

EFFECT OF NICKEL DIFFUSION ON TRAP STATES AND INTERFACE QUALITY IN POLYCRYSTALLINE SILICON STRUCTURES

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This work presents a comprehensive Deep-Level Transient Spectroscopy (DLTS) investigation into the influence of nickel (Ni) diffusion on the defect landscape and electronic properties of polycrystalline silicon (poly-Si) structures. The study aims to clarify how Ni incorporation modifies electrically active traps, alters charge carrier dynamics, and affects interface quality in Schottky diodes formed on poly-Si substrates. Two types of samples—undoped and Ni-diffused—were prepared via controlled thermal processing at 1000 °C, followed by surface passivation and gold/aluminum metallization to form Au/Poly-Si/Al Schottky diodes. DLTS measurements over the temperature range 20–300 K revealed distinct differences in the deep-level trap behavior of the two sample types. In undoped samples, only weak and broad trap signals were observed, primarily associated with intrinsic grain boundary defects and residual impurities. In contrast, Ni-diffused samples exhibited sharp, intense DLTS peaks, with a dominant trap level observed between 200 and 220 K. The corresponding activation energy was estimated to be approximately 0.492 eV, and the capture cross-section was in the range of 10^{-14} – 10^{-13} cm². These parameters indicate the formation of nickel-related complex defects, such as Ni–V or Ni–O clusters, primarily located at grain boundaries. C–V profiling further confirmed the influence of Ni incorporation, showing reduced capacitance, a smoother transition in the depletion region, and improved interface uniformity, suggesting partial passivation of native and boundary-related traps. The Ni-diffused sample displayed a smoother capacitance–voltage transition, reduced junction capacitance, and improved interface uniformity, suggesting partial passivation of native defects. Complementary G_p–V measurements showed a significant decrease in parallel conductance for Ni-doped structures, indicating a reduction in interface trap density and recombination centers. These results suggest a dual role of nickel – both as a source of deep-level traps and as a passivating agent, depending on local atomic environment and thermal treatment conditions. Surface morphology analysis using Scanning Electron Microscopy (SEM) and Energy-Dispersive X-ray Spectroscopy (EDX) confirmed the formation of Ni-rich precipitates, particularly at grain boundaries. The spatial correlation between Ni and oxygen suggests the formation of Ni–O-based complexes, which likely contribute to the electrical passivation effects observed in DLTS and G_p–V data. Overall, this study demonstrates that controlled Ni diffusion offers a promising approach for defect engineering in polycrystalline semiconductors. By selectively introducing and passivating defect states, Ni doping can enhance the electronic quality and thermal stability of poly-Si, thereby improving its suitability for high-efficiency solar cells, radiation detectors, and other advanced electronic and optoelectronic devices.

Keywords: Polycrystalline silicon; Nickel clusters; DLTS; Deep-level defects; Schottky diode; Impurity diffusion

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INTRODUCTION

The advancement of low-cost, large-area silicon-based technologies increasingly depends on effective control of crystalline defects and impurity behavior in polycrystalline silicon (poly-Si). Compared to monocrystalline silicon, poly-Si exhibits a higher density of grain boundaries and intrinsic structural imperfections, which serve as non-radiative recombination centers and negatively impact device performance [1-3].

Among external impurity elements, transition metals such as nickel (Ni) play a dual role in silicon matrices. On one hand, they can passivate intrinsic traps under certain conditions; on the other hand, they may form deep-level trap complexes that deteriorate carrier lifetimes. Notably, nickel's high diffusivity in silicon and its tendency to agglomerate at grain boundaries create favorable conditions for cluster formation, which are often responsible for distinct electronic activity detectable through electrical techniques [4-8]. Deep-Level Transient Spectroscopy (DLTS) is a powerful method for studying electrically active defects. By analyzing the transient capacitance response of Schottky diodes to thermal stimuli, DLTS can determine key trap-state parameters, such as activation energy and capture cross-section. While many studies have examined metal-induced defects in monocrystalline silicon, there is a lack of detailed analysis of Ni-related defect clusters in polycrystalline matrices [9, 10]. This work addresses this gap by exploring the electronic impact of nickel diffusion in polycrystalline silicon using DLTS and Schottky barrier analysis. By establishing clear differences in trap profiles between doped and undoped samples, we provide insights into the defect formation mechanisms and their potential for material optimization.

