EAST EUROPEAN JOURNAL OF PHYSICS. **1.** 203-207 (2026)
DOI:10.26565/2312-4334-2026-1-20 ISSN 2312-4334

EFFECT OF IMPURITY CLUSTERS ON OPTICAL PROPERTIES OF NICKEL AND COPPER DOPED SILICON

Sirajidin Z. Zainabidinov[1], **N.A. Turgunov**[2], **Akramjon Y. Boboev**[1],
Shuhratjon K. Akbarov[1], **Raymash M. Turmanova**[2], **Abdukakhor Arikov**[1],
Muqaddas O. Kuchkarova[1], **Bakhrikhon Tolanova**[1], **Markhabo B. Rasulova**[1]
[1]Andijan state university named after Z.M. Babur, Andijan, Uzbekistan
[2]Research Institute of Semiconductor and Microelectronics Physics at the National University of Uzbekistan, Tashkent
**Corresponding Author e-mail: aboboevscp@gmail.com*

Received June 16, 2025; revised October 28, 2025; in final form February 2, 2026; accepted February 17, 2026

This paper deals with the influence of impurity atoms on optical properties of single crystal silicon doped with nickel and copper during high-temperature diffusion doping. And also, the processes of formation of various chemical compounds with participation of oxygen and carbon atoms with atoms of nickel, copper and silicon. By means of FTIR spectrometry and X-ray diffraction analysis it was revealed that the concentration of optically active oxygen and carbon in the volume of silicon samples doped with nickel and copper significantly increases compared to the original samples.

Keywords: *Silicon; Nickel; Copper; Diffusion; Impurity; Oxygen; Carbon; Clusters*
PACS: 78.30.Am

INTRODUCTION

The control and characterization of background impurities such as oxygen and carbon in silicon single crystals is a critical task for modern microelectronics and optoelectronic device fabrication. These impurities, particularly when optically active, can significantly alter the electrical, optical, and structural properties of silicon, affecting charge carrier lifetime, recombination rates, and overall device efficiency [1]. Optically active oxygen and carbon atoms are known to interact with substitutional or interstitial impurities and contribute to the formation of electrically active complexes and extended defects, especially under thermal or radiation processing conditions [2].

Fourier-transform infrared (FTIR) spectroscopy remains a powerful and non-destructive analytical tool for the precise quantification of light elements such as oxygen and carbon in silicon matrices. Its high sensitivity to vibrational modes of impurity atoms enables accurate detection of characteristic absorption peaks corresponding to bond-specific interactions [3]. In particular, absorption at 1106 cm^{-1} is attributed to interstitial oxygen (O_i) stretching modes, while peaks in the 607–620 cm^{-1} region correspond to substitutional carbon (Cs) modes [4].

In the present study, we aimed to determine the concentration of optically active oxygen and carbon in both intrinsic n-type silicon and in silicon samples doped with transition metals such as nickel and copper. The samples were analyzed using a Fourier-transform infrared spectrometer FSM 2201, operating in the range 370–7800 cm^{-1} with a spectral resolution of 1 cm^{-1}. A DLATGS pyrodetector was employed for enhanced signal sensitivity. The oxygen and carbon concentrations were calculated from the respective IR absorption intensities at room temperature, applying standard calibration methods [5].

To complement the FTIR analysis and gain deeper insight into the structural rearrangements induced by metallic dopants, we also conducted X-ray diffraction (XRD) studies. These investigations were essential for identifying the formation of metallic impurity complexes, dislocation loops, or secondary phase precipitates within the silicon lattice. The XRD measurements were performed using a high-resolution Malvern Panalytical Empyrean diffractometer with CuKα radiation ($\lambda = 0.15405$ nm), operated in step-scan mode to ensure accurate peak identification and lattice parameter extraction [6].

Such integrated spectroscopic and diffraction-based analysis enables a more comprehensive understanding of impurity-induced modifications in silicon, which is crucial for the optimization of material parameters in semiconductor device engineering.

