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Theory of optical properties of 6.1 Å III−V superlattices: The role of the interfaces

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Interfacial interdiffusion in quantum wells and superlattices could alter the interfacial strain, band alignment, and even the atomic symmetry at the interface, thus potentially changing the electronic and optical properties. We consider the InAs/GaSb system describing the interdiffused interfaces via

by different growers. Vurgaftman and Meyer[9] showed that there are conspicuous differences between the band gaps derived using data from different growers. In some cases they found differences as large as 200 meV in the predicted VBO for the InAs/GaSb system, even for structures nominally quite similar. Experiments have also shown that, besides interfacial disorder effects, even the nature of the interfacial bonds has a conspicuous effect on the band gap energy. Bennett *et al.*[10] measured the band gaps of InAs/GaSb superlattices grown in such a way so to have or almost pure InSb-like or almost pure GaAs-like interfaces and found a difference of 40 meV for superlattices with a nominal period $n=8$. In particular, gaps $E_g=209$ and 216 meV have been measured for two samples with In–Sb-like interfaces, whereas a gap $E_g=253\,\mathrm{meV}$ was measured for a sample with only GaAs-like interfaces. Clearly, the atomic-level structure at the interface controls the band gap.

We have previously shown[11] that the ‘‘standard model’’ based on continuum-like effective-mass **k·p** approaches is insufficient to describe the electronic structure of such thin superlattices, even if they are assumed to be abrupt. A good theory should take into account the effects on the band structure of segregation and interfacial atomic intermixing to provide accurate values.

In this article, we use a kinetic model of interfacial segregation during molecular beam epitaxy MBE) growth. We find the atomic positions near the interface after segregation at a given growth temperature and deposition rate. We, then, use these atomic concentration profiles in a pseudopotential environment considering only the nearest-neighbor environment. In the quaternary $(AC)(BD)$ systems, the C and D anions can be surrounded by A_nB_{4-n} cations, where $n=0$, 1, 2, 3, and 4. Analogously, the A and B cations can be surrounded by C_nD_{4-n} anions. Our EPM has been obtained by fitting the properties of only the pure binary compounds corresponding to environments $n=0$ and $n=4)$. To improve the transferibility to other environments, we assume a linear interpolation between these limits as

$$
\begin{aligned}
&v_{\mathrm{A}}\ C_nD_{4-n})=\frac{n}{4}v_A\ AC)+\frac{4-n}{4}v_A\ AD),\\
&v_{\mathrm{B}}\ C_nD_{4-n})=\frac{n}{4}v_B\ BC)+\frac{4-n}{4}v_B\ BD),\\
&v_{\mathrm{C}}\ A_nB_{4-n})=\frac{n}{4}v_C\ AC)+\frac{4-n}{4}v_C\ BC),\\
&v_{\mathrm{D}}\ A_nB_{4-n})=\frac{n}{4}v_D\ AD)+\frac{4-n}{4}v_D\ BD).
\end{aligned}
\qquad 2)
$$

AC, BC, AD, and BD are the four binary compounds, in our case GaSb, GaAs, InSb, and InAs, whose properties have been directly fitted to extract the atomic pseudopotential parameters. This procedure leads to a potential for the InAs monolayers closer to the interface different from the potential of the InAs monolayers in bulk InAs, in agreement with the results of more accurate self-consistent calculations.

An empirical pseudopotential calculation requires: a) to determine a reliable equilibrium atomic configuration for the system, and b) to calculate the band structure relative to that given atomic configuration. To determine the atomic positions $R_{n\alpha}$ we minimize the elastic energy corresponding to a given atomic arrangement in the system, via the valence force field approach.[20] For b) we expand the wave functions $\psi_i(r)$ in a plane-wave basis. The Hamiltonian matrix elements are calculated in this basis with no approximation, then the Hamiltonian matrix is diagonalized via the folded spectrum method.[21]

