Interface Heterobond Effects in \((hkl)\) InAs/GaSb Superlattices Solved by Bond Orbital Model

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Abstract

For the \((hkl)\)-oriented InAs/GaSb superlattices: the in-plane spin splitting and the Dresselhaus-like spin splitting are found in the presented paper. Moreover, it is due to the microscopic symmetry reduction, which originates from the existence of heterobonds (In-Sb and Ga-As) inside the interfacial unit-cells.

Introduction

It is realized that a considerable difference \([1]\) exists in the interfaces between the no-common-atom (NCA) superlattices, such as \((\text{InGa})\text{As/InP}\) and \((\text{InAs/GaSb})\), and the common-atom (CA) superlattices, such as \((\text{AlGa})\text{As/GaAs}\). The NCA superlattices \((\text{well=C1-A1, barrier=C2-A2})\) do not share common atoms, because both the cations \((\text{C1,C2})\) and anions \((\text{A1,A2})\) in the host materials are different. For the NCA superlattices, the heterobonds \((\text{C1-A2 and C2-A1})\) existing at successive interfaces result in interface perturbation and symmetry reduction.

Due to the unit-cell-scale basis, the oversymmetric bond orbital model (BOM) \([2]\) could not be used to solve the lower symmetric heterostructure system at the interfaces. According to the concept of \(H_{BF}\) \([1]\), a modified bond orbital model (MBOM) \([3]\) is then proposed to solve the microscopic interface effects. Those \(s\)- and \(p\)-like bond orbitals (unit-cell-scale basis) of Chang are expanded in terms of the tetrahedral (anti)bonding orbitals of Harrison \([4,5]\). By the interaction between the microscopic basis function and the potential operator in the \(\text{Schrödinger}\) equation at the proposed model, the microscopic consequences will be extracted from this framing.

Through consideration of the three degenerate band \((\Gamma_6^1\ and \Gamma_6^2)\) approximations, the Hamiltonian for each monolayer can be expressed in terms of the \(6 \times 6\) MBOM matrix formalism. Away from the heterojunction, all the off-diagonal matrix elements of the potential matrix \(V_{6 \times 6}\) are zero, and this diagonal matrix has the same scalar potential \(V\) as usual of the BOM. Therefore, the \(V_{6 \times 6}\) potential matrix can be separated into the scalar potential \(V\) of host materials by adding an additional potential matrix \(\Delta V_{6 \times 6}\), i.e., \(V_{6 \times 6} = V + \Delta V_{6 \times 6}\). In the low symmetry NCA heterostructures, the key difference between the MBOM and the BOM is the non-zero \(\Delta V_{6 \times 6}\) matrices at the interfaces.

In-plane Spin Splitting

In this \((10,10)\) InAs/GaSb superlattice grown along the [001] direction, one can find Ga-As and In-Sb heterobonds with alternately successive existences at the interfaces. According to the MBOM, one needs to put the additional potential matrix \([\omega_{1/2}, \omega_{-1/2}, u_{3/2}^{3/2}, u_{-3/2}^{3/2}, u_{1/2}^{3/2}, u_{-1/2}^{3/2}, u_{-3/2}^{3/2}]\) to the original BOM matrix at the interfaces as

\[
\Delta V_{6 \times 6} = \begin{bmatrix}
\frac{1}{2} \Delta U & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{2} \Delta U & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{2} \Delta V & 0 & \frac{i}{2\sqrt{3}} \Delta V & 0 \\
0 & 0 & 0 & \frac{1}{2} \Delta V & 0 & \frac{i}{2\sqrt{3}} \Delta V \\
0 & 0 & \frac{-i}{2\sqrt{3}} \Delta V & 0 & \frac{1}{2} \Delta V & 0 \\
0 & 0 & 0 & \frac{-i}{2\sqrt{3}} \Delta V & 0 & \frac{1}{2} \Delta V
\end{bmatrix}
\]

(1)

where \(\Delta U\) and \(\Delta V\) denote the difference of potential energy of conduction and valence bands between the heterobond species and the host material at each interfacial monolayer, respectively. In the MBOM model, \(\Delta U\) and \(\Delta V\) are expressed as the fitting parameters. \(\Delta U = -0.36\text{eV}\) and \(\Delta V = -0.56\text{eV}\) are used for the InSb/InAs junction; \(\Delta U = -0.16\text{eV}\) and \(\Delta V = 0.56\text{eV}\) for the GaAs/GaSb junction.

In contrast to Fig.1(a) solved by the BOM, the MBOM band structure of InAs/GaSb superlattice is then calculated and shown in Fig.1(b). The sizable differences of the band structures can be seen between the BOM
Figure 1: Subband structures of a (10,10) InAs/GaSb [001]-grown superlattice, (a) calculated with BOM method, (b) calculated with MBOM method. Note that the zero energy of band structure is at valence band top of GaSb. Where d is the thickness of superlattice period.

