

Nitrogen passivation and Chemical Trends of Defects at Al₂O₃:GaAs/InAs/InP/GaSb Interfaces

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1. Introduction

The III-V compound semiconductors GaAs, InAs, InP and GaSb are promising high mobility channel materials for advanced metal-oxide-semiconductor field-effect transistors (MOSFETs) [1-4]. The use of III-Vs in MOSFETs has been hindered by our inability to properly passivate their surfaces so that the Fermi level could be moved freely across the whole band gap. Further development of III-V MOSFETs requires a better understanding of defects at the dielectric:semiconductor interface [2,4,5] and how to passivate them. Here we calculate the chemical trends of various intrinsic interfacial defects of InAs, InP and GaSb compared to GaAs using ab-initio methods [6].

We also find that Nitrogen is a very effective passivant because the interfacial configurations that are proposed to form gap states [1] such as As-As dimers, As dangling bonds (DBs) or some As-O bonds are unstable or do not produce gap states when As atoms are replaced by N.

2. Calculation and Results

Fig. 1 shows the relaxed atomic structure at the defect-free Al₂O₃:GaAs (100) interface. All interfaces are built to satisfy the electron-counting rule and suppress the quantum confinement effects. To obtain band offsets without the DFT band gap problem, we use the sX hybrid functional to calculate band structures. We consider various defects such as like-atom bonds (dimers), dangling bonds (DBs), and Ga or As sites with the wrong number of oxygen neighbors. We also varied electron occupancies of DB and dimer states, which can bring states into the gap.

Fig 2b,c shows the relaxed atomic structure and defect state for the Ga DB, when it is empty or filled with 1 electron. In GaAs, the Ga DB energy level lies outside the gap for an empty DB, Fig 2a. When partly occupied, the DB state comes into the gap, because the Ga bond angle relaxes towards pyramidal. Taking the transition state as mid-way between the level for empty and part-filled case, then it lies above the conduction band minimum (CBM). Fig 3a shows the As DB state on HfO₂: GaAs(110). A similar defect occurs on (100). For the filled DB, the state lies below the VB edge, Fig 3b. When partly empty, the As site becomes flatter, and this state rises into the gap at +0.2 eV (not shown), causing gap states. There is similar behavior of As or In DBs in all the III-Vs.

Fig 4 shows the interfacial anion dimers for GaAs, InAs, InP and GaSb. For GaAs, the As dimer antibonding state

σ^* lies near the CBM, Fig 4d. If filled by 1 electron, the bond weakens, and the state drops into the gap. In InAs, the As-As σ^* state lies at the same energy as in GaAs - well above InAs's CBM. For InP, the P-P bond is stronger, so its σ^* state lies well above the CBM. In GaSb, the Sb-Sb bond is weaker, but with the small band gap of GaSb, the Sb-Sb σ^* state is also above the CBM. This confirms the trends derived earlier based on tight-binding [6,7]. Therefore in InAs, InP, and GaSb the dimer antibonding states are all above the CBM (Fig 5) and do not contribute to Fermi level pinning. These states do become important if E_F enters the CB under strong drive [8]. The absence of gap states for InP explains why InP capping layers are beneficial [9].

If the last layer of As in the III-V is replaced by nitrogen, by an MOCVD process or plasma nitridation, this causes a substantial change in behavior. III-N bonds are stronger and more ionic than the equivalent III-As bond. On the other hand, N-N single bonds are less stable than P-P or As-As bonds. We find that N-N dimers are unstable and will not form (Fig 6). Any N excess on the surface will not form dimers. The nitrogens instead form pyramidal 3-fold sites with N states well below the VB top, leaving no states in the gap or near the CB edge. Similarly, N dangling bond sites give states well below the VB edge. This removes two of the main sources of possible gap states, anion dimers and anion dangling bonds.

Direct Ga-N or Al-N bonds are very stable due to the higher ionicity than Ga-As bonds, giving a larger local band gap. Only certain types of N-O bonds are stable.

Thus, our results suggest that N passivation with metal first ALD is a good combination to form a well passivated III-V -oxide interface. It could be used as an alternative to InP-capped quantum well channel as used by Radosavljevic et al [9]. It might be more controllable than S or Si passivation.

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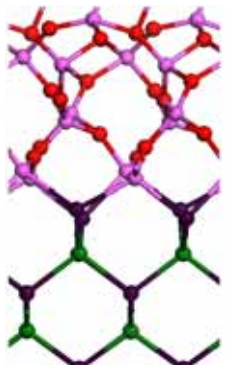


Fig. 1(a). Relaxed structure of Al-terminated Al_2O_3 :GaAs(100) interface

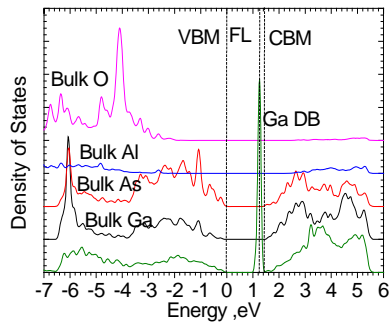


Fig. 2a PDOS of empty Ga dangling bond at Al_2O_3 :GaAs(100) interface.

