



Understanding of the Bonding Configurations at SiC/III-V Semiconductor Interfaces

by Zheng Jin-Cheng, Wang Hui-Qiong, A.T.S. Wee and C.H.A.Huan Dept of Physics

"...The other important effect comes from band-structure components. When the bonding configuration is unfavorable, localized interface states occur in the main band gap, pushing the Fermi level up and causing the bands to shift upward..."

There has been increasing interest in silicon carbide (SiC) due to its favorable electronic properties, extreme elastic and thermal properties. The technological realization of self-aggregating wires and quantised homostructures make it one of the most promising materials for nanodevices, microelectronics, sensors, and high-power, high-temperature devices. An understanding of the SiC/substrate interface is important for the growth of high quality SiC films.

In this study, the linear-muffin-tin-orbital (LMTO) band structure method and local-density-functional (LDA) theory are used to study the bonding configuration between SiC and 16 III-V semiconductors. The supercell approach is employed to calculate the total energies, electronic structures and properties of SiC/(III-V) superlattices, and to compare two different bonding configurations, i.e. Si-V and C-III for Model A, and Si-III and C-V for Model B, as shown in Fig 1. Most calculations are performed on the Cray J916 and SGI Origin 2000 at the Computer Center, National University of Singapore.

Normally, the stable bonding configuration at the interfaces between SiC and many III-V compounds is through Si-V and C-III, where III-V = BN, AlN, AlP, AlAs; GaN, GaP, GaAs; InN, InP, InAs, InSb. However, for some other III-V, our results show a preference to form the surprising "anomalous" Si-V & C-III (model A) bonding configuration at the SiC/III-V interface. We note that the SiC/(III-V) formation energy of model A increases, while that of model B decreases, as the group V element descends from "N" to "Sb". The same trend is observed in the energy difference between models A and B, as shown in Fig 2 (a). Our predictions of different bonding configurations at SiC/III-V (001) interfaces significantly change the growth of SiC thin film on III-V (001) substrates and vice versa.

The origin of stable bonding configurations can be explained in terms of the ionicity of III-V semiconductors, electrostatic effects, charge distribution and band-structure component. For electrostatic effects, the cation-anion bonding is expected to preside at bonding configuration for SiC/(III-V) interfaces. The charge distributions of III-V semiconductors reflect their ionicity and clearly relate to the bonding configurations, as shown in Fig 2 (b). We note that in SiC, Si acts as the cation (+1.166 lel positive charge) and C as the anion (-1.166 lel negative charge)



Zheng Jin-cheng



Wang Hui-qiong



A/P A.T.S Wee



A/P C.H.A Huan

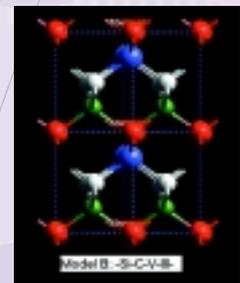
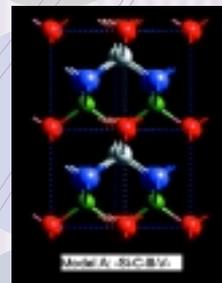


Figure 1: Two different bonding configurations.

because lower valence levels are associated with the carbon atom. From electrostatic arguments, cations prefer to bond to anions at the interface between two compounds. The charge distribution in III-V semiconductors is clearly consistent with the predicted bonding configurations at the SiC/(III-V) interface except in the case of III-V = InSb.

The other important effect comes from band-structure components. When the bonding configuration is unfavorable, localized interface states occur in the main band gap, pushing the Fermi level up and causing the bands to shift upward. For example, SiC/BN with favorable bonding configuration (Si-N, C-B) shows semiconductor characteristics, while the unfavorable model (Si-B, C-N) exhibits anomalous metallic properties.

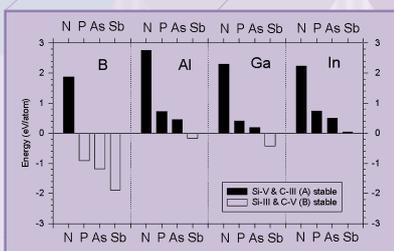


Figure 2a: Energy Difference.

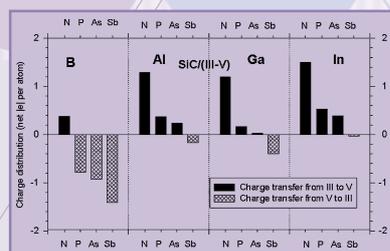


Figure 2b: Charge Distribution.