JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **17** No 5, 05011(4pp) (2025)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **17** № 5, 05011(4cc) (2025)

OPEN ACCESS

REGULAR ARTICLE

Comparative Analysis of the Properties of Manganese Silicide

A.T. Mamadalimov[1], M.Sh. Isaev[2,3*] ✉, S.R. Kodirov[4], T.U. Atamirzaev[5] M.N. Mamatkulov[6], U.T. Asatov[6]

[1] *Institute of Semiconductor Physics and Microelectronics at the National University of Uzbekistan, 100057 Tashkent, Uzbekistan*
[2] *National University of Uzbekistan named after Mirzo Ulugbek, 100174 Tashkent, Uzbekistan*
[3] *Cyber University of Uzbekistan, Nurafshan city, Uzbekistan*
[4] *Urgench State University, 220100 Urgench city, Uzbekistan*
[5] *Namangan State Technical University, Namangan, Uzbekistan*
[6] *Tashkent Institute of Chemical-Technology, Tashkent, Uzbekistan*

(Received 25 July 2025; revised manuscript received 23 October 2025; published online 30 October 2025)

In this paper, a comparative analysis of the main physical, structural, thermoelectric and magnetic properties of various phases of manganese silicides is presented: mono- (MnSi), di ($MnSi_2$) and higher silicides ($MnSi_{1.75}$), obtained by the diffusion doping method. The temperature dependences of electrical conductivity, mobility, as well as thermoelectric properties, including the Seebeck coefficient and thermal conductivity, are studied. It is shown that manganese disilicide is an *n*-type semi-conductor with a band gap of $\Delta E_g = 0.35 \div 0.45$ eV. The Seebeck coefficient is 100 μV/K at $T = 150 \div 200$ K. It was established that the monosilicide has *n*-type conductivity, with a concentration of $\sim 10^{21} \div 10^{22}$ cm^{-3} and a mobility of $2 \div 5$ cm^2/V·s, the disilicide has *p*-type conductivity, with a concentration of $10^{16} \div 10^{17}$ cm^{-3} and a mobility of 1 cm^2/V·s, the higher silicide has *n*-type conductivity, with a concentration of $5 \cdot 10^{20} \div 7 \cdot 10^{20}$ cm^{-3} and a mobility of $0.5 \div 2$ cm^2/V·s. It is shown that each of these phases has a unique combination of crystallographic forms, electronic structure and technological capabilities, which determines their application in microelectronics, nanoelectronics and thermoelectric devices.

Keywords: Manganese silicides, Thermal conductivity, Electrical conductivity, Mobility, Temperature dependence, Phase composition, Diffraction pattern, Symmetry, Hall effect, ThermoEMF.

DOI: 10.21272/jnep.17(5).05011 PACS numbers: 61.05.cp, 61.82.Fk, 73.43.Qt

1. INTRODUCTION

The study of physical processes occurring both in the volume and on the surface, and in the near-surface layers of a single-crystal semiconductor, in particular, silicon in the process of diffusion doping with impurities that create deep levels and obtaining compensated materials with specified electrophysical, thermoelectric, photoelectric and optical properties are urgent tasks of today [1-7].

A well-developed technology for growing single-crystal silicon, a planar technology for creating integrated devices based on it, a fundamentally new technology for creating low-dimensional objects in silicon, modifying the properties of Si by various methods, as well as discovering new physical phenomena in the surface of silicon that are not characteristic of its volume, attract close attention of researchers as an active material for the needs of micro- and nanoelectronics. At present, transition metal silicides are becoming the base material for new, promising integrated circuits of the next generation due to their resistance to aggressive environments and high-temperature treatments [8-11].