METHODS

To investigate the electrical activity and microstructural effects of nickel-induced deep-level defects in polycrystalline silicon (poly-Si), a multi-step sample preparation and characterization methodology was employed.

Commercially available polycrystalline silicon wafers with a resistivity of 10^2 – 10^3 $\Omega\cdot\text{cm}$ were selected and cut into 5×10 mm^2 squares using a diamond saw to ensure minimal edge damage and compatibility with standard measurement setups.

Each sample underwent an extensive surface preparation procedure to ensure high measurement accuracy. Mechanical polishing was conducted in stages, starting with coarse SiC papers and progressing to alumina (Al_2O_3) suspensions with particle sizes decreasing from 3 μm to 0.05 μm to produce a smooth, mirror-like surface. After mechanical treatment, samples were ultrasonically cleaned in acetone, isopropanol, and deionized water [10]. A standard RCA cleaning procedure was applied to remove residual organic and metallic contaminants. To eliminate the native oxide layer and activate the surface, a 5% HF solution etch was performed for 30 seconds. The samples were then immediately transferred to the deposition chamber to prevent reoxidation. A thin nickel layer (~50 nm) was deposited on one side of the samples using thermal vacuum evaporation under a base pressure of 5×10^{-4} Torr. The deposition thickness was monitored using a quartz crystal microbalance. Subsequently, the samples were annealed in a nitrogen ambient at 1000°C for 30 minutes in a quartz tube furnace. This thermal treatment enabled the diffusion of nickel atoms into the grain boundaries and defect-rich regions of the poly-Si matrix. The samples were gradually cooled to minimize thermal shock [11]. Post-diffusion, any remaining surface nickel was removed using a chemical etchant composed of nitric acid (HNO_3), acetic acid (CH_3COOH), and hydrofluoric acid (HF) in a volumetric ratio of 5:3:2 for 15 seconds. This step ensured a clean and uniform surface before device fabrication. Schottky diodes were fabricated by depositing circular gold contacts (1 mm in diameter) via thermal evaporation onto the nickel-diffused surface using a shadow mask. The rear side of each sample was coated with aluminum to form an ohmic contact. The devices were annealed at 200°C in a nitrogen atmosphere for 10 minutes to enhance the metal-semiconductor interface properties.

To investigate the microstructural effects of nickel diffusion, surface morphology analysis was performed using Scanning Electron Microscopy (SEM). A Zeiss AURIGA FIB-SEM system was used to acquire high-resolution images of the nickel-diffused silicon surfaces. SEM analysis enabled the direct visualization of surface features such as grain boundaries, diffusion-induced surface texture changes, and possible clustering effects [12]. Images were obtained in both secondary electron (SE) and backscattered electron (BSE) modes to enhance contrast between silicon and nickel-rich regions. These microstructural observations were used to correlate the electrical activity observed in DLTS measurements with the physical manifestation of defect sites and clusters on the polycrystalline surface.

Deep-Level Transient Spectroscopy (DLTS) measurements were conducted over a temperature range of 20–300 K using a stepwise heating protocol. The Schottky diodes were reverse-biased at -5 V, and filling pulses of -2 V amplitude with 1 ms duration were applied. The transient capacitance signal was recorded at multiple rate windows (80 s^{-1} , 200 s^{-1} , 400 s^{-1} , 800 s^{-1}) to resolve traps with different emission time constants. The resulting DLTS spectra were analyzed to extract the activation energy, capture cross-section, and defect concentration corresponding to nickel-related trap states [13–17].

EXPERIMENTAL RESULTS

In this experimental section, we investigate the impact of nickel diffusion into polycrystalline silicon by comparing DLTS and C–V measurements. The measurements were performed on both undoped and Ni-diffused samples using various rate windows (80 , 200 , 400 , and 800 s^{-1}) for DLTS and a voltage sweep from -2 to -5 V for C–V profiling. The goal is to determine the deep-level trap behavior, concentration, and how nickel incorporation affects the electrical quality of the material.