III. RESULTS

A. Superlattices with abrupt interfaces

Figure 1 shows the electron $E1$ and hole HH1,LH1,HH2) levels of $(\mathrm{InAs})_n/(\mathrm{GaSb})_n(001)$ superlattices as a function of n. We see that as n is reduced from infinity, the $E1$ level moves up, while HH1, LH1, and HH2 move down, all states becoming more and more confined within the corresponding wells. When $n<28$ the superlattices acquire a semiconducting gap with the first electron state $E1$ localized in the InAs layer and the first hole state HH1 localized in the GaSb layer. At $n\geqslant 28$ the energy of the $E1$ level becomes lower than the energy of the hole HH1 state. At $n\approx 28$ the $E1$ level and the HH1 level should cross. However, because of the reduced C_{2v} symmetry of the superlattices, the two levels anticross. The anticrossing gap opens at $k_{\parallel}=0$ and its calculated value is $E_A^{\mathrm{HH1},E1}=11\,\mathrm{meV}$. We find a strong wave-function mixing at the $\mathrm{HH1}-E1$ anticrossing. The superlattice period at which the anticrossing gap occurs is in good agreement with other calculations.[22]

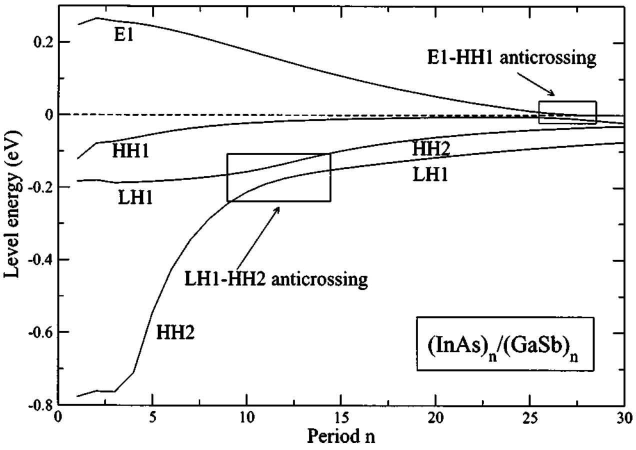

FIG. 1. Level energies of the $E1$, HH1, LH1, and HH2 states of $(\mathrm{InAs})_n/(\mathrm{GaSb})_n$ superlattices as a function of layer thickness n. Dashed line denotes the VBM of bulk GaSb.

In addition to $E1-\mathrm{HH1}$ coupling and anticrossing we also find anticrossing between the hole levels LH1 and HH2 around $n=13$ see Fig. 1). For superlattice periods n close to $n=13$ the wave functions of the two hole states strongly intermix. The calculated anticrossing gap is $E_A^{\mathrm{LH1,HH2}}=40\,\mathrm{meV}$. This causes the appearance of new transitions $\mathrm{LH1}\leftrightarrow E2$ and $\mathrm{HH2}\leftrightarrow E1$ in the spectra that become allowed because of this mixing. These effects are due to the superlattice low spatial symmetry and are not taken into account in the standard envelope function approaches.

At $n>28$, one expects a metallic state. However, even for superlattices with a InAs layer large enough for the $E1$ level to fall well *below* the HH1 level at $k_{\parallel}=0$, a small anticrossing gap is found at some in-plane wave vectors $\mathbf{k}_{\parallel}^{*}$. Figure 2 describes the band structure of the $(\mathrm{InAs})_{46}(\mathrm{GaSb})_{14}$ superlattice. On the right side, we show the in-plane dispersion along the [1,1,0] direction $(k_x=k_y)$ corresponding to the

