Extended Abstracts of the 2008 International Conference on Solid State Devices and Materials, Tsukuba, 2008, pp. 994-995

E-10-5

ZnO/Si Heterostructured Light-emitting Diodes by MOCVD

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1. Introduction

ZnO with a strong exciton binding energy (60 meV) and wide direct bandgap (3.37 eV) is a promising candidate for short-wavelength optoelectronic devices.[1] The capability of fabricating ZnO at a lower temperature (500~800^{o}C) and the feasibility of wet-chemical etching make the integration of ZnO with Si technology highly feasible.[2] It has motivated tremendous research activities on ZnO-based materials in the past few decades. However, reliable and high quality *p*-type ZnO films are difficult to achieve and have stumbled many researchers. ***The lack of p-type ZnO films has always been a major challenge for fabricating p-n homojunction optoelectronic devices.*** [3,4]

In this work, we present a promising ZnO/Si heterostructured light - emitting diode that emits UV light (~380nm) at room-temperature. Moreover, epitaxial grown n-ZnO/MgO/TiN/n$^+$-Si LED has been demonstrated. The device fabrication, device structures and origin of the electroluminescence shall be discussed.

2. Experiments

The ZnO films used in this work were deposited by a shower-head injector metal-organic chemical-vapor deposition (MOCVD).[5] Au electrodes were deposited on the surface of ZnO film and the backside of Si wafers by a direct-current magnetic sputtering. The schematic of *n*-ZnO/SiO$_x$/*n,p*-Si LEDs and *n*-ZnO/MgO/TiN/*n*$^+$-Si LEDs were depicted together with the cross-sectional transmission electron micrographs in **Fig. 1** and **Fig. 5**, respectively. HRXRD, HRTEM, IV, PL, and EL were used to characterize the performance of the devices.

3. Results and Discussion

The native SiO$_x$ (~3nm) functions as a carrier blocking layer for the LEDs, as shown in **Fig. 1**.

The typical I-V characteristics of the ZnO/Si heterostructured diodes are shown in **Fig. 2**. Ohmic contact was established for Au/*n*-ZnO, as shown in the inset of **Fig. 2**. *n*-ZnO/*p*-Si heterostructured diodes show diode-like rectification characteristics with a low breakdown voltage (~3V) at reverse bias. On the other hand, the I-V curve of ZnO/*n*-Si heterostructured diodes shows rectifying characteristics at both positive and negative bias. The native SiO$_x$ at the ZnO/Si interface acts as a double Schottky barrier for both *n* layers and the junction can be considered as a series of two back-to-back Schottky diodes.

Fig. 3 shows the RT EL of *n*-ZnO/SiO$_x$/*n*-Si LED when Si is positively biased. The EL spectrum consists of a UV band peaking at 380nm and a defect band centered at ~600nm. The field-induced inversion layer in the *n*-Si was proposed to be responsible for the hole injection and hence photon emission, as shown in **Fig. 4**.

By adopting a MgO/TiN buffer layer, ZnO can be epitaxially grown on Si, despite of its large lattice mismatch (~15.4%). **Fig. 5** shows the cross-sectional HRTEM of the ZnO/MgO/TiN/Si heterostructure. A well-defined MgO layer below ZnO and a thin TiN layer between MgO and Si can be found in the HRTEM. The crystal quality of ZnO film was further investigated by HRXRD. **Fig. 6(a)** shows a θ/2θ scan of XRD, in which only a sharp diffraction peak of (0002) can be found, indicating the ZnO film is strictly grown along c-axis. The Φ-scan was performed on the ZnO $(10\bar{1}0)$ and Si (220) planes, as shown in **Fig. 6(b)**. Six sharp Φ-scan peaks at 60^O intervals confirm that the epitaxial ZnO exhibits a single-domain wurtzite structure with hexagonal symmetry. Moreover, Φ-scan also indicates that the surface lattice of ZnO (0002) and Si (111) are exactly overlapped without any rotation, with an in-plane epitaxial relationship as $\langle 10\bar{1}0\rangle_{ZnO} \parallel \langle 11\bar{2}\rangle_{Si}$. The ω-scan rocking curve of ZnO (0002) shows a symmetric Gauss peak, with the full width at half maximum (FWHM) of 0.8^O, as illustrated in **Fig. 6(c)**.

