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Identity of the conduction-band minimum in $(AlAs)_1/(GaAs)_1$ (001) superlattices: Intermixing-induced reversal of states

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First-principles pseudopotential calculations on the (001) $(AlAs)_1/(GaAs)_1$ superlattice (SL) shows that *partial* intermixing of the Al and Ga atoms relative to the abrupt case lowers its formation energy, making this SL even stabler at low T than the fully randomized $Al_{0.5}Ga_{0.5}As$ alloy. Concomitantly, the conduction-band minimum (CBM) reverts from the GaAs L-derived state, to the X^{xy}-derived AlAs state. The previously noted discrepancy between theory (pertinent to abrupt SL's and yielding an L-derived CBM) and experiment (yielding an X^{xy}-derived CBM) is therefore attributed to insufficient interfacial abruptness in the samples used to date in experimental studies.

The recent perfection of atomic-scale control over nucleation and growth has made possible laboratory synthesis of $(AC)_p/(BC)_p$ superlattices (SL's) with periods p in the 1–3 monolayer regime. These systems exhibit a number of spectroscopic features that are not predicted by effective-mass and particle-in-a-box models, which retain only the kinetic energy of the particles, but neglect explicit potential energy (i.e., band-structure) effects. Band-structure calculations predict that the $p=1$ [001] AlAs/GaAs SL has two unexpected features: (i) The $\bar{\Gamma}_{1c}$ conduction state has a *lower* energy than that of the $p=2$ SL.[1] Kinetic-energy confinement arguments predict a monotonic decrease of energy with increasing SL size, i.e., $\bar{\Gamma}_{1c}$ should be higher in the $p=1$ SL than in the $p=2$ SL. (ii) The L_{1c} state of the $Al_{0.5}Ga_{0.5}As$ alloy is predicted[1–9] to split by ~ 1 eV in the $p=1$ SL. This makes the L_{1c}-derived state the conduction-band minimum (CBM) —even though L_{1c} is 0.3 eV above X_{1c} in the alloy. The L_{1c}-derived state of the SL is also predicted to exhibit conduction-band localization, even though the effective masses and barrier heights are small.[10] Prediction (i) has been confirmed experimentally.[11,12] But, in recent experiments, Ge and co-workers[13] showed that the CBM behaves like an X-derived state, in contradiction with prediction (ii). In this paper we show that although the experimental results conflict with the theoretical predictions for the *abrupt* SL, they agree well with the theoretical predictions for an SL in which the layers are *partially intermixed*. We show that intermixing lowers the SL formation energy, while preserving the [001] SL diffraction spots. In what follows we first describe the symmetry and the folding of the SL states, then the theoretical predictions for the ordering of these states and the discrepancy with the ordering deduced from experiment. Finally, we present our theoretical results for partially intermixed SL's. We conclude that currently available SL samples may be insufficiently ordered to exhibit the spectroscopic level sequence of an atomically abrupt SL.

SYMMETRY CONSIDERATIONS

The first two columns of Fig. 1 show how the energy levels of the $Al_{0.5}Ga_{0.5}As$ alloy (shown in angular brackets) are predicted to evolve into the $p=1$ (001) SL energy levels. Denoting SL states by an overbar, followed by the zinc-blende states from which they originate in parentheses, the basic symmetry compatibility relations are

$$\langle X^{x,y,z}_{1c}\rangle \rightarrow \bar{M}_{5c}(X^{x,y}_{1c}) + \bar{\Gamma}_{4c}(X^{z}_{1c}), \quad (1)$$

$$\langle L_{1c}\rangle \rightarrow \bar{R}_{1c}(L_{1c}) + \bar{R}_{4c}(L_{1c}), \quad (2)$$

$$\langle X^{z}_{3c}\rangle + \langle \Gamma_{1c}\rangle \rightarrow \bar{\Gamma}^{(1)}_{1c}(\Gamma_{1c}+X^{z}_{3c}) + \bar{\Gamma}^{(2)}_{1c}(\Gamma_{1c}+X^{z}_{3c}). \quad (3)$$

Their symmetry properties will now be explained.