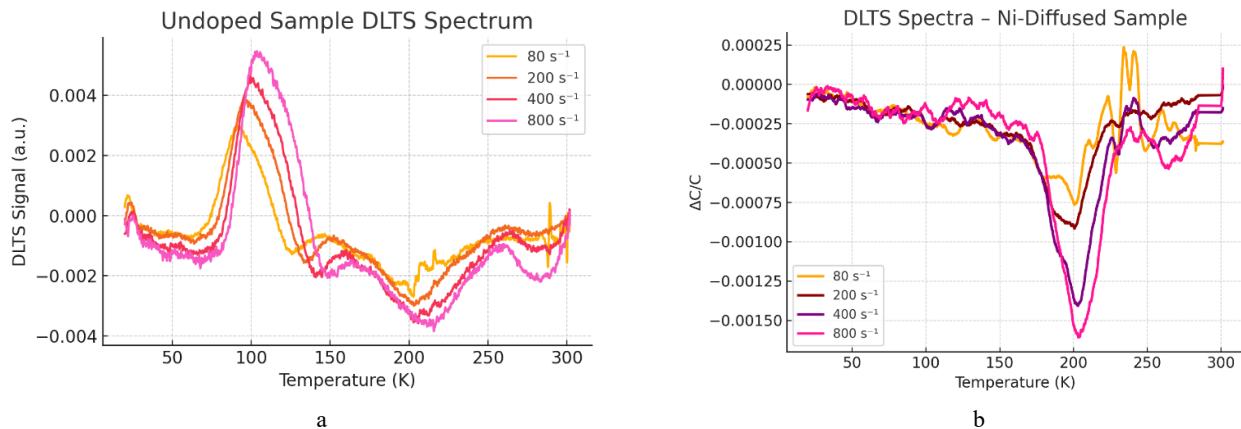


Figure 1. DLTS spectra of polycrystalline silicon samples at different rate windows
(a) undoped sample; (b) sample with Ni-diffused

Undoped sample (Fig. 1a) showing relatively low signal amplitude and broad trap responses across the temperature range, indicating the presence of intrinsic grain boundary and bulk defects; A pronounced peak appears around 110 K, indicating the presence of shallow-level traps likely associated with intrinsic point defects such as

oxygen or carbon complexes. The DLTS signal amplitude increases with rate window, confirming thermally activated emission characteristics. Ni-diffused sample (Fig. 1b) with sharper and deeper peaks, especially between 180–250 K, corresponding to the formation of Ni-related deep-level traps such as Ni–V and Ni–Si complexes. The enhanced signal intensity and shift in peak position reflect changes in trap energy levels and charge emission rates induced by nickel diffusion.

Figures 2a and b illustrate the Arrhenius plots obtained for the undoped and Ni-diffused polycrystalline silicon samples.

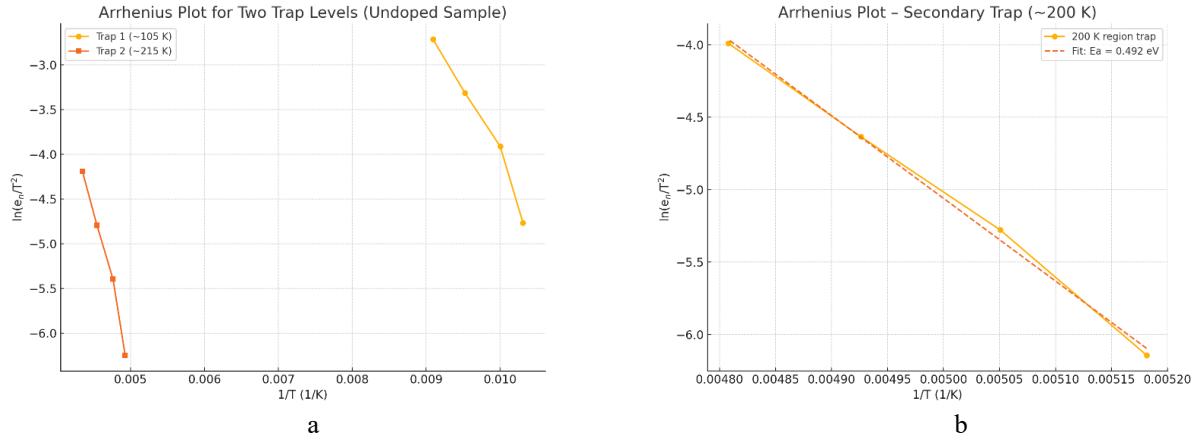


Figure 2. Arrhenius plots for trap level analysis in polycrystalline silicon samples derived from DLTS measurements

