First-principles Study on As Antisites in InGaAs Alloys, GaAs and InAs

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INTRODUCTION

Due to the high electron mobility of III-V materials, they have been studied as a promising next-generation semiconductor material. However, if there are mid-gap defects, those significantly degrades the device performance. In particular, As antisite is a critical trap state which usually forms their states in the band gap. In this work, we perform first-principles study to rigorously calculate the defect energy level of As antisites in bulk structures of GaAs, InGaAs, and InAs. In addition, we evaluate the energy level while varying the ratio between In and Ga atoms in InGaAs alloys.

SIMULATION AND RESULT

III-V Bulk Structures. We perform density functional theory (DFT) simulations using SIESTA [1] on bulk structures of GaAs, InGaAs and InAs. We first optimize their lattice vectors in conventional unit cells (Fig. 1). We consider various InGaAs alloys such as $In_{0.25}Ga_{0.75}As$, $In_{0.5}Ga_{0.5}As$ and $In_{0.75}Ga_{0.25}As$ with randomly distributed In and Ga atoms. We apply the DFT-1/2 technique [2] to compensate for the fact that general DFT calculations underestimate the band gaps of semiconductor materials as shown in Fig. 2. The relaxed bulk structures with $2\times2\times2$ supercell of the conventional unit cells are obtained and their band structures are shown in Fig. 3. This shows that the band gap decreases as the ratio of In atoms to Ga atoms increases.

Modeling of As Antisite. We model an As antisite in various III-V materials such as GaAs, $In_{0.25}Ga_{0.75}As$, $In_{0.5}Ga_{0.5}As$, $In_{0.75}Ga_{0.25}As$ and InAs. To minimize the effects of a defect to the near cell, $2\times2\times2$ supercell with 64 atoms is used. Then we change an In or a Ga atom to an As atom (As_{In} and As_{Ga}, respectively.). Then we relax the structures with the defect (Fig. 4).

Analysis on As Antisite. As shown in Fig. 5, when compared to defect-free structure(Fig 5 (a)), the band structures of both As_{In} (Fig 5 (b)) and As_{Ga} (Fig 5 (c)) have a trap band, which is in the band gap (above the valence band). Also, it can be seen that the distribution of their density of states (DOS) is almost similar between the conduction band and the valence band (Fig 5 (d)). In the same way, we demonstrated the energy levels of As antisites (both As_{In} and As_{Ga}) in five materials (Fig. 6). For all cases, the energy levels of As antisites are located closer to the valence band than the conduction band. Also, in various InGaAs alloys, the energy level of As_{In} is higher than that of As_{Ga} but the difference of them decreases as the ratio of In atom increases.

CONCLUSION

We performed first-principles simulations for As antisites in several III-V materials. The results show the energy level difference between As_{In} and As_{Ga} is larger in $In_{0.25}Ga_{0.75}As$ than that in $In_{0.75}Ga_{0.25}As$. However, an important finding is that As antisites form a mid-gap state for all the cases we experimented. This means As antisites have the potential to have a fatal effect on device performance by causing leakage current.

REFERENCES

[1] Soler, et al., *"The SIESTA method for ab initio order-N materials simulation."* Journal of Physics: Condensed Matter (2002).

[2] Ferreira, et al., *"Approximation to density functional theory for the calculation of band gaps of semiconductors."* Physical Review B (2008).

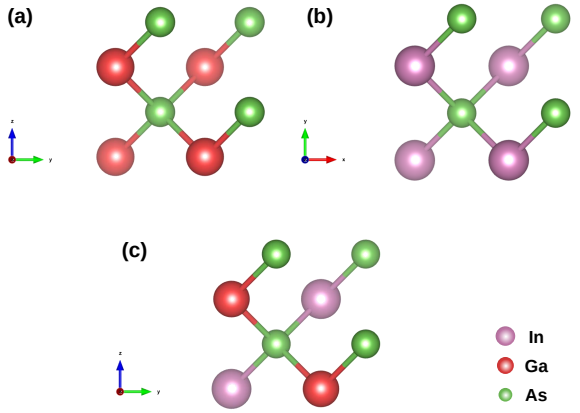

Fig. 1. Atomic structures of conventional unit cells of (a) GaAs, (b) InAs (c) $In_{0.5}Ga_{0.5}As$.