MATERIALS AND METHODS

Growing silicon single crystals by the Czochralskii method, which is the most frequently used in modern semiconductor production, involves a number of important parameters, such as melt temperature, drawing speed, rotation speed of the crystal and seed, composition and purity of the initial polysilicon, mainly determine the quality of the obtained single crystal. In the technological process of growing single crystals of silicon, depending on the conditions of growth, to exclude the penetration of oxygen and carbon atoms in the composition of the growing material is virtually impossible.

Cite as: S.Z. Zainabidinov, N.A. Turgunov A.Y. Boboev, Sh.K. Akbarov, R.M. Turmanova, Abdukakhor Arikov, M.O. Kuchkarova, B. Tolanova, M.B. Rasulova, East Eur. J. Phys. 1, 203 (2026), https://doi.org/10.26565/2312-4334-2026-1-20

Therefore, in the volume of single crystalline silicon, obtained by this method, oxygen and carbon atoms are present in high enough concentrations up to 10^{17}-10^{18}cm^{-3}. These two contaminating impurities in single crystals of silicon are called background impurities, because when using the existing installations of the Czochralski method, their entry into the melt can not be excluded. Numerous studies have shown that oxygen and carbon atoms participate in complexation processes in single crystal silicon [7]. Often extensive precipitates or microinclusions of impurity atoms [8-11], which are formed during very large-scale or ultra-large-scale integrated fabrication, can be critical to device quality and performance. Oxygen precipitates can be useful by allowing the deposition of transition metals and strengthening the wafer by preventing plastic deformation during processing. However, if they form in active regions, they act as defects, degrading device performance [12].

RESULTS AND DISCUSSION

Initial n-Si samples and doped n-Si <Ni,Cu> samples were fabricated for the studies. As an initial sample for experiments, single-crystalline silicon of KEF grade, grown by the Czochralski method, with a resistivity of 0.3 Ohm·cm was used. The samples prepared in the form of a rectangular parallelepiped with dimensions 10x5x2 mm were pre-cleaned by chemical methods [13]. Using a VUP-4 vacuum sputtering system unit, in which the vacuum value was 10^{-4}Torr, nickel atoms were deposited on the previously prepared silicon samples on one side by sputtering with a thickness of 0.4 μm. And on the other side, copper atoms with a thickness of 0.6 μm were deposited on the same samples. Simultaneous diffusion of nickel and copper atoms in silicon was carried out in a horizontal SUOL-4 furnace at temperature T=1473 K for 5 hours. The furnace temperature was controlled within ±3 K using a platinum-platinum-rhodium thermocouple. After diffusion annealing, the samples were cooled by rapid cooling method, where the cooling rate was υ_{col}=200 K/s. Fig. 1. shows a fragment and spectrograms of the change in the concentration of optically active oxygen in the original sample and in the n-Si <Ni,Cu> sample

Calculations of the value of optically active oxygen concentration were carried out using the following formula [14]:

$$N_O^{opt} = 3.3 \cdot 10^{17} \cdot \frac{1}{d} ln \frac{I}{I_0}, \quad (1)$$

Where: *I* and *I₀* are the intensities of incident and transmitted light, *d* is the thickness of the sample

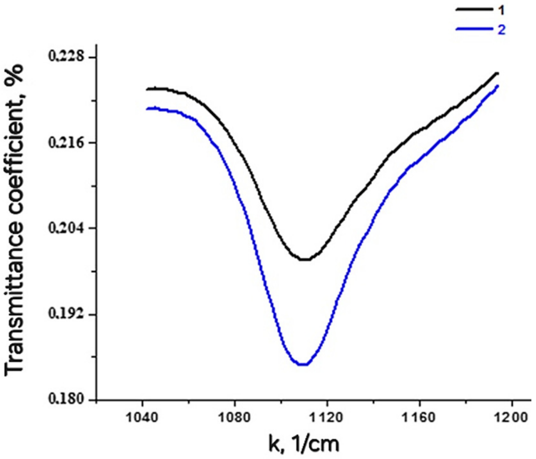


Figure 1. Dependence of transmittance on wavenumber (*k*, cm^{-1}): 1 - n-Si; 2 - n-Si<Ni,Cu>

The concentration of optically active oxygen in the original sample and in the n-Si< Ni,Cu> samples is n = 2.5·10^{17}cm^{-3} and n= 3.9·10^{17}cm^{-3}, respectively. Calculations show that the concentration of optically active oxygen in the n-Si<Ni,Cu> samples is 1.6 times higher compared to the original samples.

