Applicability of the k·p method to modeling of InAs/GaSb short-period superlattices

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We investigate the long-standing controversy surrounding modeling of the electronic spectra of InAs/GaSb short-period superlattices (SPSLs). Most commonly, such modeling for semiconductor heterostructures is based on the **k**·**p** method. However, this method has so far failed to predict the band structure for type-II InAs/GaSb SPSLs. Instead, it has systematically overestimated the energy gap between the electron and heavy-hole minibands, which led to the suggestion that the **k**·**p** method is inadequate for these heterostructures. Our results show that the physical origin of the discrepancy between modeling and experimental results may be the *graded* and *asymmetric* InAs/GaSb interface profile. We have performed band-structure modeling within the **k**·**p** method using a realistic interface profile based on experimental observations. Our calculations show good agreement with experimental data, both from our own measurements and from the published literature.

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I. INTRODUCTION

InAs/GaSb superlattices have a type-II "broken gap" band alignment, where the conduction-band minimum in InAs is below the valence-band maximum in GaSb. By tailoring the superlattice period, this antimonide-based system provides great potential for optical devices in a wide wavelength range, including the technologically useful 3–5 μm midinfrared atmospheric window. InAs/GaSb short-period superlattices (SPSLs) with a period of 4–12 monolayers (MLs) have recently attracted a lot of interest because they have optical transitions in this wavelength region. Indeed, promising results have been reported for InAs/GaSb SPSLs operating within the 3–5 μm range.[1–3]

The **k**·**p** method within the envelope-function approximation has been widely used in calculations of the electronic spectra for semiconductor nanostructures. Its simple input requirements (such as dimension, orientation, and basic parameters from bulk materials) have made it so popular that it is termed as the "standard method."[4,5] It has been successfully used in modeling for quantum wells and superlattices, especially for electronic states close to the Γ point of the Brillouin zone. However, this method has not been successful for InAs/GaSb SPSLs.[6,7] Instead, it was found to overestimate the fundamental energy gap between the electron and heavy-hole minibands by as much as 60 meV.[5,8] Apart from fundamental limitations of the **k**·**p** method (such as assumption of equal Bloch functions in InAs and GaSb), many authors have suggested that this is due to the lack of a common atom at the interfaces between the two materials.[6,7] Indeed, the two interfaces (GaSb-on-InAs and InAs-on-GaSb) have chemically distinct bonds: the former has Ga-Sb and In-Sb bonds, while the latter has In-As and Ga-As bonds. As a result, the system is of the lower C_{2v} point group of symmetry, instead of D_{2d} which is implicitly assumed in the **k**·**p** method.

Since the standard **k**·**p** method did not provide accurate results, the atomistic calculations such as using the pseudopotential method, were suggested as the only viable alternative.[6,7] However, the amount of calculation involved is massive and the size of the structure is limited. Simultaneously, some modifications to the **k**·**p** method were proposed. In some publications, a deltalike potential at the interface was suggested to account for the effect of extra In-Sb and Ga-As chemical bonding.[9] The results were in better agreement with experimental data, even within a single-band model.[2,9] However, it was achieved at the cost of using an additional fitting parameter which does not have a real physical meaning.

II. INTERFACE

Other than the lack of a common atom, another important issue for the physical structure of InAs/GaSb interfaces is the effect of segregation, in particular, that of antimony. Interface roughness and layer composition profiles are difficult to control due to the exchange reaction between As and Sb during growth.[10,11] Segregation of Sb largely contributes to degradation of the interfacial abruptness and to formation of asymmetrical interfaces.[6,7,10] For large period superlattices, the effect of the interface disorder may be relatively small. Indeed, the overestimation of the energy gap by the **k**·**p** method reduces with the superlattice period.[5] However, for short-period superlattices, modifications of the band profile around the interfaces can have a deleterious effect on the band structure. This leads to a suggestion that the overestimate may be due to modification of the interface band profile caused by segregation.