The typical I-V characteristics of the diode are shown in **Fig. 7**. The MgO acts as a double Schottky barrier for both *n*-ZnO and *n*$^+$-Si and the heterojunction can be considered as a series of two back-to-back Schottky diodes. **Fig. 8(a)** shows the typical PL spectrum from the ZnO/MgO/TiN/Si heterostructure. **Fig. 8(b)** illustrates the EL photo and spectra of the heterostructured LED at RT under injection current from 40 to 192mA. The output light from the LED is clearly observed by naked eyes, with a yellow-whitish color, when a positive voltage was applied on the back electrode of Si substrates.

4. Summary

In summary, we have demonstrated *n*-ZnO/SiO$_x$/*n,p*-Si and *n*-ZnO/MgO/TiN/*n*$^+$-Si LEDs by MOCVD. The distinct RT EL can be observed from the diodes when a positive bias applied on Si substrate. Such ZnO/Si based heterostructured diodes are promising for the development of low-cost and high performance optoelectronic devices integrated on Si.

References

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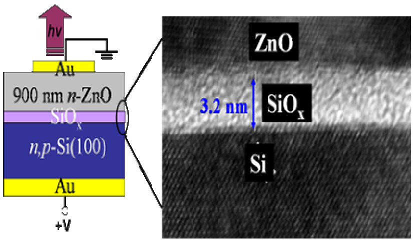

Fig. 1 A schematic diagram of ZnO/Si heterostructured LEDs and its cross-sectional TEM image.

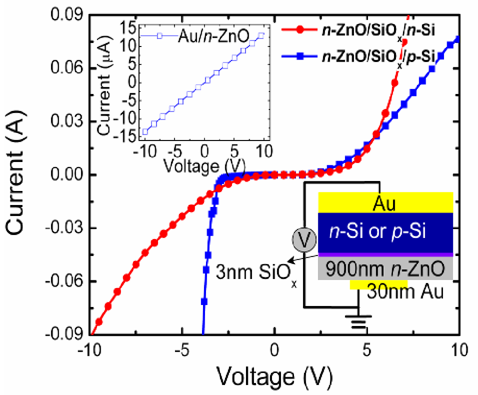

Fig. 2 IV characteristics of ZnO/Si heterostructured diodes. Top inset shows the ohmic characteristic of Au/*n*-ZnO.

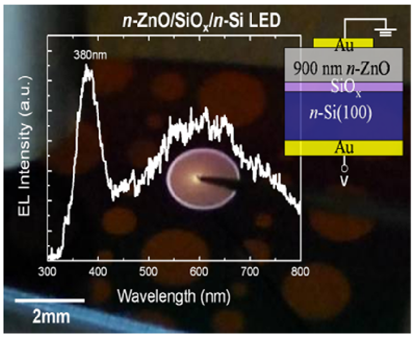

Fig. 3 Room-temperature EL of the *n*-ZnO/SiO$_x$/*n*-Si LEDs.

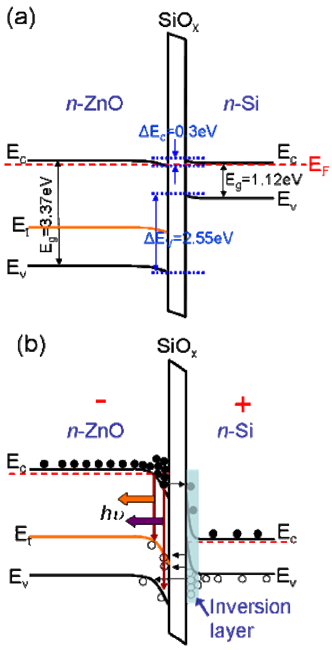

Fig. 4 Energy band diagrams of the *n*-ZnO/SiO$_x$/*n*-Si LEDs.

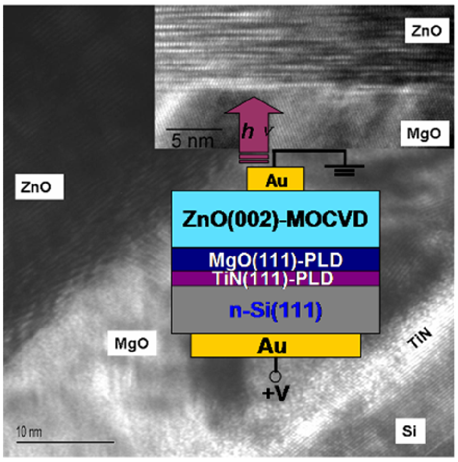

Fig. 5 A schematic diagram of ZnO/MgO/TiN/Si heterostructured LEDs and its cross-sectional TEM.

