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# Band alignment of lattice-mismatched $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$ heterojunction determined by x-ray photoemission spectroscopy

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## AFFILIATIONS

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**Note:** This paper is part of the Special Topic on: Highly Mismatched Semiconductors Alloys: from Atoms to Devices.

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## ABSTRACT

X-ray photoelectron spectroscopy and ultraviolet photoelectron spectroscopy were used to measure the band structure for high lattice-mismatched  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$ . The valence band offset was determined to be 0.43 eV, which is in agreement with the theoretical values based on the previous analysis. Together with a conduction band offset of 0.44 eV, it is indicated that a type-I band structure forms at the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  heterojunction. The precise determination of the band structure of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  is crucial for future device design and performance improvement. Besides, the valence band offset of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{GaAs}$  was estimated to be 0.24 eV, which also presents a type-I band alignment.

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## INTRODUCTION

Heterojunctions offer a means to tailor the transport, band alignments, and optical and electrical properties. Their carrier limitation and high carrier injecting ratio properties caused by the difference in bandgap make it possible for the realization of advanced functional devices.<sup>1,2</sup> The main parameters that govern the transport properties in the heterojunctions are the valence and conduction band discontinuities at the interfaces. Detailed knowledge of valence band offset (VBO) and conduction band offset (CBO) in InGaAs material systems is vital for assessing the degree of carrier confinement and understanding the electronic properties. Thus, an investigation on the band offset at InGaAs heterojunctions is important for device design, modeling, and performance prediction.<sup>3</sup>

The band offsets of InGaAs heterojunctions were studied and analyzed earlier, but most of the measurements were focused on lattice-matched systems. The typical experimental VBOs and CBOs are summarized here. For  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ , I-V and C-V profiles

yielded a CBO of  $0.22 \pm 0.02$  eV;<sup>4</sup> low temperature-photoconductivity gave a CBO of 0.23 eV;<sup>5</sup> and admittance spectroscopy gave a VBO of  $0.346 \pm 0.010$  eV and a CBO of  $0.250 \pm 0.010$  eV.<sup>6</sup> Low-temperature optical data gave a VBO of 0.38 eV and x-ray photoelectron spectroscopy (XPS) gave a VBO of 0.34 eV.<sup>7,8</sup> For  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{In}_{0.52}\text{Al}_{0.48}\text{As}$ , a CBO of 0.52 eV was obtained by thermionic emission,  $0.50 \pm 0.05$  eV was achieved by C-V profiling, Sugiyama *et al.*<sup>12</sup> reported a CBO of  $0.533 \pm 0.020$  eV, and Sandhu *et al.*<sup>13</sup> gave a value of  $0.51 \pm 0.02$  eV.<sup>9–11</sup> For InGaAs lattice-mismatched systems, there are few experimental reports and studies compared with the lattice-matched ones. This may be attributed to the difficulties in dealing with the band discontinuities due to the misfit strain. For the lattice-mismatched  $\text{In}_{0.17}\text{Ga}_{0.83}\text{As}/\text{Al}_{0.32}\text{Ga}_{0.68}\text{As}$ , photoluminescence yielded a VBO of  $0.157 \pm 0.025$  eV,<sup>2</sup> which was in good agreement with the observations made by Wilkinson *et al.*<sup>14</sup> Waldrop *et al.* measured a VBO of AlAs/InP but produced a result of  $-0.27$  eV by ignoring the misfit strain effect.<sup>21</sup>

Extended wavelength InGaAs heterojunctions with high In content have gained wide attention due to their extensive applications in near-infrared detection. However, inadequate experimental data and high uncertainties still exist on the band offsets for lattice-mismatched  $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{InP}$ . The lack of detailed knowledge about band structure will hinder the energy band control and device design in the future. Only when we get a full understanding of the band structure can we manipulate the band structure and obtain an effective performance optimization and design.

There are many ways for determining the band offset, such as C-V, XPS, admittance spectroscopy, internal photoemission, thermionic emission, and low-temperature photoluminescence.<sup>4–13</sup> C-V and XPS are the most used methods. C-V profiling was demonstrated to be an effective method to measure the band offset for the heterojunction by Kroemer, and it was soon used extensively.<sup>15,16</sup> Besides, XPS was used to precisely determine the VBOs in semiconductor heterojunctions, and it has proven to be a direct and powerful tool for band offset measurements.<sup>18</sup> In this study, XPS was used to measure the VBO of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$ , then the CBO was calculated from the VBO, and finally, the band alignment diagram was presented. In addition, the influence of misfit strain on the band offset was discussed and analyzed.