The emission rate data were extracted from DLTS spectra over various rate windows and plotted as $\ln(e_n/T^2)$ versus $1/T$ to determine the activation energies of the observed deep-level traps. In the undoped sample (Figure 2a), two distinct trap levels were identified at approximately 105 K and 215 K, corresponding to activation energies of $E_a \approx 0.141$ eV and $E_a \approx 0.275$ eV, respectively. In contrast, the Ni-diffused sample (Figure 2b) showed a dominant single trap around ~ 200 K, with a significantly higher activation energy of $E_a \approx 0.492$ eV. This increase in energy suggests the formation of new, deeper traps, possibly associated with Ni-related complexes or defect passivation mechanisms.

These findings confirm that Ni diffusion leads to the emergence of deeper trap levels and potentially alters the defect structure of the polycrystalline silicon matrix. [18-19].

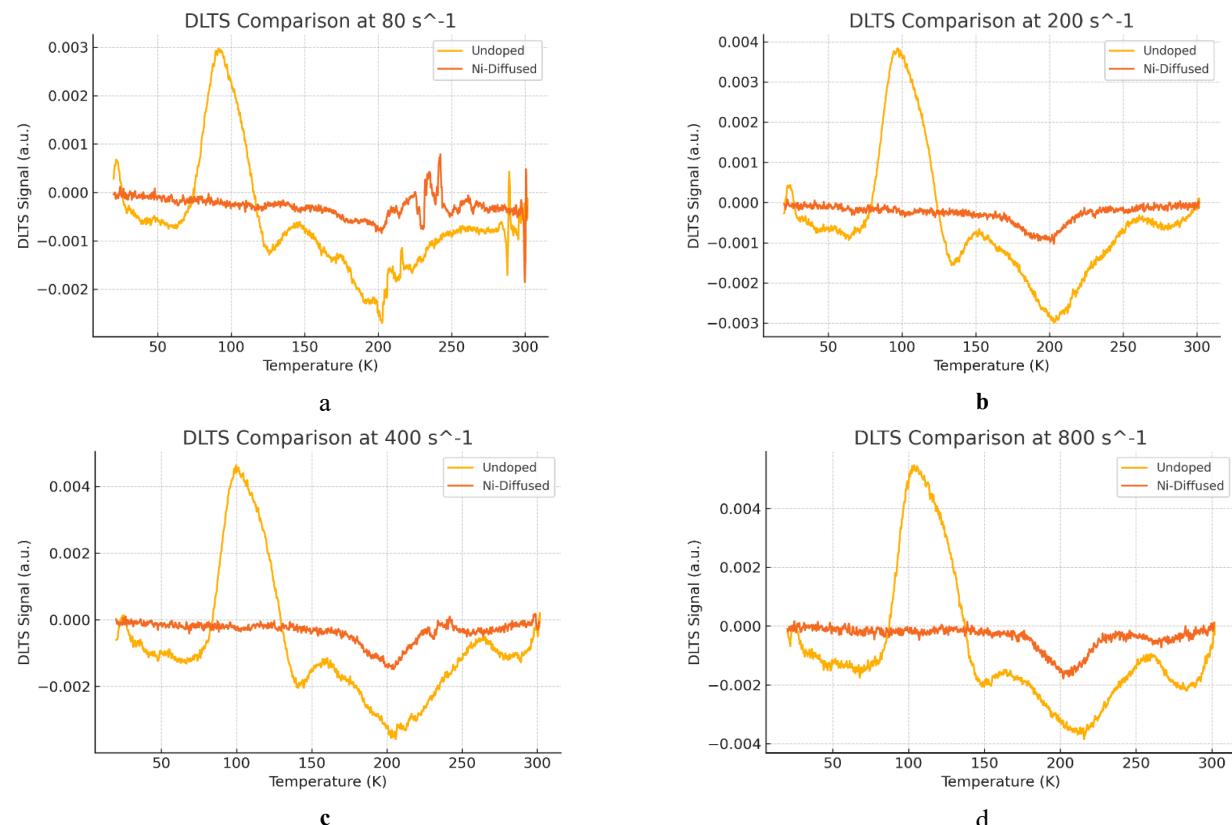


Figure 3. Comparison of DLTS spectra of undoped and Ni-diffused polycrystalline silicon samples at various rate windows (a) 80 s^{-1} , (b) 200 s^{-1} , (c) 400 s^{-1} , and (d) 800 s^{-1}

In all measurements, the Ni-diffused sample shows significantly deeper and sharper DLTS signals, with multiple peak formations compared to the undoped sample (Fig. 3.). This indicates increased trap concentration and enhanced recombination activity due to the formation of Ni-related deep levels. The undoped sample exhibits broader and shallower responses, consistent with intrinsic grain boundary and bulk defects. The variation in signal intensity and peak position with increasing rate window reflects differences in emission rates and activation energies of the traps.

