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Magnetic Behaviour of Silicon with Paramagnetic Centers Introduced by Impurity Atoms

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Abstract. One promising route to achieving magnetic functionality in silicon is the introduction of paramagnetic transition-metal impurities, particularly iron (Fe) and nickel (Ni). In this study, we investigate the formation of magnetically active silicon by diffusion doping with Fe and Ni atoms. Monocrystalline *p*-type silicon with resistivities of ρ=5 Ω·cm and ρ=0.5 Ω·cm was used as the substrate material. Diffusion temperature–time conditions were optimized to ensure that the doped samples remained highly compensated *p*-type after thermal treatment. The experimental results reveal pronounced magnetoresistive behavior in Fe- and Ni-doped silicon. In Si<Fe> samples, the magnitude of negative magnetoresistance (Δρ/ρ) increases monotonically with decreasing temperature, reaching values of approximately 100–120% at T = 100 K. Conversely, Si<Ni> samples exhibit positive magnetoresistance that also increases upon cooling and attains Δρ/ρ values of about 10–15% at T = 100 K. These contrasting responses indicate different scattering mechanisms associated with Fe- and Ni-related impurity centers in the silicon lattice. Overall, the findings confirm that diffusion doping with Fe and Ni modifies the charge-transport behavior of silicon through the formation of magnetic impurity centers, making these materials promising candidates for semiconductor systems with tunable magnetic properties relevant to spintronic applications.

INTRODUCTION

The development of magnetic semiconductor materials for modern spintronic technologies relies heavily on understanding how transition-metal impurities modify the electronic and magnetic behavior of silicon [1-3]. Among the various paramagnetic impurities considered in earlier studies, iron (Fe) and nickel (Ni) are of particular interest due to their relatively high spin states and their ability to form magnetically active centers within the silicon lattice. Their electronic configurations and key physical parameters, presented in Table 1, indicate that both Fe and Ni can introduce localized magnetic moments capable of influencing charge-carrier transport and spin-dependent scattering processes [4,5].

A well-known limitation associated with Fe and Ni doping is their relatively low solubility in electrically active states; however, their incorporation pathways in silicon offer several advantages. Previous investigations [6-8] have shown that Fe and Ni atoms may occupy both interstitial and substitutional sites in the silicon crystalline lattice, allowing for the formation of diverse impurity complexes with distinct magnetic signatures. Unlike many other transition-metal dopants, the charge state and spin configuration of Fe- and Ni-related centers are highly sensitive to the thermal history of the material [9,10]. Consequently, the concentration of electrically active Fe and Ni atoms is strongly governed by diffusion parameters and cooling rates.

Rapid quenching techniques have been demonstrated to stabilize a larger fraction of electrically active impurity atoms [11,12], particularly for Fe, which tends to form deep-level centers that significantly affect magnetotransport properties. Similarly, Ni incorporation may lead to the formation of impurity clusters or defect complexes that enhance magnetic interactions on the nanoscale. These characteristics make Fe- and Ni-doped silicon promising candidates for engineering magnetic semiconductor systems suitable for spintronic applications.

In addition, the electrically inactive fraction of dissolved impurities – present in the silicon lattice in the form of interstitial atoms, dimers, nanoclusters, microclusters, precipitates, or magnetic silicides – may also exhibit magnetic behavior. However, magnetic properties arising from microclusters, precipitates, or silicides are generally unsuitable for spintronic applications due to the strong spatial non-uniformity of their magnetic response. Nickel is a characteristic example of such behavior. Owing to its high tendency to form microclusters, precipitates, and silicides, the electrically inactive concentration of Ni near the silicon surface can reach 10^{20}–10^{21} cm^{-3} [13-15]. At the same time, the electrically active solubility of nickel does not exceed ~10^{16} cm^{-3}, meaning that Ni doping produces only a minor change in the resistivity of silicon samples [16,17]. From a spintronics perspective, silicon materials containing magnetic nanoscale clusters – particularly those formed by transition-metal impurity complexes – are considered more promising. In contrast to Ni, iron (Fe) plays a more favorable role in this regard: Fe can form impurity complexes and nanoscale magnetic centers that influence spin-dependent transport without creating large-scale inhomogeneities. As a result, Fe-related nanoclusters or defect complexes can provide a controllable magnetic contribution suitable for semiconductor-based spintronic device design.

