain nanoscale multi-component layers on the surface of films of metals, semiconductors and dielectrics.

Therefore, this paper attempts to obtain three-component Co - Si - O nanofilms by implanting O_2^+ ions into $CoSi_2$/Si(111) films in combination with annealing and investigate their morphology, composition and electronic properties.

2. Method of experiment

Ion bombardment, temperature annealing, as well as the study of the composition and structure of the studied samples was carried out in the same experimental device under ultra-high vacuum ($P = 10^{-7}$ Pa). Monocrystalline films $CoSi_2/Si$ (111) with thickness of 10 - 50 nm, obtained by molecular beam epitaxy, were used as objects of investigation. The energy of O_2^+ ions varied within $E_0 = 1 - 5$ keV. To obtain solid films, implantation was carried out at a dose of $D \geq D_{sat} \approx 4 \cdot 10^{16}$ cm^{-2}. The research was carried out using the following methods: Auger Electron Spectroscopy (AES), Ultraviolet Photoelectron Spectroscopy (UPS), Characteristic Electron Energy Losses Spectroscopy (CEELS), removal of energy dependencies of secondary electron emission factors, scanning electron microscopy (SEM).

3.The results of the experiments and their discussion

The analysis of AES spectra showed that after the implantation of O_2^+ ions in $CoSi_2$, Co - Si, Co - O, Si - O compounds of the Co - Si type are formed in the near-surface region and there are also unbound Co, Si and O atoms. Only after heating at $T \approx 900$ K does a three-component polycrystalline film of CoSiO type, consisting of individual crystals with dimensions of 20 - 50 nm, is formed (Fig. 1). Between the blocks there are nanopores with sizes 10 - 20 nm and a depth of 40 - 50 Å (Fig. 1, dark areas).

Fig. 1 SEM of $CoSiO/CoSi_2$ film surface image (100).

Fig. 2 shows concentration profiles of atoms O, Si and Co distribution obtained after heating at $T \approx 900$ K of $CoSi_2/Si$ film (111) implanted with ions O_2^+ with $E_0 = 1$ keV at $D = 6 \cdot 10^{16}$ cm^{-2}. It can be seen that in the surface layer with a thickness of 35 - 40 Å the concentrations of atoms of these elements differ little from each other and lie within the range of ~ 30 - 38 atoms. That is, we can assume that this creates a thin polycrystalline film with an approximate composition of CoSiO.

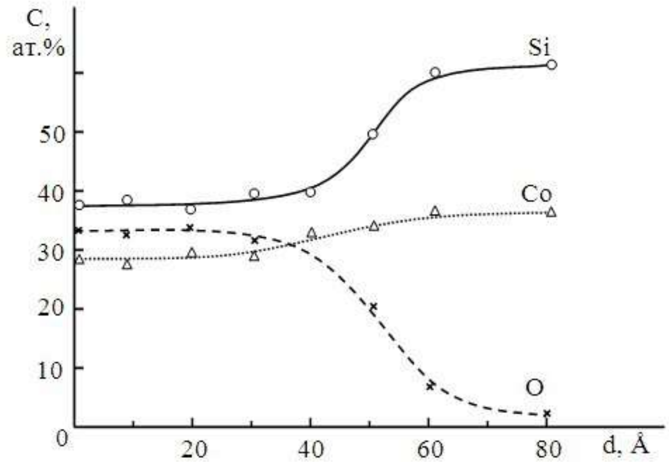

Fig. 2. Concentration distribution profiles of Si, Co, O atoms by depth of $CoSi_2$ film obtained after heating at T = 900 K of $CoSi_2$ film implanted with O_2^+ ions with $E_0 = 1$ keV at $D = 6\cdot10^{16}$ cm^{-2}.

In Fig. 3 shows photo electronic spectra for pure Si (111), $CoSi_2$/Si (111) and CoSiO films with thickness 35 - 40 Å. We can see that EV values for Si, $CoSi_2$ and CoSiO are 5.1; 4.7 and 5.9 eV, respectively. In the case of pure Si, these features are due to the excitation of electrons from the surface states (SS) and M_{23}(3p), M_{23}+M_1(3p+3s) of the valence electrons state. In the case of CoSi2 film with θ≈120 Ǻ (fig.4 curve 2) three peaks are detected. Based on the results of [9, 10] the presence of these peaks can be explained by hybridization of M_1, M_2 and M_3 states Si with M_4 and M_5 states $CoSi_2$. The curve structure, i.e., the density of the valence electrons state of CoSiO film differs significantly from that of Si and $CoSi_2$. In the CoSiO spectrum intensive peaks A, B, C are formed at energies E_c = -0.2; -1.3; -3.4 eV, respectively.

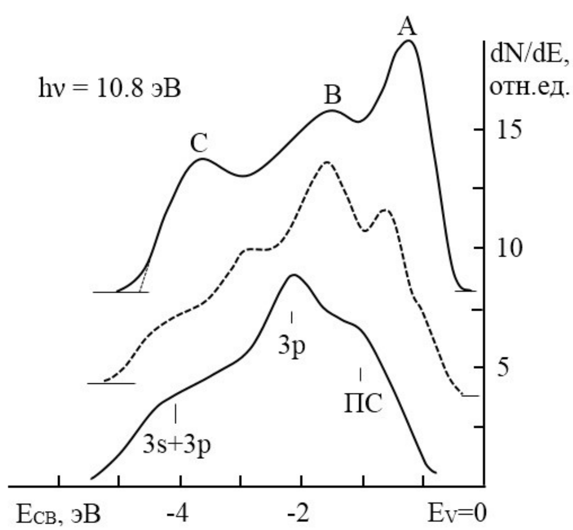

Fig. 3. Photoelectronic spectra: 1 - Si (100); 2 - $CoSi_2$/Si (111); 3 - CoSiO/ $CoSi_2$ nanofilms (111) with thickness of 35 - 40 Å.

We can assume that peak A is formed by hybridization of M_3 - silicon state, M_5 - cobalt state and L_3 oxygen state, and peak B is formed by hybridization of M_2 - silicon state, M_3 cobalt state and L_3 oxygen state, while peak C is formed by hybridization of M_1 - silicon state, M_4 - cobalt state and M_2 - oxygen state.
We determined the composition and parameters of the energy zones $CoSi_2$ and CoSiO nanofilm (Table 1) based on the analysis of the AES spectra, dependence curves $\delta(E_p)$ and $R(E_p)$, and photon spectra (Fig. 3).

Table 1. Composition and parameters of energy zones

Films	Composition, at.%			χ, eV	E_g, eV
	Co	Si	O		
$CoSi_2$	34	65	1	4,0	0,5
CoSiO	29	38	33	3,5	2,4

The table shows that the E_g value for CoSiO is ~ 2.4 eV. Therefore, the CoSiO/Si/$CoSi_2$ system may have prospects in the development of solar energy devices.

4.Conclusions

1. For the first time, the composition, structure and properties of CoSiO/Si/$CoSi_2$ nanofilm heterostructures were obtained and studied by implanting O_2^+ ions into $CoSi_2$/Si film;
2. Zone energy parameters $CoSi_2$ and CoSiO were determined;
3. It is shown that the three-layer structure absorbs light rays in the energy range from 0.6 eV to 3 eV.

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