# ELECTRICAL PROPERTIES AND DUAL BARRIER PHENOMENA IN Au/3% AND 5% Ni-DOPED PVP/n-Si SCHOTTKY DIODES : ROLE OF INTERLAYER ENGINEERING

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We investigated the electrical characteristics of Au/Ni-doped polyvinylpyrrolidone (PVP)/n-Si Schottky diodes to evaluate the effect of Ni concentration on barrier formation and charge transport. Current–voltage (I–V) measurements were performed in the range of −3.5 V to +3.5 V at room temperature (RT) (300 K). Key diode parameters, including ideality factor (n), reverse (saturation) current ($I_s$), and effective barrier heights ($\Phi_{B0}$), were extracted using thermionic emission (TE) theory. The Ln(I)–V characteristics of Ni-doped devices revealed two distinct linear regions, confirming the presence of a second barrier mechanism arising from the polymer interlayer. Increasing Ni content from 3% to 5% improved the interface quality, leading to higher barrier heights (0.631eV →0.833eV), lower saturation currents ($2{,}26\times10^{-6}$A→$9.63\times10^{-10}$ A), and reduced ideality factors (3.14 → 1.44). These results demonstrate that Ni doping modulates the double-barrier transport behavior, enhancing rectifying performance and providing a tunable approach for polymer–semiconductor hybrid Schottky devices.

**Keywords:** Schottky diode; Thermionic emission, Metal Polymer semiconductors (MPS), double-barrier transport behavior, polyvinylpyrrolidone, polyvinyl alcohol.
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## INTRODUCTION

Metal–Polymer–Semiconductor (MPS) diodes, particularly Au/Polymer/n-Si (Schottky diodes), have attracted considerable research interest owing to their adaptable electrical characteristics, straightforward fabrication, and mechanical flexibility, which make them promising candidates for sensors, photovoltaic devices, and rectifiers [1-6]. These devices offer cost-effective and tunable performance, where the choice of polymer interlayer and the incorporation of specific dopants play a crucial role. Incorporating metals such as Al, Ni, or Ag into polymer layers can effectively reduce gas and vapor permeability, enhancing the device's environmental stability. Critical diode parameters—including barrier height ($\Phi_{B0}$)), ideality factor (n), and reverse saturation current ($I_s$)—are strongly influenced by the doping level of donor or acceptor atoms ($N_d$ or $N_a$), as well as the homogeneity of the interfacial barrier and polymer layer [6-8].

Among the available polymer materials, polyvinylpyrrolidone (PVP) and polyvinyl alcohol (PVA) stand out due to their excellent film-forming ability, chemical durability, and mechanical compliance. As interlayers, these polymers not only improve the structural integrity of the device but also tailor charge transport, which is vital for long-term operational stability [5-12]. Their chemical resistance mitigates environmental degradation at the interface, while their amorphous nature introduces intrinsic trap states that can temporarily capture charge carriers. In undoped form, these traps significantly influence forward current conduction, allowing the polymers to act as charge-modulating layers without adding excessive resistance, unlike conventional insulating layers. Additionally, the inherent flexibility of PVP expands its suitability to flexible electronic applications [9-16]. Alternative interlayer materials, such as metal oxides like $In_2O_3$**,** $SnO_2$, and MgO can enhance barrier height but often at the cost of increased series resistance, which impedes efficient current transport and leads to power losses. This trade-off limits their widespread use in high-performance rectifying devices [14,17,18].

Despite the recognized advantages of polymer interlayers, the electrical properties of Au/Ni-doped PVP/n-Si structures remain largely unexplored. Modern PVP-based systems, which exhibit notable stability in ambient conditions, can be further engineered by blending with dopants to achieve desired electronic behavior. In this study, we focus on investigating the influence of both pure and Ni-doped PVP interlayers on the electronic characteristics of Au/n-Si Schottky diodes. Current–voltage (I–V) measurements were conducted over a wide voltage range (−3.5 V to +3.5 V) to extract key parameters and reveal the role of Ni doping in modulating the device's performance.

## EXPERIMENTAL DETAILS

In this study, Au/n-Si Schottky diodes (SDs) were fabricated with and without polyvinylpyrrolidone (PVP) interlayers, including pure, 3% Ni-doped, and 5% Ni-doped PVP films, using identical n-type silicon (phosphorus-doped) wafers. The wafers had a (100) orientation, approximately 350 μm thickness, and a resistivity of 1–10 Ω·cm. Initially, each wafer was cleaved into two segments and subjected to a cleaning sequence to eliminate the native oxide layer and surface impurities. The cleaning process involved immersion in an ammonium peroxide solution for 1 minute, followed by dipping in an acidic solution of $H_2SO_4$:$H_2O_2$:$H_2O$ (3:1:1) for 3 minutes. The wafers were then thoroughly rinsed with high-purity deionized water (18 MΩ·cm) for 10 minutes and dried using nitrogen ($N_2$) gas.