TABLE 1. The electronic structure and key parameters of Fe and Ni impurity atoms in silicon.

Element	Electronic structure	Spin	Total solubility limit, sm^{-3}	Electrically active fraction of the solubility limit, sm^{-3}	Energy levels in silicon
Fe	$3d^6 4S^2$	2	$4 \cdot 10^{16}$	$2 \cdot 10^{14}$	Ec – 0.14 Ec – 0.51 Ec – 0.40
Ni	$3d^8 4S^2$	1	$7 \cdot 10^{17}$	$7 \cdot 10^{14}$	Ev + 0.35 Ev + 0.23

Magnetic structure formation in semiconductors can be achieved using several techniques, such as chemical vapor deposition, molecular beam epitaxy, or ion implantation. Ion implantation of silicon with transition-metal ions including Fe and Ni has been widely employed to create magnetic nanoclusters and metal silicides within the lattice. In this work, we investigate the possibility of producing silicon with magnetic properties through diffusion doping with Fe and Ni impurities.

EXPERIMENTAL RESEARCH

To obtain silicon doped with Fe and Ni impurity atoms, monocrystalline *p*-type silicon substrates were employed. For Fe diffusion, *p*-type silicon with a resistivity of ρ = 5 Ω·cm was used, whereas Ni diffusion was carried out using *p*-type silicon with a resistivity of ρ = 0.5 Ω·cm. The diffusion temperature–time regimes were selected to ensure that, after thermal annealing, the Fe-doped samples remained strongly compensated p-type, providing stable conditions for the formation of Fe-related deep centers and magnetic complexes. For Ni doping, the diffusion parameters were optimized to promote the incorporation of Ni atoms while minimizing the formation of electrically inactive large-scale silicide precipitates, which are known to degrade magnetic uniformity. Prior to and after diffusion, all samples underwent both mechanical and chemical surface treatments. The cleaning procedure included peroxide–ammonia solution processing followed by a one-minute etching step in an HF + HNO_3 mixture (1:3), ensuring the removal of surface contaminants and mechanically induced defects. This preparation was essential for achieving reproducible diffusion profiles and reliable magnetotransport measurements. The magnetoresistance of the doped samples was measured using an experimental setup capable of generating magnetic fields in the range of 0.1–2 T and applying electric fields from 0.1 to 1000 V/cm over a temperature interval of T = 100–300 K [18]. This configuration allowed for the precise evaluation of spin-dependent scattering mechanisms associated with Fe- and Ni-related impurity centers. Low-temperature magnetization measurements were performed using a SQUID magnetometer, enabling the detection of weak magnetic signals and the characterization of possible nanoscale magnetic clusters formed by Fe and Ni impurities. These measurements provided valuable insights into the magnetic behavior of the doped silicon systems and their potential applicability in spintronic devices.

RESEARCH RESULTS

TABLE 2. Electrophysical parameters of the obtained samples. Electrophysical parameters of silicon doped with Fe and Ni atoms

Samples	*ρ*, Ohm·sm	Type of conductivity	Charge carrier concentration, sm^{-3}	Charge carrier mobility, $sm^2/V\cdot c$
Si<Fe>	$(5\div7)\cdot10^3$	*p*	$4{,}2\cdot10^{12}$	200÷250
Si<Ni>	0,5	*p*	$4\cdot10^{16}$	250÷350

Table 3 presents the magnetoresistance (Δρ/ρ) values of the samples at T = 300 K, obtained under identical electric (E = 200 V/cm) and magnetic field conditions (approximately 2 T).

