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Band offset measurements of ZnO/6H-SiC heterostructure system

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The conduction band offset of n-ZnO/n-6H-SiC heterostructures fabricated by rf-sputtered ZnO on commercial n-type 6H-SiC substrates has been measured by a variety of methods. Temperature dependent current-voltage characteristic, photocapacitance, and deep level transient spectroscopy measurements showed the conduction band offsets to be 1.25, 1.1, and 1.22 eV, respectively.


ZnO is under consideration for a variety of optical devices owing to its large exciton binding energy (60 meV), relative ease of bulk material growth, and the possibility of growing highly conductive layers. Because high quality, reproducible p-type ZnO layers are not yet available, p-n junctions are fabricated that take advantage of heteroepitaxy.1 Heteroepitaxial structures are also of interest on their own merits because of advantages provided by the valence and conduction band offsets.2 Various heteroepitaxial structures have been used as the p-type layer for device fabrication. For example, ZnO has been used as a channel for high quality field-effect transistors by several groups.3,4 The component materials of the heterojunction can have a large impact on device performance.

One of the vital criteria in heteroepitaxial based devices is to match the lattice parameters, and from this point of view GaN and its alloys with aluminum have been considered by many authors as one of the best candidates for such device fabrication.5–9 Another good candidate for ZnO based heterostructure devices is SiC, which matches the wurtzite crystal structure and has a relatively small lattice mismatch of ~4% with ZnO.10–13 Recently, we demonstrated high quality and highly reproducible n-ZnO/p-6H-SiC heterojunction diodes with a very good rectifying behavior and with a leakage current less than 1 × 10−4 A/cm² at −10 V, a forward current of 4 A/cm² at 8 V, and a breakdown voltage greater than 20 V.10,11 In Ref. 11 it was shown from electroluminescence measurements that electron injection takes place primarily from ZnO into SiC without substantial hole injection into the ZnO. Although this is not beneficial for light-emitting diode applications (because ZnO would not be the active photon emission layer in this case), it would be of interest for applications in which ZnO would serve as the emitter, such as photodiodes and n-p-n-type heterostructure bipolar transistors.

To better understand heterostructure device performance, knowledge of the band offset between materials forming the heterostructure is necessary. No report on the band offset in ZnO/SiC heterostructure is available. In this letter we have measured the conduction band offset of this material system by studying n-ZnO/n-6H-SiC isotype heterodiodes with Ohmic contacts by temperature dependent current-voltage characteristic (I-V-T), photocapacitance, and deep level transient spectroscopy (DLTS) measurements.

The n-ZnO/n-SiC heterostructure samples were fabricated by growing 0.3 μm thick undoped ZnO film by rf sputtering on 300 μm commercial n-type 6H-SiC substrates. ZnO layers were deposited directly on 6H-SiC substrates at 750 °C by rf magnetron sputtering in an Ar+O₂ ambient atmosphere. Electron concentration of n-6H-SiC was 2.6 × 10¹⁷ cm⁻³. The chamber process pressure and plasma power were 4.20 mTorr and 100 W, respectively. After growth ZnO layers were annealed at 950 °C for 1 h to improve film crystal quality. It should be noted that we observed earlier that such treatment of ZnO on SiC leads to significant improvement of ZnO crystal quality.12 The 250 μm diameter mesa structures were fabricated by conventional photolithography method. The Ohmic contacts to n-ZnO and n-SiC were formed by depositing Au/Al (300/300 Å) and Au/Ti/Ni (300/300/300 Å) metal layers, respectively, with subsequent rapid temperature annealing at 800 °C for 2 min. The I-V-T and DLTS measurements were performed in the temperature range of 80–700 K. The photocapacitance spectroscopy was taken at 80 K using a xenon lamp and monochromator.

In Fig. 1 the typical I-V characteristics of the diodes at 300 and 80 K are shown. As seen from the figure, the I-V characteristic exhibits a clear rectifying behavior, and at room temperature the forward current at 3 V is 1 × 10⁻² A while the reverse current at −3 V is 1 × 10⁻⁷ A. Both reverse
The forward bias current from Eq. 1 is given by

\[ I = I_s \left[ \exp \left( \frac{qV}{nkT} \right) - 1 \right], \]

where \( I_s \) is the saturation current, \( n \) the ideality factor, \( k \) the Boltzmann constant, and \( T \) the absolute temperature. The saturation current in Eq. (1) is given by

\[ I_s = A^* T^2 \exp \left( -\frac{\phi_B}{kT} \right), \]

where \( A^* \) is the effective Richardson constant and \( \phi_B \) the barrier height. The forward bias current from Eq. (1) was fitted for the saturation current at each temperature. A plot of \( \ln(I_s/T^2) \) vs \( 1/kT \) has a slope of \( -\phi_B \), which is 1.25 eV.

Adjustments can be made to account for the position of the Fermi level relative to the conduction band in each component material, but the shallow carrier activation energy in each is similar and small compared to the band offset. The band offset in a \( n-n \) heterojunction is

\[ \Delta E_c = qV_D - \delta_1 + \delta_2. \]  

(3)

\( V_D \) is the sum of the band bending in each material, and \( \delta_1 \) and \( \delta_2 \) are the Fermi level positions with respect to the conduction band in each material. The band bending in the ZnO will also be very small compared to the band bending in the SiC, proportional to the ratio of dopant in SiC to conduction band density of states in ZnO. A calculation of the band bending based on a band offset of 1.25 eV and carrier concentrations of \( 6 \times 10^{17} / \text{cm}^3 \) in ZnO and \( 1 \times 10^{18} / \text{cm}^3 \) in SiC is shown in the inset of Fig. 2.

Photocapacitance measures the change in capacitance when monochromatic light with energy near the barrier height is incident on the diode. Figure 3 presents the results of photocapacitance measurements for a \( n-ZnO/n-6H-SiC \) diode as a function of photon energy taken at 80 K. As seen from the figure, the spectrum has a peak at 1.1 eV, which corresponds to the energy necessary to overcome the energetic barrier due to the band offset at the \( n-ZnO/n-6H-SiC \) interface.

The temperature dependence of thermionic emission over the barrier was also measured using DLTS to determine the band offset. The filling pulse was 1 V for 100 ms, and the measurement bias was −3 V. The filling pulse bias required to bring the Fermi level above the bottom of the triangular well at the heterojunction was determined from an abrupt increase in the emission amplitude as the filling pulse was increased. The spectrum for a rate window of 278/s is shown in Fig. 4. A conventional rate window analysis was performed to obtain the energy. The energy from a rate window analysis is 1.2 eV. This is the thermionic emission energy over the heterojunction barrier.

In conclusion, the conduction band offset of \( n-ZnO/n-6H-SiC \) diode with Ohmic contacts has been measured by three different methods: \( I-V-T \), photocapacitance, and DLTS. The measured band offsets using each method are 1.25, 1.1, and 1.2 eV, respectively.

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