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INVESTIGATION OF THE BEHAVIOR OF NICKEL IMPURITY ATOMS IN THE SILICON LATTICE BASED ON FIRST PRINCIPLES

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This work presents a comprehensive theoretical and experimental study of the behavior of nickel impurity atoms in the silicon crystal lattice. The focus is on analyzing diffusion mechanisms, the energetic characteristics of interstitial nickel atoms, their interaction with defects and other impurities, as well as the formation of stable clusters within the crystal volume. First-principles quantum mechanical modeling was employed using the QuantumATK software, applying the Linear Combination of Atomic Orbitals (LCAO) method and the Local Density Approximation (LDA) exchange-correlation functional. Special attention was given to calculating the binding energy of nickel atoms in interstitial sites and estimating the activation energy for their migration along various crystallographic directions ([100] and [010]). The modeling results revealed that nickel atoms predominantly diffuse in interstitial positions with an activation energy around 0.31 eV, which aligns well with previously reported experimental data. It was found that interactions of nickel with oxygen, carbon impurities, and point defects have a minimal impact on diffusion processes. However, interactions with vacancies lead to the formation of stable nickel silicides and cause an increased concentration of nickel near the surface. The experimental part of the study confirmed the formation of nickel clusters under high-temperature treatments. Scanning Electron Microscopy (SEM), Secondary Ion Mass Spectrometry (SIMS), and Infrared (IR) microscopy revealed a high density and uniform distribution of clusters throughout the crystal volume. Cluster sizes ranged from 20 to 100 nm, with concentrations reaching approximately 10^{10} cm^{-3}. These findings demonstrate that nickel acts as an effective gettering impurity, enhancing the electrophysical properties of silicon. The results provide valuable insights for optimizing the fabrication processes of high-efficiency silicon solar cells and microelectronic devices.
Keywords: *Nickel; Silicon; Diffusion; Clusters; Interstitial atoms; First-principles; Activation energy; Quantum mechanical modeling; Gettering; Semiconductors*
PACS: 68.37.Rt, 68.37.Ps

INTRODUCTION

Silicon is a key semiconductor material widely used in microelectronics, photonics, and solar energy. The electrophysical properties of silicon are largely determined by the level of crystalline purity and the presence of impurity atoms. Of particular importance is the influence of such impurities on the lifetime of minority charge carriers - a critical parameter that determines the efficiency of solar cells. Transition metals, in particular nickel, form deep energy levels in the silicon bandgap, acting as recombination centers and reducing the carrier lifetime, which leads to degradation of semiconductor device performance. At the same time, nickel exhibits pronounced gettering properties, facilitating the removal of contaminating impurities from the active region, which conversely increases carrier lifetime and improves photovoltaic parameters.

The present study aims to investigate the behavior of nickel atoms in silicon, their impact on recombination processes, gettering effects, as well as the stability and durability of silicon structures. Using quantum-mechanical modeling methods based on first principles, the microscopic mechanisms of interaction between nickel and the crystal lattice are analyzed, enabling the proposal of new approaches to improve the efficiency and reliability of semiconductor devices. Previous studies [1-3] and foreign researchers [4-7] have examined the diffusion mechanisms of nickel impurities, the state of impurity atoms in the lattice, and their influence on the electrical parameters of silicon. The majority of nickel atoms diffuse in silicon in an electronically neutral state and primarily occupy interstitial positions. The maximum solubility of nickel atoms is nearly two orders of magnitude higher (see Table 1) than that of other transition group elements. To deepen the understanding of the diffusion processes of nickel impurity atoms in silicon, this work performs first-principles calculations of the activation energy of interstitial nickel atoms in the silicon crystal lattice.

The diffusion coefficient of interstitial nickel atoms depends weakly on temperature and is approximately $\sim 10^{-5} \div 10^{-4}$ cm^2/s. To calculate the diffusion coefficient of nickel in silicon, the equations given in Table 2 can be used.