The interface composition profile is strongly affected by the growth conditions, which are different between the samples. Therefore, to take segregation into account, it is necessary to identify the profile parameters which are common for real heterostructures grown under typical conditions. Experimental studies of the interface profile in the InAs/GaSb superlattices have been performed using scanning tun-

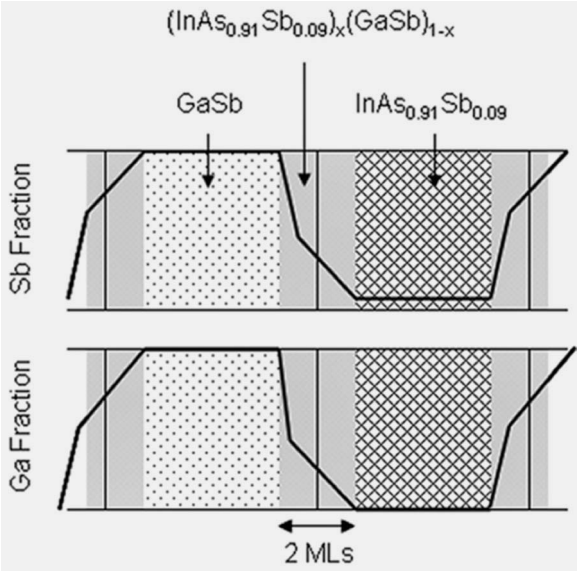

FIG. 1. Segregated composition profile for the GaSb/InAs interface. A ternary $InAs_{0.91}Sb_{0.09}$ compound is used instead of the nominal InAs layer.

neling microscopy (STM) (Refs. 7 and 12) and transmission electron microscopy (TEM).[10,11] They have revealed that the interface disorder has two major components, the interface roughness (uneven surface due to formation of steps) and the interfacial diffusiveness (intermixing due to stochastic processes and exchange reactions).[10,11] From these reports, it follows that there is an identifiable common parameter, which is the *graded interface* with a thickness of 2–6 MLs.

Next, the dominating interface-disorder mechanisms for the two interfaces (GaSb on InAs and InAs on GaSb) are different, resulting in the different physical structure. Antimonides have a lower binding energy than arsenides,[10] so Sb atoms are more diffusive. Because of this, exchange reactions tend to occur more for arsenides (in this case, InAs) grown on antimonides (GaSb), reducing the surface energy during growth. In particular, strong segregation of Sb has been observed in the case of InAs grown on GaSb, e.g., by as much as 25% Sb and for up to 6 MLs into the InAs.[7,10,12] Moreover, about 5% of Sb has been reported even beyond 6 MLs into the InAs.[7,12] For GaSb grown on InAs, although minor exchange still occurs, the graded interface is mainly due to interface roughness with an average interface region thickness of up to 2 MLs dependent on growth conditions. This leads to *physical asymmetry* in the composition profiles between the two interfaces. Such asymmetry has been observed using both STM and TEM techniques and is supported by modeling.[7,12]

Using this information, a simplified segregated composition profile was constructed, which is shown in Fig. 1. It corresponds to the STM-studied profile reported in Ref. 7 for the growth temperature of 450 °C. The interface layer comprises 2 MLs of material with graded composition, with 1 ML taken from the InAs and the other from GaSb. Strictly speaking, this material is a quaternary $Ga_xIn_{1-x}As_ySb_{1-y}$, in which x and y may be independent. However, for simplicity we use $(InAs_{0.91}Sb_{0.09})_x(GaSb)_{1-x}$ instead, which is lattice matched to GaSb and for which the band parameters are well known.[13] Also, for a very short superlattice period (with the nominal thickness of InAs up to 5 MLs), we use the ternary compound $InAs_{0.91}Sb_{0.09}$ in place of pure InAs. This simulates the effect of strong Sb segregation into the InAs layer. As illustrated in Fig. 1, the Sb fraction is always nonzero in this case.

III. METHODS

For our calculations, the finite-element method was employed, using a COMSOL multiphysics commercial package. First, the strain tensors were calculated within the continuum-elasticity approximation using elastic constants from Ref. 14. Next, the electronic structure was modeled using the standard eight-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian.[15,16] The effects of strain are included in the Hamiltonian, based on the standard deformation potential theory. All band parameters are taken from Ref. 13.

