



COMPOSITION AND STRUCTURE OF THE INTERFACIAL BOUNDARY Si/Al(111) AND Si/Cu(111)

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Abstract:

In this work, we found the results of experimental studies on the formation of an interfacial boundary during the deposition of Si and Ge on the surface of Al(111) and Cu(111) single crystals. Optimal modes of deposition and annealing are established for obtaining semiconductor-metal systems. Some consequences of implantation of barium ions on the composition, morphology, electronic and crystal structure of the Si(Ge)/Cu(Al) system. The optimal temperature for creating the Si-CuSi-Cu nanoheterostructure is shown. According to the OES and CFE data, it was established that, when Si is deposited on the Al surface and ignition is detected, the bond between Si and Al atoms is impossible. Special parameters of the CuSi energy band.

Keywords: heterostructure, nanofilms, nanophases, single crystal, energy losses by electrons, intensity, plasma oscillations, photoelectrons.

Introduction

The use of nanoscale materials in the creation of various heterostructures for modern electronic devices requires obtaining the most complete information about the concentration of impurity atoms on the surface and their distribution in depth. Therefore, nanofilms and nanocrystals of metal silicides and other semiconductor compounds obtained by various methods under ultra-high vacuum conditions on the Si surface, as well as multilayer Si–Me–Si–Me systems, on the basis of which modern micro- and nanoelectronics devices are being developed, are being widely studied [1–5].

In particular, nanophases and nanolayers of metal silicides and germanides have prospects in the creation of microwave transistors and integrated circuits, and $GexSi_{1-x}/Si$ heterostructures in the creation of light-emitting diodes, photodetectors, laser sources, optical and electronic devices [6–13].

In this paper, the results of experimental studies of the regularity of the formation of the interfacial boundary during the sputtering of Si and Ge on the surface of single crystals Al(111) and Cu(111), the establishment of optimal modes of deposition and





annealing for the production of semiconductor-metal systems, the effect of ion implantation and adsorption of barium atoms on the composition, morphology, electronic and crystal structure of the Si(Ge)/Cu(Al) system are presented. Prior to the start of this work, no such studies had been conducted.

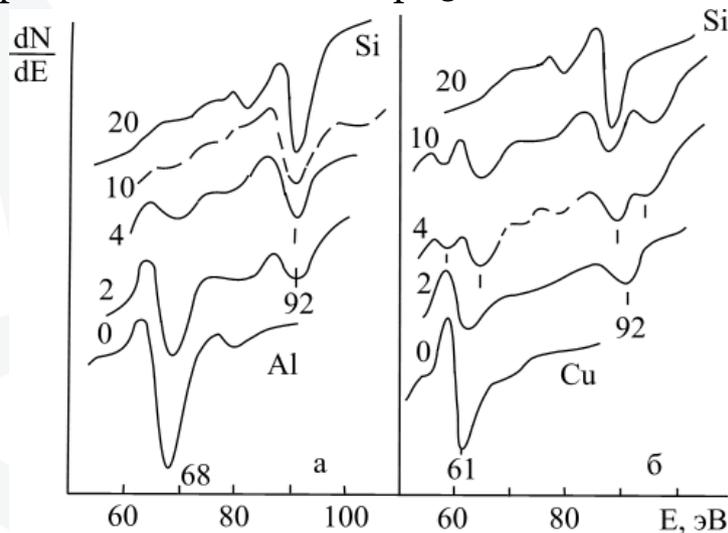
High-purity monocrystalline samples of Al(111) and Cu(111) were chosen as substrates. Prior to Si spraying, these samples were degassed at $T=850$ K and 900 K, respectively, under a vacuum of 10^{-7} Pa for 3-4 hours. Further cleaning was carried out by etching the surface of Ar⁺ with an energy of 1 keV in combination with short-term annealing to 950 (Al) and 1000 K (Cu). At the same time, the surface concentration of oxygen was ≥ 1 at.%, and carbon - 0.5 at.%. Sputtering of Si with a thickness of 1 to 20 monolayers was carried out at a vacuum of 10^{-6} Pa. Changes in the composition and electronic structure of the surface of Al(111) and Cu(111) during Si deposition were studied by the methods of Auger-electron spectroscopy, spectroscopy of characteristic energy losses by electrons, and ultraviolet photoelectron spectroscopy under vacuum - 10^{-7} Pa.

