East European Journal of Physics. **3.** 328-332 (2024)
DOI:10.26565/2312-4334-2024-3-36 ISSN 2312-4334

ANALYSIS OF THE INFLUENCE OF FORMATION OF Pd SILICIDES ON SURFACE LAYERS OF Si ON THE DIFFUSION OF ATOMS OF CONTACTING METAL

D.A. Tashmukhamedova[a], X.E. Abdiev[a]*, S.T. Gulyamova[a], E.A. Rabbimov[b], B.E. Umirzakov[a]
[a]Tashkent State Technical University named after Islam Karimov, Tashkent, 100095 Republic of Uzbekistan
[b]Jizzakh Polytechnical Institute, Jizzakh, 130100 Republic of Uzbekistan
**Corresponding Author e-mail: abdiev.xasan.92@bk.ru*
Received April 30, 2024; revised June 14, 2024; accepted June 17, 2024

4-probe measurements of surface resistivity, measurements of dark and light current-voltage characteristics, the possibilities of using a thin PdSi film to obtain perfect nano-sized ohmic contacts on the Si(111) surface have been investigated using Auger electron spectroscopy methods in combination with ion etching of the surface. It has been shown that the depth of Ni diffusion in the Ni-Si (111) system is 400 - 500 Å at indoor temperature, and 70 – 80 Å in the Ni-PdSi-Si (111) system. The quality of the ohmic contact in the latter case does not change up to T = 800 K and withstands luminous flux illumination up to F = 1100 lux. It is shown that the resistivity of the PdSi film passes through a minimum at T = 900 – 1000 K. An analysis of the results obtained will be given in the article.
Keywords: *Atomic diffusion; Ohmic contact; Luminous flux illumination; Auger spectrum; Resistivity; Sputtering; Luminous flux; Current-voltage characteristic*
PACS: 61.72.uj, 68.55.Ln

INTRODUCTION

Physics of multilayer film structures of nanoscale thickness on various substrates has been intensively developing recent years. Such structures can be obtained by molecular beam and gas-phase epitaxy [1, 2], sputtering [3 – 5], ion beam deposition [6] and ion implantation [7 – 9]. Using reflection electron diffraction in combination with layer-by-layer chemical etching, the structure of the Pd-Si interface subjected to heat treatment in the temperature range 330-870 K was studied in [10]. It was revealed that a transition layer (TL) consisting of an amorphous region is formed at the phase interface and the adjacent region of elastically deformed silicon of nanometer thicknesses. The total thickness of the TL is determined by the heat treatment temperature. Three-phase amorphization model was proposed.

The most used type of ethanol vapor sensors are semiconductor-based resistive gas sensors at present time. The use of porous silicon, for example por-Si/Pd, formed by metal-stimulated etching, as a sensitive structure allows the formation of a sensitive element and electronic wiring in a single technological process. The possibility of forming resistive gas sensors using the method of metal-stimulated chemical etching of silicon is presented in [11, 12]. Experimental samples based on porous silicon of p- and n-type conductivity were prepared. An empirical explanation of ethanol sensitivity mechanism of the investigated structures is presented. The possibility of forming a sensitive structure and electronic wiring in a single technological process is shown.

When creating various multilayer and thin-film systems, it is very important to obtain nano-sized contacts with small transition layers [13–15]. Contact systems based on silicides have been used in the development of semiconductor devices, along with traditional ones (nickel, titanium, palladium, platinum, etc.) recent years [16, 17].

It was created an active Pd-Si interface with tunable electronic metal-substrate interaction (EMSI) by growing a thin permeable silica layer on the surface of a non-reducible oxide ZSM-5 (named Pd@SiO 2/ZSM-5) in [18]. The active Pd-Si interface is shown to enhance charge transfer from deposited Si to Pd, creating an electron-rich Pd surface that significantly reduces the activation barriers to O_2 and H_2O.

The authors of [19, 20] showed that low-energy ion implantation is an effective means of creating barrier layers on the Si surface, which allows reducing the penetration depth of the contacting metal into Si.