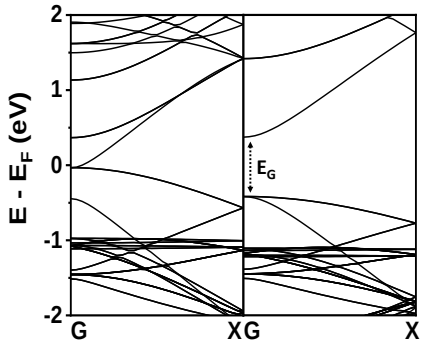

Fig. 2. Band structures of (left) $In_{0.5}Ga_{0.5}As$ and (right) $In_{0.5}Ga_{0.5}As$ with DFT-1/2 technique. E_G is the band gap.

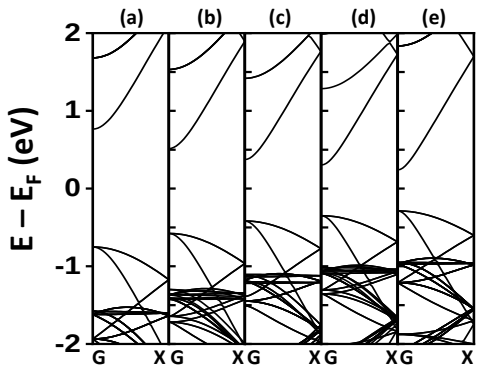

Fig. 3. Band structures of (a) GaAs, (b) $In_{0.25}Ga_{0.75}As$, (c) $In_{0.5}Ga_{0.5}As$, (d) $In_{0.75}Ga_{0.25}As$ and (e) InAs.

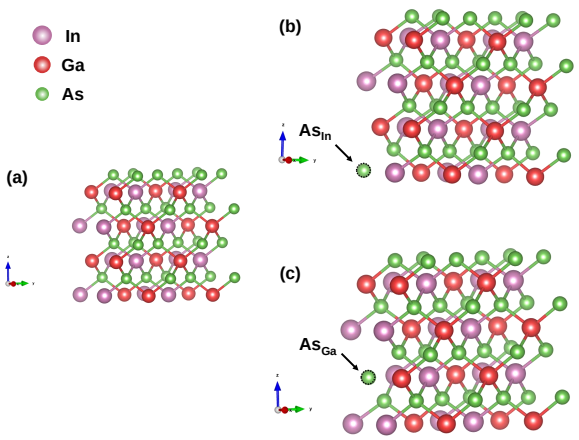

Fig. 4. Relaxed atomic structures of (a) defect-free, (b) w/ As_{In} and (c) w/ As_{Ga} in $In_{0.5}Ga_{0.5}As$.

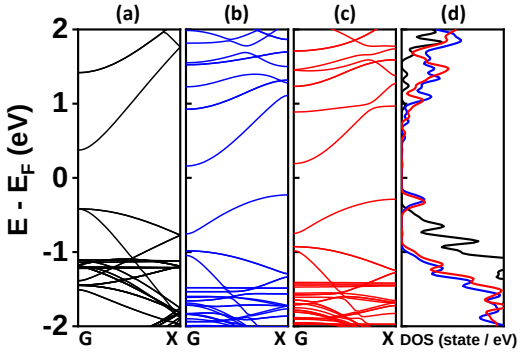

Fig. 5. Band structures of $In_{0.5}Ga_{0.5}As$ (a) defect-free, (b) w/ As_{In} ,(c) w/ As_{Ga} and (d) their density of states (DOS).

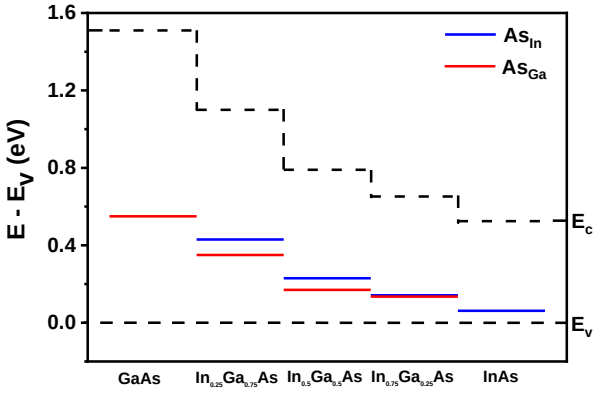

Fig. 6. Charge transition levels of As antisites in various InGaAs alloys.