This means that in the process of diffusion at T=1473 K oxygen atoms form a bond with impurity atoms, forming a metal oxide. Because of this, the concentration of optically active oxygen in the doped samples increases.

Fig. 2. shows fragments of IR spectrograms of the change in the concentration of optically active carbon in the original n-Si sample and in the n-Si <Ni,Cu> sample.

The concentration of optically active carbon was calculated by the following formula [14]:

$$N_C^{opt} = 1{,}1 \cdot 10^{17} \cdot \frac{1}{d} ln \frac{I}{I_0}, \quad (2)$$

Where: *d*-thickness of the sample, *I* - and *I₀*- of incident and transmitted light.

The results obtained showed that the concentration of optically active carbon in the original sample and in the n-Si< Ni,Cu> samples respectively are n= 6.6·10^{17}cm^{-3} and n= 8.84·10^{17}cm^{-3}. From the results obtained, it is found that the value of optically active carbon concentration in the n-Si<Ni,Cu> samples is 1.33 times more as compared to the original sample.

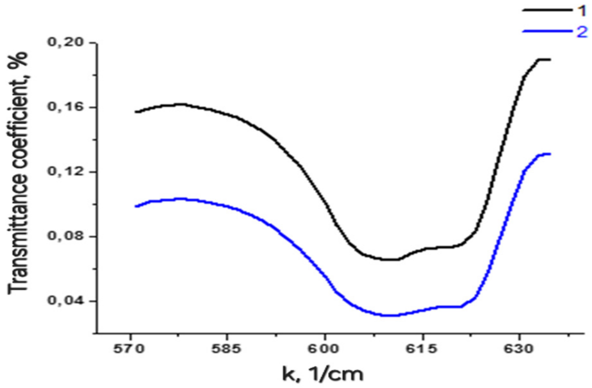


Figure 2. Graphs of dependence of transmission coefficient on the wave vector: 1 – n-Si, 2 – n-Si<Ni,Cu>

In order to further clarify and confirm the presented results, we carried out X-ray diffraction analyses of all samples. The obtained results were analyzed as follows. In Fig. 3. shows the X-ray diffraction patterns of the original sample and the n-Si <Ni,Cu> sample. Using the obtained results, the interplanar distance in the crystal can be determined from the Wolf-Bragg equation [15].