Development and assessment of the catalytic activity of electrode nanocomposites platinum-porous silicon and palladium-porous silicon, obtained by chemical reduction in microemulsions with a nonionic surface active substances (SAS, or surfactants) - Triton X-100 were carried out in [21]. The thermal stability of thin PdSi films was studied in the temperature range from 300 to 700 °C in [22]. PdSi, in contact with crystalline Si, transforms into Pd_2Si and Si at a temperature of 500–700 °C, which contradicts the equilibrium phase diagram. It has been established that the transformation rate depends on the structure and orientation of Si. When heated above 750 °C, Pd_2Si again transforms into PdSi. However, PdSi is resistant to annealing when in contact with Pd_2Si or an inert SiO_2 substrate. The authors suggest that the transformation of PdSi to Pd_2Si and Si in the presence of crystalline Si occurs due to the lower energy of the Pd_2Si interface compared to the PdSi-Si interface.

During the solid-phase reaction of the Ni(Pd) alloy with Si(100), phase separation of binary silicides Ni and Pd occurs [23]. PdSi monosilicide nucleates at temperatures well below the widely accepted temperature of nucleation of the

Cite as: D.A. Tashmukhamedova, X.E. Abdiev, **S.**T.Gulyamova, E.A.Rabbimov, B.E. Umirzakov, East Eur. J. Phys. 3, 328 (2024), https://doi.org/10.26565/2312-4334-2024-3-36

binary system. The decrease in nucleation temperature is due to the presence of isomorphic NiSi, which reduces the nucleation interface energy of PdSi. Despite the mutual solubility of NiSi and PdSi, these two binary compounds coexist in the temperature range of 100 °C. Solid solution form of $Ni_{1-x}Pd_xSi$ can be formed only above 700°C, which, in turn, delays the $NiSi_2$ formation process to a higher temperature due to the entropy of mixing. The authors highlight the general importance of interface energy for nucleation in ternary systems.

The possibility of using a PdSi nanofilm (≤ 250 Å) to create a barrier layer between the contacting metal (Ni) and single-crystalline silicon has been investigated for the first time in this research.

EXPERIMENTAL TECHNIQUE

Single-crystal samples of Si (111) KEF (K – Silicon, E – Electronic conductivity, F – Phosphorus)-4.5 with dimensions of 10×10×1 mm^3, polished and treated in hydrofluoric acid, were used as a substrate. Before the studies, the Si (111) surface was degassed at T = 1200 K for 4–5 hours in combination with short-term heating to T = 1500 K in a vacuum of no worse than 10^{-7} Pa. Then Pd atoms were deposited onto the Si (111) surface using the SPE method with a thickness of d ≈ 100 Å. The film deposition rate was preliminarily determined using the AES method in combination with ion etching and was ~0.5 Å/min.

Deposition of Pd atoms, heating samples, studies of their composition and parameters of energy bands using the methods of Auger electron and ultraviolet photoelectron spectroscopy (AES and UVES) and measurement of the coefficient of light passing through the sample K have been carried out in the same device, created by the authors of this research at based on the UUVI (Universal ultra-high vacuum installation), under ultra-high vacuum conditions ($P = 10^{-7}$ Pa).

The depth distribution profiles of atoms were determined by the AES method in combination with surface sputtering with Ar^+ ions with E_0 = 1 keV at an angle of 10 – 15° relative to the surface.

EXPERIMENTAL RESULTS AND DISCUSSION

Polycrystalline Pd_2Si films were obtained in a vacuum of ~ 10^{-6} Pa by deposition of Pd on a Si(111) surface, followed by heating at T = 1050 K for 40 minutes. The PdSi film thickness was ~200 Å. Then, Ni atoms with a thickness of d = 600 Å were deposited onto the surface of pure Si(111) and PdSi/Si(111). Figure 1 shows the dependence of the concentration of nickel atoms C_{Ni} over depth h for the Ni/Si(111) system, obtained after heating the system at different T. Heating of each T is ~ 40 min. It can be seen from Fig. 1 that noticeable interdiffusion of atoms occurs at the Ni/Si(111) interface at indoor temperature. The penetration depth of h Ni into Si is ~ 400 – 500 Å. After heating the system to T = 900 K, h increased by 3–4 times.