It was established that silicon samples doped with Ni exhibit predominantly weak positive magnetoresistance (PMR), typically not exceeding 6%. This behavior is attributed to the formation of Ni-related impurity complexes and electrically inactive clusters, which introduce scattering mechanisms that weakly enhance the resistivity in the presence of a magnetic field. In contrast, Fe-doped silicon samples demonstrate negative magnetoresistance (NMR), although the magnitude is relatively small, with Δρ/ρ values on the order of 5–7%. The observed NMR in Si<Fe> is commonly associated with spin-dependent scattering at Fe-related deep centers, whose contribution becomes more pronounced at lower temperatures and under stronger electric (E) and magnetic (B) fields [19,20].

TABLE 3. Values of resistivity and magnetoresistance of the samples at T = 300 K

Samples	***ρ*** **(Ohm·sm)**	**Maximum Δρ/ρ, %**	**Type of magnetoresistance in the magnetic field range (0–2 T)**
Si<Fe>	$5{,}5\cdot10^3$	-7	Weak negative
Si<Ni>	0,5	6	Weak positive

To gain further insight into the magnetotransport behavior of Fe- and Ni-doped silicon, the temperature dependence of the magnetoresistance Δρ/ρ was investigated over the interval T = 100–380 K. These measurements were performed under applied fields of E = 210 V/cm and B = 2 T, enabling the characterization of field-enhanced spin-dependent transport mechanisms (Fig. 1). The obtained results reveal distinct temperature-driven trends for Fe and Ni dopants. In Si<Fe> samples, the magnitude of negative magnetoresistance increases gradually with decreasing temperature, reflecting enhanced localization effects and stronger spin–carrier interactions at lower energies. Conversely, the positive magnetoresistance observed in Si<Ni> samples also increases with decreasing temperature but remains relatively small in magnitude, consistent with Ni's known tendency to form clusters or silicide-related states that do not significantly contribute to strong spin-dependent scattering. Overall, the comparative analysis of Fe- and Ni-doped silicon demonstrates that Fe introduces more pronounced magnetic scattering centers capable of producing measurable NMR, whereas Ni leads primarily to weak PMR due to its clustering behavior and limited electronic activity. These findings help to clarify the distinct roles of Fe and Ni impurities in determining the magnetotransport properties of silicon.

The experimental results demonstrate clear differences in the magnetoresistive behavior of Fe- and Ni-doped silicon. In Si<Fe> samples, the magnitude of negative magnetoresistance (NMR) increases monotonically with decreasing temperature. At T = 100 K, the NMR reaches Δρ/ρ ≈ 100–120%, indicating strong spin-dependent scattering associated with Fe-related deep centers. Importantly, across the entire investigated temperature range, no sign inversion of magnetoresistance is observed in Si<Fe>. This means that the material consistently exhibits negative magnetoresistance, unlike certain other transition-metal-doped silicon systems where a transition from NMR to positive magnetoresistance (PMR) may occur. The absence of sign inversion suggests that Fe introduces stable magnetic scattering centers that remain dominant over competing temperature-dependent mechanisms [21].

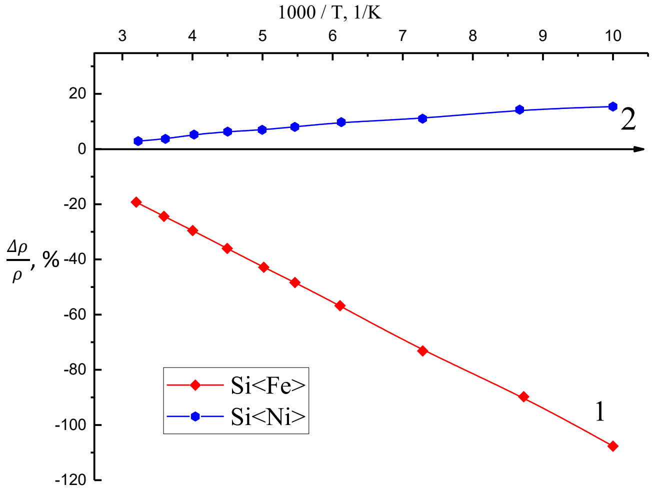

FIGURE 1. Temperature dependence of magnetoresistance for the samples: 1 – Si<Fe>, 2 – Si<Ni> at E = 210 V/cm and B = 2 T.

