Influence of titanium nitride thin films on the electrical properties of isotype *n*-TiN/*n*-Si heterostructures

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Introduction

It is known that crystalline silicon is the main material of modern semiconductor electronics. The band gap (E_g = 1.12 eV), which is in the range of optimal values for photoelectric conversion of solar energy and the possibility of obtaining electron and hole type conductivity with the required concentration of charge carriers (≈ 10^{16} cm^{-3}) ensure the use of silicon in solar cells with high coefficient useful action 27.8% [1]. The efficiency of photoconverters, based on both crystalline and amorphous Si, is largely determined by the properties of transparent conductive oxides (TCO), which are used in these solar cells as front and rear contacts. Thin TiN films can be an alternative material for use in high-performance silicon-based solar cells due to the following parameters: large band gap (E_g = 3.4 eV), high transmittance in the visible and near-infrared spectral regions (T = 70 – 80 %), significant concentration of electrons ($n = 10^{18} – 10^{19}$ cм$^{-3}$) [2]. Therefore, the study of physical processes in the field of *n*-TiN/*n*-Si isotype heterojunctions is relevant and can be used in solar energy.

Experimental technique

Polycrystalline silicon of electronic conductivity type was used to fabricate *n*-TiN/*n*-Si heterojunctions. The values of specific conductivity, concentration and Hall mobility of charge carriers at T = 294 K were σ = 1.0 Ohm^{-1}·cm^{-1}, $n = 4.7\cdot10^{15}$ cm^{-3}, μ_H = 1330 cm^2/V·s, respectively. The deposition of thin TiN films was carried out in a Leybold-Heraeus L560 universal vacuum unit by the method of reactive magnetron sputtering. The pure titanium target was sprayed in an atmosphere of a mixture of nitrogen and argon at constant voltage. The substrate temperature was 573 K. The thickness of the studied films ~ 100 nm was determined from the microphotographs obtained with a scanning electron microscope. The obtained thin TiN films were *n*-type conductivity. Their specific conductivity and charge carrier concentration at T = 294 K were σ = 0.17 Ohm^{-1}·cm^{-1}, $n \approx 5\cdot10^{18}$ cm^{-3}, respectively.

Ohmic contact to titanium nitride films was formed by thermal deposition of indium at a substrate temperature of 150 °C. Ohmic contact to *n*-Si was obtained by pre-doping with phosphorus of the near-surface layer of the semiconductor, which led to the formation of *n*+-region. Then, layers of chromium and nickel were successively applied to the surface by thermal evaporation.

Experimental results and their discussion

The study of *I-V*–characteristics of isotype *n*-TiN/*n*-Si heterojunctions at forward (positive potential on the TiN) and reverse (positive potential on *n*-Si) voltages in the temperature range T = 299 – 342 K (Fig. 1) indicate rectifying properties of structures. The rectifying ratio at |V| = 1.5 V and T = 294 K was ~ 10^3. The series resistance: R_S = 23 Ohm.