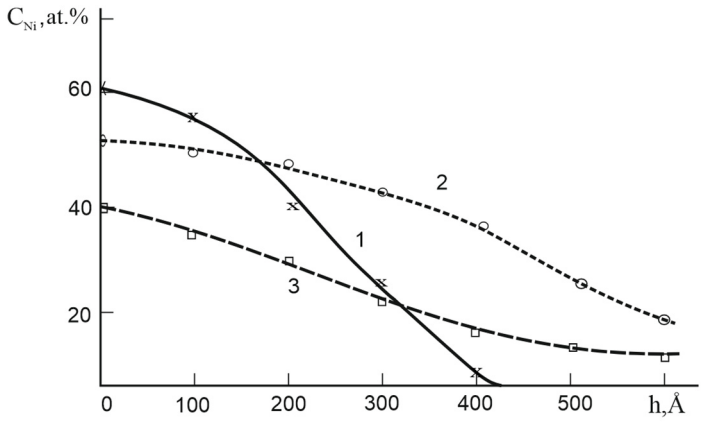

Figure 1. Dependence of C_{Ni} on h for the Ni/Si(111) system, obtained after heating at temperatures T, K: 1-300, 2-600, 3-900

The penetration depth of Ni into the PdSi/Si system is only 70 – 80 Å in the case of the Ni – PdSi – Si system at indoor temperature (Fig. 2). In this case, no noticeable diffusion of Pd into Ni occurs, and Si atoms penetrate into Ni up to 20 – 30 Å. The penetration depth of Ni into Si increases to 130 – 150 Å after heating at T = 800 K. Here, the concentration of Si in the Ni film increases noticeably, and Pd atoms are also detected. It should be noted that PdSi films were obtained at T = 1050 K. Therefore, the appearance of Pd atoms in the Ni film can be explained as follows. During heating, a significant amount of Ni penetrates into PdSi, which apparently leads to a weakening of the Pd + Si bond and the appearance of a certain number of unbound Pd and Si atoms, consequently their diffusion to Ni. However, this does not lead to a noticeable change in the quality of contact. A significant change in composition and thickness occurs at the Ni/PdSi/Si(111) contact region at T = 1000 K. In this case, Ni atoms partially penetrate (Fig. 2, curve 3) into Si.

The dependence $\rho_{PdSi}(T)$ in the region T from 400 to 1200 K on the resistivity of the contacting layer was studied to clarify the effect of changes in composition at the PdSi/Si interface during heating (Fig. 3). The heating time was ~40 min. at each T. It can be seen that the value of ρ up to T = 1000 K practically does not change, and then decreases, passing

through a minimum (ρ = 20 - 30 μΩ·cm) it increases sharply at T = 1000 K. Results of Fig. 3 can be explained as follows. The composition of the film does not change noticeably up to T = 900 K, therefore $\rho_к$ does not change significantly until this temperature.

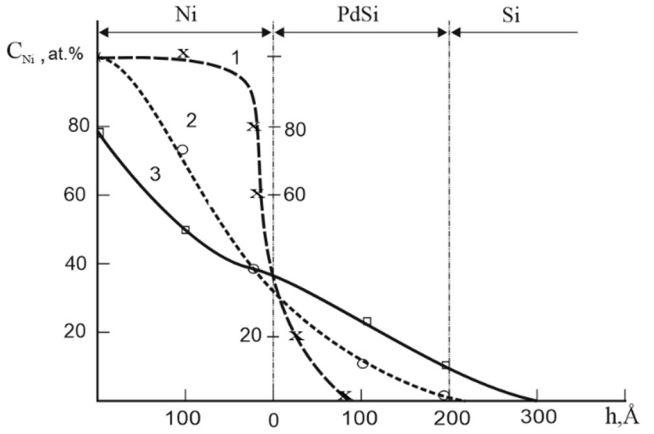

Figure 2. Dependence of C_{Ni} on h for the Ni/PdSi/Si system, obtained after heating at T, K: 1-300, 2-800, 3-1000.

