

## Fabrication and Characterization of n-ZnO/n-Si Heterojunction

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### Abstract

The n-ZnO/n-Si heterojunction are fabricated by depositing ZnO films on n-Si (111) films substrate using magnetron sputtering Al doped ZnO ceramic target. The structures of n-ZnO films, analyzed by X-ray diffraction (XRD) spectroscopy, and the preferential orientation of the ZnO grains is observed along the (101) and (100) axis aligning with the growth direction. The photoelectric properties, charge carrier transport properties and conductive mechanism were studied by testing the I-V, C-V characteristics with illumination and without illumination. Current-voltage (I-V) measurements of n-ZnO/n-Si heterojunctions show good diode characteristics and photovoltaic effects with illumination. The forward conduction is respectively determined by carrier recombination in the space charge region, defect-assisted tunneling and exponential distribution trap-assisted space charge limited current mechanism with the increase of forward voltage. Also, a band diagram of n-ZnO/n-Si heterojunctions has been proposed to explain the transport mechanism. As the conduction band and valence band offset in the ZnO/n-Si heterojunction is too big, the current transport mechanism is dominated by the space-charge limited current (SCLC) conduction at the forward voltage exceed 0.8 V. The results suggest the existence of a large number of interface states in ZnO/n-Si heterojunction, and the interface states can be reduced and the photoelectric properties can be further improved.

**Keywords:** ZnO/n-Si heterojunction, the characteristics of I-V, the characteristics of C-V, the built in potential

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### 1. Introduction

Wide band gap of zinc oxide (ZnO) thin film has very good electrical and optical properties, as an excellent transparent electroconductive film material [1-3]. Low cost of ZnO/n-Si heterojunction solar cells, ZnO/n-Si heterojunction light emitting diodes have become research hotspot in recent years [4-6]. In addition, ZnO/n-Si heterojunction can also be used in many areas of the photoelectric detection, short-wave optoelectronic devices [7-9]. In recent years, ZnO/n-Si heterojunction is a research hotspot in the field of electro-optic conversion, but the basic theoretical research on the ZnO/n-Si heterojunction are not formed a complete systems theory, and the theoretical study of the characteristics and mechanism is still immature.

In this paper, ZnO/n-Si heterojunction are fabricated by magnetron sputtering of Al doped ZnO ceramic targets deposited on the p-Si film, and n-type conductivity of the ZnO thin film prepared. The current transport properties of the heterojunction are also investigated by means of current-voltage measurements and capacitance voltage method.

### 2. Experiment Method

#### 2.1. ZnO Thin Films Preparation

The mixture of the analytically pure Al<sub>2</sub>O<sub>3</sub> powder and ZnO powder in the molar ratio 1% is pressed into  $\Phi$  60 mm × 5 mm wafer embryoid bodies using a tableting machine under a pressure of 10MPa, under the conditions of an air atmosphere sintered into a ceramic at 1350°C, incubated for 2 hours followed by furnace cooling. Prepared Al-doped ZnO ceramics used as a ceramic target for sputtering ZnO film.

The surface textured Si wafer is used as a n-type ZnO thin film deposition substrate. The resistivity of the Si wafer is 50  $\Omega$ . Si wafer in the mixed solution of ammonia water, hydrogen peroxide, and deionized water (volume ratio of 1:2:5) was boiled for 8 minutes, and then in the mixed solution of hydrochloric acid, hydrogen peroxide and deionized water (volume ratio of 1:2:8) was boiled for 8 minutes, followed in ethanol ultrasonic cleaning by 15 minutes, and finally in deionized water ultrasonic cleaning and drying with argon. Used in this paper the n-type Si film samples were cut into 1 cm<sup>2</sup> size.

Sputtering of ZnO film in an argon atmosphere and 0.6 Pa atmospheric pressure. A DC sputtering power is 300 W, 15 minutes of sputtering. Purity Al film was deposited on back of the n-type Si by sputtering purity Al target as back field, and 4 hours in an argon atmosphere, 400°C annealing.

## 2.2. Characterization and Measurements

The phase composition of the samples was characterized by X-ray powder diffraction (XRD, RINT-2100V, Rigaku, Cu K $\alpha$ ). Current-voltage (*I-V*) characteristics of the ZnO/n-Si heterojunctions were measured using a Agilent sourcemeter (model 4156C). Capacitance-voltage (*C-V*) characteristics were measured using a Agilent LCR meter (model 4824A). Electrical resistivity of the films was measured by a four-point method (4 PROBES TECH China RTS-9).