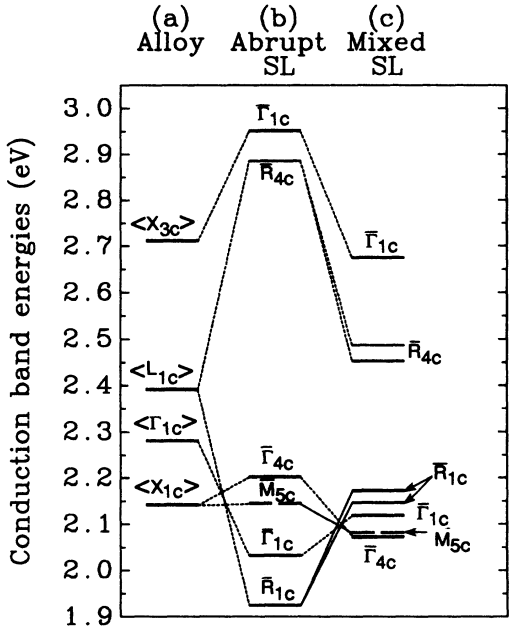

FIG. 1. Calculated (LDA and spin-orbit corrected) energy levels of (a) the bulk $Al_{0.5}Ga_{0.5}As$ alloy [from the virtual crystal approximation (Ref. 3)], (b) the abrupt (001) $(AlAs)_1/(GaAs)_1$ superlattice, and (c) the $\frac{1}{3}$ intermixed superlattice with a (3×1) interfacial unit cell. The X_3-derived $\bar{M}_{1c}$ and $\bar{M}_{2c}$ levels are not shown. The intermixed SL actually used has lower symmetry than the abrupt SL, but the symmetry labels of the abrupt case are retained for clarity.

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X_{1c}-folded states [Eq. (1)]

Of the three degenerate x,y,z zinc-blende X_{1c} valleys, X^x_{1c} and X^y_{1c} (whose $\mathbf{k}$ vectors lie in the SL plane) fold in the SL into the doubly degenerate $\bar{M}_{5c}(X^{x,y}_{1c})$ state, while X^z_{1c} (whose $\mathbf{k}$ vector is in the growth direction) folds into the "pseudodirect" $\bar{\Gamma}_{4c}(X^z_{1c})$ state. Since the members of the X_{1c}-folded states $(\bar{M}_{5c}+\bar{\Gamma}_{4c})$ have different symmetries and $\mathbf{k}$ vectors, they do not interact. Both states have cation-pd and anion-s character, with zero cation-s character.

L_{1c}-folded states [Eq. (2)]

The four zinc-blende L_{1c} valleys at $k=2\pi/a$ $(\frac{1}{2}, \pm\frac{1}{2}, \pm\frac{1}{2})$ fold into the $p=1$ SL states $\bar{R}_{1c}$ and $\bar{R}_{4c}$. These states have different point symmetries, and hence cannot interact. $\bar{R}_{1c}$ is a (Ga-s)+(As-s) state with zero s character on the Al site, while the complementary $\bar{R}_{4c}$ state has (Al-s)+(As-s) character with zero s character on the Ga site. Since the $\bar{R}_{1c}$ wave function is commensurate with the Ga-s component of the potential whereas $\bar{R}_{4c}$ is commensurate only with the Al-s component, the $\bar{R}_{1c}-\bar{R}_{4c}$ energy splitting reflects the potential difference $V_s(\mathrm{Ga})-V_s(\mathrm{Al})$ and oscillates with the period p. Hence, while the L_{1c} alloy wave function "sees" the *average* of the cation-s potentials (so the alloy state is extended on both sublattices), in the $p=1$ SL there is a symmetry-mandated segregation of the amplitude of the L_{1c}-derived wave functions into distinct atomic sublattices: $\bar{R}_{1c}$ on GaAs and $\bar{R}_{4c}$ on AlAs. Since this feature depends sensitively on symmetry, we will see below that it also depends on the degree of atomic abruptness at the SL interface.