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Table 1. Solubility of nickel atoms in silicon [2]

State of atoms	Calculation formula	Solubility at T=1250 °C, cm^{-3}
in nodes	$Ni_s(T)=10^{26}\cdot\exp(-3.1\ eV/kT)$	$5\cdot10^{14}$
in the internodes	$Ni_i(T)=1.23\cdot10^{24}\cdot\exp(-1.68\ eV/kT)$	$7\cdot10^{17}\div10^{18}$
	$N_i(T) = 1{,}4\times10^{25}\ \exp(-2.3\ eV/kT)$	$7\cdot10^{17}$

Table 2. Diffusion coefficient of nickel atoms in silicon [3]

Temperature range T, °C	Calculation formula	D, cm^2/c
900÷1300	$D(Ni_i)=2.3\cdot10^{-3}\cdot\exp(-0.47\ eV/kT)$	$(3\div8)\times10^{-5}$
600÷900	$D(Ni_i)= (1.69\pm0.74)\times10^{-4}\ \exp(-0.15\ eV/k_BT)$	$(2\div4)\times10^{-5}$

RESEARCH METHODOLOGY

In this work, the behavior of the energy of an interstitial nickel atom in the silicon crystal lattice was studied. For this purpose, based on first principles, the dependence of the lattice energy on the position of the interstitial nickel atom was analyzed. Figure 1 shows the primitive unit cell of the silicon crystal.

To calculate the dependence of the lattice energy on the position of the interstitial nickel atom, a minimal region of the silicon lattice was selected, constructed based on the primitive unit cell. For this, a lattice slice (lattice projection) in the (100) direction was considered (Fig.2). To form the first coordination sphere around the Ni atom, the cell shown in Figure 2 was translated in the Y direction (Fig.3).

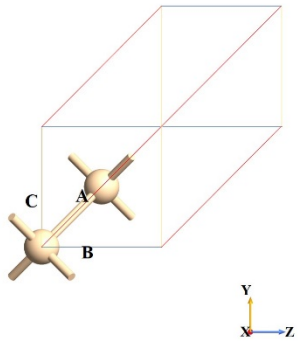


Figure 1. Primitive unit cell of the silicon crystal

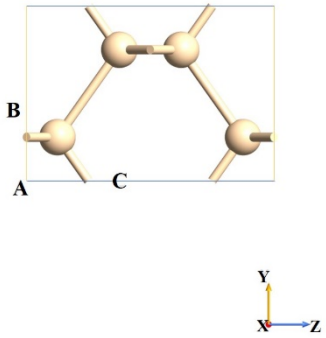


Figure 2. Section of the silicon lattice in the (100) direction

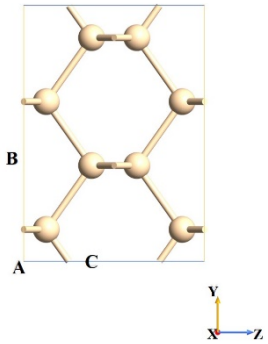


Figure 3. A silicon lattice cell obtained by translating the cut shown in Fig. 2 in the direction of the Y axis

The position of the nickel atom was considered relative to point O at the center of the obtained cell (Fig.3), so atoms located farther from this region, which did not belong to the first coordination sphere, were removed (Fig.4).

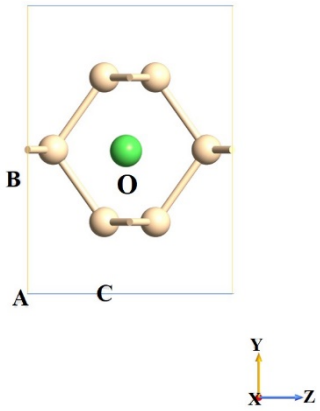


Figure 4. Cell and silicon atoms included in the first coordination sphere for the nickel impurity atom located in the region around point O

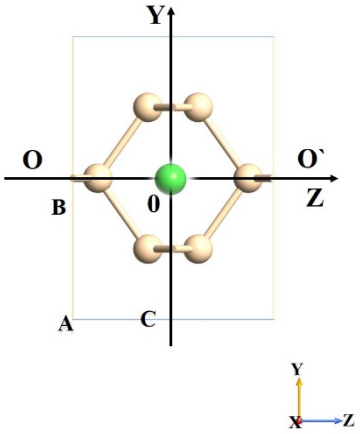


Figure 5. Illustration of the OO' axis (Z-axis direction) along which various positions of the interstitial Ni atom were considered

