Current transport in ZnO/Si heterostructure grown by laser molecular beam epitaxy*

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The n-ZnO/p-Si heterojunction was fabricated by depositing high quality single crystalline aluminium-doped n-type ZnO film on p-type Si using the laser molecular beam epitaxy technique. The heterojunction exhibited a good rectifying behavior. The electrical properties of the heterojunction were investigated by means of temperature dependence current density–voltage measurements. The mechanism of the current transport was proposed based on the band structure of the heterojunction. When the applied bias V is lower than 0.15 V, the current follows the Ohmic behavior. When 0.15 V $< V <$ 0.6 V, the transport property is dominated by diffusion or recombination in the junction space charge region, while at higher voltages ($V >$ 0.6 V), the space charge limited effect becomes the main transport mechanism. The current–voltage characteristic under illumination was also investigated. The photovoltage and the short circuit current density of the heterojunction aproached 270 mV and 2.10 mA/cm^2, respectively.

Keywords: ZnO/Si heterostructure, current transport, laser molecular beam epitaxy

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1. Introduction

ZnO is an attractive wide-band-gap (3.37 eV) oxide semiconductor with a large exciton binding energy of 60 meV. It has been extensively investigated due to its potential applications in ultraviolet (UV) optoelectronic devices, light-emitting diodes, field emission devices, transparent conducting electrodes, etc.[1−4]

Generally, undoped ZnO thin films exhibit typically n-type conductivity due to the native defects, such as oxygen vacancies and zinc interstitials.[5] Since the reproducible and high quality p-ZnO is not obtainable yet, the fabrication of effective ZnO p–n homojunction remains a challenge to be accomplished. As an alternative way, ZnO-based heterojunctions can be constructed by depositing n-ZnO on various p-type semiconductor layers, such as Cu_2O, SiC, and Si.[6−8]

The n-ZnO/p-Si heterojunction is of particular interest in the integration of optoelectronic devices utilizing the hybrid advantages of the ZnO thin film and the cheapness of the Si substrate. Moreover, the heterojunction can efficiently collect the solar light through the double-band structure, high energy photons in the ultraviolet region can be absorbed by ZnO, while low-energy photons in the visible range are collected at the depletion region of p-Si after they have passed through the ZnO layer. Recently, quite a lot of research groups have devoted to the fabrication of ZnO/Si.[8−12] Mridha *et al.*[9] fabricated an n-ZnO/p-Si heterojunction by using the sol–gel method and demonstrated the strong responsivity of the heterojunction for both visible and UV photons under reverse and forward bias conditions. Ibrahim *et al.*[11] prepared ZnO/Si junction solar cells with the conversion efficiency of 6.6% by using the spray pyrolysis method. Analyses of the electrical properties of the heterojunction revealed that the efficiency improvement might be due to the recombination of the charges or due to the structure of the ZnO film.

However, at present, the efficiency of ZnO/Si heterojunction is still very low. It is important to understand the physical properties and the current transport mechanisms of the junction. A proper characterization of the photoelectric properties requires high-quality ZnO films. The laser molecular beam epitaxy (LMBE) technique is especially useful for fabricating higher-quality films of oxides. The layer-by-layer epitaxial growth can be controlled, and the composition of films can be tailored without contamination.

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In the present study, we fabricated highly oriented aluminium-doped n-ZnO films on p-Si by using the LMBE technique. The electrical characters of the ZnO/Si heterojunction were studied, and the mechanism of carrier transport was investigated in detail.

2. Experiment

Al-doped n-ZnO thin films were deposited on B-doped p-Si (001) substrates using the LMBE technique. A pulsed XeCl excimer laser with an energy density of about 1 J/cm^2 was used to ablate the targets at a repetition rate of 3 Hz. The target used for deposition was synthesized using high purity ZnO (99.99%) and Al_2O_3 (99.99%) powders in the standard solid state reaction route, and the target-to-substrate distance was 50 mm. The base pressure was kept at 1×10^{-4} Pa during the film growth, while the substrate temperature was 450 °C. Under such experimental conditions, the thickness of the film was about 200 nm. The atomic force microscopy measurements indicated that the deposited films were very uniform.

For the current density–voltage (J–V) and the photo voltaic properties measurements, two indium electrodes with the size of 0.4 mm^2 were deposited on ZnO and Si respectively. The J–V curves were measured over the temperature range from 216 K to 276 K using a Keithley sourcemeter in dark, and the photovoltaic properties measurements were performed.