Fig. 1 shows the Auger spectra obtained by spraying Si on the surface Al(111) (Fig. 1, a) and Cu(111) (1, b). The thickness of the θ films in the monolayers is shown in the curves. It can be seen that in the case of the Si/Al(111) system, the adsorption of Si starting from $\theta_{Si}=2$ monolayers is accompanied by the appearance and increase of the intensity of the Auger-peak of silicon L₂₃VV ($E=92$ eV) and the attenuation of the intensity of the Auger-peak L₂₃VV Al ($E=68$ eV). With increasing film thickness, Si positions and shapes of Auger-peaks Si and Al practically does not change, only their intensities change. Starting from the thickness of $\theta_{Si} = 3-4$ of the monolayer, there is a sharp decrease in the intensity of the Al peak, which is explained by the formation of a continuous film of Si. The complete disappearance of the Auger-peak Al is observed at $\theta_{Si} \geq 10$ monolayers. The concentration of Si in this film is $\sim 35-40$ at.%. Analysis of the ECO results shows that up to $\theta_{Si} = 8-10$ monolayers, there is an intense mutual diffusion of Si atoms in Al and Al in Si. At $\theta \geq 12-15$ monolayers, the intensity of the SiL₂₃VV peak practically does not change.

A different picture was observed in the Auger spectra of the Si/Cu(111) system (1, b). At $\theta_{Si} = 2$ monolayers, a peak of L₂₃VV Si appears in the Auger spectrum, the intensity of the Cu MVV peak ($E=61$ eV) decreases and its width increases slightly. Starting from $\theta \approx 3-4$ monolayers, the peak Si with $E=92$ eV splits into two peaks: 90 and 94 eV [14], and instead of the peak Cu with $E=61$ eV, peaks with energies of 59 and 63 eV appear. A number of low-intensity peaks also appear. These The results show that in this case the chemical compounds Cu+Si are formed [15]. Analysis of changes in the intensity of high-energy peaks Cu (ELMM=922 eV) and Si



(ELMM=1620 eV) and calculations using the formula $C_x = \alpha C_{\text{table}}$ showed that $\theta \approx 12$ monolayers form an amorphous film (Fig. 1.b) of copper silicide with a thickness of $\theta \approx 24$ -26 monolayers (60-65 Å) with an approximate composition of CuSi. With a thickness of $\theta_{\text{Si}} \geq 12$ -15 monolayers, a film of "pure" silicon is formed. Warming up the system Si/ Cu(111) with $\theta_{\text{Si}} \approx 12$ monolayers at $T = 810$ K for 30-40 minutes led to the formation of a polycrystalline film (Fig. 1.b) CuSi with a good stoichiometric composition, and at $T \approx 900$ K, an island monocrystalline film was formed. In the case of $\theta_{\text{Si}} \geq 15$ -20 monolayers, heating at $T=750$ K led to an increase in the thickness of the CuSi film by 2-3 monolayers, and the surface film Si had a structure close to monocrystalline. When the temperature is increased to 900 K, the morphology of the Si film surface changes, due to the formation of islands in the CuSi film. Thus, the optimal temperature for the creation of the nanoheterostructure of Si-CuSi-Cu is 750-800 K. In the case of Si films with $\theta_{\text{Si}} \geq 25$ -30 monolayers at a temperature of 900 K, a monocrystalline film Si(111) was formed, the composition, structure and properties of which do not differ for massive films (Fig. 1.b). Spectra of CPEE Al and Cu with a film Si with a thickness of $\theta_{\text{Si}} \approx 8$ and $\theta_{\text{Si}} \approx 20$ monolayers, respectively, are shown in Figs. 1a and 1b. Spectra are obtained at $E_p=310$ eV.



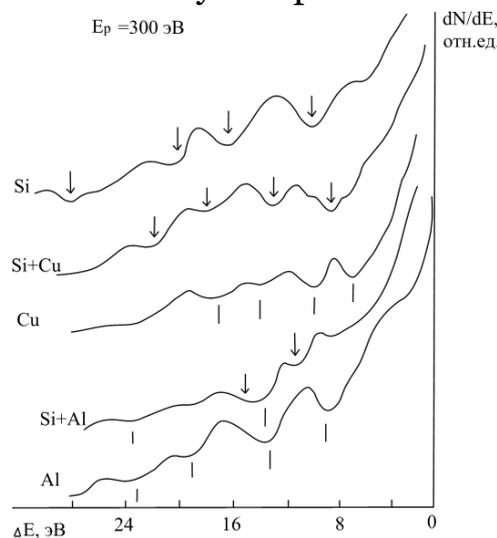
Rice. 1. Auger spectra Si sprayed on the surface Al(111) (Fig. 1, a) and Cu(111) (Fig. 1, b). Digits for the thickness curves of Si films in monolayers.