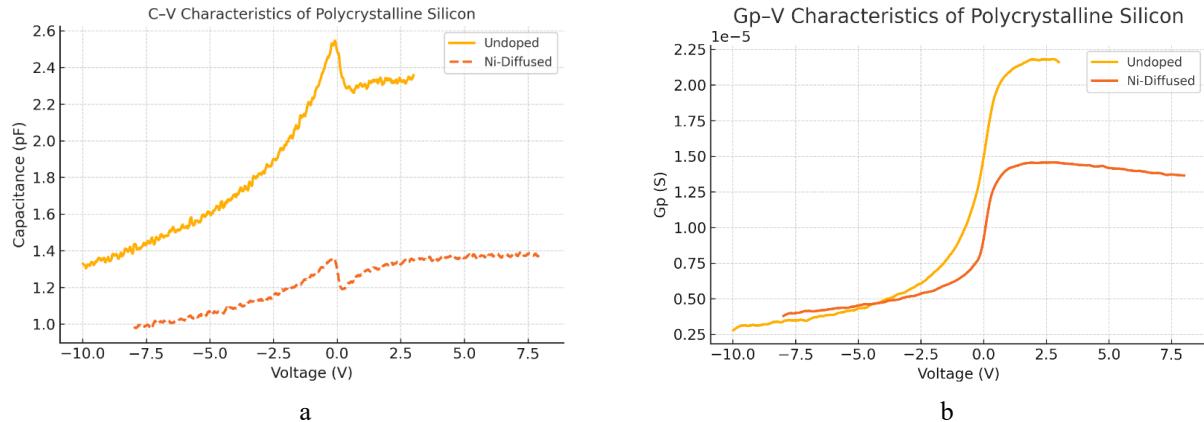


Figure 4. a) Capacitance–Voltage (C–V) characteristics of undoped and Ni-diffused polycrystalline silicon samples.
b) Gp–V characteristics of undoped and Ni-diffused polycrystalline silicon samples.

The undoped sample (Figure 4a) exhibits higher capacitance values and a sharper transition in the depletion region, which may be attributed to a lower defect density and more abrupt junction interface. In contrast, the Ni-diffused sample shows a reduced capacitance with a smoother voltage response, indicating an increased trap concentration and possible passivation of grain boundaries. The shift in capacitance behavior reflects the changes in dopant distribution and interface quality resulting from nickel diffusion. The Ni-diffused sample (Figure 4b) shows a reduced parallel conductance across the voltage range, indicating effective passivation of interface and grain boundary states. In contrast, the undoped sample exhibits higher G_p values, especially in the depletion region, which suggests a greater density of interface traps and enhanced recombination activity. The suppression of G_p in the doped structure confirms that nickel incorporation reduces the density of electrically active defects and improves the junction quality.