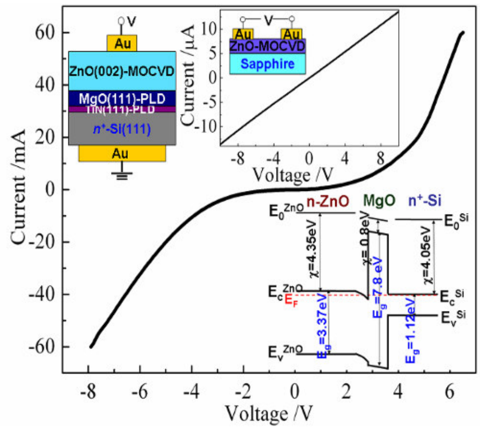

Fig. 7 Typical IV characteristic of ZnO/MgO/TiN/Si heterostructured LEDs

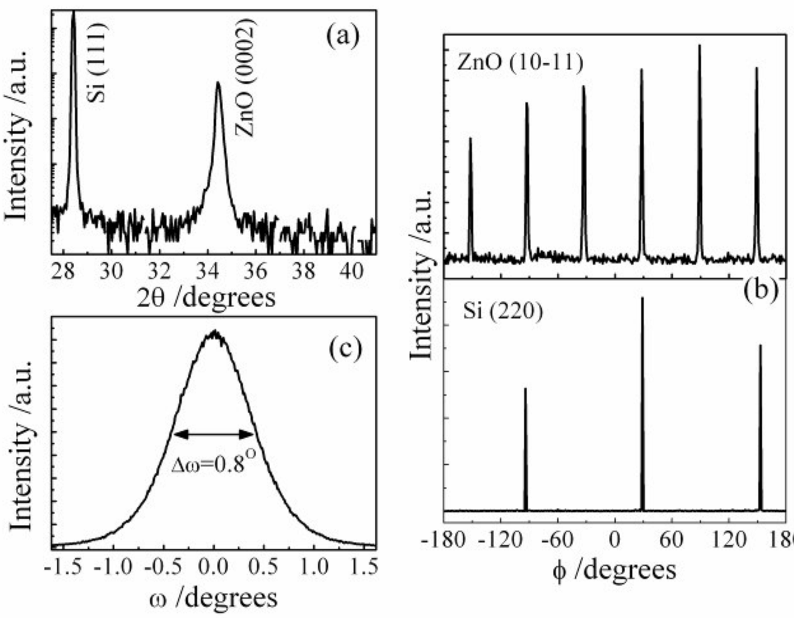

Fig. 6 XRD spectrum of the epitaxial ZnO film on MgO/TiN buffered Si(111): (a) θ/2θ scan, (b) Φ-scan for ZnO (10$\bar{1}$1) and Si (220), and (c) ω-scan rocking curve of ZnO (0002).

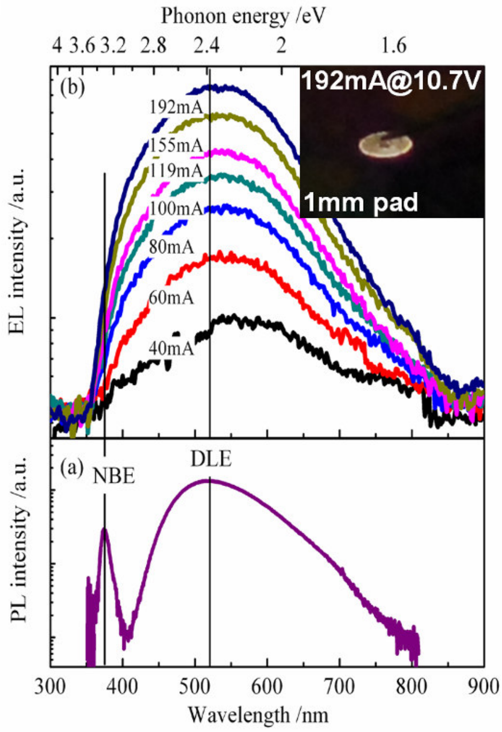

Fig. 8 Room-temperature (a) PL, (b) EL of ZnO/MgO/TiN/Si heterostructured LEDs.