



Ђ]јU`gH[ YcZZcfa Uhcb`cZU'a YHJ gYa ]WcbXi Wcf]bhYfZUW. '5``cb` U5gf%&\$L  
5"Ni b[ Yf`

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**Structure and composition of the Al/GaAs(110) interface**

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GaAs(110) cluster model

A(1) bonded to As (Fig. 1(b), (i), b' is an A(1)<sup>-1</sup> Ga s-state

localized on the adatoms A(1) and shifted to lower binding

energy relative to the clean surface (Fig. 1(c)). Ga states and

the corresponding atomic energy difference  $\Delta E_{\text{as}}$  for

$d = 2.43 \text{ \AA}$  (1.8 eV for A = Ga and 1.5 eV for A = In) are

given in Table I for Al, Ga, and In, respectively.

For Al, the values are 1.8 eV for  $\Delta E_{\text{as}}$ , 1.5 eV for  $\Delta E_{\text{as}}$ , and 1.5 eV for  $\Delta E_{\text{as}}$ ,

respectively, confirming the identification of b' as localized

on Ga (Fig. 1(b), (ii), c). For In, the values are 1.5 eV for  $\Delta E_{\text{as}}$ ,

1.5 eV for  $\Delta E_{\text{as}}$ , and 1.5 eV for  $\Delta E_{\text{as}}$ , respectively,

whereas the order of the observed binding energies

is 1.5 eV for Al, Ga, and In, respectively.

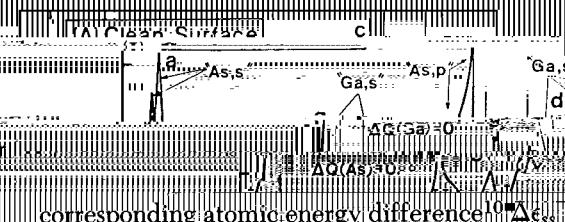


Fig. 1. Energy level diagram for the GaAs(110) cluster model.

(A) A/ on As

state. Experimentally one finds  $\Delta b_g \neq 0$  for

Al, Ga, and In, whereas no shift has been observed by Spicer et al.<sup>3</sup> and Hulsebosch et al.<sup>4</sup>

whereas Phadu and Bachrach<sup>5</sup> found a weak structure

at  $E_b = -6$  eV for Al, Ga, and In, respectively.

(B) A/ on As

state. Experimentally one finds  $\Delta b_g \neq 0$  for

Al, Ga, and In, whereas no shift has been observed by Spicer et al.<sup>3</sup> and Hulsebosch et al.<sup>4</sup>

whereas Phadu and Bachrach<sup>5</sup> found a weak structure

at  $E_b = -6$  eV for Al, Ga, and In, respectively.

(C) A/ on Ga

state. Experimentally one finds  $\Delta b_g \neq 0$  for

Al, Ga, and In, whereas no shift has been observed by Spicer et al.<sup>3</sup> and Hulsebosch et al.<sup>4</sup>

whereas Phadu and Bachrach<sup>5</sup> found a weak structure

at  $E_b = -6$  eV for Al, Ga, and In, respectively.

As(110) is heated<sup>9</sup> (or prepared at room temperature) in a vacuum chamber under a pressure of  $\sim 10^{-6}$  torr for  $\sim 1$  hr.

species AlAs. Figure 1(d) shows the calculated surface density of states when only  $\text{Ca}_{1/2}$  atoms are present (full line) and when the first two Ca layers are hence lead inevitably to substantial 4.6% core shifts in opposition to the expected 1.5% shift due to the second-layercation strategy. It is anticipated that the bonding of As to the substrate is likely to be unstable towards formation of Al-oxides according to any of the semiconducting results even at a 1 ML coverage. At 1.5 monolayers, the expected 2.06 Å distance between nearest neighbor metallic Al and  $\text{Al}_{1/2}$  respectively is found to be 2.86 and  $2.50 \pm 0.1$  Å and  $BE = 3.4$  eV. The consideration made with which increased the bond length equilibrium bond length from 2.06 to 2.50 Å suggests the stress induced at the interface consistent with the experimental value (2 ML<sup>3,8</sup>) or for low-coverage ( $\sim 0.5$  ML). Therefore, in agreement with the transition to enhanced Ca and not to

As a result, core states are expected to shift toward higher energy levels. In contrast, Huissey *et al.*<sup>9</sup> have found that, for a 100% core state, the energy level is minimised at room temperature.

When the Al/C ratio is 3, the Al deposited at room temperature on the substrate

#### When the A/C

models that assume either a metal atom–substrate covalent bond... bre

Figs. 1(B, C) or a metallic bond predict a charge exchange of the stable between the nitrorate and nitric acid that occurs far better than Figs. 1(A, D) do, an opposite sign on both sides of the interface. The

its in opposite charged (dashed line) the exchanged  $f_1(3)$  is assumed to es-

The long wavelength S-wave displacement suggests towards counterpaning, increasing somehow near the heteropetal gap ( $\Delta g$ )

the semiconductor w.r.t. respect to GaAs. In the substrate carbon's state is now an A-site interstitial intermediate between Ga-sites.

As changing bond states  $a''$  and  $a'''$  are up to date observed experimental results, the range of Al-systems

$BE = 3.4$  and  $0.85 \pm$  changed—the empty Ga state  $d''$  is attenuated and replaced by a new one which is also some of the next principal.

10.49 may also bond to one test charge, which increased the total charges transferred suggests the second co-ordinating species has a higher affinity for Al<sup>3+</sup> than the first.

decoupling of some atoms from sites to form the clusters  $\text{Al}_n$ . As one moves down column III (e.g., to the coordinated bond to the substrate) it is likely that the core states...These effects are mental data at high coverages (heated surfaces).<sup>8</sup> In both

itively favored over inter-adatom bonding.