## 3. Results and Discussions

### 3.1. Structural Characterization

Figure 1 shows the XRD spectra of the as-grown ZnO films on n-Si is presented. The observed inter-planer distance “*d*” is compared with JCPDS data which is in good agreement with the standard “*d*” values. Analyses of XRD data reveal peaks corresponding to (111) and (101) planes of the Si crystal structure, and different peaks of ZnO corresponding to planes (100), (002), (101), (102), (110), (103), (200) and (112) of hexagonal structure have been identified. The preferential orientation of the ZnO grains is observed along the (101) and (100) axis aligning with the growth direction. The presence of a number of peaks in XRD pattern is the indication of polycrystalline nature of the ZnO.

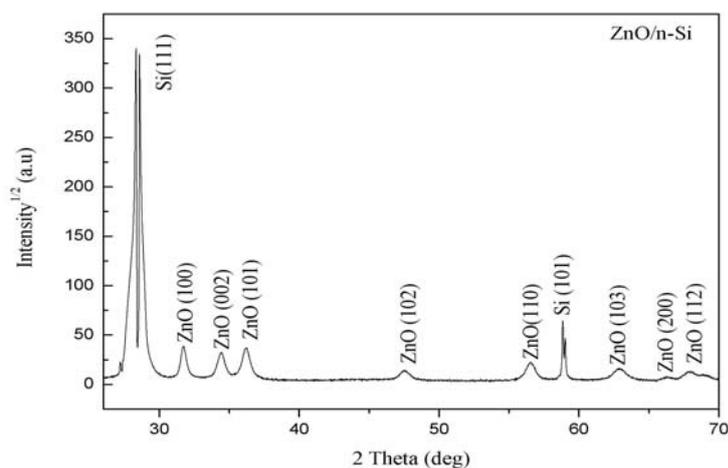


Figure 1 X-ray diffraction spectra of ZnO/n-Si heterojunction

### 3.2. Electrical Characteristics

The n-Si is connected to the negative electrode, ZnO is connected the positive electrode. The *I-V* characteristic of the ZnO/n-Si heterojunction in Figure 2 exhibits a good photoelectric effect and rectifying behavior with a  $I_F / I_R \sim 204$  at 5 V indicating formation of a diode ( $I_F$  and  $I_R$  stand for the forward and reverse currents, respectively). Under light irradiation, forward current increases, the reverse current hardly changes.

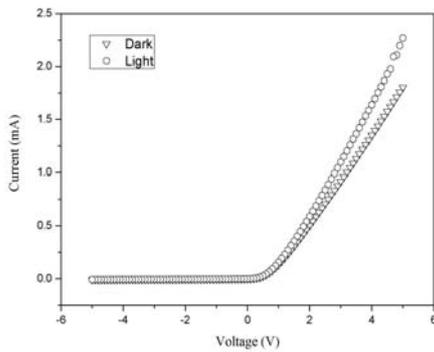


Figure 2. I-V Curve for the ZnO/n-Si Heterojunction with Illumination and no Illumination

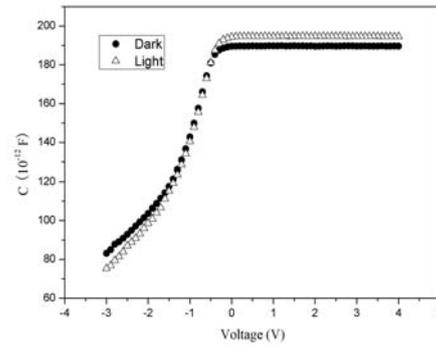


Figure 3. The C-V Curve of the ZnO/n-Si Heterojunction Diode Measured at 500 kHz with Illumination and no Illumination

The capacitance (C) - voltage characteristics of the ZnO/n-Si heterojunction is measured at a frequency of 500 kHz conditions with illumination and no illumination in Figure 3. As can be seen from the diagram, when the reverse voltage, light-induced capacitance decreased; when plus the forward voltage, the light-induced capacitance increased.

The  $1/C^2$  versus voltage curve of the ZnO/n-Si heterojunction diode was shown in Figure 4. Can be seen from Figure 4, under no illumination, the  $1/C^2$  versus voltage curve of the ZnO/n-Si with the extension line of the voltage variation curve in the V-axis of the intercept 0.15 V. Illumination to cause  $1/C^2$ -V curve extension cord becomes smaller in the V-axis intercept.

