Band alignment of Ga_2O_3/6H-SiC heterojunction*

Chang Shao-Hui(常少辉), Chen Zhi-Zhan(陈之战), Huang Wei(黄 维), Liu Xue-Chao(刘学超),†
Chen Bo-Yuan(陈博源), Li Zheng-Zheng(李铮铮), and Shi Er-Wei(施尔畏)

Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, *China*

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A high-quality Ga_2O_3 thin film is deposited on an SiC substrate to form a heterojunction structure. The band alignment of the Ga_2O_3/6H-SiC heterojunction is studied by using synchrotron radiation photoelectron spectroscopy. The energy band diagram of the Ga_2O_3/6H-SiC heterojunction is obtained by analysing the binding energies of Ga 3d and Si 2p at the surface and the interface of the heterojunction. The valence band offset is experimentally determined to be 2.8 eV and the conduction band offset is calculated to be 0.89 eV, which indicate a type-II band alignment. This provides useful guidance for the application of Ga_2O_3/6H-SiC electronic devices.

Keywords: band alignment, Ga_2O_3/6H-SiC, synchrotron radiation photoelectron spectroscopy

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1. Introduction

Silicon carbide (SiC) is an extremely promising semiconductor material for the fabrication of electronic and opto-electronic devices.[1] Due to its wide band gap (4H: $E_g = 3.2$ eV, 6H: $E_g = 3.0$ eV), it is quite suited for fabricating high power, high frequency and high temperature devices.[2] The recent progress in large scale high quality SiC wafers increases the possibility of fabricating SiC-based devices.[3,4] The β-Ga_2O_3 is a typical transparent conductive material in the deep ultraviolet (UV) region due to its wide band gap ($E_g = 4.9$ eV).[5] High-quality Ga_2O_3 thin films and single crystals have been reported.[5,6] They are good materials to be used as the electrodes in wide band gap semiconductor devices, such as SiC UV detectors and photo-electric switches. Trinchi *et al.*[7] reported a Ga_2O_3/SiC gas sensor with good performance. Besides, the lattice mismatch between 6H-SiC ($a = b = 3.08$ Å) and Ga_2O_3 ($a = 12.23$ Å, $b = 3.04$ Å) is less than 1.5%.[4] For the Ga_2O_3/SiC heterojunction structure, the band alignment is quite necessary for further applications. The band alignment parameters of a heterojunction can be experimentally or theoretically obtained.[8] In the present paper, we perform in-depth study on the electronic structure of the Ga_2O_3/6H-SiC heterojunction. The valence band offset (VBO), the conduction band offset (CBO) and the band alignment of the Ga_2O_3/6H-SiC heterojunction are experimentally determined by using the synchrotron radiation photoelectron spectroscopy (SRPES).[9]

2. Experiment

The Ga_2O_3/6H-SiC heterojunction was prepared by depositing Ga_2O_3 thin film on a 6H-SiC substrate through the radio frequency magnetron sputtering. Before deposition, the sputtering chamber was evacuated down to 5.0×10^{-5} Pa and the substrate was heated to 500 °C. The Ga_2O_3 film was grown with the argon plasma at a fixed pressure of 1.0 Pa for 10 min. The thickness of the Ga_2O_3 film was found to be 12 nm, which was characterized by transmission electron microscopy. The X-ray diffraction (XRD) showed that the Ga_2O_3 film was polycrystalline with β (–201) orientation. The carrier concentration and the Hall mobility were 2.7×10^{16} cm^{-3} and 246 cm^2/V·s for the n-type 6H-SiC substrate, respectively.