## MATERIALS AND METHOD

XPS and ultraviolet photoelectron spectroscopy (UPS) were used to determine the VBO of the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  heterojunction. To obtain the VBO values and the band structure, three samples were prepared before XPS measurements were taken: a commercial epi-ready InP 2 in. wafer was used as the InP bulk sample and the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  (1.4  $\mu\text{m}$ ) bulk sample and  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  (5 nm)/InP sample were grown by metal organic chemical vapor deposition (AIXTRON 200/4) at low pressure (76 Torr) with purified  $\text{H}_2$  as the carrier gas, and the deposition temperature set at 650  $^{\circ}\text{C}$  for all samples. Trimethylindium (TMIn), trimethylgallium (TMGa), and pure arsine ( $\text{AsH}_3$ ) were used as the In, Ga, and As precursors, respectively. Here, we introduced the interfacial sample because although the VBO could be roughly estimated from the difference between valence band maximum (VBM) of the two bulk materials, it contained an appreciable error since the effect of the dipole that existed at the interface was not accounted for.<sup>17</sup>

Scanning electron microscopy (SEM, Hitachi S4800) was used for the surface morphology investigation. XPS and UPS measurements were performed on the ESCALAB 250 system by using a monochromatized Al K $\alpha$  x-ray source ( $h\nu = 1486.6$  eV) and a He I source ( $h\nu = 21.22$  eV), respectively. The size area of the x-ray spot was about 500  $\mu\text{m} \times 500 \mu\text{m}$ . The ESCALAB 250 system was equipped with the MAGCIS dual beam Ar ion source, which could operate in both monatomic and gas cluster modes, and all we needed to do was to choose the mode we wished to use in the experiment. The damage of the cluster ion source to the surface is negligible when eliminating the surface contamination. All samples were vacuum-packed with aluminum foil during transportation. Before XPS measurements were taken, all samples were bombarded with an  $\text{Ar}^+$  ion gun (3 kV, 3  $\mu\text{A}$ ) to prevent surface contamination. The cleanness of the samples was verified by checking for C 1s and

O 1s peaks as measured by XPS. The electric field caused by charge accumulation can affect the measured kinetic energy of photoelectron during the tests, so an electron source co-axial equipped with an analyzer input lens was used to achieve charge compensation. The binding energy was calibrated by adjusting the peak position of C 1s core level (CL) to 284.8 eV for each sample before measurement.

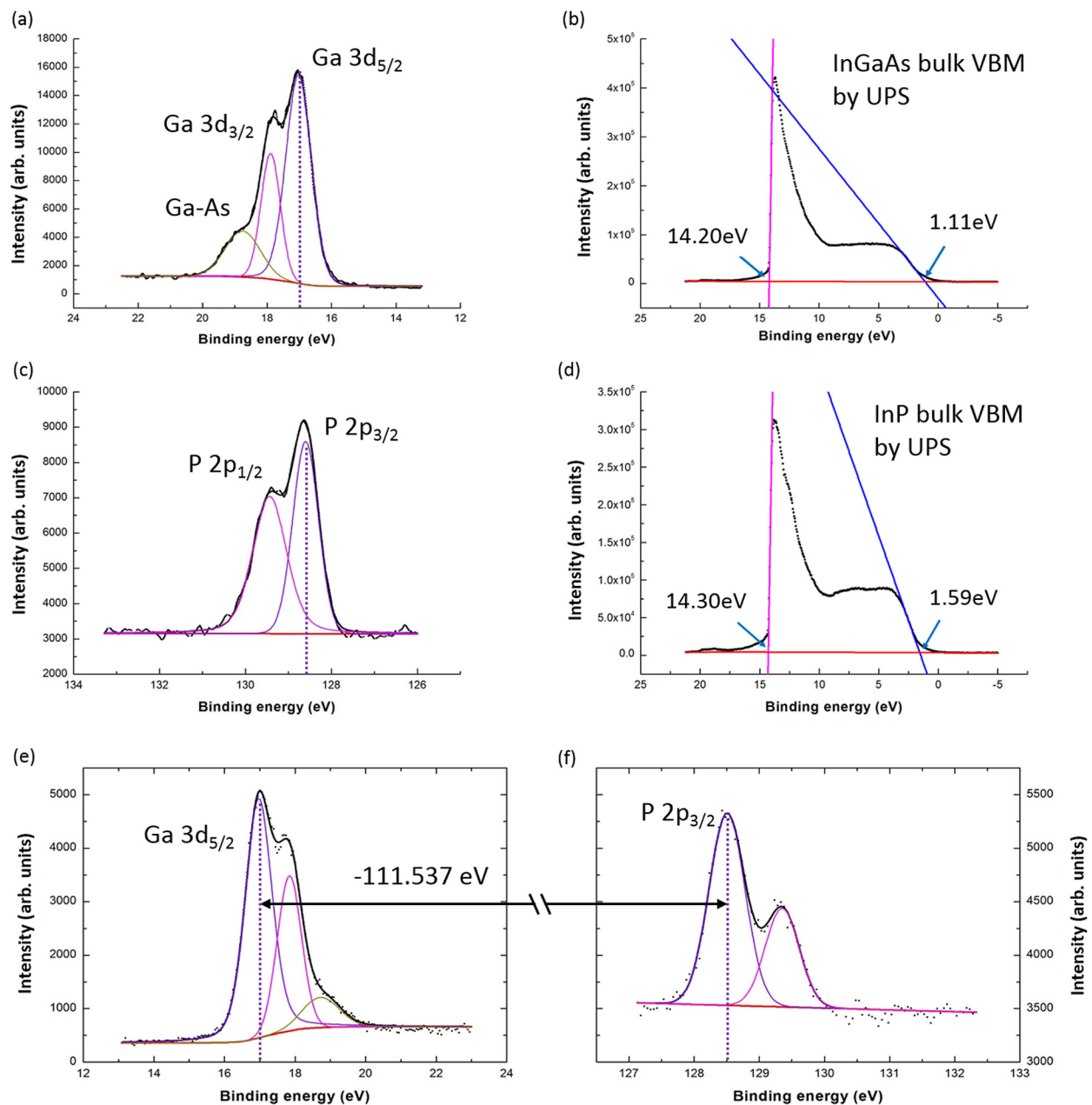
The VBO ( $\Delta E_V$ ) of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  can be evaluated from the energy separation between Ga 3d and P 2p core levels and the VBM can be determined from the formula:<sup>18</sup>