Subsequently, 150 nm of 99.99% pure gold (Au) was thermally evaporated onto the entire backside of each wafer under a high vacuum of $10^{-6}$ Torr to form the ohmic contact. This was followed by annealing at

550°C for 5 minutes in a nitrogen environment to ensure stable and low-resistance contact formation. On the front side of the first wafer segment, circular Au dots with an active area of 7.85 × $10^{-3}$ cm² were thermally deposited to produce reference Au/n-Si Schottky diodes. For the second wafer segment, solutions of 3% and 5% Ni-doped PVP were prepared and deposited on the front surface via the electrospinning technique, creating uniform polymer interlayers. After deposition, Au dots of the same dimensions were thermally evaporated onto the polymer layers, forming Au/(3% or 5% Ni-PVP)/n-Si metal–polymer–semiconductor (MPS) diodes. Electrical characterization was conducted by connecting the front and back electrodes using silver-coated copper wires. Both the rectifying front contacts and the ohmic back contacts were fabricated using a high-vacuum thermal evaporation system equipped with a stainless-steel sample holder. The thickness of the evaporated Au layers was continuously monitored throughout the process using a precision metal thickness monitor.

## RESULTS AND DISCUSSIONS

The electrical properties of Au/n-Si, Au/Pure PVP/n-Si and Ni-doped PVP/n-Si SDs were evaluated using various methods including TE theory. Once the voltage is higher than 3kT/q, the essential electrical properties of these SDs can be derived from the linear region using TE theory as shown in Fig. 1. The values of $n$ and $I_s$ were calculated from the slope and intercept of the ln(I) vs V graphic (Fig 1) for the MS and MPS. Then the value of $\Phi_{B0}$ was calculated using the calculated $I_s$ and diode area (A) as following equation 1(a-b) [1,3,5,9,13,16,18-22]:

$$n = \frac{q}{kT}\left(\frac{d(V-IR_s)}{d(\ln I)}\right) \tag{1a}$$

$$\phi_{B0} = \frac{kT}{q}\ln\left(\frac{AA^{*}T^{2}}{I_s}\right) \tag{1b}$$

The lower ideality factors (1.44 for 5% Ni-doped and 1.62 for 3% Ni-doped) confirm near-ideal behavior, suggesting that the Ni-doped diodes follow thermionic emission theory closely, with minimal contributions from recombination or tunneling [3,18-22]. In contrast, the higher ideality factors of undoped and other materials highlight non-idealities such as defect states and high surface recombination. There are two barrier heights for Ni doped structures as shown in Fig. 1, and the higher barrier heights in Ni-doped diodes (0.712 eV for 5% and 0.665 eV for 3%) further emphasize the positive impact of Ni doping**,** resulting in better control of the Schottky junctions and reduced reverse leakage current showing in Table 1.

Table 1

Electrical properties of MPS from TE theory at RT.

| Au / Polymer / n-Si MPS type SDs: | From Thermionic Emission (TE) Theory | | | | | |
|---|---|---|---|---|---|---|
| | *n* | | *I<sub>s</sub>(A)* | | *Φ<sub>B0</sub> (eV)* | |
| Au/n-Si | 4.19 | | $5.59\times10^{-6}$ | | 0.608 | |
| Au/Pure PVP/n-Si | 3.88 | | $2.26\times10^{-6}$ | | 0.631 | |
| Au/3%Ni doped :PVP/n-Si | 1.62 | 3.14 | $6.34\times10^{-9}$ | $6.25\times10^{-7}$ | 0.784 | 0.665 |
| Au/5%Ni doped :PVP/n-Si | 1.44 | 2.53 | $9.63\times10^{-10}$ | $1.03\times10^{-7}$ | 0.833 | 0.712 |

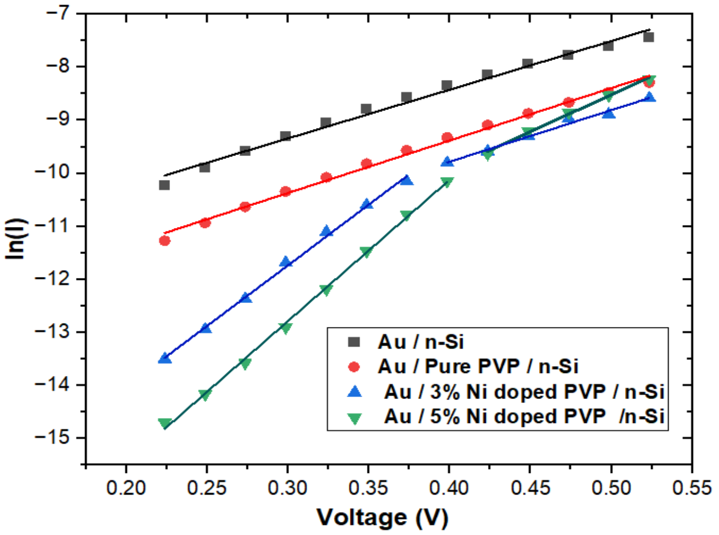

*Fig. 1.* Semilogarithmic ln(I)–V plots of Au/n-Si and Au/Pure and Ni doped PVP/n-Si MPS for short forward voltage interval.