The SRPES measurement was performed using an ultra-high vacuum (5×10^{-8} Pa base pressure) photoelectron spectroscopy beamline in the National Synchrotron Radiation Laboratory (NSRL) in Hefei, China.[10] The SRPES system consisted of a VG ARIPS 10 angle-resolved energy analyzer and a monochromatic radiation that was monochromatized

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†Corresponding author. E-mail: xcliu@mail.sic.ac.cn

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by a variable angle spherical grating monochromator and refocused by a toroidal mirror. The spectra were collected in the normal emission with an incoming photon energy of 150 eV. Before the SRPES measurement, the as-grown sample was subjected to a surface clean procedure by using the Ar^+ bombardment at 2 keV. Alfieri *et al.*[11] proposed that after the ion implantation, the conduction band edge might shift and thus change the band gap (this change was relieved after an annealing). Their samples were irradiated with 15 MeV electrons and the change of the band gap was only 0.06–0.10 eV. The energy used in our measurement was much lower, so the effect of the ion bombardment could be negligible. The positions of the valence band maximum (VBM) and the Ga 3d core level (CL) were measured on a cleaned Ga_2O_3 film surface. After that, the film was thinned to $\sim$4 nm to obtain the Ga 3d and the Si 2p CLs at the interface. Then the film was totally removed from the SiC substrate, no peak related to Ga 3d was detected. Then, information about Si 2p and the VBM in 6H-SiC was obtained.

3. Results and discussion

The relative energy differences $E_{\mathrm{Ga3d}}^{\mathrm{Ga_2O_3}} - E_{\mathrm{VBM}}^{\mathrm{Ga_2O_3}}$, $E_{\mathrm{Si2p}}^{\mathrm{SiC}} - E_{\mathrm{VBM}}^{\mathrm{SiC}}$, and ΔE_{CL} can be directly measured, and then the VBO (ΔE_{V}) is calculated from the following equation:

$$\Delta E_{\mathrm{V}} = (E_{\mathrm{Si2p}}^{\mathrm{SiC}} - E_{\mathrm{VBM}}^{\mathrm{SiC}}) - \Delta E_{\mathrm{CL}} - (E_{\mathrm{Ga3d}}^{\mathrm{Ga_2O_3}} - E_{\mathrm{VBM}}^{\mathrm{Ga_2O_3}}), \quad (1)$$

where $E_{\mathrm{Si2p}}^{\mathrm{SiC}} - E_{\mathrm{VBM}}^{\mathrm{SiC}}$ and $E_{\mathrm{Ga3d}}^{\mathrm{Ga_2O_3}} - E_{\mathrm{VBM}}^{\mathrm{Ga_2O_3}}$ are the VBM energies relative to the CL positions of the bulk SiC and the thin Ga_2O_3 film, respectively. They can be obtained by the SRPES measurements of the SiC substrate and the thin Ga_2O_3 film. The $\Delta E_{\mathrm{CL}} = (E_{\mathrm{Si2p}}^{\mathrm{SiC}} - E_{\mathrm{Ga3d}}^{\mathrm{Ga_2O_3}})$ is the energy difference between Si 2p and Ga 3d CLs, which is measured at the interface of the heterojunction

The synchrotron radiation source provides a high-brightness incident photon flux. The accuracy of the VBM position, which is limited mainly by the accuracy of the linear fitting of the valence band edge in the photoelectron spectra, is quite good due to the excellent signal-to-noise characteristics. Since the fitted line and the original measured data are in good agreement with each other, the uncertainty of the CL position should be lower than 0.02 eV, which is evaluated by numerous fittings with different parameters.

The CL spectrum of Ga 3d recorded on a cleaned surface is shown in Fig. 1(a). The spectrum is fitted using a Voigt (mixed Lorentzian–Gussian) line with a Shirley background by employing the XPS peak software.[12] The prominent peak located at 21.53 ± 0.02 eV corresponds to the Ga–O bond. The value is slightly different from that given in the literature due to the different preparation methods.[13–15] The other peak is shifted by 1.21 eV toward the lower binding energy and is assigned to a lower oxidation state.[13] The VBM position of Ga_2O_3 is determined by linearly extrapolating the leading edge of the VB spectrum, as shown in Fig. 1(b).[16] The energy reference is $E_{\mathrm{VBM}}^{\mathrm{Ga_2O_3}} = 4.41 \pm 0.02$ eV. The energy difference between Ga 3d and Ga_2O_3 VBMs, $E_{\mathrm{Ga3d}}^{\mathrm{Ga_2O_3}} - E_{\mathrm{VBM}}^{\mathrm{Ga_2O_3}}$, is calculated to be 17.12 ± 0.04 eV.