$$\Delta E_V = \Delta E_{CL} - (E_{\text{Ga}3d_{5/2}}^{\text{InGaAs}} - E_{\text{VBM}}^{\text{InGaAs}}) + (E_{\text{P}2p_{3/2}}^{\text{InP}} - E_{\text{VBM}}^{\text{InP}}), \quad (1)$$

where  $\Delta E_{CL} = [E_{\text{Ga}3d_{5/2}}^{\text{InGaAs}}(i) - E_{\text{P}2p_{3/2}}^{\text{InP}}(i)]$  is the binding energy difference between P 2p and Ga 3d core level from the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  (5 nm)/InP interface.  $(E_{\text{Ga}3d_{5/2}}^{\text{InGaAs}} - E_{\text{VBM}}^{\text{InGaAs}})$  and  $(E_{\text{P}2p_{3/2}}^{\text{InP}} - E_{\text{VBM}}^{\text{InP}})$  are the VBM energy with reference to the core level (CL) peaks in  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  (1.4  $\mu\text{m}$ ) and InP (epi-ready substrate) thick film, respectively.

Ga 3d CL spectra for the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  and  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  samples, P CL 2p spectra for the InP and  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  samples, and the valence band (VB) spectra for both the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  and InP samples are shown in Fig. 1. All CL peaks were fitted to Voigt (mixed Lorentzian-Gaussian) line shape by employing a Shirley background. The VB spectra were measured by UPS to overcome the measurement accuracy of XPS caused by the low signal to noise ratio. The VBM was determined by the intersection between the linear fitting to the leading edge of the spectrum and the background.

As shown in Fig. 1(a), for the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  sample, the Ga 3d<sub>5/2</sub> CL peak is located at 17.02 eV, which was de-convoluted with Gaussian curves constrained by known spin-orbit splitting. Ga 3d<sub>3/2</sub> is located at 17.90 eV, and the leftmost peak in the picture can be attributed to Ga-As, which is at 18.80 eV. Figure 1(b) shows the VB spectra of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$ ; the VBM was calculated to be -8.13 eV by subtracting the width of He I UPS spectra from the excitation energy (21.22 eV).<sup>19</sup> Therefore, the binding energy difference between Ga 3d<sub>5/2</sub> and  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  VBM,  $(E_{\text{Ga}3d_{5/2}}^{\text{InGaAs}} - E_{\text{VBM}}^{\text{InGaAs}})$ , can be determined to be 25.15 eV. For the InP sample, the P 2p<sub>3/2</sub> CL peak was located at 128.60 eV, as Fig. 1(c) shows, and the leftmost was P 2p<sub>1/2</sub> at 129.43 eV. InP VB spectra were shown in Fig. 1(d), and the VBM was calculated to be -8.51 eV with the same method as that of the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  sample. So, the binding energy difference between P 2p<sub>3/2</sub> and InP VBM,  $(E_{\text{P}2p_{3/2}}^{\text{InP}} - E_{\text{VBM}}^{\text{InP}})$ , was determined to be 137.11 eV. The interfacial core level offset,  $\Delta E_{CL} = [E_{\text{Ga}3d_{5/2}}^{\text{InGaAs}}(i) - E_{\text{P}2p_{3/2}}^{\text{InP}}(i)]$ , was measured by XPS, as shown in Figs. 1(e) and 1(f). It was found that both the CL peak positions had different shifts towards the low binding energy direction, and Ga 3d<sub>5/2</sub> and P 2p<sub>3/2</sub> CL peaks were located at 16.97 eV and 128.50 eV, respectively. Therefore,  $\Delta E_{CL}$  was determined to be -111.53 eV. According to formula (1) and the measured values above, the VBO value was calculated to be 0.43 eV. The summary of the energy of the CL peaks measured by XPS and UPS is shown in Table I. Finally, the conduction band offset (VBO) can be determined by  $\Delta E_C = E_g^{\text{InP}} - \Delta E_V - E_{\text{In}_{0.82}\text{Ga}_{0.18}\text{As}}^g$ . Using the bandgap values  $E_g^{\text{InP}} = 1.35$  eV and  $E_{\text{In}_{0.82}\text{Ga}_{0.18}\text{As}}^g = 0.48$  eV,<sup>20</sup>  $\Delta E_C = 0.44$  eV