A thin dielectric interface layer is considered in the metal–semiconductor contact model. In accepted model, the applied voltage is distributed between the dielectric interface layer and the depletion layer, as shown in equation 2[21].

$$V = V_1 + V_2 \tag{2}$$

where $V_1$ and $V_2$ correspond to the voltages in the dielectric interface layer and depletion layer, respectively [20]. Current transfer through the contact can occur through several mechanisms, which is reflected in the current–voltage characteristics. The analysis of the diode's current-voltage characteristics revealed two different potential barrier values. It is likely that the contact between the semiconductor and the dielectric layer in the 3% and 5% Ni doped PVP diodes forms an isotype heterojunction illustrated in Fig. 2.

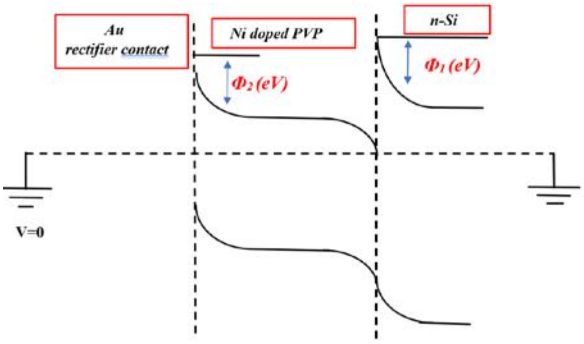

*Fig. 2.* Heterojunction contact scheme between the semiconductor and the dielectric layer in the 3% and 5% Ni doped PVP diodes.

As reported in the literature, pure PVP exhibits extremely low electrical conductivity [2]. However, the incorporation of various substances enhances the conductivity of the polymer [7,9-18]. The value of the band gap of the doped polymer is comparable to the value of the band gap of silicon. This band gap is much larger than the thermal energy at (~0.025 eV), resulting in very few thermally excited charge carriers, which explains the low intrinsic conductivity of pure polymers. The mechanism of conductivity in polymers involves three main steps: the generation of free charge carriers, their movement through polyconjugated regions, and their transfer from one conjugation site to another. It is suggested that polymers are electronically inhomogeneous systems, with conductive polyconjugated regions separated by dielectric areas. The transition of carriers across these dielectric layers creates an activation barrier. In this context, the polymer behaves like a semiconductor, allowing electrons to be injected from the connected silicon. The metal-semiconductor junction, forming the second barrier, occurs at the interface between Au and the 3% or 5% Ni-doped PVP, as shown in Table 1

Electrical properties of MPS from TE theory at RT. The results of the study showed that doping the polymer with nickel improves the barrier properties of the contact structure: the barrier height increases from 0,608 eV, 0,631eV to 0,784 eV, 0,833 eV, the ideality factor from 4.19, and 3.88 to 1,62 and 1.44, the saturation current from $5{,}59\times10^{-6}$ A and $2{,}26\times10^{-6}$ A to $6{,}34\times10^{-9}$ A and 9,63x10-10 A for Au/n-Si and Au/Pure/n-Si and Au/3% or 5% Ni-PVP/n-Si respectively. The low value of the second barrier is due to the effect of series resistance and activation of surface states.

## CONCLUSION

Au/PVP/n-Si and Au/Ni-doped PVP/n-Si Schottky diodes were successfully fabricated, and their electrical characteristics were investigated within the voltage range of –3.5 V to +3.5 V at 300 K. The current–voltage measurements showed that the insertion of a PVP interlayer and its Ni doping significantly affected the diode parameters, including the ideality factor (n), barrier height (ΦB), and saturation current (Is). In contrast to conventional insulators, Ni-doped PVP interlayers caused more significant variations. For the 3% Ni-doped PVP diode, the ideality factor was 1,62, the barrier height increased to 0.784 eV, and the saturation current decreased to $6.34 \times 10^{-9}$ A. At 5% Ni doping, the ideality factor decreased to 1.44, the barrier height increased to 0.83 eV, and the saturation current further decreased to $9.63 \times 10^{-10}$ A.

Analysis of the Ln(I)–V plots revealed a second linear region in the 3% and 5% Ni-doped diodes, confirming the presence of a secondary barrier at the metal/polymer/semiconductor interface. This secondary barrier became more prominent with increasing Ni concentration, which likely enhanced the density of localized states in the PVP layer, facilitating multi-step tunneling or thermionic emission through traps. The formation of this second barrier explains the observed non-ideal behavior and the increase in ideality factors. In summary, Ni doping in the PVP interlayer effectively modulates the barrier height, saturation current, and overall charge transport characteristics, while inducing the appearance of a second barrier that strongly influences the rectifying performance. These results indicate that Ni-doped PVP layers provide a useful approach for tuning the electronic properties of metal–polymer–semiconductor structures, offering potential for applications in sensors and rectifier devices.

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