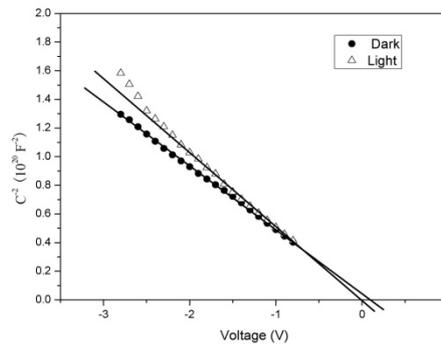


Figure 4. The  $1/C^2$  Versus Voltage Curve of the ZnO/n-Si Heterojunction Diode Measured at 500 kHz with Illumination and no Illumination

### 3.3. Carrier Transport Mechanism

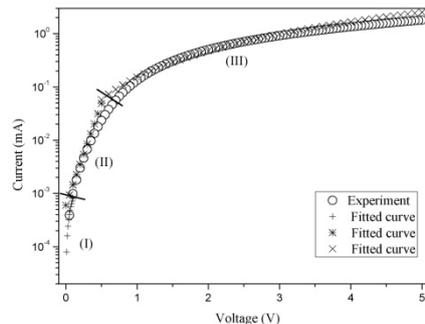


Figure 5 The I-V curve for the ZnO/n-Si heterojunction in forward bias

In Figure 5, we presented the dark current as a function of junction-voltage in forward bias. At lower forward voltage (I,  $0 < V < 0.2$  V),  $I$ - $V$  characteristic comply with the linear Ohm behavior ( $I \sim V$ ), which is mainly caused by hot carrier tunneling effect [10]. In the II range, the current increased exponentially with voltage submissive relationship formula  $I$  to  $\exp(\alpha V)$ , which is mainly due to the tunnel - caused by the recombination mechanisms, which is prevalent in the broadband p-n heterojunction phenomenon [11-14].

When the forward voltage exceeds 1 V (III,  $0.8 < V < 5$  V),  $I$ - $V$  characteristic was deviated from the ideal thermionic emission and behaved as  $I \sim V^2$  relation, which was attributed to the space-charge limited current (SCLC) conduction [15-18]. This SCLC mechanism is a normal phenomenon in the wide band gap semiconductors due to single-carrier injection [17, 18].

Figure 6 shows the theoretically expected equilibrium energy band diagram of the ZnO/n-Si heterojunction according to the Anderson model. Under the assumptions that (i) the interface states can be neglected and the Fermi level in the Si and ZnO lies at the Si conduction band edge and ZnO valence band edge, respectively.

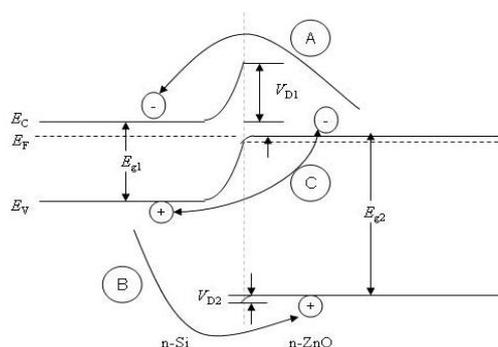


Figure 6. The Energy Band Diagram of ZnO/n-Si Heterojunction

From Figure 6, we know that the  $\Delta E_C$  and  $\Delta E_V$  for this heterojunction are very large. The potential barrier for electrons transport from the bottom of conduction band in n-Si to the bottom of conduction band in ZnO and the holes transport from the top of value band in ZnO to the top of value band in n-Si are very large, so the difficulties for transport of electrons and holes in forward bias is increased. Since the difference between  $\Delta E_C$  and  $\Delta E_V$ , the energetic barrier was much higher for holes than electrons. In the region III at Figure 5, the current is dominated by electrons.

#### 4. Conclusion

In summary, ZnO/n-Si heterojunction diode are prepared at a low cost by chemical method, and shows a good photoelectric effect and rectifying behavior with a  $I_F / I_R \sim 204$  at 5 V. The prepared ZnO film is polycrystalline nature. At lower forward voltage (I,  $0 < V < 0.2$  V),  $I$ - $V$  characteristic comply with the linear Ohm behavior ( $I \sim V$ ), which is mainly caused by hot carrier tunneling effect. In the II range, the current increased exponentially with voltage submissive relationship formula  $I$  to  $\exp(\alpha V)$ , which is mainly due to the tunnel - caused by the recombination mechanisms. When the forward voltage exceeds 1 V (III,  $0.8 < V < 5$  V),  $I$ - $V$  characteristic was deviated from the ideal thermionic emission and behaved as  $I \sim V^2$  relation, which was attributed to the space-charge limited current (SCLC) conduction. This heterojunction diode can be good used for photoelectric devices and detectors.

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