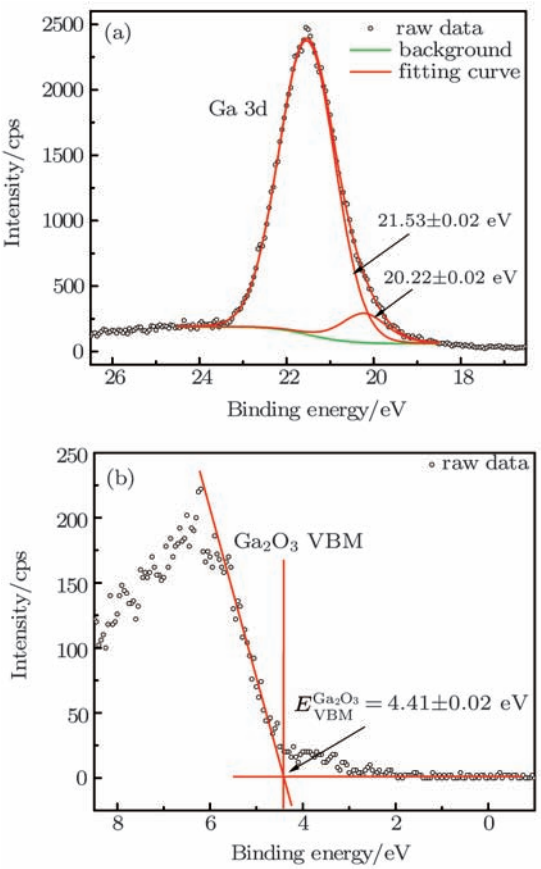


Fig. 1. (colour online) The SRPES of a cleaned surface of the Ga_2O_3/6H-SiC heterojunction obtained with an incident photon energy of 150 eV: (a) Ga 3d spectrum and (b) VBM of Ga_2O_3 film. The CL peak is simulated to the Voigt line shapes using a Shirley background. The VBM value is determined by using a linear extrapolation of the leading edge to the base line.

Figure 2 shows the interface SRPES of the Ga_2O_3/6H-SiC heterojunction. Both Si 2p and Ga 3d CLs are clearly seen in the detected photoelectron energy range as shown in Fig. 2(a). Detailed Si 2p

and Ga 3d CLs for accurate peak fittings are shown in Figs. 2(b) and 2(c), respectively. It can be seen that the Si 2p CL peak consists of two components according to the Voigt fitting. The prominent one is located at 100.81±0.02 eV. It stems from the Si emitter within the 6H-SiC substrate,[17] which has four bonds to the carbon atoms. The other one is shifted by 1.74 eV toward the higher binding energy. It is attributed to the Si^+ emitter atom,[18] which is located at the surface of the 6H-SiC substrate with one bond to the oxygen and three bonds to the carbon atoms. This result accords well with that given in the literature.[15,17] Similarly, the Ga 3d CL peak also consists of two components. The prominent one located at 20.26 ± 0.02 eV corresponds to the Ga–O bond at the interface. The other one shifted by 1.39 eV toward the lower binding energy is assigned to the lower oxidation state. It can be seen that the value of Ga 3d in Fig. 2(c) is different from that in Fig. 1(a). This may be caused by the change from the Ga–O bond at the surface into the Ga–O–Si bond at the interface of the heterojunction. The energy difference between Si 2p and Ga 3d on the interface, $E^{\mathrm{SiC}}_{\mathrm{Si2p}} - E^{\mathrm{Ga_2O_3}}_{\mathrm{Ga3d}}$, is calculated to be 80.55 ± 0.04 eV.