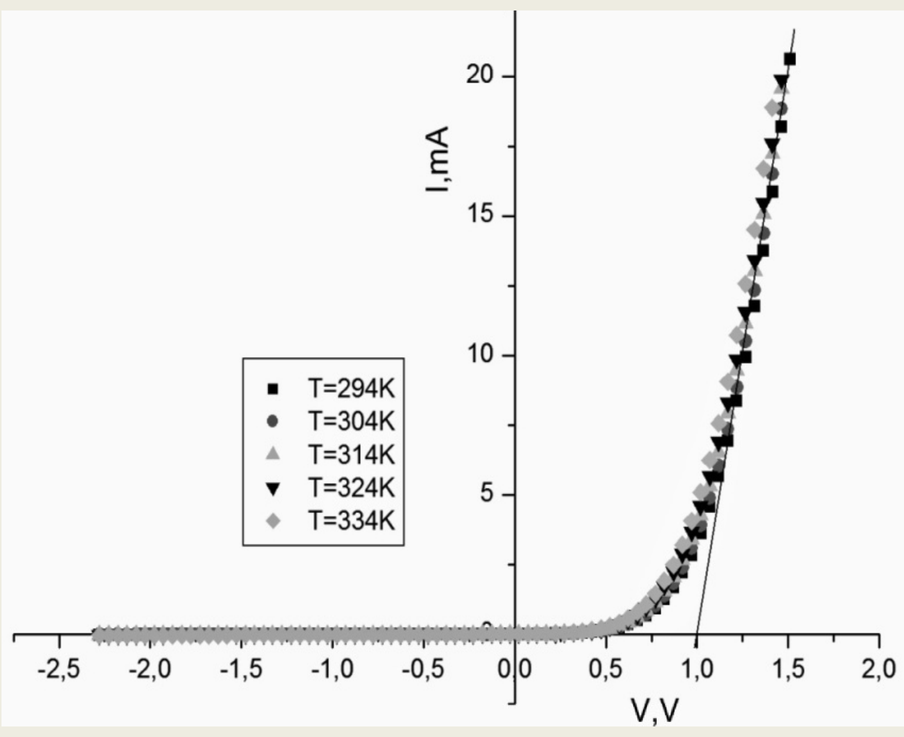

Fig. 1. *I-V*–characteristics of the investigated isotype *n*-TiN/*n*-Si heterostructure at different temperatures.

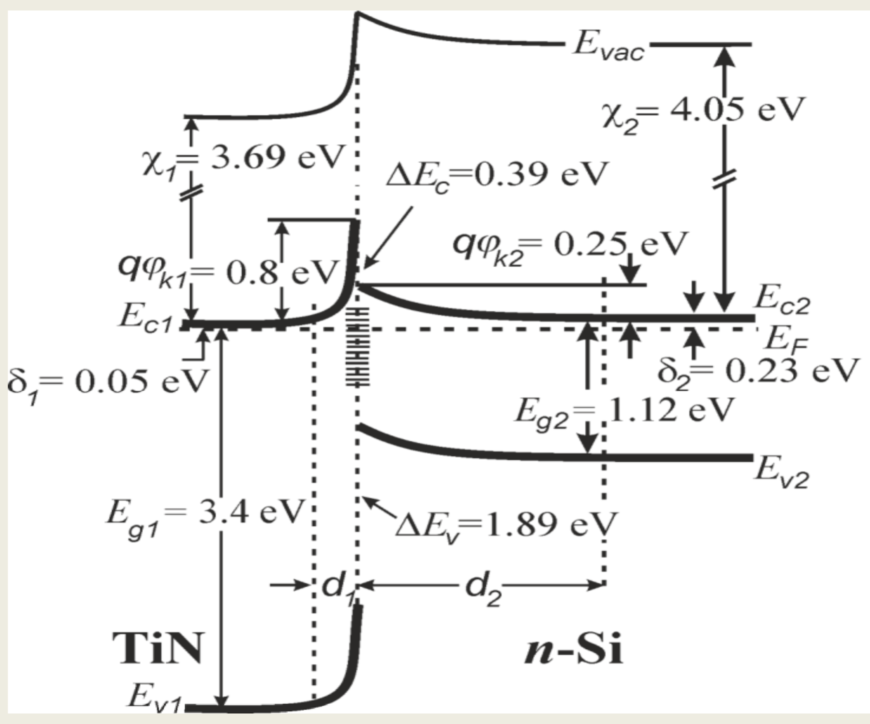

Fig. 2. Energy diagram of the isotype *n*-TiN/*n*-Si heterojunction taking into account the influence of a negative charge on the heterocontact interface.

Characteristic of the dependences $C = f(V)$, measured in the region of low (f = 10 – 90 kHz) and high (f = 300 – 1000 kHz) frequencies of the excitation variable signal is the presence of two regions, which are manifested in reverse and forward (V > 0.8 V) biases.