3. Results and discussion

Figure 1 shows the X-ray diffraction (XRD) θ–2θ scan of a ZnO thin film on the Si substrate measured by a Philips X'Pert4-circle diffractometer with the Cu $K\alpha$ radiation. It is clearly seen that apart from the substrate peaks, both the XRD peaks correspond to the wurtzite-structure ZnO, indicating that a phase-pure film with the c axis normal to the film surface is obtained. Figure 2 shows the photoluminescence (PL) spectrum of ZnO using the 325 nm UV light from an He–Cd laser at room temperature. Only a sharp UV emission peak at the wavelength of $\sim$ 371 nm is observed. According to a relevant study, there are two obvious emission bands in the typical PL spectrum of the undoped ZnO film, a dominant UV emission band and a wide green emission band. The UV emission mainly originates from the excitonic transition between valance and conduction bands. The green emission is due to the recombination of electrons in oxgen vacancies with photoexcited holes in the valence band.[13] It is also previously observed that introducing Al into ZnO thin films results in the depression of the PL from the oxygen defects.[14] It is reasonable to assume that the Al doping leads to a decrease in the defect concentration and then improves the quality of the ZnO film. The resistivity and the carrier density of the ZnO film are measured to be about 6.80×10^{-4} Ω·cm and 1.03×10^{20} cm^{-3}, respectively.

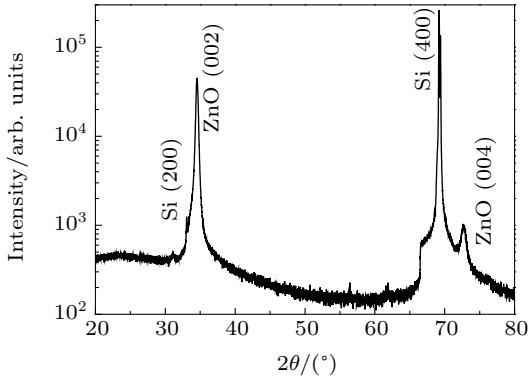


Fig. 1. X-ray diffraction pattern of the ZnO film.

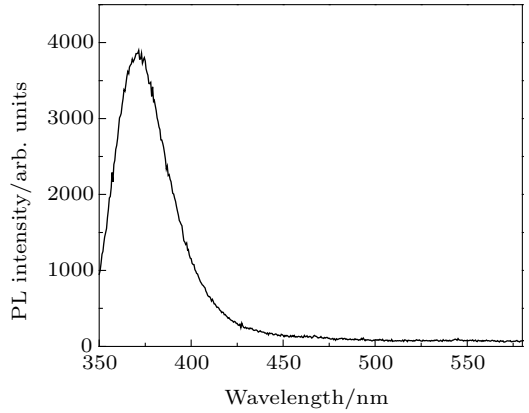


Fig. 2. PL spectrum of the ZnO film.

The linear J–V behavior between the two electrodes on the surface of the ZnO film shown in Fig. 3 indicates a good Ohmic contact. The distance of the two In electrodes on the ZnO film is 1 cm.

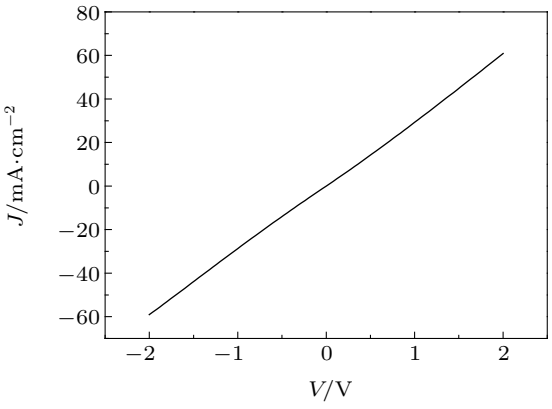


Fig. 3. The J–V characteristic of the ZnO film.

The room temperature J–V characteristic of the n-ZnO/p-Si heterojunction in dark is shown in Fig. 4(a). The convention of the applied bias polarity is defined as negative at the ZnO side and earthed at the p-Si side. It can be seen that the curve shows the well-defined rectifying diode-like behavior. The room temperature rectification ratio is about 4×10^2 at ± 2.5 V, and the reverse current density is equal to 1.4×10^{-4} A/cm^2. Figure 4(b) shows the semilogarithmic plots of the J–V characteristics of the n-ZnO/p-Si heterojunction in dark at different temperatures (from 216 K to 276 K). All plots have the same J–V behavior. The current increases with the increasing temperature at the same applied voltage, indicating a negative temperature coefficient for the resistivity. The leakage current density in the reverse bias direction is extremely low. We note that the current density varies differently with the applied bias in different voltage regions, which indicates that the currents are dominated by different mechanisms.