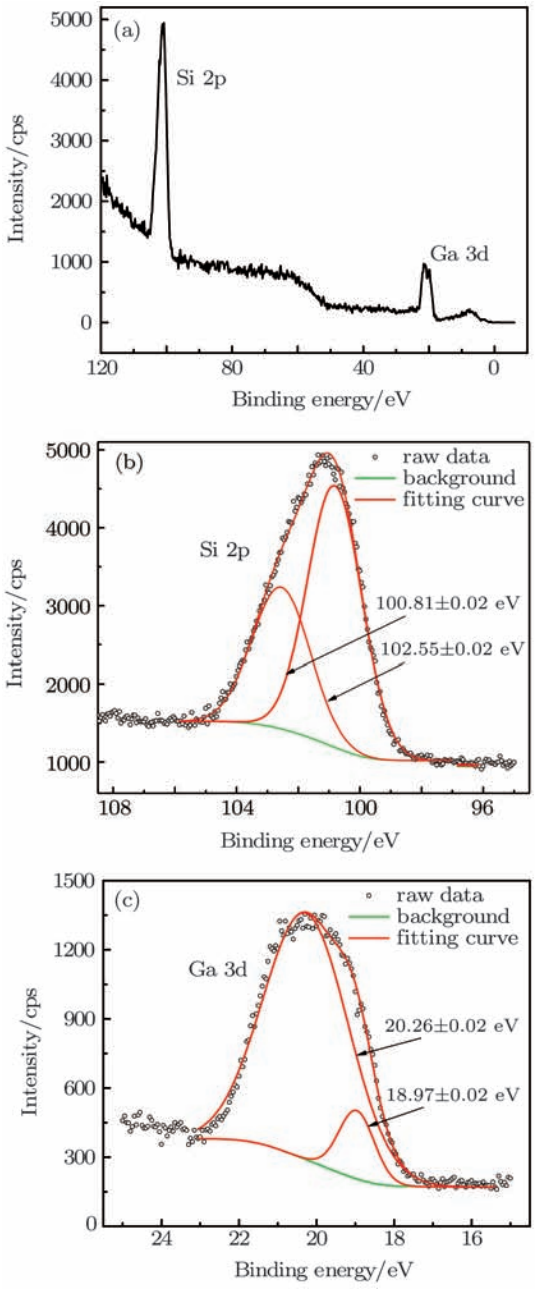


Fig. 2. (colour online) The interface SRPES of Ga_2O_3/6H-SiC heterojunction obtained with an incident photon energy of 150 eV: (a) Si 2p and Ga 3d spectra (b) Si 2p spectrum, and (c) Ga 3d spectrum. The CL peaks are fitted to the Voigt line shapes using a Shirley background.

Figure 3 shows the SRPES of the 6H-SiC substrate. It can be seen that the Si 2p CL peak consists of two components according to the Voigt fitting shown in Fig. 3(a). The prominent one is located at 100.54 ± 0.02 eV. It stems from the Si emitter within the 6H-SiC substrate, which has four bonds to the carbon atoms. The other one is shifted by 1.40 eV