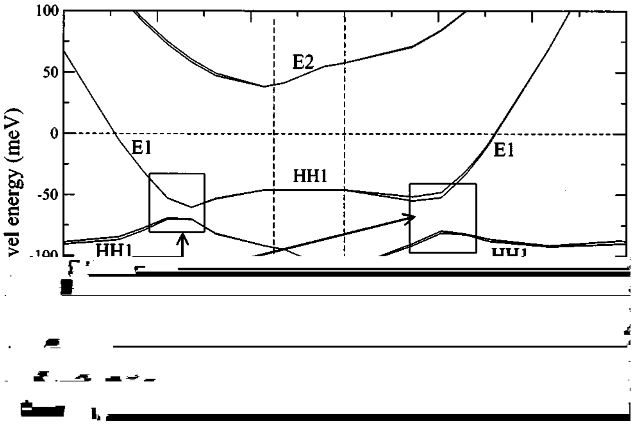

FIG. 2. Dispersion relations for the $(\mathrm{InAs})_{46}/(\mathrm{GaSb})_{14}(001)$ superlattice. Indicated by arrows and encircled by boxes are the hybridation minibands formed by the $E1$ and HH1 anticrossing away from the Brillouin zone center. Dashed line indicates the energy of the GaSb VBM.

$k_z = 0$ plane, while on the left side we show the in-plane $(k_x = k_y)$ dispersion corresponding to $k_z = \bar{Z}$ where $\bar{Z}$ $= \ /60a$, a being the lattice parameter. In the central part we give the dispersion with k_z from $\bar{\Gamma}$ to $\bar{Z}$, where $\bar{Z}$ is the point at the border of the Brillouin zone along the k_z direction. Thus, we still have a semiconducting superlattice SL) because of the overlap of the hybridization minigaps formed along different directions of the Brillouin zone.

Moving in the Brillouin zone towards and across the hybridization minigaps, one observes that the wave functions

As plane of InAs with an progressively with T_g) higher fraction of Sb atoms occurs at the same inverted interface. The mechanism here is different and it is due, instead, to As segregation which is made possible by the small value of $\Delta_{\mathrm{Sb/As}}$. Thus, we can see that the combination of a large $\Delta_{\mathrm{In/Ga}}$ for cation segregation and a small $\Delta_{\mathrm{Sb/As}}$ for anion segregation causes the narrowing of the InAs electron well with increasing T_g. The calculated profiles closely agree with the STM images of the anion sublattice of Ref. 7, where it is seen that the normal interface is rougher and broader than the inverted interface. This is due to the anion intermixing which is much larger at the normal interfaces than at the inverted interfaces where only the one monolayer shift of a GaSb layer into InAs takes place). These results are in good agreement with many experimental findings.[7,26,27]

E. Blueshift of the band gap of segregated InAs/GaSb superlattices versus ideal structures

Through the kinetic model of MBE growth we can obtain realistic composition profiles for the segregated superlattices along the growth direction. Next, we need to build the entire superlattice atomistic structure. No experimental information is available on the atomistic arrangement in the planes perpendicular to the growth direction. We, thus, assume random arrangements in these planes, consistent with the planar composition profile dictated by the growth (Thro4vsiti.9(W)Tc)-292.6(gcoin)-252e av sdeermixnd stem from the different treatment of the interfacial regions. The Dente–Tilton approach describes the interface through a step function, which leads to a very abrupt potential change at the interface between the InAs potential and the GaSb potential.[29] In our approach, instead, the change is more gradual and the interfacial Ga–As and In–Sb bonds are correctly described.

ii) While the Dente and Tilton approach fit the experimental gap versus thickness curve for *abrupt* superlattices, our atomistic pseudopotential fits the experiment well only for segregated superlattices. Since interfacial intermixing is an experimental fact, the agreement of the theory for intermixed SLs with the experiment is gratifying.

iii) The envelope function calculation by Lau *et al.*[30] with interfacial terms added to optimize the agreement with the experiment fits the experiment well for $n \lesssim 16$. At larger n approaches our result for the band gaps of abrupt interfaces. However, this approach is also not predictive i.e., one parameter was adjusted to obtain agreement with the same gaps versus GaSb thickness experimental data).

iv) The predicted blueshift of the band gap with respect to GaSb thickness n is only 47 meV for the EFA approach and 49 meV for the pseudopotential approach of Dente *et al.*, considerably smaller than the experimental value, 70 meV. Our predicted blueshifts for the same superlattices are 64 meV for segregated interfaces, and 95 meV for abrupt interfaces.

IV. CONCLUSIONS

We have presented in this article a fully atomistic ap-