Γ_{1c} and X_{3c}-folded states [Eq. (3)]

The zinc-blende X^z_{3c} state folds into the SL $\bar{\Gamma}$ point, creating there a $\bar{\Gamma}^{(2)}_{1c}$-type state. Since it has the same symmetry representation as the original zinc-blende Γ_{1c} state, we now have a pair of *equal-symmetry* members $\bar{\Gamma}^{(1)}_{1c}$ and $\bar{\Gamma}^{(2)}_{1c}$. By symmetry, both $\bar{\Gamma}_{1c}$ states have zero p character on the cations. Unlike the "segregating states," these "repelling states" can interact (hence repel) each other. This repulsion depresses $\bar{\Gamma}^{(1)}_{1c}$. As the repeat period p increases, this repulsion diminishes; hence, the nonmonotonic behavior of $\bar{\Gamma}^{(1)}_{1c}$ with p.

CALCULATED ENERGY LEVELS

While symmetry considerations provide specific relations between the atomic structure and the character of the ensuing states, assessment of the actual level ordering requires a quantitative calculation of the coupling with the self-consistent potential. This was done here by calculating the SL band structure using the first-principles nonlocal pseudopotential approach within the local-density approximation (LDA), avoiding effective-mass approximations. Careful convergence tests[14] assured an internal precision of 0.05 eV; spin-orbit corrections and corrections to the LDA were carried out[14] as described by Dandrea and Zunger[3] and Wei and Zunger.[1] The calculated energies of the abrupt SL are within 0.06 eV of the quasiparticle calculation of Zhang *et al.*[5] The results for the abrupt SL [Fig. 1(b)] display the following trends:

(i) The $\bar{R}_{1c}$ and $\bar{R}_{4c}$ states are strongly localized on the GaAs and AlAs sublattices, respectively, and accordingly the level splitting $E(\bar{R}_{4c})-E(\bar{R}_{1c})\simeq V_s(\mathrm{Al})-V_s(\mathrm{Ga})$ reflects the $\sim$1-eV atomic energy difference between Al, s and Ga, s. This large $\bar{R}_{1c}-\bar{R}_{4c}$ splitting makes $\bar{R}_{1c}$ the CBM, in spite of the fact that in the alloy the $\langle L_{1c}\rangle$ state, from which $\bar{R}_{1c}$ is derived, is about 0.3 eV above $\langle X_{1c}\rangle$ [Fig. 1(a)]. This result was found in a number of first-principles calculations, e.g., pseudopotential calculations by Bylander and Kleinman,[7] Srivastava and co-workers,[6] Dandrea and Zunger,[3] Wood, Wei, and Zunger,[2] and Nakayama and Kamimura;[4] all-electron calculations of Wei and Zunger[1] and Gopalan, Christensen, and Cardona,[8] and the quasiparticle calculations of Zhang *et al.*[5] The non-self-consistent local empirical pseudopotential calculations of Gell *et al.*[15] and Andreoni and Car[16] are not accurate enough to capture this effect; they result in other CBM symmetries, in contrast with all first-principles calculations.

(ii) The far smaller splitting between the atomic p energy levels (as opposed to the s levels) of Al and Ga results in a small $(0.06\pm0.05$ eV) $\bar{M}_{5c}(X^{xy}_{1c})-\bar{\Gamma}_{4c}(X^z_{1c})$ splitting in the SL. Like the parent zinc-blende X_{1c} state, these superlattice states are delocalized in the interstitial volume *between* atoms.[2] The dominance of potential over kinetic-energy effects is highlighted here by the fact that the X^z-derived $\bar{\Gamma}_{4c}$ state is *above* the X^{xy}-derived $\bar{M}_{5c}$ state despite the fact that kinetic-energy arguments[17] would place the heavier (longitudinal) mass X^z state *below* the lighter-mass X^{xy} state.