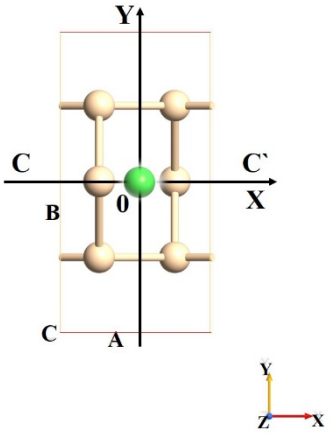


Figure 6. Illustration of the CC' axis (X-axis direction) along which various positions of the interstitial Ni atom were considered

The lattice energy was calculated for various positions of the interstitial Ni atom along the OO' axis (direction along the Z-axis) passing through the center of the formed cell (Fig. 5). The origin of the coordinate system was taken as the point corresponding to the center of volume O of the considered lattice cell. The dependence of the total energy on the position of the nickel atom was analyzed along two mutually perpendicular directions: along the OO' axis (direction along the Z-axis) and perpendicular to it along the CC' axis (direction along the X-axis), which also passes

through the center of the volume of the considered lattice (Fig. 6). The origin along this axis was also taken as the point corresponding to the center of the volume of the considered lattice.

When examining the energetic behavior of nickel impurity atoms, the most important characteristic is the binding energy of nickel atoms in the silicon lattice. To determine the binding energy of a Ni atom in the silicon lattice cell, it is necessary to subtract the total energy of the silicon cell and the Ni atom from the total energy of the system:

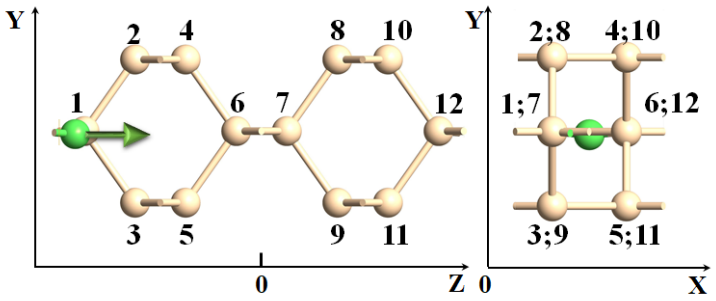
$$E_{binding} = E_{total} - E_{Si} - E_{Ni}$$

By performing these calculations for each position of the Ni atom within the silicon unit cell, one can obtain the dependence of the Ni atom's binding energy as it moves both along the OO' direction (Z axis) and along the CC' direction (X axis).

The calculations were carried out from first principles using the QuantumATK software. The molecular orbital method was employed, specifically the LCAO method (Linear Combination of Atomic Orbitals). To determine the electronic structure, the exchange-correlation functional Local Density Approximation (LDA) was chosen. The interatomic interactions were modeled using the PseudoDojo pseudopotential.

To increase the accuracy of the electronic density calculation, the density cutoff parameter of the computational grid was set to 75 Ry. The k-point mesh was chosen with a density of 4 × 4 × 0 $Å^{-1}$, which is an optimal choice for electronic property calculations.

To study the behavior of the nickel atom during its transition from one cell to a neighboring one, the energy behavior was considered during movement along two adjacent cells both in the OO' (OZ) direction and in the CC' (OX) direction (Figs. 7 and 8). In the calculations, 12 silicon atoms were fixed, while the movement of the nickel atom was restricted to only one direction at a time, with the other two directions left free.