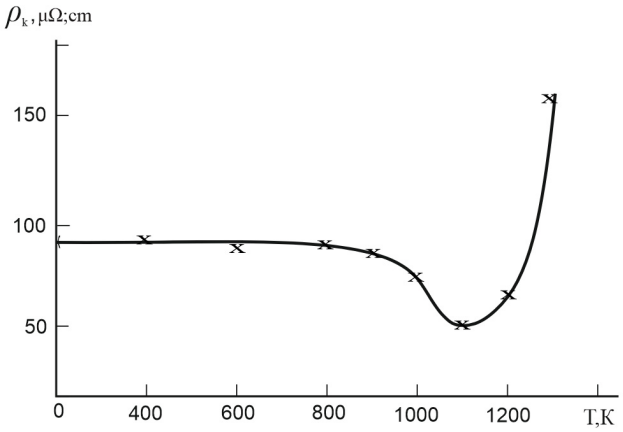

Figure 3. Dependence of the resistivity of the surface of layers of the PdSi/Si(111) system on the heating temperature. Heating time at each T is 40 minutes.

The decrease of ρ in the range 900 – 1000 K can be associated with some ordering of the structure of the PdSi film and its enrichment with Ni atoms. The sharp increase in ρ of the film at T ≥ 1000 K is explained first by the formation of PdSi islands, and then by the decomposition of PdSi into components and their evaporation.

Figure 4 shows the dark and light (curves 2 – 4) current-voltage characteristics of the Ni/PdSi/Si(111) system. The measurements were carried out at indoor temperature. It can be seen that at zero illumination (E_L = 0), the forward and reverse branches of the current dependence on voltage overlap each other, i.e. there is an ohmic contact.

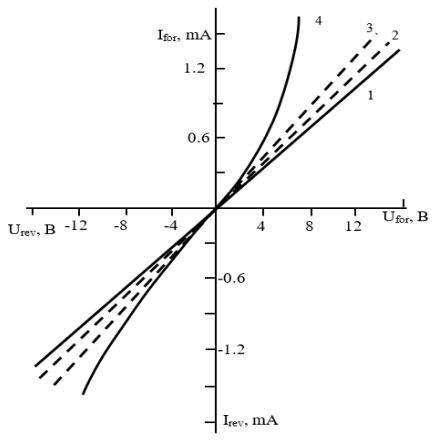

Figure 4. Dependence of $p_к$ on the illumination density, dark and light current-voltage characteristics for the Ni/PdSi/Si system

A slight decrease in contact resistance R_k is observed as E_L increases, which was estimated using the equation:

$$R_k = \left(\frac{\partial I}{\partial U}\right)^{-1} = \frac{\Delta U}{\Delta I} \quad (1)$$

The value of R = 6 kOhm at E_L = 0. Illumination of the surface with a luminous flux of up to 1100 lux does not affect the appearance of the curves. Starting from E_L = 1300 lux, a sharp change in the current-voltage characteristic (CVC) occurs, i.e. the ohmic contact is destroyed.

CONCLUSIONS

It has been discovered for the first time that the presence of a thin layer (≤ 200 Å) of palladium silicide on the Si surface sharply reduces (up to 5–6 times) the penetration depth of atoms of the contacting metal (Ni) into Si.

It has been shown that up to T = 850 – 900 K the properties of the ohmic contact do not change noticeably.

The dependence of the resistivity ρ of the PdSi film on the heating temperature of the PdSi/Si (111) system has been studied. It has been shown that ρ of the film decreases to a minimum at T = 950 – 1000 K and then increases sharply. The latter is explained first (at T = 1000 – 1100 K) by the transition of a continuous film to an island film, and then (at T ≥ 1100 K) by the decomposition of PdSi into components and their evaporation.

