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Initial stage of formation of a metal–semiconductor interface: Al on GaAs(110)

A. Zunger

Image formation of a metal-semiconductor interface: Al on GaAs(110)

A. Zunger

Solar Energy Research Institute, Golden, Colorado 80401

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GaAs(110) cluster model

A(I) *bonded to As* Fig. 1(b): (i) b' is an A(I) Ga s-state localized on the adatoms A(I) and shifted to lower binding energy relative to the clean surface [Fig. 1(a)] Ga states and

[illegible] Theoretical values: 2.5 eV for A_I = Al (d = 2.43 Å), 1.8 eV for A_I = Ga[3] and 1.5 eV for A_I = In.[5] The corresponding atomic energy difference [illegible]

spectively, confirming the identification of b' as localized [illegible] state. Experimentally one finds $\Delta_{b'g}$ to be [illegible] eV for In [illegible] shift has been observed by Spicer *et al.*[7] and Hollis [illegible] eV ($\Delta_{b'g} \simeq 1.5$ eV) which was not reproduced [illegible] whereas Chadi and Bachrach[3] found a weak structure [illegible] at E_b = −6 riments. However, even if experimentally [illegible] in the other ex the order of the observed binding energies [illegible] $\Delta_{b'g} \neq 0$ for A

As(110) is heated[9] (or prepared at room ... for ~1/3 ML of Al deposited at room temperature, the substrate ... When the Al/G

... and Al is exchanged for the substrate Ga to form layers ... models that assume either an adatom–substrate covalent bond ...

species AlAs. Figure 1(d) shows the calculated ... or a metallic bond predict a charge exchange ... of the stab

... between the substrate and ...

... an opposite sign on both sides of the interface. ...

hence lead inevitably to (substantial[4,6]) core shifts in opposite ... changed (dashed line); the exchanged Ga is assumed to es-

... counterpart, increasing somewhat the heteropolar gap ...

ed ... d(Al–Al) = 2.86 and 2.50 ± 0.1 Å and BE = 3.4 and 0.85 ± ... changed—the empty Ga state d''' is attenuated and repla

consistent with the experi- ... will induce decoupling of some atoms from sites to form the ... As core states. These effects a

2 ML[3,8]) or for low-coverage ... stabler clusters Al_n. As one moves down column III (e.g., to ... mental data at high coverages (

... In, Tl) ...

... be initially favored over inter-adatom bonding ... 4 that these results pe