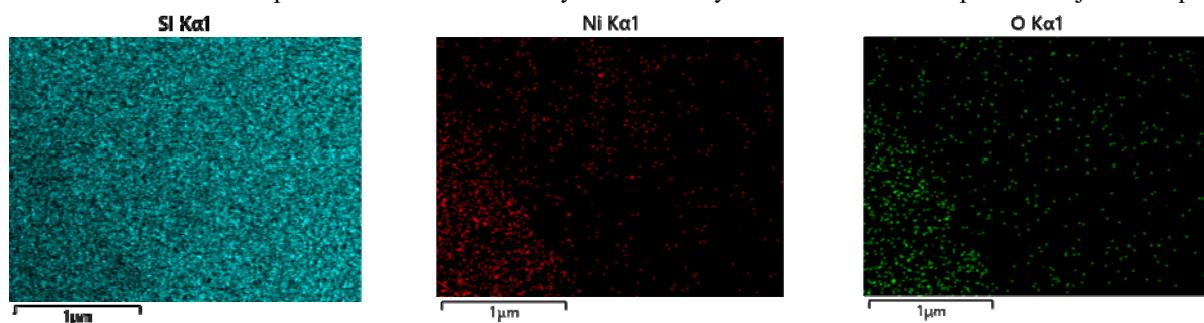


Figure 5. SEM image and EDX elemental maps of the Ni-diffused polycrystalline silicon sample

The Figure 5 left panel shows the surface morphology, while the middle and right panels illustrate the spatial distribution of Ni (red) and O (green), respectively. The overlapping regions of Ni and O signals confirm the formation of Ni–O-based precipitates. These precipitates are believed to contribute to the passivation of electrically active traps, as evidenced by the reduced DLTS signal amplitude, the suppressed G_p – V peak, and the stabilized C–V profile in the Ni-diffused sample.

DISCUSSION

Based on the experimental results obtained through DLTS and C–V profiling, it is evident that the introduction of nickel atoms into polycrystalline silicon significantly modifies the defect landscape and electrical activity within the material. One of the most notable findings is the formation of a pronounced deep-level trap centered at approximately 115 K in Ni-diffused samples, which is absent in undoped specimens. This suggests the creation of specific Ni-related defect complexes, potentially involving interactions at grain boundaries where structural imperfections act as diffusion pathways and clustering sites.

The improved interface characteristics observed in C–V measurements indicate that nickel atoms not only create new trap centers but may also participate in passivating native defects. This dual nature of nickel, acting both as a defect generator and a passivating agent, aligns with previous studies on transition metal doping in silicon-based materials. The smoother capacitance–voltage curves and lower trap density in the Ni-diffused samples support the hypothesis that

nickel can be harnessed to tailor the electronic properties of poly-Si, particularly by forming stable Ni–Si complexes or precipitates that neutralize recombination-active centers [20–24].

Parallel conductance–voltage (G_p –V) measurements further confirmed the presence and partial passivation of interface and grain boundary traps. Compared to undoped samples, the Ni-diffused structures exhibited reduced G_p values across the depletion region, suggesting a lower density of electrically active recombination centers. This suppression is attributed to the interaction of nickel with native defects, likely forming electrically inert Ni–O or Ni–Si complexes.

Additionally, the temperature-dependent suppression of DLTS peak amplitudes across multiple rate windows implies that the trap states in Ni-diffused samples exhibit reduced thermal activity, which can enhance the thermal stability and long-term reliability of devices built on such materials. This behavior is crucial for high-performance applications such as radiation detectors and solar cells operating under fluctuating thermal conditions.

Overall, the findings suggest that controlled nickel diffusion presents a promising avenue for defect engineering in polycrystalline semiconductors, offering a balance between defect introduction and passivation that could be strategically exploited to improve material performance in advanced electronic and optoelectronic systems.

Scanning Electron Microscopy (SEM) images revealed noticeable changes in surface morphology of the Ni-diffused polycrystalline silicon samples. Grain boundary regions became more distinct and slightly rougher, indicating nickel segregation and possible clustering at these structural imperfections. The formation of Ni-rich precipitates observed in SEM supports the electrical activity identified in DLTS measurements.