**FIG. 1.** (a) and (e) CL spectra of Ga 3d from  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  (1400 nm) and  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  (5 nm)/InP samples, respectively. (c) and (f) CL spectra of P  $2p_{3/2}$  from the InP (epi-ready substrate) and  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  (5 nm)/InP samples, respectively. The dashed lines mark the Ga  $3d_{5/2}$  and P  $2p_{3/2}$  CL peak positions for each sample. (b) and (d) VB spectra of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  (1400 nm) and InP (epi-ready substrate) measured by UPS, the intersections of the tangents with the baseline give the edges of the UPS spectra from which the UPS width is determined.

was obtained. Thus, the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  interface exhibits a type-I band structure, as shown in Fig. 2. The band alignment strategy depicted here for the lattice-mismatched  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  agrees with the results obtained by Waldrop *et al.*,<sup>8</sup> who also

derived a type-I band structure from the XPS data for the lattice-matched  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ .

As a further check on the results above, the VBO was also determined by the As 3d and P 2p CL peaks. Therefore,

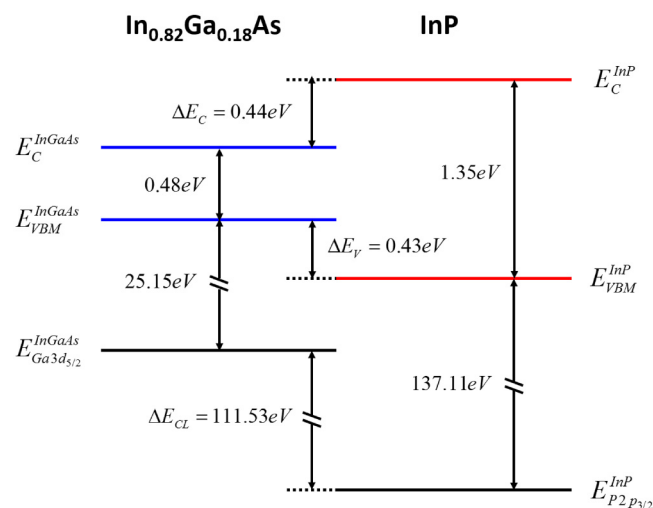
**TABLE I.** Binding energy of the XPS CL spectra fitting results; the VBM was obtained by the intersection between linear fitting to the leading edge of the VB spectrum and the background.

Samples	States	Binding energy (eV)
$\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$	Ga 3d <sub>5/2</sub>	17.02
	Ga 3d <sub>3/2</sub>	17.90
	Ga-As	18.80
	As 3d <sub>5/2</sub>	40.55
	As 3d <sub>3/2</sub>	41.25
	VBM	−8.13
InP	P 2p <sub>3/2</sub>	128.60
	P 2p <sub>1/2</sub>	129.43
	VBM	−8.51
$\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$	Ga 3d <sub>5/2</sub>	16.97
	As 3d <sub>5/2</sub>	40.48
	P 2p <sub>3/2</sub>	128.50

formula (1) now changes into

$$\Delta E_V = \Delta E_{CL} - (E_{\text{As}3d_{5/2}}^{\text{InGaAs}} - E_{\text{VBM}}^{\text{InGaAs}}) + (E_{\text{P}2p_{3/2}}^{\text{InP}} - E_{\text{VBM}}^{\text{InP}}), \quad (2)$$

where  $\Delta E_{CL} = [E_{\text{As}3d_{5/2}}^{\text{InGaAs}}(i) - E_{\text{P}2p_{3/2}}^{\text{InP}}(i)]$  is the binding energy difference between P 2p and As 3d CL of the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  interface. As shown in Fig. 3(a), the As 3d<sub>5/2</sub> CL peak is located at 40.55 eV. VB spectra of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  are shown in Fig. 3(b) and the VBM was calculated to be −8.13 eV. The interfacial CL offset was measured as shown in Figs. 3(c) and 3(d): the  $\Delta E_{CL}$  of −88.02 eV was deduced from As 3d<sub>5/2</sub> and P 2p<sub>3/2</sub> CL peaks, which were located at 40.48 eV and 128.50 eV, respectively. As a result, the



**FIG. 2.** Schematic band diagram for the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  interface; it presents a type-I straddling gap band structure; VBO and CBO are marked in the schematic.