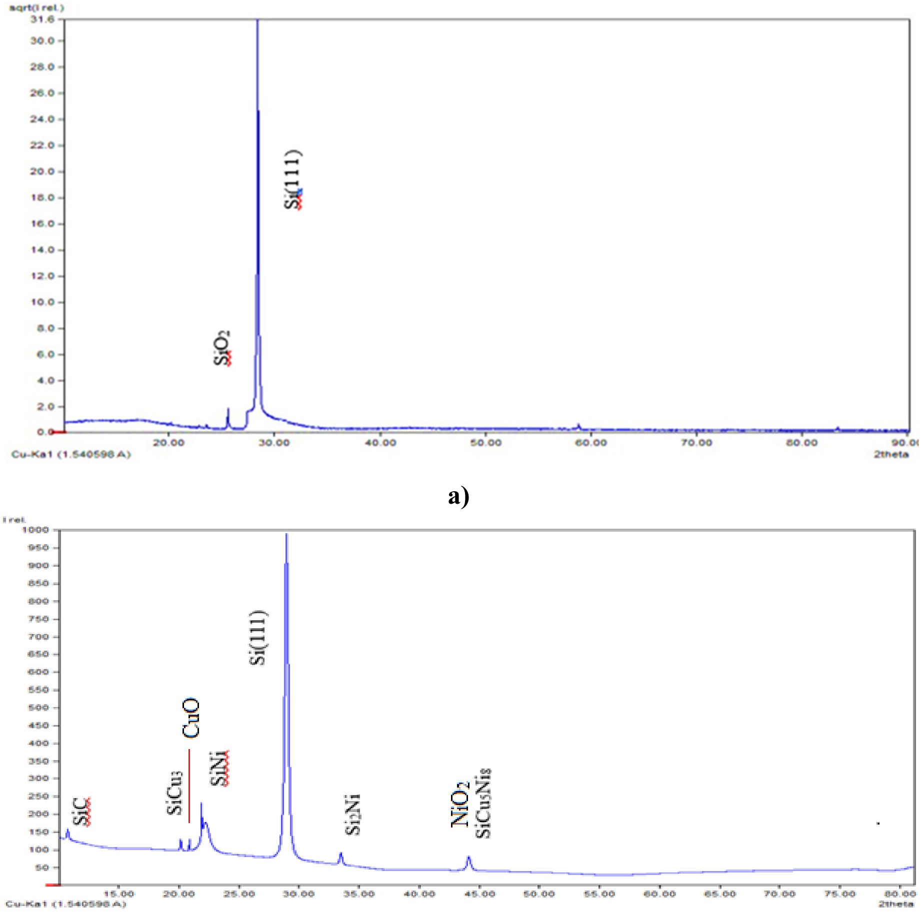
$$n\lambda = 2d sin\theta, \tag{3}$$

where d is the interplanar distance, θ is the Wolf-Bragg angle n-order of diffraction maximum, λ = 0.15405 nm is the wavelength of CuK_α-radiation.

The average size of crystallites of different planes was determined by Scherrer's formula [15]:

$$L = \frac{K\lambda}{\beta cos\theta}, \tag{4}$$

Where, K is the dimensionless particle shape factor (Scherrer's constant); λ = 0.15405 nm - wavelength of CuK_α-radiation; β - reflex width at half-height, θ - Wolf-Bragg angle, L - average crystallite size (nm).



a)

b)

Figure 3. Plots of the dependence of the transmittance coefficient on the wave vector for the samples: 1 – n-Si; 2 – n-Si<Ni,Cu>

The largest peak of them corresponds to single-crystalline silicon with crystal orientation (111). In this reflection, the L value and the d value are 0.474 nm and 1.84 nm, respectively. From this calculation, it can be seen that the L value decreases almost 6 times and the d value increases almost 3 times compared to the same reflex in the original sample. These results indicate that the crystal lattice is deformed due to the penetration (introduction) of impurity atoms. The reflex observed at an angle of 10.77° , corresponds to the SiC compound. In the X-ray diagram, the third peak by order number corresponds to the copper oxide compound CuO. It reflects at an angle of 20.88° and its L and d values are 2.805 nm and 1.27 nm, respectively. And one more peak corresponds to the compound of oxygen to metal $NiO_2$and it reflects at an angle of 44.12° [16].

As can be seen from the results of X-ray diffraction analysis, several kinds of clusters involving impurity atoms of nickel and copper were formed in the silicon crystal after diffusion. In addition, from the results of X-ray diffraction analysis, the formation of various chemical compounds of oxygen atoms, carbon atoms with nickel or copper atoms, as well as with silicon atoms is observed. Consequently, it appears that in the process of high-temperature diffusion annealing, oxygen atoms form chemical compounds with the main impurity atoms and move to an optically active state. For this reason, an increase in the optically active oxygen concentrations was observed in the Fourier spectroscopy analysis compared to the original sample.

Thus, the results obtained by determining the concentration of optically active background impurities in the original samples n-Si and in samples n-Si<Ni,Cu> showed that during high-temperature diffusion doping of silicon with nickel and copper, the concentration of optically active oxygen and carbon in the volume of samples increases significantly. This increase is due to the formation of complexes of oxygen and carbon atoms with atoms of the main impurities, after which they pass to the optically active state.