At present, one of the urgent problems is the study of physical processes occurring both in the volume and on the surface and near-surface layers of a single-crystal semiconductor, in particular, silicon in the process of diffusion doping with manganese, creating deep levels (DL) [12-15]. First of all, the need for these studies is caused by the fact that in the process of diffusion doping of the semiconductor material – silicon, it is possible to obtain compensated materials with specified electrophysical, photoelectric and optical proper-ties. In diffusion-doped silicon crystals, various silicide phases of manganese are formed in the near-surface region with a thickness of 15-20 μm. Manganese silicides are intermetallic compounds formed between manganese and silicon at various stoichiometric ratios. The most studied phases are monosilicide (MnSi), disilicide ($MnSi_2$) and higher silicide ($MnSi_{1.75}$), each of which has unique structural, electrical and thermoelectric characteristics [16-18].

* Correspondence e-mail: isayevmahmud02@gmail.com

Cite this article as: A.T. Mamadalimov et al., *J. Nano- Electron. Phys.* 17 No 5, 05011 (2025) https://doi.org/10.21272/jnep.17(5).05011

Due to the combination of metallic and semiconductor nature, they are used in microelectronics, spintronics and thermoelectric converters.

The purpose of this work is to conduct a systematic comparative analysis of the properties of various manganese silicides, identify common and distinctive features, and determine the most promising materials for practical application.

2. EXPERIMENTAL PARTS

Manganese has a large diffusion coefficient in silicon, so we used the diffusion doping method. This method has a number of other advantages: 1) the relative simplicity of the technology; 2) the possibility of studying the effect of annealing temperature on the initial parameters of the crystal; 3) the possibility of controlling the concentration of electrically active manganese, chromium and cobalt atoms by changing the temperature [19]. Manganese silicides were obtained by the diffusion method on p-type silicon of the KDB-10 brand and n-type silicon of the KEF-35 brand, grown by the Czochralski method. Measurements of the specific resistance and mobility of charge carriers were carried out on a four-probe method setup.

IR spectroscopic studies were carried out on an IR-Fourier Inventio-S device (Bruker, Germany) in the wavenumber range from 400 to 4000 cm^{-1}, resolution – 4 cm^{-1}, sensitivity signal: noise ratio – 30000:1, scanning speed – 16 spectra per second.

Structural studies were carried out by scanning electron microscopy (scanning electron microscope Jeol (Japan) brand IT200) at room temperature.

X-ray studies were carried out on an X-ray diffractometer Miniflex 600 (Rigaku) with monochromatic CuKa radiation. The Seebeck coefficient was measured by measuring the thermoelectric power at the ends of the sample with a voltmeter with high input resistance and by measuring the temperature difference at the ends of the sample using thermocouples.

3. RESULTS AND DISCUSSION

The phase diagram of the Mn-Si system is characterized by the presence of several intermetallic phases depending on the ratio of elements and temperature [20-21]. The following compounds are the most stable: manganese monosilicide MnSi, atomic ratio Mn:Si = 1:1. Stable at temperatures of 900 – 1200 °C; manganese disilicide, Mn:Si = 1:2, is formed with excess silicon content (> 66 at. % Si). Stable at temperatures of 600 – 1200 °C and higher manganese silicide, Mn:Si = 1:1.75. Stable at temperatures of 850 – 1120 °C.

The crystal structures of manganese silicides are as follows. The cell parameters of silicon monosilicide at 300 K are: $a = 4.558$ Å, $b = 4.558$ Å, $c = 4.558$ Å (cubic crystal structure); disilicide: $a = b = 3.90$ Å, $c = 5.43$ Å, each Mn atom is surrounded by 8 Si atoms (octahedral positions), and each silicon atom is directly bonded to 4 manganese atoms; higher silicide: $a = 6.889$ Å, $c = 4.777$ Å (hexagonal crystal structure). Higher manganese silicide is characterized by high coordination of manganese, complex hexagonal packing, and the presence of two types of vacancies. Higher manganese silicides contain clusters where manganese atoms are in octahedral coordination.

The temperature dependences of specific resistance for three phases were investigated (Fig. 1).

As is known, specific resistance is described as

$$\rho = \frac{1}{en\mu} \quad (1)$$

where ρ is the resistivity, n is the carrier concentration, e is the carrier charge, μ is the charge carrier mobility.