Figure 2: Subband structures of a (10,10) InAs/GaSb [111]-grown superlattice, (a) calculated with BOM method, (b) calculated with MBOM method.

and MBOM. The spin splitting at non-zero in-plane wave vector in the MBOM calculation cannot be found in the BOM result. The crossing of HH and LH subbands along the wave vector of growth direction [00ζ] (ζ=0-1) can be seen in the BOM, but not in the MBOM. These problems originate from the perturbation of interface heterobond, i.e. the so-called NCA effect. Owing to not considering the interface heterobonds, the BOM makes a different band structure of the InAs/GaSb superlattices with respect to that of the MBOM.

For the (10,10) InAs/GaSb superlattice grown along the [111] direction, it has the same order of atomic planes as the (001) superlattice. Similarly, one needs to put the additional potential matrix to the original BOM matrix at the interfaces as

\[ \Delta V_{6 \times 6} = \begin{bmatrix}
\frac{1}{4} \Delta U & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{4} \Delta U & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{2} \Delta V & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2} \Delta V & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix} \]  

(2)

The band structures of [111] grown direction solved by the BOM and MBOM are shown in Fig.2(a) and 2(b). The crossing of LH1 and HH3 subbands still exists in the central panel [00ζ] in Fig.2(b) as same as Fig.2(a). The spin splitting at non-zero in-plane wave vector is from the asymmetric interface potential.

Due to not considering atomic-scale phenomena, the BOM cannot distinguish a C2v symmetric NCA superlattice such as InAs/GaSb from a D2d symmetric CA superlattice such as AlAs-GaAs at the (001)-oriented
Figure 3: A (10,10) (110)-oriented InAs/GaSb superlattice. (a) Subband structure calculated with the BOM method. (b) Subband structure calculated with the MBOM method.

Figure 4: The InAs/GaSb superlattice band structures along the growth direction are calculated with the MBOM method. (a) A (10,10) (001)-oriented InAs/GaSb superlattice. (b) A (10,10) (111)-oriented InAs/GaSb superlattice. (c) A (15,15) (113)-oriented InAs/GaS super lattice. (d) A (20,20) (115)-oriented InAs/GaSb superlattice.

heterostructures. The (111) CA superlattices have the $D_{3d}$ symmetry. When considering the inversion asymmetry effect at the interfaces, the (111) NCA superlattices have a symmetry reduction from $D_{3d}$ to $C_{3v}$. The difference between the CA and NCA superlattices stems from the inequivalence of the interfaces between the well and barrier host materials.

**Dresselhaus-like Spin Splitting**

For the (u,u) InAs/GaSb superlattices grown along the [110] direction, each interface has an equal number of heterobonds (In-Sb and Ga-As). Therefore, the additional potential matrix $\Delta V_{6\times6}$ in the spin-orbit coupling bond orbital basis at the interfaces is given as

$$\Delta V_{6\times6} = \begin{bmatrix} \frac{1}{2}\Delta U & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2}\Delta U & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2}\Delta V & \frac{\pm 1}{2\sqrt{3}}\Delta V & \frac{\pm 1}{2\sqrt{3}}\Delta V & 0 \\ 0 & 0 & \frac{\pm 1}{2\sqrt{3}}\Delta V & \frac{\pm 1}{2\sqrt{3}}\Delta V & \frac{\pm 1}{2\sqrt{3}}\Delta V & 0 \\ 0 & 0 & 0 & \frac{3}{2}\Delta V & 0 & \frac{3}{2}\Delta V \\ 0 & 0 & 0 & 0 & \frac{1}{2}\Delta V & \frac{1}{2}\Delta V \end{bmatrix},$$

Note that the upper sign of the additional matrices is used for the Mth and Nth interfacial monolayers with $N=M+u$, and the lower sign is used for the $(M+1)$th and $(N+1)$th monolayers.

For the (10,10) InAs/GaSb superlattice grown on the (110) substrate, the band structure in the growth direction calculated by the BOM and MBOM is illustrated in Fig.3(a) and 3(b), respectively. Moreover, the
spin splitting along the growth direction is shown in the MBOM band structure.

The degeneracy bands of the zinc-blende bulk are lifted [6] except for the wave vectors along the <001> and <111> directions, and this is the so-called Dresselhaus effect. Along the growth direction of the NCA superlattices, the microscopic symmetry reduction at the interfacial unit-cells is found due to the existence of heterobonds. This microscopic potential perturbation leads to the bulk-like or Dresselhaus-like spin-splitting which is an intracell phenomenon. Therefore, the results of the Dresselhaus-like effect are shown in Fig.4(a) to 4(d) for various growth directions of InAs/GaSb superlattices.

**Conclusion**

The possibility of tailoring the electronic and optical properties of semiconductor devices can be obtained through symmetry breaking. In addition to the growth direction, the structure asymmetry, and the strain effect, the interface heterobonds may offer another degree of freedom for varying the symmetry. It may open a new frontier for future application.

**REFERENCES**