Fig.2 shows that in the spectrum of pure Al(111) intense peaks with energies $\Delta E \geq 9.2; 13; 18; 23.2$ eV due to excitation of surface plasmons $\hbar\omega_s$ and $2\hbar\omega_s$, volumetric plasmons and hybrid plasmons ($\hbar\omega_s + 2\hbar\omega_s$, plasma oscillations). When Si is sputtered with $\theta_{\text{Si}} \approx 2$ monolayers, the intensity of the peaks of CPEE Al decreases and a wide peak with $\Delta E \approx 12$ eV appears. However, the position of the peaks of CPEE Al practically does not change.



At $\theta_{\text{Si}} \approx 4$ monolayers, the intensity of the Al peaks associated with surface plasma oscillations disappears, and the intensity of the peak $\hbar\omega_v$ decreases sharply and widens. Already at $\theta_{\text{Si}} \approx 10$ monolayers, the main peaks of collective oscillations of the valence electrons Si are detected in the spectrum: 10.6 ($\hbar\omega_s$); 16.7 ($\hbar\omega_v$); 21 ($2\hbar\omega_s$) and 28.3 eV ($\hbar\omega_v + \hbar\omega_s$).

In the case of the Si/Cu(111) system, peaks with $\Delta E = 7.2$ ($\hbar\omega_s$), 9.8 ($\hbar\omega_v$), 14 eV ($2\hbar\omega_s$) and 17 eV ($\hbar\omega_s + \hbar\omega_v$) are detected in the pure Cu(111) CPEE spectrum. Sputtering Si with $\theta_{\text{Si}} \approx 2$ monolayers results in a change in the energy positions and intensity of all Cu peaks. Already at $\theta \approx 8$ monolayers, intense peaks with $\Delta E = 8.8$ eV; 13.8; 18 and 21.8 eV. Calculations have shown that these peaks correspond to the excitation of surface, volumetric and hybrid plasma oscillations of CuSi silicide.



Rice. 2. HPEE spectra: 1-Al(111); 2-Al(111) with Si film with $\theta=4$ monolayer; 3-Cu(111); 4-Cu(111) with Si film c $\theta=8$ monolayers; 5-Cu with Si films with $\theta=20$ monolayer.

From the spectra of the photoelectrons, it is possible to determine the main parameters of the zones, in particular, the photoelectron F and the thermoelectronic operation of the ϕ output (i.e., the positions of E_V and E_F), the type of conductivity of the semiconductor, and to estimate the value of the quantum output. In the case of pure Cu(111): $F = \phi = \hbar\nu - \Delta E \approx 4.4$ eV. CuSi silicides have a p-type conductivity, so that there is no shift in the position of the beginning of the spectrum relative to the E_F metal; In the case of a "thick" film, Si shifts relative to E_F towards the smaller E_{cv} by ~ 1 eV, i.e. Si has n-type conductivity. The bandgaps of Si and CuSi were determined by spectroscopy of elastically reflected electrons (Table 1).



Table 1 Parameters of energy zones.

Samples	EV, eV	EF, eV	Eg, eV	Y (at hv=10.8 eV)
With	4,4	4,4	0	$2 \cdot 10^{-5}$
CuSi	4,2	4,2	0,4	$8 \cdot 10^{-5}$
Yes	4,8	3,8	1,1	$2 \cdot 10^{-4}$

Similar patterns were observed when Ge was sputtered on the surface of Al(111) and Cu(111). Therefore, the results of the study are not given for Ge films. It should be noted that at $\theta \geq 20$ -25 monolayers, heating at a temperature of 950 K leads to the formation of a film of Si(111) and Ge(111) with a good stoichiometric composition. Thus, on the basis of the data of the ECO and CPE, it was established for the first time that when Si is sputtered on the surface of Al and subsequent annealing, no bond is formed between the atoms Si and Al. In the case of the Cu-Si and Cu-Ge systems, depending on annealing, bonds of the CuSi and CuGe types are formed. The parameters of the CuSi energy zones have been determined.

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