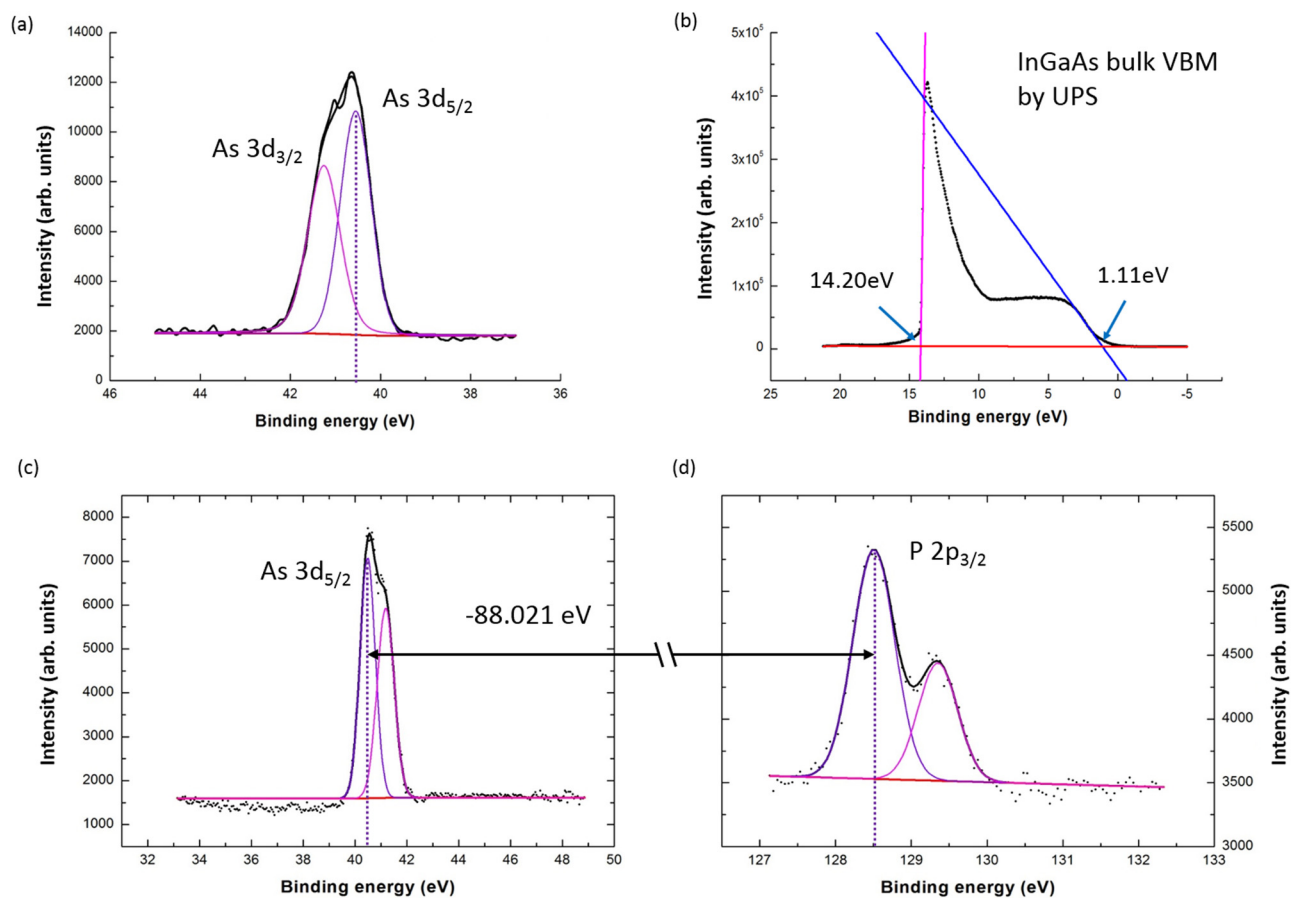
VBO is determined to be 0.41 eV, which is close to 0.43 eV obtained by using Ga 3d<sub>5/2</sub> and P 2p<sub>3/2</sub>, and the CBO is calculated to be 0.46 eV. A type-I band structure was also obtained.