The InAs/GaSb SPSL samples were grown by molecular-beam epitaxy at a temperature of 420 °C on a GaSb substrate. We have investigated two asymmetric InAs/GaSb SPSLs. The nominal layer thickness of the InAs/GaSb layers was 1.0/1.7 nm (sample A) and 0.9/2.0 nm (sample B), respectively. Photoluminescence (PL) spectra were recorded at 10 K using Fourier-transform infrared spectroscopy in step scan mode. The spectra were excited at 800 nm using a continuous-wave Ti:sapphire laser and collected by a liquid-nitrogen-cooled InSb photodetector. The excitation power density was about 5 W/cm^2.

IV. RESULTS AND DISCUSSION

We modeled the electronic structure of the InAs/GaSb SPSLs using the segregated composition profile that has been described above. We focus on short-period superlattices with layer thicknesses within the range of 4–8 MLs because the effect of the graded interface on the band energies is much more significant for short-period than for long-period structures. Modeling was performed for both asymmetric and symmetric SPSLs. Results for asymmetric structures were compared to our experimental spectra. For symmetric structures, the results were compared to the experimental data in the literature.[2,3,17,18] For comparison purposes, calculations assuming perfectly abrupt interfaces were also performed. The effect of dominant interface bonding type is not included in our model because for a graded interface, it is much less relevant than it would be for an abrupt interface. Nor is the exciton binding energy taken into account in the calculations because it is small (less than a few meV).[19]

Figure 2 shows normalized PL spectra obtained from our samples. The spectra show the peaks due to transitions between the electron and hole minibands at 0.415 and 0.440 eV for the two samples. Dashed arrows show calculated energy gaps assuming perfectly abrupt interfaces. One can see that in this case, the transition energies are hugely overestimated, by 50–60 meV. Agreement between the modeling results and experimental data is significantly improved if segregation is taken into account. The modeled transition energies in this

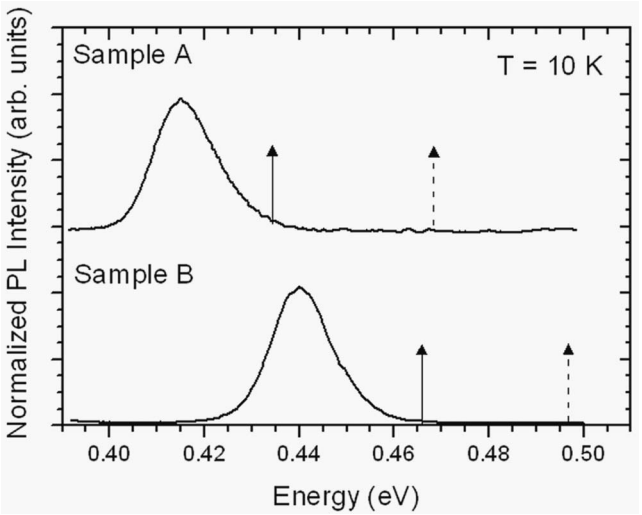

FIG. 2. PL spectra from asymmetric InAs/GaSb SPSLs. Samples A and B have InAs/GaSb layer thicknesses of 1.0/1.7 and 0.9/2.0 nm, respectively. The spectra are offset for clarity. Arrows indicate the calculated energy-gap values: dashed lines for abrupt interfaces and solid lines for graded interfaces.

case are shown by solid lines. The calculated energy gap is reduced by 30–35 meV, with the discrepancy decreasing almost threefold. Still, some overestimate remains, probably because the real composition profile of the samples deviates from the one used for calculations.

Data for symmetric structures are shown in Fig. 3. The symbols show the experimental data from literature.[2,3,17,18] One can see that there is a scatter for samples even with same nominal structure, which is due to different growth conditions and resulting interface parameters. The calculations were performed using band parameters at 80 K for better comparison with the experimental data. Modeling results using graded interfaces are shown by the solid line; the dashed line shows results for the abrupt interface. In the