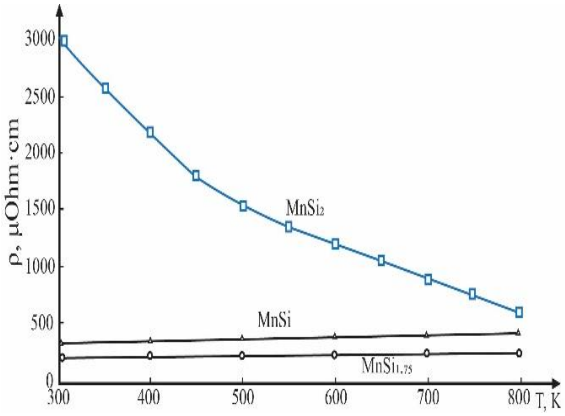

Fig. 1 – Temperature dependences of resistivity of various phases of manganese silicides

In manganese monosilicide, the specific resistance increases with increasing temperature according to the law:

$$\rho(T) = \rho_0 + AT^n \quad (2)$$

where $n = 1 \div 2$, typical for scattering on phonons. This metallic dependence is dominated by scattering of electrons on phonons at high temperatures. The conductivity type is almost metallic.

In manganese disilicide at low temperatures ρ is high (at T = 300 K, $\rho = 300$ μOhm·cm), conductivity is weak. With increasing temperature, the specific resistance falls exponentially (thermogeneration of charge carriers):

$$\rho(T) \sim \exp\left(\frac{\Delta E_g}{2kT}\right) \quad (3)$$

where ΔE_g is the band gap ($\Delta E_g = 0{,}6 - 0{,}8$ eV). The conductivity type is semiconductor (activated).

In higher manganese silicide, the specific resistance increases slightly with temperature. The specific resistance is low due to the scattering of charge carriers on phonons, due to phase transitions and defects. The conductivity type is mixed: metallic and semiconductor.

Fig. 2 shows the temperature dependences of the concentration of different phases of manganese silicides. In manganese monosilicide, the concentration of charge carriers remains almost unchanged, typical of metals. In manganese disilicide, the concentration increases sharply with increasing temperature, as:

$$n \sim \exp\left(-\frac{\Delta E_g}{2kT}\right) \quad (4)$$

where k is the Boltzmann constant.

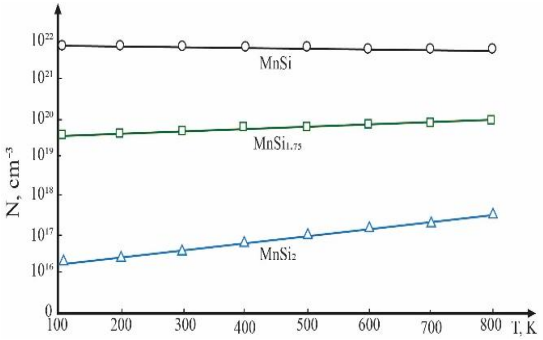

Fig. 2 – Temperature dependences of concentration of various phases of silicides

The behavior of $n(T)$ is like that of a semiconductor. In the higher manganese silicide, the concentration of charge carriers increases slightly with temperature.

Fig. 3 shows the temperature dependences of the mobility of charge carriers of different phases of manganese silicides.

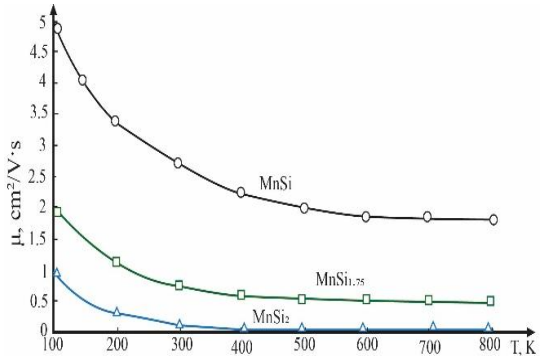

Fig. 3 – Temperature dependences of the mobility of charge carriers of different phases of manganese silicides

As is known, the mobility depends on the scattering mechanism:

$$\mu \sim \frac{1}{T^m}, \text{ where } m = 1 \div 2 \quad (5)$$

In manganese monosilicide, the mobility decreases with temperature as $\mu \sim T^{-1,5}$, which is explained by the scattering of charge carriers on phonons (the Drude model). At low temperatures, the mobility is high.