(iii) The repelling $\bar{\Gamma}^{(1)}_{1c}$ and $\bar{\Gamma}^{(2)}_{1c}$ states are localized, respectively, on the GaAs and AlAs sublattices. The large (0.9 eV) splitting between them places $\bar{\Gamma}^{(1)}_{1c}$ below $\bar{M}_{5c}$. Since the Γ_{1c}(GaAs)-X^z_{3c}(AlAs) coupling that determines this splitting [Eq. (3)] diminishes as the GaAs-AlAs layers become spatially separated, the splitting is reduced in the $p=2$ SL. This causes $\bar{\Gamma}^{(1)}_{1c}$ of the $p=2$ SL to lie *above* $\bar{\Gamma}^{(1)}_{1c}$ of $p=1$. This nonmonotonicity of energy *versus* p contrasts with the simple monotonic decay with p anticipated from kinetic-energy (e.g., Kronig-Penney) models.

EXPERIMENTAL ASSIGNMENT OF LEVELS

Spectroscopic studies are able to clearly distinguish between the X^z-derived $\bar{\Gamma}_{4c}$ state and the X^{xy}-derived $\bar{M}_{5c}$ state. Because the $\bar{M}_{5c}(X^{xy})$ state is indirect, it exhibits a slow photoluminescence (PL) decay time, and a low quantum efficiency. $\bar{M}_{5c}$ also moves *up* in energy under compressive (001) strain, and exhibits strong, X-like phonon sidebands with weak no-phonon lines. Transitions from $\bar{\Gamma}_{4c}(X^z)$ have precisely the reverse behavior: fast decaying PL with high quantum efficiency, downward shift with strain, weak-phonon sidebands and strong no-phonon lines. Spectroscopic studies by Ge and co-workers[13] revealed that in $p=1$–3 SL's, the $\bar{M}_{5c}(X^{xy}_{1c})$ state is indeed below $\bar{\Gamma}_{4c}(X^z_{1c})$, as found theoretically here [Fig. 1(b)] and in Refs. 1, 4, 5, 7, 9, and 12. [The order is reversed

for $4 \leq p \leq 11$ SL's, or, for shorter period SL's under compressive (001) strain.] Similarly, experiments by Garriga *et al.*[11] and Jiang *et al.*[12] have shown that the $\bar{\Gamma}_{1c}^{(1)}$ level *increases* in energy in going from $p=1$ to 2 SL's, as found in first-principles calculations.[1] However, the experimental studies of Ge and co-workers[13] revealed two clear discrepancies relative to theory: (a) Ge and co-workers[13] show that the lowest radiative conduction band in the $p=1$ SL is the AlAs X-derived $\bar{M}_{5c}$ state while our own and other first-principles calculations[1-9] clearly show that CBM is the GaAs L-derived $\bar{R}_{1c}$ state. The calculated $\bar{M}_{5c}-\bar{R}_{1c}$ energy difference (0.22 eV) is considerably larger than the theoretical uncertainty, so the conflict with experiment is real. Experiment therefore characterizes the $p=1$ SL as "type II" (VBM on GaAs, CBM on AlAs), while theory characterizes it as "type I" (VBM and CBM on GaAs). (b) The $\bar{\Gamma}_{1c}^{(1)}$ state too appears in the present calculation (and in those of Refs. 1-3) below $\bar{M}_{5c}$, while the experiments of Ge and co-workers place it higher in energy, above $\bar{\Gamma}_{4c}$ and $\bar{M}_{5c}$. The calculated 0.10 eV $\bar{\Gamma}_{1c}-\bar{M}_{5c}$ difference is again outside the theoretical error bar.