CONCLUSIONS

As can be seen from the results of X-ray diffraction analysis, several types of clusters containing nickel and copper impurity atoms formed in the silicon crystal after diffusion. In addition, from the results of X-ray diffraction analysis, the formation of various chemical compounds of oxygen atoms, carbon atoms with nickel or copper atoms, as well as with silicon atoms, is observed. Consequently, it appears that during high-temperature diffusion annealing, oxygen atoms form chemical compounds with the main impurity atoms and become optically active. For this reason, an increase in the optically active oxygen concentrations was observed in the Fourier spectroscopy analysis compared to the original sample.

Thus, the results obtained by determining the concentration of optically active background impurities in the original samples n-Si and in samples n-Si<Ni,Cu> showed that during high-temperature diffusion doping of silicon with nickel and copper, the concentration of optically active oxygen and carbon in the volume of samples increases significantly. This increase is due to the formation of complexes of oxygen and carbon atoms with atoms of the main impurities, after which they pass to the optically active state.

Funding

The present research work was financed under the project FZ-292154210 granted by the Ministry of Innovative Development of the Republic of Uzbekistan

ORCID

S.Z. Zainabidinov, https://orcid.org/0000-0003-2943-5844; **N.A. Turgunov,** https://orcid.org/0000-0003-3481-5622
A.Y. Boboev, https://orcid.org/0000-0002-3963-708X; **Sh.K. Akbarov,** https://orcid.org/0009-0008-4193-8659
R.M.Turmanova, https://orcid.org/0009-0005-7346-0571; **A. Artikov,** https://orcid.org/0009-0001-3911-3999
M.O. Kuchkarova, https://orcid.org/0009-0005-4053-0414; **B. Tolonova,** https://orcid.org/0009-0004-4944-1672
M.B. Rasulova, https://orcid.org/0009-0003-1068-7651

REFERENCES

[1] S.Z. Zainabidinov, Sh.K. Akbarov, N.A. Turgunov, N.B. Khaytimmetov, and R.M. Turmanova, "Formation of impurity accumulations in silicon doped with nickel and copper," E3S Web of Conferences. **632**, 03004 (2025). https://doi.org/10.1051/e3sconf/202563203004

[2] S.Z. Zaynabidinov, A.Y. Boboev, N.Y. Yunusaliyev, and M.B. Rasulova, "X-ray diffraction analysis, optical characteristics and electro-physical properties of the n-ZnO/p-NiO structure grown by the spray pyrolysis method," New Materials, Compounds and Applications, **8**(3), 411–421 (2024). https://doi.org/10.62476/nmca83411

[3] Y. Yamashita, *et al*., "Effect of metal impurities on recombination lifetime in Si," J. Appl. Phys. **127**, 075701 (2020). https://doi.org/10.1063/1.5140424

[4] S. Sarti, *et al*., "FTIR characterization of carbon in silicon," Materials Science in Semiconductor Processing, **21**, 78–83 (2014).

[5] M. Fahelelbom, A. Saleh, M. M. A. Al-Tabakha, and A. A. Ashames, "Recent applications of quantitative analytical FTIR spectroscopy in pharmaceutical, biomedical, and clinical fields: A brief review," Rev. Anal. Chem. **41**(1), 21–33 (2022). https://doi.org/10.1515/revac-2022-0030

[6] J.H. Linn, and K.L. Hanley, "Quantitative infrared spectroscopy of interstitial oxygen in silicon wafers using multivariate calibration," Applied Spectroscopy, **47**(12), 2102–2107 (1993). https://doi.org/10.1366/0003702934066361

[7] J. Kozuch, K. Ataka, and J. Heberle, "Surface-enhanced infrared absorption spectroscopy," Nat. Rev. Methods Primers, **3**, 1 (2023). https://doi.org/10.1038/s43586-023-00253-8

[8] B. Talanin, and I. Talanin, "High-temperature precipitation of impurities in metals," Physics of the Solid State, **64**(3), 340–346 (2022). https://doi.org/10.1134/S1063783422030270.