In manganese disilicide, the mobility is high at low temperatures, and with increasing temperature, μ decreases exponentially due to phonon scattering as $\mu \sim T^{-1} \div T^{-2}$.

In higher manganese silicide, it is high at low temperatures. At high temperatures, the mobility decreases due to phonon scattering and the presence of structural defects.

The temperature dependence of the thermoelectric power coefficient of manganese silicides was studied (Fig. 4).

For manganese monosilicide, the thermoEMF is small (5 ÷ 10 μV/K), thermal conductivity $æ = 12 \div 14$ W/m·K at 300 K. It increases slightly with increasing temperature. The small value of the thermoEMF coefficient is due to the metallic nature of electrical conductivity. For higher manganese silicide, a weak increase in α is observed with increasing temperature. At temperatures $T > 500$ K, the growth of α slows down, thermal conductivity $æ \approx 10 \div 12$ W/m·K. For manganese disilicide $\alpha = 115 - 160$ μV/K, æ = 5 ÷ 7 W/m K. With increasing temperature, the thermoEMF value up to $T = 500$ K increases almost linearly, and at $T > 500$ K its growth slows down, which is typical for semiconductors.

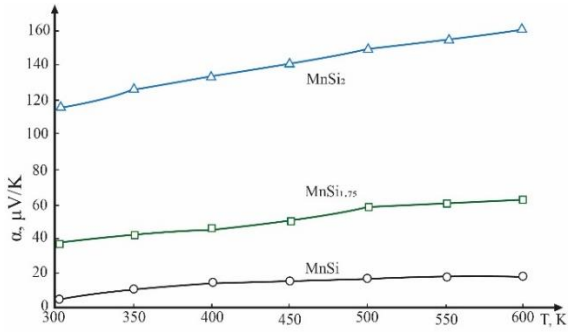

Fig. 4 – Temperature dependences of thermoEMF of different phases of silicides

Fig. 5 shows the temperature dependence of the quality factor of different phases of manganese silicides. The quality factor is determined by the formula

$$Q = ZT = \frac{\alpha^2 \sigma T}{æ} \quad (6)$$

For manganese monosilicide $Q = 0.01$ due to low α (at $T = 300$ K, $\alpha = 10$ μV/K). MnSi has high thermal conductivity due to metallic bonding.

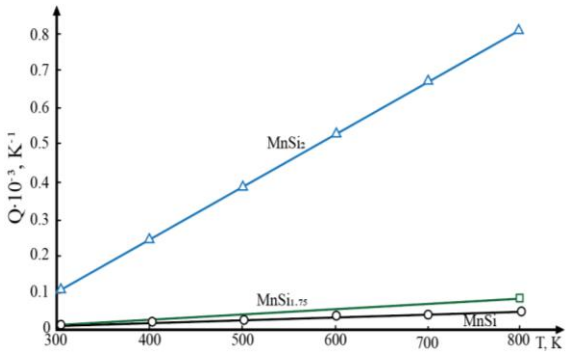

Fig. 5 – Temperature dependence of Q

For higher manganese silicide $Q = 0.05$, the thermal conductivity is high due to the metallic bond, but the presence of clusters partially reduces the thermal conductivity. For manganese disilicide $Q = 0.66 \div 0.8$ at $T = 700 - 800$ K due to $\alpha > 155$ μV/K and reduced $æ < 5$ W/m·K. If we suppress the phonon thermal conductivity to 1 ÷ 1.2 W/m K, we can obtain Q close to unity.