LOCALLY INTERMIXED SL's

We next examine the possibility that these significant differences between theory and experiment result from insufficient interfacial quality in the samples used to date.[13] To test this, we have calculated the total energy, diffraction pattern, and band structure of the $(AlAs)_1/(GaAs)_1(001)$ SL where the abrupt (1×1) interface in the xy plane is replaced by larger (2×1), (3×1), and (4×1) interfacial unit cells and a fraction ($\frac{1}{2}$, $\frac{1}{3}$, or $\frac{1}{4}$) of the Al atoms on the AlAs side is exchanged with Ga atoms on the GaAs side. We first calculate the changes in total energy due to this local atomic intermixing. The pseudopotential calculated[18] excess enthalpy of an *abrupt* $(AlAs)_1/(GaAs)_1$ SL taken with respect to bulk GaAs+AlAs is 13.7 meV/$AlGaAs_2$-unit, while the mixing enthalpy of the random $Al_{0.5}Ga_{0.5}As$ alloy is calculated to be 10.6 meV/$AlGaAs_2$. Hence, the ordered, abrupt $p=1$ SL is less stable at $T=0$ than the random alloy. However, total-energy calculations for the $\frac{1}{2}$ fraction intermixed $(4\times1)p=1$ SL show that the excess enthalpy is lowered to 5.5 meV/$AlGaAs_2$. The lowest-energy exchanges for the $\frac{1}{3}$ and $\frac{1}{4}$ fraction exchanges are 7.3 and 8.8 meV/$AlGaAs_2$, respectively. Hence, local atomic mixing at the interface stabilizes the $p=1(001)$ SL with respect to the random alloy.

We next examine whether the locally intermixed $p=1$ (001) SL still possesses the characteristic superlattice x-ray reflections observed[19] in such samples. The random alloy and the zinc-blende constituents have, by symmetry, a zero x-ray structure factor $\rho(\mathbf{G})$ for the momentum $\mathbf{G}=2\pi/a$ (0,0,1) where 1 is an odd integer. In contrast, an (001) SL has $\rho(0,0,1)\neq0$ ("superlattice spots"). Our calculated (normalized) $\rho(0,0,0)/\rho(0,0,1)$ was 191 for the abrupt SL and 572 for the SL with $\frac{1}{3}$ of the Al exchanged with Ga. Hence, this type of local atomic intermixing in the (001) plane still exhibits superlattice diffraction features in the growth direction. Note also that the intermixing patterns used still exhibit the fundamental symmetry inequivalence of the [110] and [1$\bar{1}$0] direction [as well as the existence of a unique (001) axis] so that the basic spectroscopic selection rules and strain behavior associated with this inequivalence[13] remain intact.

The calculated energy levels for the (3×1) intermixed SL are shown in Fig. 1(c). Comparison with Fig. 1(a) shows that the intermixed SL is indeed not an alloy. We see that (a) reconstruction removes the symmetry constraint that led the "segregating" behavior of $\bar{R}_{1c}$ and $\bar{R}_{4c}$ and consequently to their large energy splitting. The $\bar{R}_{1c}$ level is split and both components move up by 0.23 eV. The CBM is now either $\bar{M}_{5c}$ or Γ_{4c} (the energy splitting is only 5 meV). The position of the CBM is now at 2.08 eV, close to the experimentally-determined (zero-phonon) CBM at 2.07 eV.[13] (b) The s-like $\bar{\Gamma}_{1c}^{(1)}$ level also moves up in energy; it is now 40 meV *above* $\bar{M}_{5c}$. Both changes [(a) and (b)] remove the conflicts between experiment and the theoretically calculated levels of the abrupt SL.

To examine if these results depend sensitively on the assumed reconstruction, we examined two exchange patterns for each of the three ($\frac{1}{4}$, $\frac{1}{3}$, $\frac{1}{2}$) exchange fractions. Figure 2 shows the eigenvalue differences between the $\bar{R}_{1c}$ and $\bar{\Gamma}_{4c}$ points and between the $\bar{M}_{5c}$ and $\bar{\Gamma}_{4c}$ points for the abrupt SL and for these different exchanged SL's. The $L-\Gamma$ difference increases monotonically with the fraction exchanged, while the $X-\Gamma$ difference is less than 15 meV for all of the exchanges. The experimental results are compatible with a fraction of $\sim\frac{1}{3}$ of the atoms intermixed across the interface. A minor discrepancy remains: experiment finds $\bar{\Gamma}_{4c}(X_{1c}^{z})$ to lie 15 meV *above* $\bar{M}_{5c}(X_{1c}^{xy})$ while the calculation for the intermixed SL [Fig. 1(c)] places it 5 meV below. This is a strain effect: the calculation neglected the small lattice mismatch between GaAs