In contrast, the behavior of Si<Ni> samples is markedly different. The magnetoresistance remains positive throughout the explored temperature interval, confirming the predominance of PMR in Ni-doped silicon. As the temperature decreases, the PMR increases gradually and reaches Δρ/ρ ≈ 10–15% at T = 100 K. This relatively small magnitude of PMR is consistent with the known tendency of Ni atoms to form impurity clusters or silicide phases, which influence the electronic structure but do not produce strong spin-dependent scattering. Additionally, the PMR observed in Si<Ni> shows only a weak dependence on external electric and magnetic fields, suggesting that the underlying scattering mechanisms are governed primarily by structural and defect-related factors rather than field-enhanced spin interactions [22, 23].

Overall, the comparative analysis highlights a fundamental contrast between Fe and Ni doping in silicon. Fe introduces strong, temperature-enhanced magnetic scattering centers resulting in significant negative magnetoresistance, whereas Ni produces weak but steadily increasing positive magnetoresistance consistent with its clustering behavior. These differences are crucial for selecting dopant species for specific magnetotransport and spintronic applications.

CONCLUSIONS

1. The diffusion doping of silicon with Fe and Ni fundamentally alters its magnetotransport properties. The study demonstrates that introducing Fe and Ni atoms into the silicon lattice through diffusion leads to the formation of paramagnetic centers that significantly modify charge-carrier scattering mechanisms. Iron atoms, in particular, create deep-level centers that intensify spin-dependent scattering, resulting in pronounced negative magnetoresistance. In contrast, nickel tends to form electrically inactive clusters and silicide phases, which produce only a weak magnetic response. This distinction indicates that Fe and Ni interact with the silicon lattice through fundamentally different physical mechanisms.

2. The strong negative magnetoresistance observed in Fe-doped silicon confirms its potential for spintronic applications. In Si<Fe> samples, the negative magnetoresistance reaches Δρ/ρ ≈ 100–120%, which suggests the presence of strong spin-coupling effects associated with Fe-related centers. This behavior remains stable across the entire temperature range studied, and the absence of magnetoresistance sign inversion confirms that Fe centers are structurally stable and uniformly distributed in the silicon matrix. Such high and persistent NMR values make Fe-doped silicon a highly promising material for spin-injection devices, spin filters, and low-temperature spintronic sensors.

3. The weak magnetic response in Ni-doped silicon is directly linked to its tendency to form clusters. Si<Ni> samples exhibit only 6–15% positive magnetoresistance, which is explained by the strong tendency of Ni atoms to form electrically inactive nanoclusters and silicide phases. Although these structures may exhibit magnetic properties, they do not significantly contribute to spin-dependent transport. Therefore, Ni-doped silicon is less effective in magnetotransport applications, but it still holds potential for the development of cluster-based magnetic nanocomposites or localized magnetic field sources.

4. Comparing the effects of Fe and Ni impurities reveals opportunities for engineering magnetically tunable semiconductor materials. The results show that Fe-doped silicon forms homogeneous magnetic centers responsible for strong spin-dependent scattering, whereas Ni-doped silicon exhibits a weaker magnetoresistive response due to its cluster-related structural defects. Understanding these contrasting mechanisms enables controlled tuning of the magnetic and electronic properties of silicon by selecting appropriate diffusion parameters and dopant species. This opens a pathway toward designing optimized semiconductor platforms for advanced spintronic systems.