The dark and light current-voltage characteristics of the Ni/PdSi/Si(111) system have been studied. It is shown that the perfection of the ohmic contact practically does not change when illuminating the surface with a luminous flux up to E_L = 1100 lux.

ORCID

D.A. Tashmukhamedova, https://orcid.org/0000-0001-5813-7518; **X.E. Abdiev,** https://orcid.org/0000-0003-3843-1503
S.T. Gulyamova, https://orcid.org/0009-0005-4074-2310; **E.A. Rabbimov,** https://orcid.org/0000-0002-3046-2025
B.E. Umirzakov, https://orcid.org/0000-0002-9815-2111

REFERENCES

[1] L.L. Chang, and K. Ploog, *Molecular beam epitaxy and heterostructures*, Part of the book series: NSSE, vol. 87 (1985). https://doi.org/10.1007/978-94-009-5073-3
[2] D.A. Tashmukhamedova, Izvestiya Akademii Nauk. Ser. Fizicheskaya, **70**(8), 1230 (2006). https://elibrary.ru/item.asp?id=9296378. (in Russian)
[3] Z.Yu. Gotra, *Technology of microelectronic devices: Handbook*, (Radio and communication, Moscow, 1986). https://rutracker.org/forum/viewtopic.php?t=6090709 (in Russian)
[4] B.E. Umirzakov, Zh.Sh. Sodikjanov, D.A. Tashmukhamedova, A.A. Abduvayitov, and E. Rabbimov, Technical Physics Letters, **47**(8), 620-623 (2021). https://doi.org/10.1134/S1063785021060262
[5] D.A. Tashmukhamedova, and M.B. Yusupjanova, Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques, **10**(6). 1338-1340 (2016). https://doi.org/10.1134/S1027451016050438
[6] L.B. Gulina, and V.P. Tolstoy, *Synthesis by ion layering*, in: Intl. conf. Glass and solid electrolytes, (St. Petersburg, 1999). pp. 149.
[7] B.E. Umirzakov, D.A. Tashmukhamedova, and Kh.Kh. Kurbanov, Tech. Phys. **58**, 841 (2013). https://doi.org/10.1134/S1063784213060261
[8] Kh.Kh. Boltaev, D.A. Tashmukhamedova, and B.E. Umirzakov, Journal of Surface Investigation. Xray, Synchrotron and Neutron Techniques, **8**(2). 326 (2014). https://doi.org/10.1134/S1027451014010108
[9] Y.S. Ergashov, D.A. Tashmukhamedova, and B. E. Umirzakov, J. Surf. Invest.: X-ray, Synchrotron Neutron Tech. **11**, 480 (2017). https://doi.org/10.1134/S1027451017020252
[10] P.N. Krilov, A.B. Fedotov, and I.V. Fedotova, "The formation of Pd-Si multilayer interface during heat treatment", Journal Chemical Physics and Mesoscopics, **17**(2), 282–286 (2015). https://www.mathnet.ru/php/archive.phtml?wshow=paper&jrnid=chphm&paperid=35&option_lang=eng&ysclid=lxbrsftlbx495807277. (in Russian)
[11] G. Li, X. Zhang, H. Lu, Yanchao, *et al*., Ethanol sensing properties and reduced sensor resistance using porous Nb_2O_5-TiO_2 n-n junction nanofibers," Sensors and Actuators B: Chemical, **283**, 602-612 (2019). https://doi.org/10.1016/j.snb.2018.12.074
[12] G.O. Silakov, E.N. Lazorkina, S.A. Gavrilov, O.V. Volovlikova, A.V. Zheleznyakova, and A.A. Dudin, Russian Microelectronics, **52**, 572–576 (2023). https://doi.org/10.1134/S1063739723070259
[13] S.V. Tomilin, and A.S. Yanovsky, Journal of Nano-and Electronic Physics, **4**(1), 01013 (2012). https://core.ac.uk/reader/14056570
[14] N.S. Boltovets, V.V. Basanets, V.N. Ivanov, V.A. Krivutsa, V.A. Fesunenko, and A.V. Tsvir, Technology and design in electronic equipment, (4), 35 (1999).
[15] L.P. Anufriev, V.V. Baranov, Ya.A. Soloviev, and M.V. Tarasikov, *Technology and design in electronic equipment*, (4), 55-56, (2005). http://dspace.nbuv.gov.ua/handle/123456789/53610. (in Russian)
[16] A.I. Blesman, and R.B. Burlakov, Omsk Scientific Bulletin, 1(163), (2019). https://doi.org/10.25206/1813-8225-2019-163-50-54
[17] V.A. Saladukha, V.A. Pilipenko, V.A. Gorushko, and V.A. Philipenya, "The impact of formation modes of platinum silicide by the quick heat treatment on Schottky diodes parameters," **119**(1), 62-66 (2019). https://libeldoc.bsuir.by/bitstream/123456789/34383/1/Solodukha_Vliyaniye.PDF (in Russian)
[18] T. Dong, *et al*., JACS Au, **3**(4), 1230-1240 (2023). 10.1021/jacsau.3c00093
[19] D.M. Muradkabilov, D.A. Tashmukhamedova, and B.E. Umirzakov, J. Surf. Invest.: X-Ray, Synchrotron Neutron Tech. **7**(5), 967 (2013). https://doi.org/v10.1134/S1027451013050376
[20] B.E. Umirzakov, Poverkhn.: Fiz., Khim., Mekh. **9**(2), 119 (1992) (in Russian)