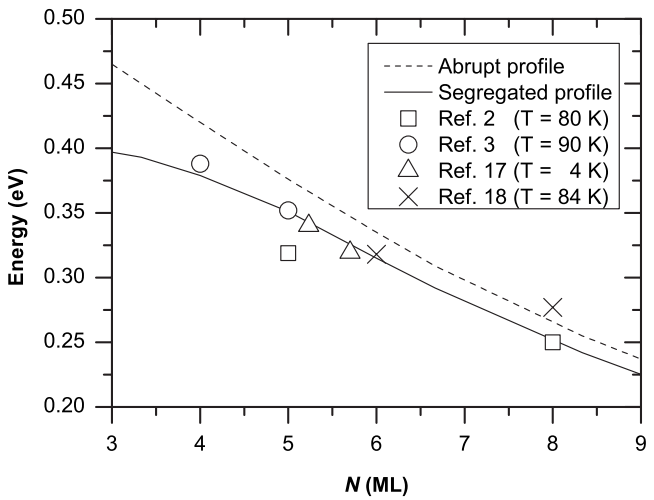

FIG. 3. Fundamental energy gap for symmetric $(InAs)_N/(GaSb)_N$. Lines show the calculation results, symbols represent the experimental data from the literature, and N is the number of monolayers in the SPSL samples.

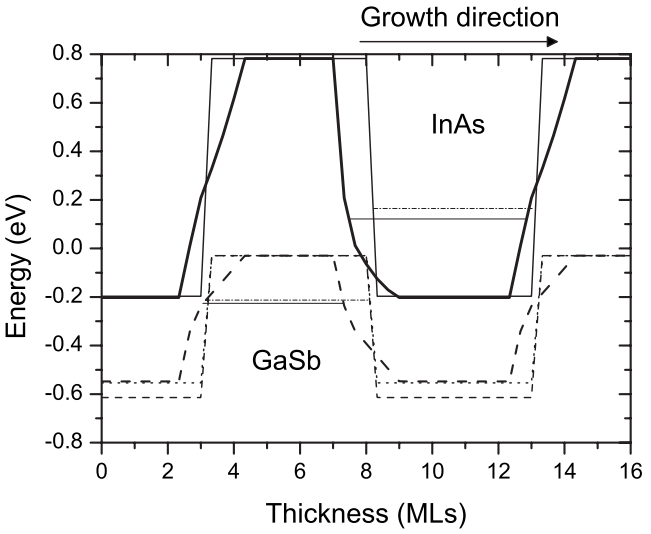

FIG. 4. Band profiles for abrupt and segregated interfaces (fine and bold lines, respectively). Conduction band, light-hole, and heavy-hole valence bands are represented by the solid, dashed and dotted lines, respectively. The ground electron and heavy-hole energy levels are shown for both segregated and abrupt profiles using solid and dash-dotted lines, respectively.

latter case, the transition energies are overestimated by 20–60 meV. With the segregated composition profile, the modeled transition energies decrease by 20–70 meV; the decrease is greater for shorter superlattice periods. In the latter case, our modeling demonstrates excellent agreement with the experimental data.

To reveal the physical mechanism by which the graded composition profile affects the optical transition energy, its effect on the band profile needs to be considered. Figure 4 shows the modification of the profile for the conduction band and the heavy-hole and light-hole valence bands. One can see that for the graded interface, the quantum well profile for electrons is wider than for abrupt interfaces. This is a direct consequence of the *physical asymmetry* in the composition profile at the interfaces due to different dominating interface-disorder mechanisms for GaSb on InAs and InAs on GaSb (as discussed in Sec. II). This results in a decrease in the size-quantization energy for the electron miniband by up to 70 meV.

Similarly, the quantum well profile for holes in the graded structure is narrower. However, the increase in size-quantization energy, which might be expected in this case, is counteracted by a reduction in the height of the barrier formed by the InAs layer. Our calculations show that the overall effect of segregation on the heavy-hole miniband is minor (less than 10 meV). As a result of these combined effects from the electron and hole confinement in graded and asymmetric quantum wells, the optical transition energy is reduced by as much as 60 meV, resulting in much better agreement with the experimental data.

V. SUMMARY

We have investigated the physical origin of the failure of the standard **k**·**p** method to model the electronic structure for

InAs/GaSb short-period superlattices. Our calculations have shown that the *asymmetric* interfacial segregation results in a significant reduction in the size-quantization energy for the electron miniband, leading to a reduction in the fundamental energy gap. Using a simplified segregated composition profile, which is based on *experimental evidence*, we obtained results in much better agreement with the experimental data. We have demonstrated that the $\mathbf{k}\cdot\mathbf{p}$ method can be used for InAs/GaSb SPSLs with a good predictive ability, as long as the real physical structure of the interface is correctly taken into account.

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