(a) (b)

Figure 7. Structure of the considered silicon crystal cell with a nickel impurity atom (colored green) and the direction of nickel atom diffusion along the OZ axis (a) and view of the cell in cross-section (b). The numbers in the Figure mean the order number of atoms

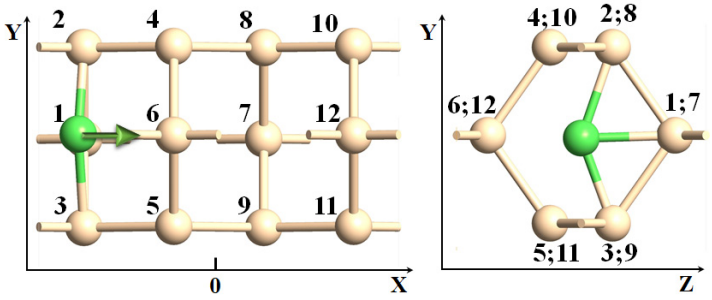


Figure 8. Structure of the considered silicon crystal cell with a nickel impurity atom (colored green) and the direction of nickel atom diffusion along the OX axis (a) and view of the cell in cross-section (b). The numbers in the Figure mean the order number of atoms

Structure optimization was also performed using the Optimize Geometry function of the program. During optimization, the force tolerance was set to 0.05 eV/Å, and the stress tolerance was set to 0.1 GPa [17, 18]. The maximum number of iterations was limited to 200, and the maximum step size was not allowed to exceed 0.2 Å. The optimization process was carried out using the LBFGS algorithm (Limited-memory Broyden-Fletcher-Goldfarb-Shanno).

For the optimized structure, the total energy was calculated, which allowed determination of the thermodynamically stable states of the system and the energetic configurations of the nickel atom in the silicon matrix. The applied methods provide high accuracy in calculating the electronic and structural properties of the system.

RESULTS AND DISCUSSION

The results of calculating the binding energy dependence of the interstitial nickel impurity atom on its position along two mutually perpendicular directions are shown in Figures 9 and 10. These graphs show that the activation

energy, defined as the energy required to transition from one equilibrium position to another, depends on the direction of movement within the lattice.

During diffusion of the nickel atom along the Z direction, several equilibrium positions appear with energies of 0.26, 0.32, 0.44, and 0.67 eV. The maximum energy required to overcome the barrier (diffusion activation energy) in this direction is 0.91 eV. During diffusion along the X direction, several equilibrium positions also appear, with approximately equal energies around 0.31 eV.

The activation energy values obtained from first-principles calculations (0.31 eV) lie between the values of 0.51 eV and 0.15 ± 0.04 eV reported in studies [8, 9], respectively.

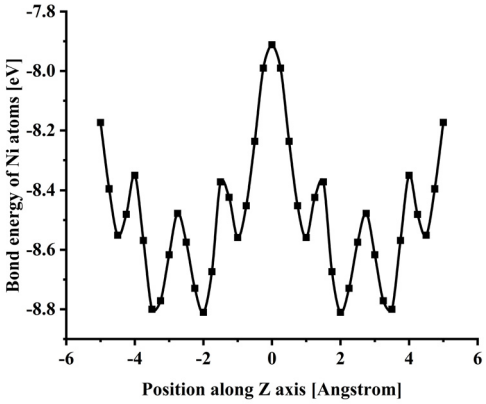


Figure 9. Dependence of the binding energy on the position of the Ni atom along the CC' axis (along the Z direction).

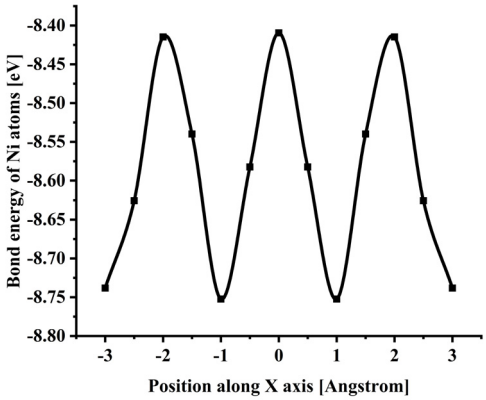


Figure 10. Dependence of the binding energy on the position of the Ni atom along the X direction.

However, when calculating diffusion parameters in real crystals, it is also necessary to take into account the influence of impurities (including electrically inactive ones) and point defects that have a significant concentration in semiconductor silicon under diffusion conditions. These include oxygen, carbon, boron, vacancies, divacancies, and interstitial silicon.