REFERENCES

1. Narang, S. B., Pubby, K. Nickel spinel ferrites: a review // Journal of Magnetism and Magnetic Materials, 2021 519, 167163. https://doi.org/10.1016/j.jmmm.2020.167163.
2. Liu, W., Zhang, H., Shi, J. A., Wang, Z., Song, C., Wang, X., Chen, N. A room-temperature magnetic semiconductor from a ferromagnetic metallic glass // Nature communications 2016. Vol. 7(1), pp. 13497. https://doi.org/10.1038/ncomms13497.
3. Kenzhaev Z. T., Zikrillaev N. F., Ayupov K. S., Ismailov K. A., Koveshnikov S. V., Ismailov T. B. Enhancing the efficiency of silicon solar cells through nickel doping // Surface Engineering and Applied Electrochemistry 2023. 59(6), pp. 858-866. https://doi.org/10.3103/S1068375523060108.
4. Ismaylov B.K., Zikrillayev N.F., Kenzhaev Z.T., Ismailov K.A. Clusters of impurity nickel atoms and their migration in the crystal lattice of silicon // Physical Sciences and Technology 2023. 10(1), pp. 13–18. https://doi.org/10.26577/phst.2023.v10.i1.02.
5. Kushiev G.A., Isakov B.O., Mukhammadjonov U.X. The Prospects of Obtaining a New Material with a Hetero-Baric Structure Ge_xSi_{1-x}-Si Based on Silicon for Photo Energy Applications // Journal of Nano and Electronic Physics Open source preview 2024. 16(3). https://doi.org/10.21272/jnep.16(3).03003.
6. Yakubov D., Sattarov O., Abdurakhmanov B., Ismailov T., Kholikova P. (2025, September). Mathematical modeling based on astronomical and physical-geometric principles for optimizing the efficiency of solar panels // In Optical and Computational Technologies for Measurements and Industrial Applications (OptiComp 2025) 2025, Vol. 13803, pp. 152-157. SPIE. https://doi.org/10.1117/12.3077879.
7. Zikrillaev N.F., Koveshnikov S.V., Trabzon L., Mavlonov G.Kh., Ismaylov B.K., Ismailov T.B., Urakova F.E. Ferromagnetic Properties of Silicon Doped Manganese Atoms // Surface Engineering and Applied Electrochemistry 2025. Vol. 61, No. 1. pp. 75–80. ISSN 1068-3755. https://doi.org/10.3103/S1068375524700571.
8. Ruziev, Z. J., Fedotova, O. M., Khasanov, O. K., Sapaev, U. K. Features of second harmonic generation of intense short laser pulses in crystals with a regular domain structure under conditions of self-action, nonstationarity, and synchronism of group velocities // Journal of Applied Spectroscopy 2021. 88(3), PP. 514-518. https://doi.org/10.1007/s10812-021-01202-7.
9. Razzokov J., Fazliev S., Yusupov, M., Sharipov A., Ruziev Z., Mamatkulov S. Effect of mutation and disulfide bond formation on the catalytic site of monomeric cytoglobin: A molecular level insight // Plasma Medicine, 2021. 11(4). https://doi.org/10.1615/PlasmaMed.2021041420.
10. Zikrillayev N., Kenzhaev Z., Ismailov T., Kurbanova U., Aliyev B. Effect of nickel doping on the spectral sensitivity of silicon solar cells // E3S Web of Conferences 2023. 434, 01036, https://doi.org/10.1051/e3sconf/202343401036.
11. Zikrillayev N.F., Mavlonov G.Kh., Trabzon L., Koveshnikov S.V., Kenzhaev Z.T., Ismailov T.B., Abduganiev Y.A. Magnetic properties of silicon with paramagnetic impurity atoms // East European Journal of Physics 2023(3), pp. 380–384, https://doi.org/10.26565/2312-4334-2023-3-40.
12. Zikrillaev N.F., Urakova F.E., Toshev A.R., Kushiev G.A., Ismailov T.B., Abduganiev Y.A., Norkulov N. Physical and magnetic properties of silicon doped with impurity germanium atoms // East European Journal of Physics 2025(1), pp. 184–189. https://doi.org/10.26565/2312-4334-2025-1-18.
13. Iliev K.M., Ismailov K. A., Kosbergenov E. Zh., Odzhaev V. B., Prosolovich V. S., Yankovsky Yu. N., Kenzhaev Z. T., Isakov B. O., Kushiev G. A. The Influence of γ-Irradiation on the Electrophysical Parameters of Nickel-Doped