## DISCUSSIONS

The determination of the band offset in semiconductor heterojunction systems should be made carefully, because the misfit strain caused by the lattice-mismatch may introduce a piezoelectric field, which could influence the measured values by XPS and lead to a wrong conclusion. In the process of the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  VBO determination, we did not take the misfit strain into account, while there was an almost 2% lattice-mismatch at the interface. Whether the misfit strain should be considered while determining the band offsets was a question that frequently cropped up.

Kraut used XPS to measure the VBO of the lattice-mismatched AlAs/InP by ignoring the misfit strain, and the obtained value of −0.27 eV was interpreted as being a characteristic of an unstrained interface.<sup>21</sup> Ding *et al.* investigated the band structure of the GaN/GaAs by synchrotron radiation photoelectron spectroscopy.<sup>3</sup> It is believed that the GaN's critical thickness is less than one atomic layer, and 1.8 nm is sufficient to relax the misfit strain. Therefore, the lattice-mismatch was ignored during the determination of the GaN/GaAs' VBO. The band offset of the InN/GaN heterostructure with a 12% lattice-mismatch was measured by XPS, and the author concluded that the piezoelectric field caused by the misfit strain at the interface is shielded by the high carrier density in InN.<sup>22</sup> Thus, the strain-induced piezoelectric effect was not considered. Zhang *et al.* also believed that the thin layers of InN on GaAs are perfectly relaxed, such that the misfit strain did not play a role in the investigation of the band offset.<sup>23</sup> Besides, the band bending effect was ignored as well. The influence of band bending and polarization on the measurement of valence bands was discussed by Xu *et al.*, and it was found that the measured VBOs display no evident discrepancy in the relaxed and the strained Al/Ga-polar AlN/GaN heterojunctions.<sup>24</sup> XPS was used to directly measure the VBO of PbSe/ZnO by Li *et al.*, and the estimated critical thickness of the PbSe film on ZnO demonstrated that a 5 nm PbSe is thick enough to be considered strain-relaxed, and therefore, the effect of the strain-induced piezoelectric effect can be ignored in the experiment.<sup>25</sup> As a result, any issues related to potential energy differences or non-idealities introduced at the interface should have a negligible effect on the VBO determination of PbSe/ZnO and therefore should be ignored.

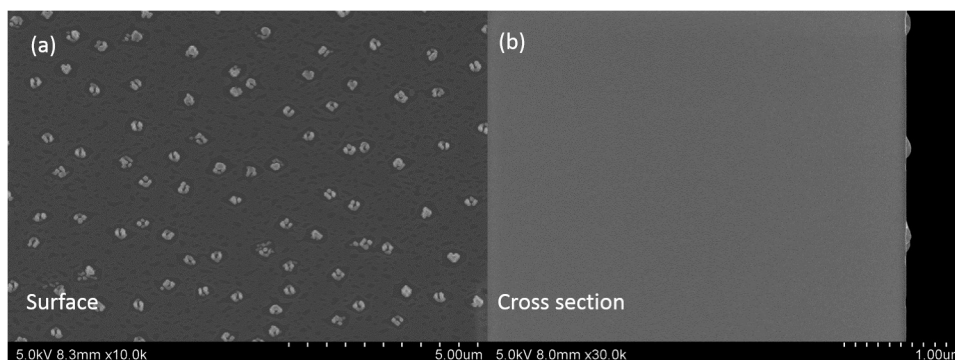
According to the previous analysis, we can conclude that if the misfit strain at the interface was perfectly relaxed, the strain-induced piezoelectric effect would be a negligible factor in band offset determination. Besides, the band bending effect, which could bend all of the energy levels by the same amount, occurs away from the interface. Thus, for the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  band offset determination, the band bending effect could be ignored, and what needs to be considered is the misfit strain relaxation at the interface. Figure 4(a) shows the surface morphology of the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  (5 nm) film with many white dots, and the cross-sectional image in Fig. 4(b) confirms the island-like crystals on the surface. The  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  epilayer shows an S-K mode growth at 650 °C, in which several strained atomic layers were deposited, with the constant being the same as InP, then followed by the 3D island growth in order to accommodate the misfit



**FIG. 3.** (a) and (c) CL spectra of As 3d<sub>5/2</sub> from In<sub>0.82</sub>Ga<sub>0.18</sub>As and In<sub>0.82</sub>Ga<sub>0.18</sub>As/InP, respectively. (d) CL spectra of P 2p<sub>3/2</sub> from In<sub>0.82</sub>Ga<sub>0.18</sub>As/InP. The dashed lines mark the As 3d<sub>5/2</sub> and P 2p<sub>3/2</sub> CL peak positions for each sample. (b) VB spectra of In<sub>0.82</sub>Ga<sub>0.18</sub>As measured by UPS.

strain caused by the lattice-mismatch. For majority determination of the band offset, the whole thin layer was always seen as the interface, so we regard the 5 nm In<sub>0.82</sub>Ga<sub>0.18</sub>As as the interface for analysis here.<sup>3,22–25</sup> It is commonly acknowledged that the strain is largely relaxed when it exceeds the critical thickness.<sup>22–25</sup> The formation of

islands is a sign of exceeding the critical thickness.<sup>26</sup> Obviously, the 5 nm In<sub>0.82</sub>Ga<sub>0.18</sub>As film in Fig. 4 has exceeded the critical thickness, and it is believed that the misfit strain has been largely relaxed. Therefore, the VBO values of In<sub>0.82</sub>Ga<sub>0.18</sub>As/InP obtained by ignoring the strain effect are reliable in terms of the analysis.