Since Ni_i is in a neutral charge state [7], there is no Coulomb attraction to small dopant impurities (such as boron).

The interaction between Ni_i and substitutional carbon (C_s) occurs with an energy of – 0.31 eV [8]. This energy is comparable to the activation energy of nickel diffusion in pure silicon, so the carbon impurity does not affect diffusion.

The interaction between Ni_i and interstitial oxygen (O_i) is very weak: the formation energy of the complex is - 0.07 eV [7]. This trapping energy is significantly lower than the activation energy of interstitial nickel atoms, which is 0.31 eV for diffusion in silicon [8,9]. Therefore, O_i does not impede Ni_i diffusion.

In work [7], the interaction of Ni_i with intrinsic interstitial silicon atoms (I_{Si}^0) and vacancies (V^0) was calculated. The interaction between interstitial nickel and silicon has little effect on nickel diffusion processes in silicon because the concentration of I_{Si}^0 is low [$\sim 10^9 \div 10^{11}$ cm^{-3}], and the binding energy is estimated to be 0.07÷0.10 eV [7].

The interaction between Ni_i and V^0 is much stronger [10], since Ni becomes substitutional and forms four covalent Ni–Si bonds:

$$Ni_i + V^0 \rightarrow Ni_s + 2.60 \text{ eV}$$

Such a reaction is highly likely to lead to the formation of chemical compounds—silicides—at the nickel-silicon interface. The flux of vacancies and divacancies from the silicon lattice volume slows down nickel diffusion and results in an increased concentration of substitutional nickel near the surface, forming a nickel-enriched layer.

The maximum nickel excess in the surface layer can reach $\exp(2.6/0.31) \approx 4\times10^3$ times the solubility of nickel in the lattice (10^{18} cm^{-3}). This allows estimating the maximum nickel concentration at the surface to be on the order of 10^{22} cm^{-3}. This roughly corresponds to experimental data [11].

During the cooling process after diffusion, the state of nickel atoms can easily change. Nickel, having high mobility in the silicon lattice, can form complexes with impurities (carbon, oxygen) and with each other, forming "nickel clusters."

As shown in [9], nickel atoms diffuse in silicon as electronically neutral atoms but with a changed quantum state ($3d^8 4s^2 \rightarrow 3d^{10} 4s^0$). According to Hund's rule, nickel atoms thus acquire a more stable state. At the same time, the atomic radius of nickel decreases from 12.5 nm to 10 nm. This enables nickel atoms to occupy interstitial sites and move through the interstitial positions without significant deformation of the silicon lattice. Since the size of the interstitial sites in silicon (12.7 nm) is larger than the radius of the nickel atom, it can be assumed that the cluster consists of electronically neutral nickel atoms located at interstitial positions in the silicon lattice and additionally bonded to each other, most likely by metallic-type bonding.

Based on the above, it can be assumed that electronically neutral nickel atoms in the clusters occupy the nearest equivalent interstitial positions and form a cubic nickel sublattice similar to the regular silicon lattice, with a lattice constant approximately equal to that of silicon.

We calculated [12] that the binding energy of nickel atoms to a nickel cluster is $\Delta E_k \approx 1.39$ eV, and the concentration of nickel atoms in the clusters is 6 to 8 orders of magnitude higher than the residual nickel concentration in the silicon lattice.

To verify the formation of clusters and silicides on the surface due to the high nickel concentration, the following studies were conducted:

Polished silicon wafers of grade KDB-0.5 were used. A layer of pure nickel, 1 μm thick, was deposited on the surface of the samples in a vacuum, followed by diffusion at T_{diff} = 800÷950°C for 30 to 60 minutes, and at T_{diff}=1000÷1200°C for 5 to 60 minutes in an air atmosphere. The samples were cooled in air at a rate of approximately 50÷60°C/sec.

To determine the composition and distribution of nickel clusters, samples with clusters were studied using scanning electron microscopy (SEM) equipped with X-ray microanalysis, as well as by SIMS and IR microscopy methods.