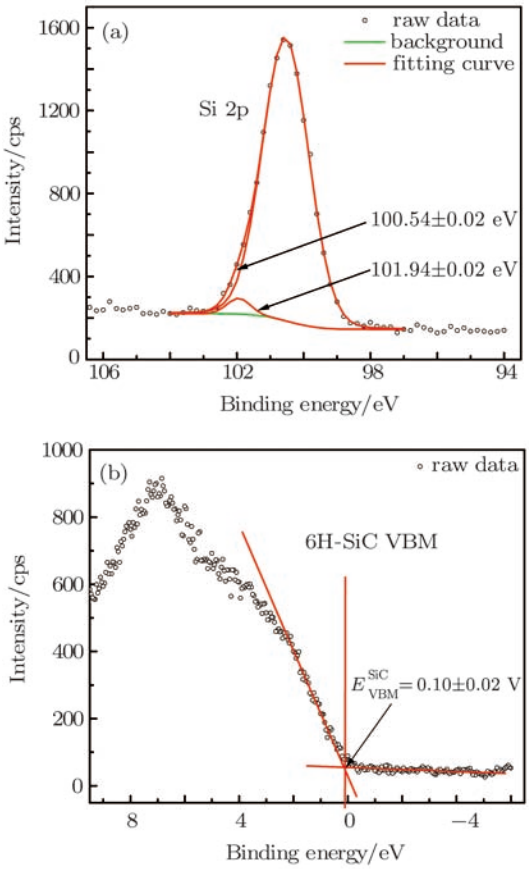


Fig. 3. The SRPES of 6H-SiC substrate obtained with 150 eV incident photon energy: (a) Si 2p spectrum and (b) VBM of 6H-SiC. The CL peak is fit to the Voigt line shape using a Shirley background. The VBM values are determined by using a linear extrapolation of the leading edge to the base line.

toward the higher binding energy. It is attributed to the Si^+ emitter atom, which is located at the surface of the 6H-SiC substrate with one bond to the oxygen and three bonds to the carbon atoms. Using the same linear extrapolation method mentioned above, we find a VBM value of 0.10 eV from the SRPES spectra given in Fig. 3(b). The energy difference between Si 2p and 6H-SiC VBMs, $E^{\rm SiC}_{\rm Si2p} - E^{\rm SiC}_{\rm VBM}$, is calculated to be 100.44 ± 0.04 eV. The VBO value is 2.8 eV obtained by substituting those values into Eq. (1). The CBO value is calculated to be 0.9 eV by using formula $\Delta E_{\rm C} = \Delta E_{\rm V} + E^{\rm SiC}_{\rm g} - E^{\rm Ga_2O_3}_{\rm g}$. By using the VBO and the CBO values, the energy band diagram of the heterojunction is obtained and shown in Fig. 4. The Ga_2O_3/6H-SiC heterojunction shows a typical type-II band alignment.

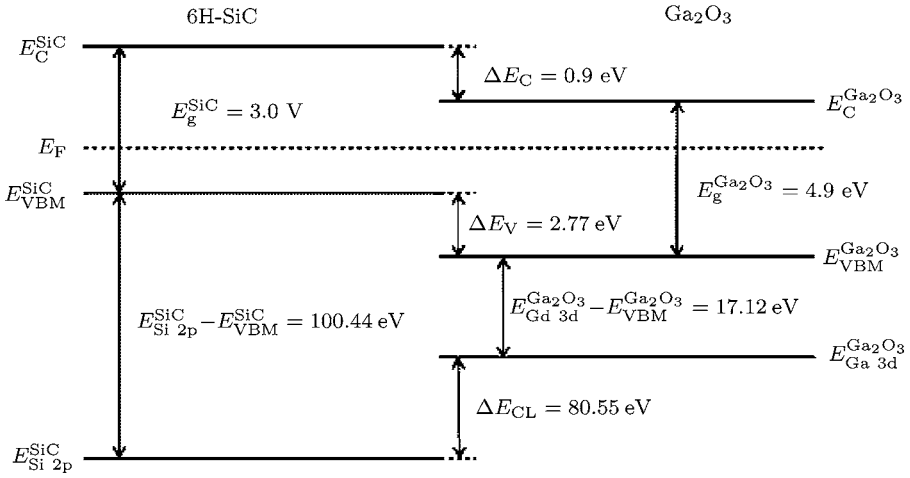


Fig. 4. Energy band diagram of Ga_2O_3/6H-SiC heterojunction.

4. Conclusion

We perform an in-depth study on the electronic structure of the Ga_2O_3/6H-SiC heterojunction by using the SRPES. The result reveals that the Ga_2O_3/6H-SiC heterojunction has a type-II band alignment with a VBO value of $\Delta E_{\rm V} = 2.8 \pm 0.1$ eV and a CBO value of $\Delta E_{\rm C} = 0.9 \pm 0.1$ eV. The results provide useful guidance for the design and the application of SiC-based devices with Ga_2O_3.

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