[9] G. Kissinger, D. Kot, F. Bärwolf, and M. Lisker, "Investigation of the Impact of Amorphous Silicon Layers Deposited by PECVD and HDP-CVD on Oxide Precipitation in Silicon," Materials Science in Semiconductor Processing, **164**, 107614 (2023). https://doi.org/10.1016/j.mssp.2023.107614

[10] N.A. Turgunov, E.Kh. Berkinov, and R.M. Turmanova, "Accumulations of impurity Ni atoms and their effect on the electrophysical properties of Si," E3S Web of Conferences, **402**, 14018 (2023).

[11] N.A. Turgunov, S.K. Akbarov, N.B. Khaytimmetov, and R.M. Turmanova, "Influence of accumulation of impurity atoms Ni and Fe on the electrophysical properties of Si single crystals," J. Nano Electron. Phys. **16**(1), 01004 (2024). https://doi.org/10.21272/jnep.16(1).01004

[12] D. Firsov, S. Khakhulin, and O. Komkov, "Fourier-transform infrared reflection anisotropy spectroscopy of semiconductor crystals and structures: Development and application in the mid-infrared," Appl. Spectrosc. **1**(4), 1–12 (2023).

[13] N.Y. Yunusaliyev, "The gas-sensitive properties of tin dioxide films" East Eur. J. Phys. **4**, 439 (2024), https://doi.org/10.26565/2312-4334-2024-4-5

[14] A. Janotti and C.G. Van de Walle, "Fundamentals of zinc oxide as a semiconductor," Reports on Progress in Physics, **72**(12), 126501 (2009). https://doi.org/10.1088/0034-4885/72/12/126501

[15] S. Zaynabidinov, *et al.*, "X-ray diffraction and electron microscopic studies of the ZnO(S) metal oxide films obtained by the ultrasonic spray pyrolysis method," Herald of the Bauman Moscow State Tech. Univ., Ser. Nat. Sci. **1**, 78 (2024). https://doi.org/10.18698/1812-3368-2024-1-78-92

[16] M. Kooti, and M. Jorfi, "Synthesis and characterization of nanosized NiO_2 and NiO using Triton X-100," Open Chemistry, **6**(1), 186–192 (2008). https://doi.org/10.2478/s11532-008-0005-9

ВПЛИВ ДОМІШКОВИХ КЛАСТЕРІВ НА ОПТИЧНІ ВЛАСТИВОСТІ КРЕМНІЮ, ЛЕГОВАНОГО НІКЕЛЕМ ТА МІДДЮ

Сіраджідін З. Зайнабідінов[1], Н.А. Тургунов[2], Акрамжон Й. Бобоєв[1], Шухратжон К. Акбаров[1], Раймаш М. Турманова[2], Абдукахор Аріков[1], Мукаддас О. Кучкарова[1], Бахріхон Толанова[1], Мархабо Б. Расулова[1]
[1]Андижанський державний університет імені З.М. Бабура, Андижан, Узбекистан
[2]Науково-дослідний інститут фізики напівпровідників та мікроелектроніки Національного університету Узбекистану, Ташкент

У цій статті розглядається вплив домішкових атомів на оптичні властивості монокристалічного кремнію, легованого нікелем та міддю, під час високотемпературного дифузійного легування. А також процеси утворення різних хімічних сполук за участю атомів кисню та вуглецю з атомами нікелю, міді та кремнію. За допомогою ІЧ-спектрометрії з перетворенням Фур'є та рентгеноструктурного аналізу було виявлено, що концентрація оптично активного кисню та вуглецю в об'ємі зразків кремнію, легованих нікелем та міддю, значно зростає порівняно з вихідними зразками.

Ключові слова: *кремній; нікель; мідь; дифузія; домішка; кисень; вуглець; кластери*