During this experiment, it was found (see Fig. 11) that the surface density of nickel clusters is approximately 5×10^6 to 10^7 cm^{-2} on the silicon surface and about $(4\div5)\times10^6$ cm^{-2} in the bulk. The distribution of clusters in the bulk is practically uniform, and their size is less than 0.5 μm (estimated by us to be from 20 to 100 nm), which confirms the results of studies [13–15].

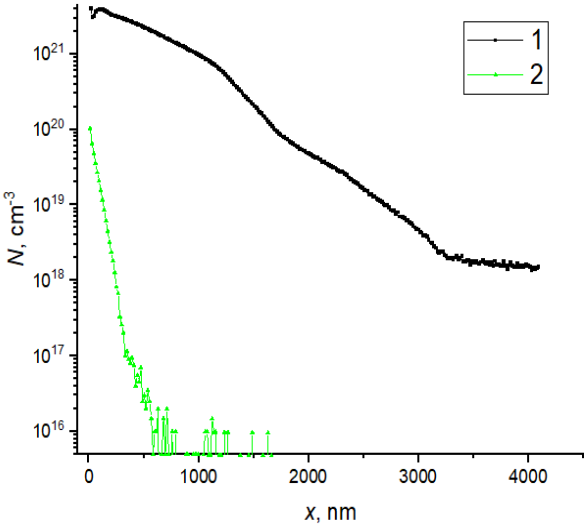


Figure 11. Distribution of nickel atoms in the front (1) and back (2) layers of silicon after diffusion from a metallic nickel film deposited on one surface of the silicon

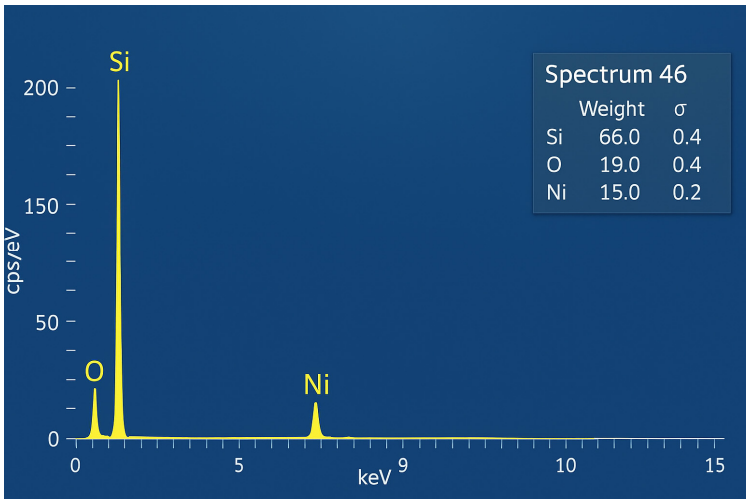


Figure 12. Spectrum and composition of clusters of nickel primium atoms on the silicon surface, obtained using a MIRA 3 TESCAN scanning electron microscope (Field-Emission Scanning Electron Microscope (FE-SEM)).

Fig. 12, shows the arrangement of nickel atom clusters on the silicon surface obtained using a MIRA 3 TESCAN (Field-Emission Scanning Electron Microscope (FE-SEM)). To verify that the observed clusters are nickel atom clusters, we studied their composition using the method (energy dispersive X-ray spectroscopy EDS).

Additional thermal annealing at relatively low temperatures should lead to the redistribution of isolated interstitial nickel atoms and to the growth of cluster sizes. The additional thermal annealing was carried out at T_{ann} = 700÷900 °C for 30 to 60 minutes in an air atmosphere. The cooling rate of the samples after annealing was not significant. The increase in cluster size makes it possible to study nickel clusters in silicon using infrared microscopy (on the INFRAM-I microscope).

As seen in Fig. 13, the nickel atoms introduced by diffusion are present in the lattice as clearly visible clusters, uniformly distributed throughout the crystal volume, which confirms the results of [16-18].