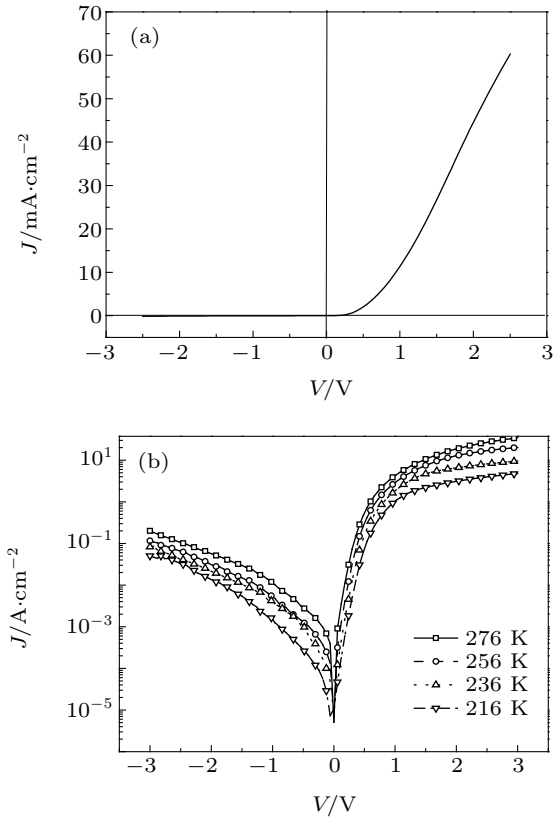


Fig. 4. The J–V characteristics of the ZnO/Si heterojunction at (a) room temperature and (b) different temperatures.

The current transport mechanisms behind the J–V characteristics can be understood based on the energy band diagram of the n-ZnO/p-Si heterojunction constructed by using the Anderson model shown in Fig. 5,[15] where E_g, ε, and χ represent the energy gap, the dielectric constant, and the electron affinity (work function), respectively. It can be seen that the barrier for electron is equal to $\Delta E_C = \chi(\text{ZnO}) - \chi(\text{Si}) = 0.3$ eV and that for hole is equal to 2.6 eV ($\Delta E_V = E_g(\text{ZnO}) + \chi(\text{ZnO}) - E_g(\text{Si}) - \chi(\text{Si}) = 2.6$ eV). Due to the differences in the electron affinities and the band gaps of the two materials, both the conduction and the valance bands have band offsets. But it is noticed that the valance band offset ΔE_V is much larger than the conduction band offset ΔE_C. As the carrier concentration of p-Si is much lower than that of ZnO, the depletion space charge region mainly locates at the p-Si side.

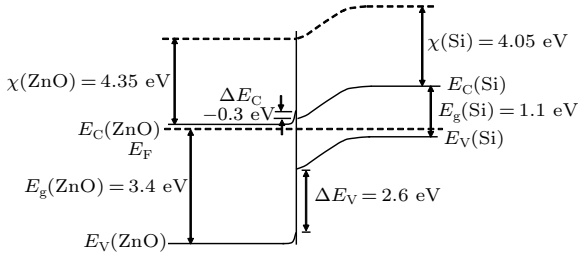


Fig. 5. Schematic energy band diagram of the ZnO/Si heterojunction.

As the n-ZnO/p-Si heterojunction is under the negative bias, the conduction band barrier will be decreased, and the electron flow from ZnO to p-Si will be enhanced. The subsequent recombination at the p-Si depletion region would give rise to the forward bias current flow. At low biases ($0 < V < 0.15$), the linearity of the forward current can be clearly observed in Fig. 6. The electrical field due to the injected carriers is negligible compare to that due to the applied bias. The J–V relation is often Ohmic, indicating that an Ohmic series resistance exists in parallel to the junction and is responsible for such a mechanism.

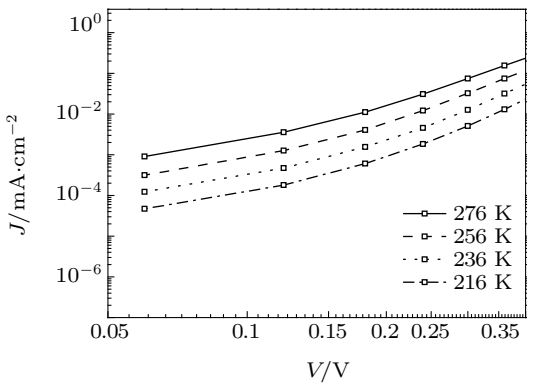


Fig. 6. The log–log plot of the J–V data for the ZnO/Si heterojunction at low biases.