Silicon Grown by the Czochralski Method // Surface Engineering and Applied Electrochemistry 2025. 61(6), PP. 854–859. https://doi.org/10.3103/S1068375525700942.
14. Kenzhaev Z.T., Iliev Kh.M., Odzhaev V.B., Mavlonov G.Kh., Prosolovich V.S., Kosbergenov E.Zh., Ismaylov B.K., Isamov S.B., Ollambergenov Sh.Z. The Effect of Gamma Irradiation on the Electrophysical Parameters of Nickel-Doped Silicon Solar Cells // Surface Engineering and Applied Electrochemistry 2024. Vol. 60, No. 6, pp. 851–856. https://doi.org/10.3103/S1068375524700467
15. Bakhadyrkhanov M.K., Ismailov K.A., Kosbergenov E.Zh. Thermal stability of electrical parameters of silicon crystal doped with nickel during growth // Semiconductor Physics, Quantum Electronics & Optoelectronics 2022. Vol. 25, No. 1, pp. 6–9. https://doi.org/10.15407/spqeo25.01.006.
16. Iliev Kh.M., Koveshnikov S.V., Isakov B.O., Kosbergenov E.Zh., Kushiev G.A., Khudoynazarov Z.B. The elemental composition investigation of silicon doped with gallium and antimony atoms // Surface Engineering and Applied Electrochemistry 2024. Vol. 60, No. 5, pp. 633–639. https://doi.org/10.3103/S106837552470025X.
17. Bakhadirkhanov M.K., Iliev Kh.M., Tursunov M.O., Isamov S.B., Koveshnikov S.V., Majitov M.Kh. Electrical Properties of Silicon Doped with Manganese via High-Temperature Diffusion // Inorganic Materials. 2021. Vol. 57, No. 7, pp. 655-662. https://doi.org/10.1134/S0020168521070013.
18. Mavlonov G. H., Isamov S. B., Koveshnikov S. V., Zikrillaev Kh. F., Abduganiev Y. A., Sattorov A. A., Ibrohimov A. B. Ordering of europium magnetic domains in silicon at room temperature// Indian Journal of Physics 2024. Vol 98.13 pp 1-7. https://doi.org/10.1007/s12648-024-03473-0.
19. Begmatova D. A., Nortojiyev A. M., Xudayberdiyev S. S., Mahmadiyorov A. Z., Nosirov N. B., Sapaev I. B. The importance of physical exercises in the training of specialists in the field of architecture and construction // In AIP Conference Proceedings 2022. Vol. 2432, No. 1, p. 030056. AIP Publishing LLC. https://doi.org/10.1063/5.0089959.
20. Ruziev Z. J., Sapaev B., Sapaev I. B., Sapaev, U. K., Amanov, R., Nazaraliev, D. On theory of approximation methods in the study of second harmonic generation of ultrashort laser pulses in periodic crystals // In AIP Conference Proceedings 2022. Vol. 2432, No. 1, p. 020008. AIP Publishing LLC. https://doi.org/10.1063/5.0089970
21. Olimov A. N., Ruziev Z. J., Yusupov D. B., Sapaev U. K. (2019). Frequency doubling of femtosecond laser pulses in nonlinear photonic crystals with account of high-order dispersion // Journal of Russian Laser Research 2019. 40(3), PP. 280-287. https://doi.org/10.1007/s10946-019-09803-6
22. Zikrillaev N.F., Mavlonov G.H., Trabzon L., Isamov S.B., Abduganiev Y.A., Ibodullaev Sh.N., Kushiev G.A. Magnetic Properties of Silicon Doped with Impurity Atoms of Europium // Journal of Nano- and Electronic Physics 2023. 15(6), 0600. https://doi.org/10.21272/jnep.15(6).06001.
23. Zikrillaev N.F., Tursunov O.B., Kushiev G.A., Development and Creation of a New Class of Graded-Gap Structures Based on Silicon with the Participation of Zn and Se Atoms // Surface Engineering and Applied Electrochemistry 2023. 59 No 5, 670. https://doi.org/S1068375523050198.