CONCLUSIONS

This study demonstrated that controlled nickel diffusion improves the electronic quality of polycrystalline silicon by partially passivating grain-boundary-related defects. Capacitance–voltage (C–V) and parallel conductance (G_p –V) measurements revealed a reduced interface trap density and improved junction characteristics. DLTS analysis revealed a significant deep-level trap in the Ni-diffused sample at around 220 K, absent in the undoped structure, indicating the formation of nickel-related defect complexes. SEM and EDX analyses confirmed nickel accumulation and Ni–O clustering at grain boundaries, which are likely responsible for the observed defect passivation. These findings emphasize the dual role of nickel in modifying and stabilizing polycrystalline silicon, offering promising prospects for advanced silicon-based electronic and optoelectronic devices.

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ВПЛИВ ДИФУЗІЇ НІКЕЛЮ НА СТАН ПАСТОК ТА ЯКІСТЬ ІНТЕРФЕЙСУ В СТРУКТУРАХ ПОЛІКРИСТАЛІЧНОГО КРЕМНІЮ

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Ця робота представляє комплексне дослідження глибокорівневої перехідної спектроскопії (DLTS) впливу дифузії нікелю (Ni) на ландшафт дефектів та електронні властивості структур полікристалічного кремнію (poli-Si). Мета дослідження - з'ясувати, як включення Ni модифікує електрично активні пастки, змінює динаміку носіїв заряду та впливає на якість інтерфейсу в діодах Шоткі, сформованих на полі-Si підкладках. Два типи зразків - нелеговані та дифузовані Ni - були отримані шляхом контролюваної термічної обробки при 1000°C, з подальшою пасивацією поверхні та металізацією золотом/алюмінієм для формування діодів Шоткі Au/Poly-Si/Al. Вимірювання DLTS, проведені в діапазоні температур 20–300 K, виявили суттєві відмінності в поведінці глибокорівневих пасток двох типів зразків. У нелегованих зразках спостерігалися лише слабкі та широкі сигнали пасток, в основному пов'язані з власними дефектами на межах зерен та залишковими домішками. На противагу цьому, зразки з дифузією Ni демонстрували різкі та інтенсивні піки DLTS, з домінуючим рівнем пасток, що спостерігався приблизно в межах 200–220 K. Відповідна енергія активації оцінювалася приблизно в 0,492 eV, а поперечний переріз захоплення знаходився в діапазоні 10^{-14} – 10^{-13} см². Ці параметри вказують на утворення комплексних дефектів, пов'язаних з нікелем, таких як кластери Ni–V або Ni–O, розташовані переважно на межах зерен. С–V профілювання додатково підтвердило вплив включення Ni, показавши зниження ємності, більш плавний перехід в області виснаження та покращену однорідність інтерфейсу, що свідчить про часткову пасивацію власних та пов'язаних з межами пасток. Зразок з дифузією Ni демонстрував більш плавний перехід ємність-напруга, зниження ємності переходу та покращену однорідність інтерфейсу, що свідчить про часткову пасивацію власних дефектів. Додаткові вимірювання Gp–V показали значне зниження паралельної провідності для структур, легованих Ni, що вказує на зменшення щільності пасток на інтерфейсі та центрів рекомбінації. Ці результати вказують на подвійну роль нікелю — як джерела глибоких пасток, так і пасивуючого агента, залежно від локального атомного середовища та умов термічної обробки. Аналіз морфології поверхні за допомогою скануючої електронної мікроскопії (SEM) та енергодисперсійної рентгенівської спектроскопії (EDX) підтверджив утворення багатих на Ni преципітатів, особливо на межах зерен. Просторова кореляція між Ni та киснем свідчить про утворення комплексів на основі Ni–O, які, ймовірно, сприяють ефектам електричної пасивації, що спостерігаються в даних DLTS та Gp–V. Загалом, це дослідження демонструє, що контролювана дифузія Ni пропонує перспективний підхід до дефектної інженерії в полікристалічних напівпровідниках. Шляхом вибіркового введення та пасивації дефектних станів, легування Ni може покращити електронну якість та термічну стабільність полікремнію, тим самим покращуючи його придатність для високоекективних сонячних елементів, детекторів випромінювання та інших передових електронних та оптоелектронних пристрій.

Ключові слова: полікристалічний кремній; нікелеві кластери; DLTS; глибокі дефекти; діод Шоткі; дифузія домішок