**FIG. 4.** (a) SEM image of the In<sub>0.82</sub>Ga<sub>0.18</sub>As (5 nm) thin film and (b) cross-sectional image of the In<sub>0.82</sub>Ga<sub>0.18</sub>As/InP heterojunction.

**TABLE II.** Spin split-off band energy, average valence band energy, and the deformation potential of GaAs, InAs, and InP.

Binary compound	$\Delta$ (eV)	$E_{V,av}$ (eV)	$a_v$ (eV)
GaAs	0.34	−6.92	1.16
InAs	0.38	−6.69	1.00
InP	0.11	−7.04	1.27

Since there are no previously reported experimental values for the VBO of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$ , it is useful to compare our measured values with what can be inferred from the theoretical calculations by others so that the accuracy could be verified. The band alignment for the  $\text{InP}/\text{In}_x\text{Ga}_{1-x}\text{As}$  heterostructures was estimated by People. On the basis of the full self-consistent interface calculation of  $\text{InAs}/\text{GaAs}$  VBO and band offset transitivity, the  $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{InP}$  VBO as a function of In content was estimated by the following formula:<sup>27</sup>

$$\Delta E_V = (0.191 + 0.282x)\text{eV}, \quad (3)$$

where  $x$  is the In content of  $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{InP}$ . There is a premise or hypothesis for this formula: the in-plane lattice constant,  $a_{\parallel}(\text{In}_x\text{Ga}_{1-x}\text{As}) = a_0(\text{InP})$ . We know that  $\text{In}_x\text{Ga}_{1-x}\text{As}$  shows an S-K growth mode, in which the atomic layer of  $\text{In}_x\text{Ga}_{1-x}\text{As}$  was deposited with a strained constant that was the same as that of the InP substrate. So, we used the formula carefully. Also, this linear interpolation was obtained by Waldrop *et al.*, in which the  $\text{In}_x\text{Ga}_{1-x}\text{As}$  lattice constant was assumed to match the InP.<sup>30</sup> For the similar  $\text{InGaAs}/\text{GaAs}$  heterostructure, the authors also indicate the linear relationship between the valence band and the In content.<sup>31</sup> For  $\text{InGaN}$  alloys, the author found that the dependence of the  $\text{InGaN}$  valence-band alignment on the In content is almost linear, and much of the nonlinearity is attributed to a downward bowing of the conduction band, not the valence band.<sup>32</sup> So, the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  VBO here was calculated to be 0.422 eV, which is in agreement with the experimental values 0.43 eV and 0.41 eV. Then, the CBO was deduced to be 0.448 eV.

Van de Walle and Martin's model solid theory (MST) was utilized to investigate the compositional dependence of the band edge alignment at the  $\text{Al}_x\text{Ga}_{1-x}\text{SbAs}/\text{InGaAs}$  and  $\text{Al}_x\text{Ga}_{1-x}\text{SbAs}/\text{InAlAs}$  heterointerfaces.<sup>28</sup> Similarly, MST was applied to the VBO estimation for  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  in the following. There are three main valence bands in a semiconductor: light-hole band, heavy-hole band, and spin split-off band; the average band energy of the three bands is defined as  $E_{V,av}$ . If the heterostructure is lattice-matched, the misfit strain does not exist at the interface, and the light-hole band edge and the heavy-hole band edge in the center of the Brillouin zone are degenerate in nature. The valence band energy will be  $E_V$ , namely, valence band edge:

