

**STUDY OF THE EFFECT OF Ni<sup>+</sup> ION IMPLANTATION ON THE NEAR-SURFACE  
LAYERS OF SILICON USING MODERN ANALYSIS METHODS**

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**Abstract**

In this work, a comparative study of the effect of Ar<sup>+</sup> and Ni<sup>+</sup> ion implantation on the structural, electronic, and optical properties of monocrystalline silicon (Si) was carried out. Ion bombardment leads to disordering of the near-surface layers and a decrease in the light transmission coefficient. After thermal annealing at T = 900 K, silicon implanted with Ni<sup>+</sup> ions forms epitaxial phases and nanofilms of NiSi<sub>2</sub> depending on the implantation dose. Modern approaches based on artificial intelligence methods for materials analysis can significantly improve the interpretation of experimental data obtained from spectroscopy and optical measurements.

**Keywords**

heterostructure, nanophase, ion implantation, silicon, nanofilms, silicide, surface morphology, artificial intelligence in materials science

**1. Introduction**

In recent years, significant attention has been devoted to studying the optical and electronic properties of semiconductor nanostructures formed in the surface layers of materials. Silicon-based nanostructures are of particular interest because reducing the crystal size to several nanometers can significantly modify the band structure and optical absorption edge.

Previous studies have shown that decreasing the size of silicon nanocrystals leads to a shift of the optical absorption edge toward higher photon energies due to an increase in the band gap width ( $E_g$ ). For nanocrystalline silicon phases with sizes of 3–4 nm, the band gap can increase up to 1.7 eV.

Modern artificial intelligence (AI) and machine learning methods are increasingly used in materials science to analyze experimental data and predict material properties. The integration of AI techniques with ion implantation experiments can significantly improve the analysis and optimization of semiconductor nanostructures.

**2. Purpose of the Work**

The main objective of this study is to investigate the effect of Ar<sup>+</sup> and Ni<sup>+</sup> ion bombardment on the formation of nanoscale phases in the near-surface region of Si(111) monocrystals, as well as their influence on electronic band structure, electrophysical properties, and optical characteristics of silicon.

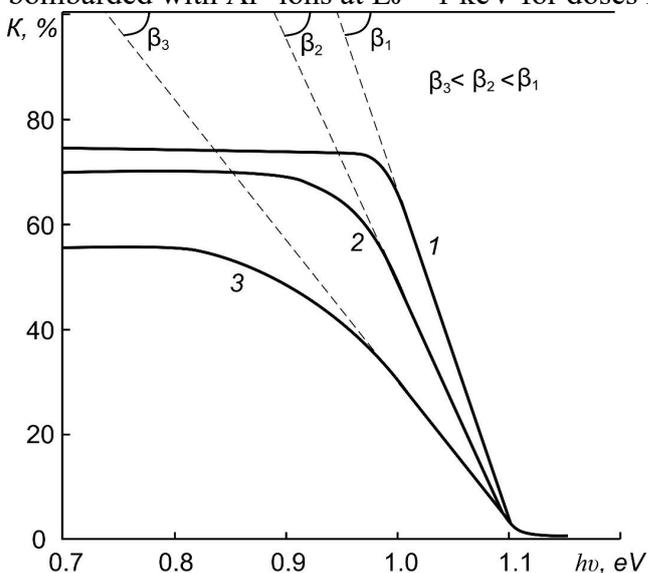
**3. Experimental Method**

Monocrystalline Si(111) samples with dimensions 10 × 10 × 0.5 mm were used as the objects of investigation. Ion implantation and surface analysis were performed using Auger Electron Spectroscopy (AES), Ultraviolet Photoelectron Spectroscopy (UPS), and optical transmission measurements.

All experiments were carried out in an ultra-high vacuum chamber with pressure  $P < 10^{-7}$  Pa. The energy of implanted ions was varied within  $E_0 = 0.5 - 2$  keV, and the implantation dose ranged from  $D = 10^{14} - 10^{17}$  cm<sup>-2</sup>.



Fig. Dependences of the light transmission coefficient  $K$  on photon energy for a Si(111) film bombarded with  $\text{Ar}^+$  ions at  $E_0 = 1$  keV for doses  $D$  ( $\text{cm}^{-2}$ ): 1 – 0; 2 –  $5 \times 10^{15}$ ; 3 –  $5 \times 10^{16}$ .



#### 4. Results and Discussion

Ion bombardment leads to disordering of the near-surface silicon layer, which results in a noticeable decrease in the optical transmission coefficient across the investigated photon energy range. Increasing the ion dose increases structural disorder and leads to the amorphization of the near-surface layer.

After annealing at 900 K, implantation of  $\text{Ni}^+$  ions leads to the formation of epitaxial  $\text{NiSi}_2$  phases in the silicon surface layer. Artificial intelligence methods may be applied to analyze spectral data and predict the formation of such nanophases.

#### 5. Conclusion

The results demonstrate that ion implantation significantly affects the structural and optical properties of silicon. The formation of  $\text{NiSi}_2$  nanophases after annealing confirms the effectiveness of ion implantation techniques for modifying semiconductor materials. The integration of AI-based analytical methods may further improve the understanding and optimization of such nanostructures.

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