4. CONCLUSION

Based on the results of this research, the following conclusions can be drawn:

1. A comparative analysis of the main physical, structural, thermoelectric properties of mono-, di- and higher manganese silicide is given.

2. A study of the temperature dependences of resistivity on temperature revealed that ρ in manganese disilicide decreases exponentially with increasing temperature, due to semiconductor conductivity, and in mono- and higher silicides ρ increases slightly with increasing temperature, due to metallic conductivity.

3. Studies of the temperature dependences of the charge carrier concentration and mobility in mono-, di- and higher manganese silicides have shown that the monosilicide has n-type conductivity, with a concentration of ~ $10^{21} \div 10^{22}$ cm^{-3} and a mobility of $2 \div 5$ cm^2/V·s, the disilicide has p-type conductivity, with a concentration of $10^{16} \div 10^{17}$ cm^{-3} and a mobility of 1 cm^2/V·s, the higher silicide has n-type conductivity, with a concentration of $5 \cdot 10^{20} \div 7 \cdot 10^{20}$ cm^{-3} and a mobility of $0.5 \div 2$ cm^2/V·s.

4. Temperature dependences of thermoEMF showed that manganese disilicide exhibits a high thermoEMF coefficient, typical of *p*-type semiconductors.

REFERENCES

1. F.Y. Wang, *Impurity Doping Processes in Silicon*, (North Holland Publishing, North Holland, 2013).
2. A.A. Lebedev, *Semiconductors* **33** No 2, 107 (1999).
3. Sh.B. Utamuradova, K.S. Daliev, Sh.Kh. K. Daliev, S.A. Muzafarova, K.M. Fayzullaev, G.A. Muzafarova. *E3s Web of Conferences* **583**, 04006 (2024).
4. Sh.B. Utamuradova, J.J. Khamdamov, J.Sh. Zarifbayev, K.M. Fayzullaev, *E3s Web of Conferences* **508**, 07009 (2024).
5. B.A. Lombos, *Can. J. Chem.* **63**, 1666 (1985)
6. S.Z. Zainabidinov, Kh.S. Daliev, K.P. Abdurakhmanov, Sh.B. Utamuradova, I.Kh. Khomidjonov, I.A. Mirzamurodov, *Modern Phys. Lett. B* **11** No 20, 909 (1997).
7. N.F. Zikrillaev, G.A. Kushiev, Sh.I. Hamrokulov, Y.A. Abduganiev, *J. Nano- Electron. Phys.* **15** No 3, 03024 (2023).
8. M. Sh. Isaev, A.I. Khudayberdieva, M.N. Mamatkulov, U.T. Asatov, S.R. Kodirov, *East Eur. J. Phys.* **4**, 297 (2024).
9. A.T. Mamadalimov, M.Sh. Isaev, T.U. Atamirzaev, Sh.N. Ernazarov, M.K. Karimov, *East Eur. J. Phys.* **2**, 358 (2024).
10. M.Sh. Isaev, I.T. Bozarov, A.I. Tursunov, *E3s Web of Conferences* **402**, 14019 (2023).
11. M.Sh. Isaev, A. Gaibov, A. Eshkulov, M. Mirkamilova, D. Shukurova, *Lecture Notes in Networks and Systems* **509,** 681 (2023).
12. M.Sh. Isaev, U.T. Asatov, M.A. Tulametov, S.R. Kodirov, A.E. Rajabov, *East Eur. J. Phys.* **2**, 341 (2024).
13. Sh.B. Utamuradova, A.V. Stanchik, D.A. Rakhmanov, A.S. Doroshkevich, K.M. Fayzullaev, *New Materials Compounds and Applications* **6** No 3, 214 (2022).
14. K.P. Abdurakhmanov, Kh.S. Daliev, Sh.B. Utamuradova, N.Kh. Ochilova, *Applied Solar Energy English Translation of Geliotekhnika* **34** No 2, 73 (1998).
15. Sh.B. Utamuradova, Sh.Kh. Daliev, S.A. Muzafarova, K.M. Fayzullaev, *East Eur. J. Phys.* **3**, 385 (2023).
16. A.T. Mamadalimov, M.Sh. Isaev, I.T. Bozarov, A.E. Rajabov, S.K. Vakhabova, *East Eur. J. Phys.* **2**, 362 (2024).
17. A.T. Mamadalimov, M.Sh. Isaev, M.K. Karimov, G.T. Badalova, Kh.T. Abdurazzakov, *Adv. Phys. Res.* **1**, 50 (2024).
18. L. Wang, J. Liu, Y. Li, G. Wei, Q. Li, Z. Fan, H. Liu, *Adv. Energy Sustain. Res.* **5** No 2, 2300240 (2024).
19. Sh.B. Utamuradova, Kh.J. Matchonov, J.J. Khamdamov, Kh.Y. Utemuratova, *New Materials, Compounds and Applications* **7** No 2, 93 (2023).
20. Sh.G. Askerov, L.K. Abdullayeva, M.G. Hasanov, *J. Semicond.* **41** No 10, 102101 (2020).
21. M.K. Bahadyrkhanov, G.Kh. Mavlonov, S.B. Isamov, Kh.M. Iliev, K.S. Ayupov, Z.M. Saparniyazova, S.A. Tachilin, *Inorgan. Mater.* **47** No 5, 479 (2011).