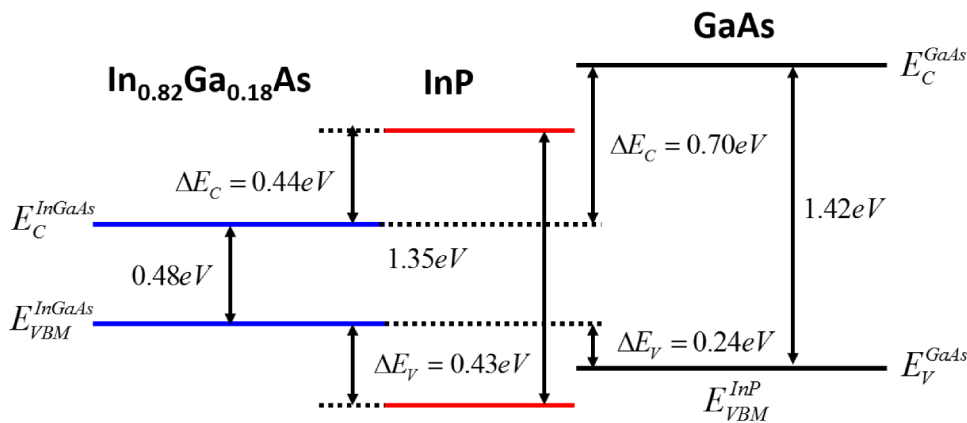
$$E_V = E_{V,av} + \frac{\Delta}{3}, \quad (4)$$

where  $\Delta$  is the spin split-off band energy and the conduction band edge  $E_C$  is obtained by  $E_C = E_V + E_g$ . For the  $\text{In}_x\text{Ga}_{1-x}\text{As}$  ternary alloy, the average valence band energy  $E_{V,av}$  is defined as

$$E_{V,av} = xE_{V,av}(\text{InAs}) + (1-x)E_{V,av}(\text{GaAs}) + 3x(1-x)[-a_v(\text{InAs}) + a_v(\text{GaAs})]\frac{\Delta a}{a_0}, \quad (5)$$

where  $a_v$  is the deformation potential,  $\Delta a = a(\text{InAs}) - a(\text{GaAs})$  is the lattice constant difference between InAs and GaAs, and  $a_0$  is the lattice constant of  $\text{In}_x\text{Ga}_{1-x}\text{As}$ , which is deduced from Vegard's law. The average valence band energy and the deformation potential of GaAs, InAs, and InP are listed in Table II.<sup>29,33</sup>

Substituting the parameters into Eq. (5),  $E_{V,av}(\text{In}_{0.82}\text{Ga}_{0.18}\text{As}) = -6.7266$  eV was obtained. The spin split-off band energy of  $\text{In}_x\text{Ga}_{1-x}\text{As}$  can be estimated to be  $\Delta(\text{In}_{0.82}\text{Ga}_{0.18}\text{As}) = 0.1243$  eV by linear interpolation from GaAs and InAs. As a result, the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  valence band edge of  $E_V(\text{In}_{0.82}\text{Ga}_{0.18}\text{As}) = -6.6023$  eV was determined by Eq. (4) under an ideal condition without strain. The InP valence band edge was also calculated to be  $E_V(\text{InP}) = -7.0033$  eV by using the parameters in Table II. If the misfit strain was ignored at the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  interface, the VBO was determined to be

**FIG. 5.** Schematic band diagram for the  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{GaAs}$  interface; it presents a type-I straddling gap band structure; VBO and CBO are marked in the schematic.

$\Delta E_V(\text{In}_{0.82}\text{Ga}_{0.18}/\text{InP}) = 0.401$  eV finally. The theoretical values are in agreement with the experimental results.

It has been noted that  $E_V$  has a transitive property, which means that if three heterojunction interfaces are formed from a group of three semiconductors A, B, and C,  $\Delta E_V$  is transitive if  $\Delta E_V(A/C) = \Delta E_V(A/B) + \Delta E_V(B/C)$ . That is, the summation of any two offsets will yield the third.<sup>8</sup>  $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$  with a high In content is a promising heterostructure in industrial applications because of its lower cost compared with  $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{InP}$ . The band structure of  $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$  is also important for device design and performance optimization. So, we roughly estimate the VBO of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{GaAs}$  through the transitivity. Using  $\Delta E_V(\text{GaAs}/\text{InP}) = 0.19$  eV reported by Waldrop *et al.*<sup>30</sup> and  $\Delta E_V(\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}) = 0.43$  eV obtained by XPS, the VBO and CBO of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{GaAs}$  were calculated to be  $\Delta E_V(\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{GaAs}) = 0.24$  eV and  $\Delta E_C(\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{GaAs}) = 0.70$  eV, respectively. The  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{GaAs}$  presents a type-I band structure, which is shown in Fig. 5.

## CONCLUSIONS

In summary, XPS and UPS have been used to measure the VBO of the lattice-mismatched  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$  heterojunction. The VBO was determined to be 0.43 eV by using Ga 3d and P 2p CL, which is in agreement with the value obtained from As 3d and P 2p CL. A type-I heterojunction forms between  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}$  and InP in the straddling configuration with a CBO of 0.44 eV. The VBO of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{GaAs}$  was estimated to be 0.24 eV by utilizing the band offset transitivity, and the interface also presents a type-I band structure that is similar to that of  $\text{In}_{0.82}\text{Ga}_{0.18}\text{As}/\text{InP}$ .

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