The cluster size depends on the presence of defects in the silicon lattice and the conditions of additional thermal treatment (degree of supersaturation). Based on the results of infrared microscopy, it can be concluded that the average cluster diameter increases to several microns after annealing, and the cluster concentration is on the order of ~10^{10} cm^{-3}.

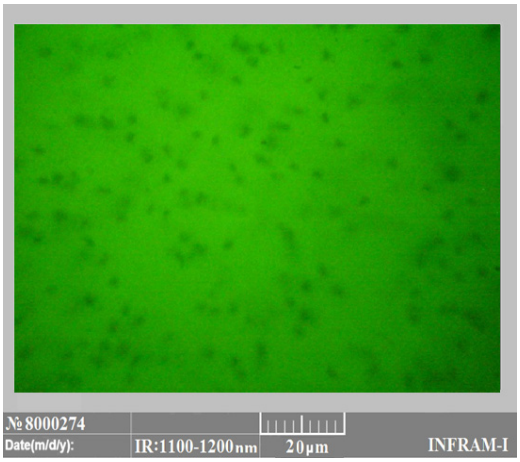


Figure 13. Clusters of impurity nickel atoms in the silicon lattice

CONCLUSION

As a result of the conducted study, it was established that nickel atoms in silicon predominantly diffuse through interstitial positions with the lowest activation energy along the crystallographic direction [100], with a value of 0.31 eV. It was found that at high nickel concentrations under thermal treatment conditions, stable clusters are formed, uniformly distributed throughout the crystal volume. These results confirm the important role of nickel as an effective gettering impurity and as a basis for controlling the recombination properties of silicon structures.

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ДОСЛІДЖЕННЯ ПОВЕДІНКИ АТОМІВ НІКЕЛЕВОЇ ПРИМІСІ В КРИСТАЛІЧНІЙ РІШІТЦІ КРЕМНІЮ НА ОСНОВІ ПЕРШИХ ПРИНЦИПІВ

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Ця робота представляє всебічне теоретичне та експериментальне дослідження поведінки атомів нікелевої домішки в кристалічній решітці кремнію. Основна увага приділяється аналізу механізмів дифузії, енергетичних характеристик міжвузлових атомів нікелю, їх взаємодії з дефектами та іншими домішками, а також утворенню стабільних кластерів у об'ємі кристала. Для моделювання з першопринципним підходом застосовувалося квантово-механічне програмне забезпечення QuantumATK із використанням методу лінійної комбінації атомних орбіталей (LCAO) та функціоналу обміну-кореляції локальної густини (LDA). Особливу увагу було приділено розрахунку енергії зв'язку атомів нікелю у міжвузлових положеннях та оцінці енергії активації їх міграції вздовж різних кристалографічних напрямків ([100] та [010]). Результати моделювання показали, що атоми нікелю переважно дифундують у міжвузлових положеннях з енергією активації близько 0,31 еВ, що добре узгоджується з раніше опублікованими експериментальними даними. Виявлено, що взаємодія нікелю з киснем, вуглецевими домішками та точковими дефектами має незначний вплив на процеси дифузії. Однак взаємодія з вакансіями призводить до утворення стабільних силіцидів нікелю та збільшення концентрації нікелю поблизу поверхні. Експериментальна частина дослідження підтвердила утворення кластерів нікелю при термічній обробці за високих температур. Методами скануючої електронної мікроскопії (SEM), вторинної іонної мас-спектрометрії (SIMS) та інфрачервоної (ІЧ) мікроскопії було виявлено високу щільність і рівномірний розподіл кластерів по всьому об'єму кристала. Розміри кластерів варіювалися від 20 до 100 нм, а концентрації досягали приблизно 10^{10} $см^{-3}$. Ці результати демонструють, що нікель виступає як ефективна геттеруюча домішка, покращуючи електрофізичні властивості кремнію. Отримані дані є цінним внеском для оптимізації технологічних процесів виготовлення високоефективних кремнієвих сонячних елементів та мікроелектронних пристроїв.

Ключові слова: *нікель; кремній; дифузія; кластери; міжвузлові атоми; першопринципне моделювання; енергія активації; квантовомеханічне моделювання; геттерування; напівпровідники*