Порівняльний аналіз властивостей силіцидів марганцю

A.T. Mamadalimov[1], M.Sh. Isaev[2,3], S.R. Kodirov[4], T.U. Atamirzaev[5] M.N. Mamatkulov[6], U.T. Asatov[6]

[1] *Institute of Semiconductor Physics and Microelectronics at the National University of Uzbekistan, 100057 Tashkent, Uzbekistan*

[2] *National University of Uzbekistan named after Mirzo Ulugbek, 100174 Tashkent, Uzbekistan*

[3] *Cyber University of Uzbekistan, Nurafshan city, Uzbekistan*

[4] *Urgench State University, 220100 Urgench city, Uzbekistan*

[5] *Namangan State Technical University, Namangan, Uzbekistan*

[6] *Tashkent Institute of Chemical-Technology, Tashkent, Uzbekistan*

У цій роботі представлено порівняльний аналіз основних фізичних, структурних, термоелектричних та магнітних властивостей різних фаз силіцидів марганцю: моно- (MnSi), ді- ($MnSi_2$) та вищих силіцидів ($MnSi_{1.75}$), отриманих методом дифузійного легування. Досліджено температурні залежності електропровідності, рухливості, а також термоелектричних властивостей, включаючи коефіцієнт термоЕРС та теплопровідність. Показано, що дисиліцид марганцю є напівпровідником n-типу із шириною забороненої зони $\Delta E_g = 0.35 \div 0.45$ еВ. Коефіцієнт термоЕРС становить 100 мкМ/К при $T \leq 150 \div 200$ К. Встановлено, що моносиліцид має n-тип провідності, з концентрацією ~$10^{21} \div 10^{22}$ см$^{-3}$ та рухливістю $2 \div 5$ см^2/В·с, дисиліцид має p-тип провідності, з концентрацією $10^{16} \div 10^{17}$ см$^{-3}$ та рухливістю 1 см^2/В·с, вищий силіцид має *n*-тип провідності, з концентрацією $5 \cdot 10^{20} \div 7 \cdot 10^{20}$ см$^{-3}$ та рухливістю $0,5 \div 2$ см^2/В·с. Показано, що кожна з цих фаз має унікальне поєднання кристалографічних форм, електронної структури та технологічних можливостей, що визначає їх застосування в мікро- і наноелектроніці та термоелектричних пристроях.

Ключові слова: Силіцид марганцю, Теплопровідність, Електропровідність, Рухливість, Температурна залежність, Фазовий склад, Ефект Холла, ТермоЕРС.