The studied *n*-TiN/*n*-Si structures belong to isotypic *n-n*–heterojunctions. According to the theory of isotype heterojunctions, this nature of the $C = f(V)$ dependence can be explained in a model in which the heterojunction is represented as two Schottky diodes connected towards each other. This model of electrical contact takes place in the presence of a significant concentration of electrically active energy states at heterointerfaces, which capture electrons from the conduction band of both semiconductors. This leads to the formation of positively charged regions on both sides of the heterojunction, and, accordingly, to the creation of two potential barriers, the capacitances of which are manifested at different polarities of the external voltage. The estimated density of surface energy levels N_{SS} at the interface between the structural components, taking into account the fact that their appearance is due to mismatch dislocations, was $N_{SS} \approx 2.7\cdot10^{13}$ cm^{-2}, which confirms the validity of the model used. The values of the height of potential barriers, both in the thin TiN film ($q\varphi_k$ = 0.8 eV) and in the base material of the structure Si ($q\varphi_k$ = 0.23 eV), determined by a known method based on high-frequency *C-V*–characteristics ($C^{-2} = f(V)$ coordinates). The concentrations of electrically active impurities in the charged regions were $N_{TiN} \approx 4\cdot10^{18}$ cm^{-3}, $N_{Si} \approx 2{,}8\cdot10^{15}$ cm^{-3}, which correlates well with the values in the initial semiconductors.

The dimensions of the space charge regions were: $d_{TiN} \approx$ 15 nm and $d_{Si} \approx$ 340 nm.

It should be noted that, according to the analysis of the work functions of semiconductors A(*n*-TiN) = 3.96 eV, A(*n*-Si) = 4.28 eV, when the *n*-TiN/*n*-Si heterojunction is formed, enrichment for *n*-Si electrons should occur and such the structure would not be characterized by rectifying properties, which contradicts the experiment and confirms the validity of the applied model of isotype heterojunction.

Analysis of the *I-V*–characteristics of the investigated heterojunctions at forward biases showed that tunneling is the main mechanism of current transfer in a wide voltage range $3kT/q < V < 1.0$ V. Due to the significant gap of the edges of the valence bands, the current is formed by the electrons of the *n*-Si conduction band. Even at low forward voltages, the zones in *n*-Si are straightened and electrons accumulate in the near-contact region (Fig. 3). The height of the barrier in the titanium nitride film increases. Electron tunneling occurs at a height of $E_{C1} + qV$ relative to the base of the barrier. The small thickness of the barrier (d_{TiN}) significantly increases the probability of the process.

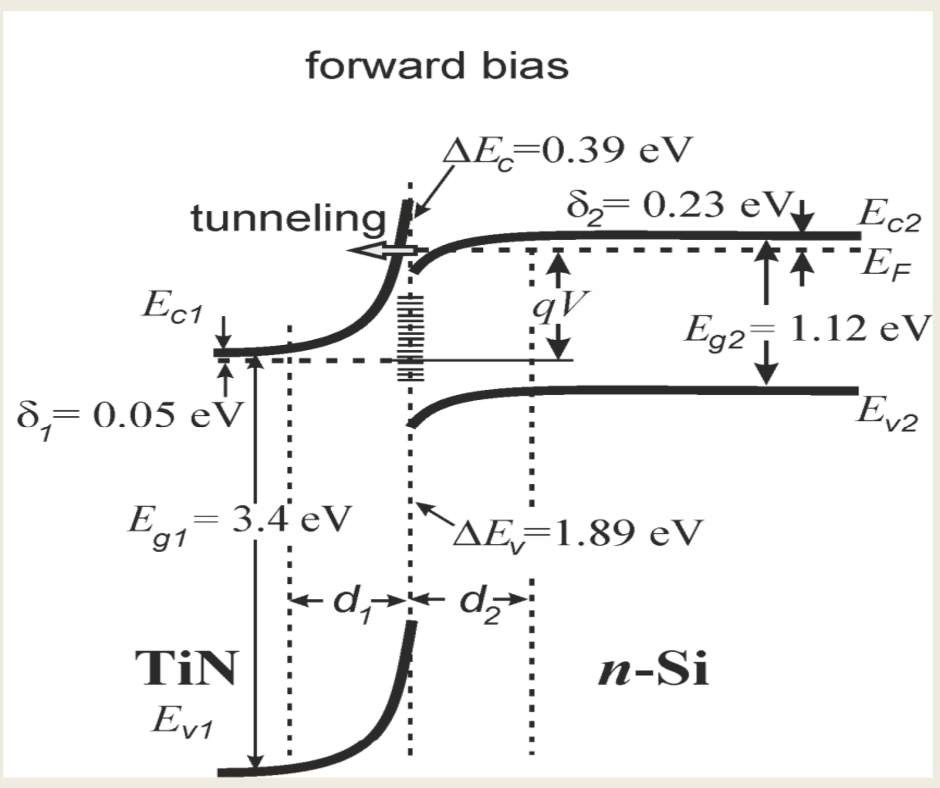

Fig. 3. Energy diagram of isotype TiN/*n*-Si heterojunction at forward bias (positive potential applied to TiN film)