In the voltage range of 0.15–0.6 V, the current density increases exponentially as a function of the applied voltage. The forward current, which corresponds to the positive potential of the substrate, can be expressed as[16]

$$J = J_0[\exp(AV) - 1], \tag{1}$$

where A is a coefficient defined by

$$A = \frac{q}{\eta kT}, \tag{2}$$

with η being the ideality factor, q is the electronic charge, and J_0 is the reverse saturation current defined by

$$J_0 = B\exp(-E_{\rm ac}/kT), \tag{3}$$

with $E_{\rm ac}$ being the activation energy. The ideality factor η is a quantity describing the deviation of the diode from an ideal p–n junction and can be evaluated by fitting the experimental data using Eq. (1). Table 1 gives the values of η obtained from the ln$J$–V curves.

Table 1. Parameters obtained by fitting the ln$J$–V curves.

T/K	A	η	m
276	12.77714	3.29	2.1
256	13.94941	3.25	2.0
236	14.72677	3.34	1.9
216	15.30214	3.51	1.8

It is known that the ideality factor η in an ideal p–n heterojunction is around 1.0 at a low voltage and up to 2.0 at a higher voltage according to the Sah–Noyce–Shockley theory.[17] Interestingly, the ideality factors in our cases are much higher than that expected from the Sah–Noyce–Shockley model. The results are in good agreement with those obtained by Lee *et al.*[18] A possible explanation for these results is related to the presence of nonlinear metal–semiconductor contact or defect states in the interface. Furthermore, the coefficient A is a linear function of the reciprocal of temperature, which indicates that the forward current is dominated by diffusion or recombination in the junction space charge region.

When the forward applied voltage is increased to be above 0.6 V, the J–V characteristics deviate from the ideal behavior. From Fig. 4(b), it can be seen that J–V follows a power law, which is generally attributed to the space-charge-limited current (SCLC) conduction for single-carrier (electron) injection observed in wide band gap semiconductors.[19−22]

In the SCLC, the relation between J and V is described by

$$J = KV^m \quad , \tag{4}$$

where K is a function of the thickness and the trap distribution. The m values obtained by linear fitting the curves of log$J$ versus log$V$ are shown in Table 1. The values are in good agreement with those obtained by Chen *et al.*[15] For the present n-ZnO/p-Si structure under the negative bias, most of the applied bias potential would drop across the ZnO film as its resistance is high. Because of the large barrier to hole injection (compared to that of electron), the injection current is mainly carried by the injected electrons, which is of the form of single carrier injection.

The J–V characteristics of the n-ZnO/p-Si heterojunction in dark and under the illumination of an incandescent lamp measured at room temperature are illustrated in Fig. 7. Typical good rectifying and photoelectric behaviors are observed for the device. Under the reverse bias conditions, the photocurrent caused by the ZnO surfaces exposing under the illumination is obviously much larger than the dark current. The light from the incandescent lamp is mostly in the visible region, and the ZnO films are highly transparent ($T > 90\%$) in the visible region. The visible light passes through the ZnO films and is absorbed primarily by the underlying p-Si. Thus, photon-induced electron–hole pairs are created only in the Si substrate at the region close to the interface where the recombination of the carriers can be neglected, and then are separated by the built-in electric field at the interface of the junction, which results in the observed photocurrent under the reverse bias conditions.[23,24] Under the forward bias conditions, the potential barrier is lowered. When the device is exposed to light, the direction of photovoltage is contrary to the bias, which further lower the barrier height of the heterojunction, therefore the forward current increases quickly. The inset in Fig. 7 shows that the photovoltage of the heterojunction is 270 mV and the short circuit current density is 2.10 mA/cm^2.

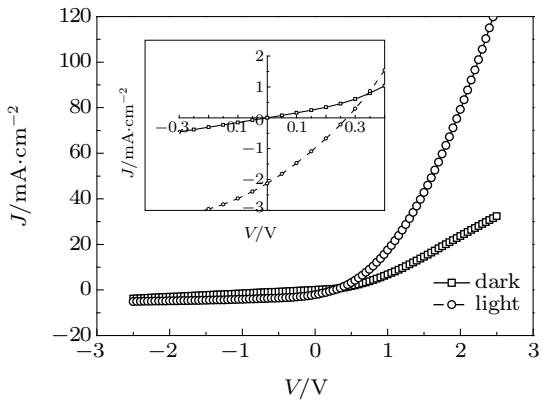


Fig. 7. The J–V characteristics of the ZnO/Si heterojunction in dark and under the incandescent lamp illumination. The inset shows the characteristics at low biases.

4. Conclusion

In summary, we have fabricated an n-ZnO/p-Si heterojunction by depositing ZnO thin film on p-type Si substrate using the LMBE technique. The heterojunction showed a good rectifying J–V behavior at room temperature. From the analysis of temperature dependence of the J–V characteristics, it has been found that in the low voltage region, the transport properties were dominated by diffusion or recombination within the junction space charge region, while at higher voltages, the space charge limited effect became the main transport mechanism. We also observed a clear photovoltaic signal when the ZnO film surface was irradiated by the incandescent lamp.

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