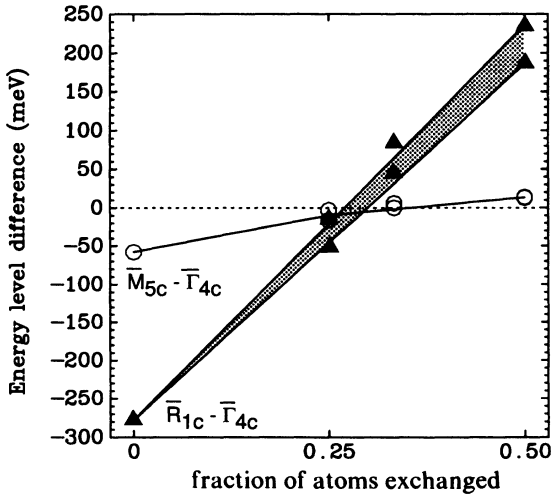

FIG. 2. Calculated $\bar{R}_{1c}-\bar{\Gamma}_{4c}$ (triangles) and $\bar{M}_{5c}-\bar{\Gamma}_{4c}$ (circles) energy splittings as a function of the fraction f of atoms exchanged across the interface. For each fraction, results of two patterns of intermixing are shown. Note that for $f\gtrsim\frac{1}{4}$ the CBM is no longer L derived. $f=0$ is the abrupt SL; $f=\frac{1}{2}$ has no [001] ordering.

and AlAs, which *raises* the energy of $\bar{\Gamma}_{4c}$ with respect to $\bar{M}_{5c}$. The energy change is 23 meV for the abrupt SL,[20] and about $\frac{2}{3}$ of that for the intermixed SL. This brings our theoretical results into full agreement with the experiment.

CONCLUSION

We conclude that a variety of interfacial roughness patterns stabilizes the $p=1$ SL and, at the same time, lead to a reversal of the identity of the CBM. There is some experimental evidence for interfacial intermixing in nominally high-quality AlAs/GaAs SL's. The $\bar{M}_{5c}$ state of $p=1$ SL's exhibits an unexpected no-phonon line, attributed by Ge and co-workers[13] to disorder effects. Similarly, the magnitude of the $X^z_{1c}-\Gamma_{1c}$ mixing,[13] the appearance of defect peaks in the PL (Refs. 11 and 13), and the fact that there are strong nonradiative decay channels in the PL for $p \leq 3$ (reflected by the fact that the total integrated emission is 1 order of magnitude weaker than in longer period SL's) all suggest the possibility of nonflat or partially disordered interfaces. The suggestion that currently available AlAs/GaAs SL's are partially intermixed is also consistent with the experimental results of Ourmazd *et al.*,[21] who used chemical-lattice imaging to show that interfaces that had been characterized optically as being perfectly abrupt were actually intermixed over two to four layers around the interface. When truly high-quality $p=1$ SL's will become available, we predict that a slowly decaying "forbidden" L_{1c}-derived PL from the CBM at 1.93 eV will be seen with its characteristic longitudinal acoustic L-phonon ($\sim$27 meV) fingerprints.

ACKNOWLEDGMENTS

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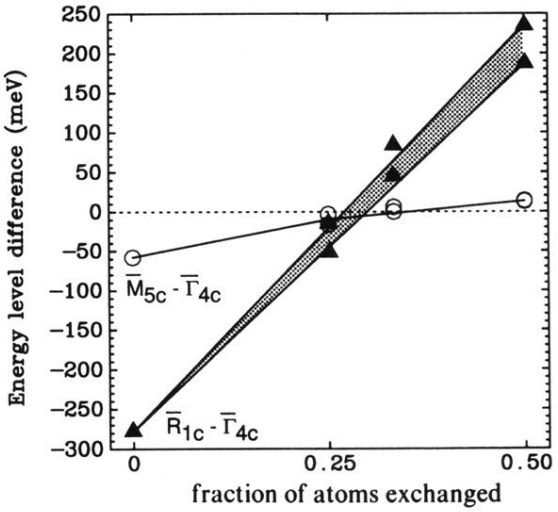

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