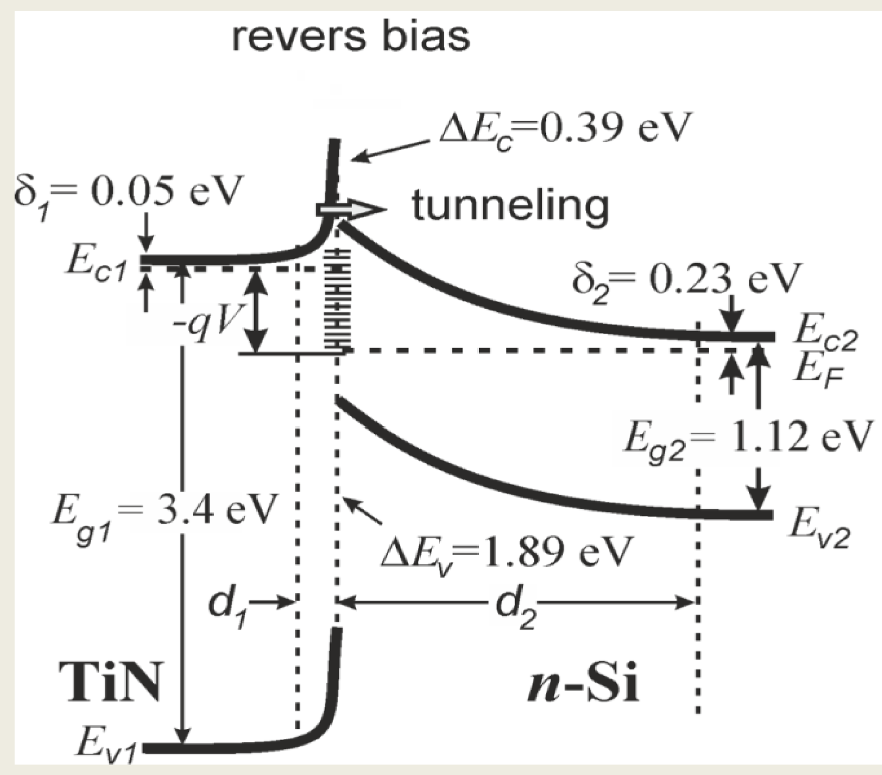

Fig. 4. Energy diagram of isotype TiN/*n*-Si heterojunction at reverse bias (positive potential applied to the *n*-Si crystal)

The *I-V*–characteristics of the investigated *n*-TiN/*n*-Si structures (plotted in $\ln I_{rev} = f(V)$ coordinates) are characterized by the presence of linear sections at reverse biases. The angle of inclination of these sections to the voltage axis does not depend on the temperature, which indicates the process of tunneling of charge carriers through the potential barrier. It should be noted that at negative voltages, most of the voltage V_2 is applied to the high-resistance *n*-Si depleted region at the *n*-TiN/*n*-Si heterojunction. Therefore, the height of the potential barrier in the TiN film (at forward bias) practically does not change ($\varphi_{k1} - V_1 \approx \varphi_{k1}$), which leads to the tunneling of electrons from the TiN conduction band through the thin barrier of the film (Fig. 4).

Conclusions

Rectifying isotype *n*-TiN/*n*-Si heterojunctions are fabricated by reactive magnetron sputtering at a constant voltage of the titanium target on the surface of polycrystalline silicon wafers. The rectifying ratio is ~ 10^3 at |V| = 1.5 V and T = 294 K. The electrical properties of the studied heterostructures are explained on the basis of a model representing an isotype *n-n*–heterojunction as two Schottky barriers with a high-conductivity interface due to a significant concentration of electrically active surface states. A model of the energy diagram of the heterostructure, which describes well the experimental electrophysical phenomena, is proposed. Tunneling through a thin potential barrier in a conductive TiN film is the main mechanism of current transfer in the obtained *n*-TiN/*n*-Si heterojunctions, both at forward and reverse biases.

References

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