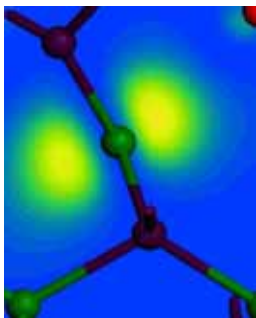


Fig 2b Relaxed atomic structure of empty Ga dangling bond at Al_2O_3 :GaAs(100).

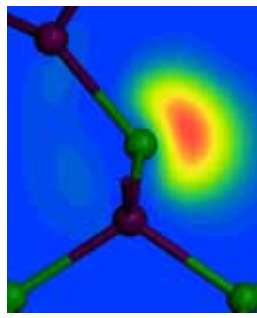


Fig 2c Relaxed structure of half-filled Ga dangling bond at Al_2O_3 :GaAs(100).

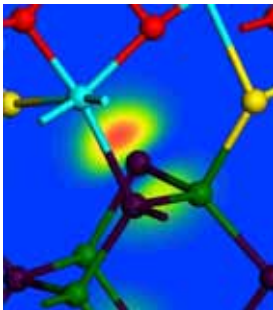


Fig 3a As dangling bond state at HfO_2 :GaAs(110)

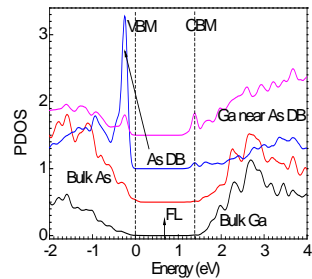


Fig 3b PDOS of As DB at HfO_2 :GaAs(110)

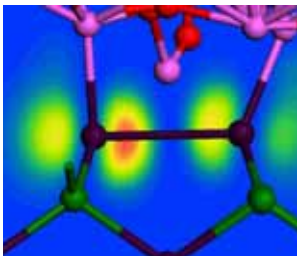


Fig 4a. Empty As-As antibonding state at Al_2O_3 :GaAs (100)

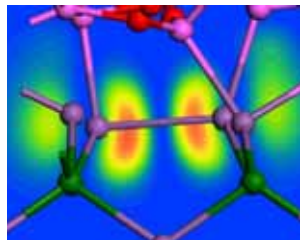


Fig 4b P-P anti-bonding state at Al_2O_3 :InP (100)

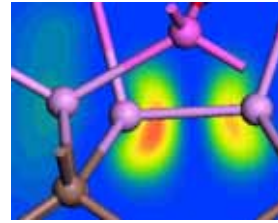


Fig. 4c Sb-Sb anti-bonding state at Al_2O_3 :GaSb (100)

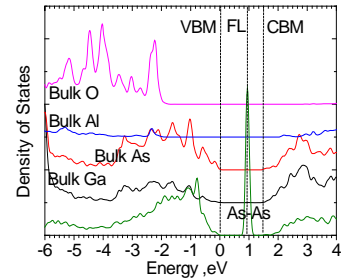


Fig 4d PDOS of As-As part filled antibonding state at Al_2O_3 :GaAs(100)

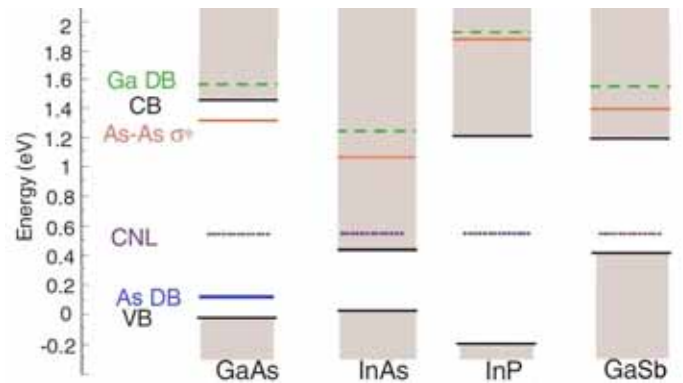


Fig 5. Alignment of empty Ga/In DBs and P-P/As-As/Sb-Sb anti-bonding levels in respect to GaAs, InAs, InP and GaSb band edges.

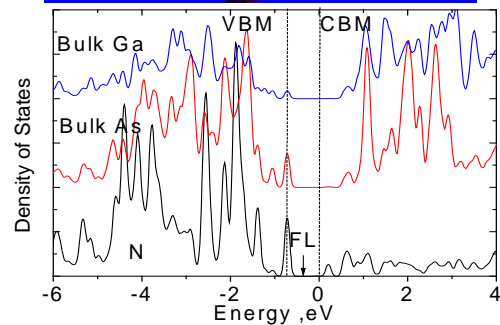
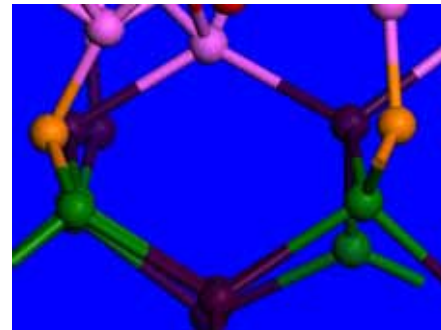


Fig 6. N-N dimers are unstable at Al_2O_3 :GaAs (100), forming 3-fold N sites. The PDOS shows no state in the GaAs gap