[21] N.A. Yashtulov, L.N. Patrikeev, V.O. Zenchenko, S.E. Smirnov, M.V. Lebedeva, V.R. Flid, Nanotechnol Russia, **10**, 910–916 (2015). https://doi.org/10.1134/S1995078015060142
[22] B.Y. Tsaur, Appl. Phys. Lett. **37**, 708–711 (1980). https://doi.org/10.1063/1.92054
[23] A. Schrauwen, J. Demeulemeester, A. Kumar, W. Vandervorst, C.M. Comrie, C. Detavernier, K. Temst, *et al.*, Journal of applied physics, **114**, 063518 (2013). https://doi.org/10.1063/1.4818333

АНАЛІЗ ВПЛИВУ УТВОРЕННЯ СИЛІЦИДІВ Pd НА ПОВЕРХНЕВИХ ШАРАХ Si НА ДИФУЗІЮ АТОМІВ КОНТАКУЮЧОГО МЕТАЛУ

Д.А. Ташмухамедова[a], Х.Е. Абдієв[a], С.Т. Гулямова[a], Є.А. Рабімов[b], Б.Є. Умірзаков[a]
[a]Ташкентський державний технічний університет імені Іслама Карімова, Ташкент, 100095 Республіка Узбекистан
[b]Джизакський політехнічний інститут, Джизак, 130100 Республіка Узбекистан

Методами Оже-електронної спектроскопії досліджено 4-зондові вимірювання питомого поверхневого опору, вимірювання темнових і світлих вольт-амперних характеристик, можливості використання тонкої плівки PdSi для отримання ідеальних нанорозмірних омічних контактів на поверхні Si(111). поєднання з іонним травленням поверхні. Показано, що глибина дифузії Ni в системі Ni-Si (111) становить 400 500 Å при кімнатній температурі та 70 – 80 Å в системі Ni-PdSi-Si (111). Якість омічного контакту в останньому випадку не змінюється до T = 800 K і витримує освітленість світлового потоку до F = 1100 лк. Показано, що питомий опір плівки PdSi проходить через мінімум при T = 900 – 1000 K. Аналіз отриманих результатів наведено в статті.

Ключові слова: *атомна дифузія; омічний контакт; освітлення світловим потоком; Оже-спектр; питомий опір; напилення; світловий потік; вольт-амперна характеристика*