Calculation of the Valence Band Structure in Strained In$_{0.7}$Ga$_{0.3}$As Devices with Different Surface Orientation

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Abstract—Using the eight-band k·p Hamiltonian approach, the valence band structure of strained In$_{0.7}$Ga$_{0.3}$As is calculated for (001), (110) and (111) orientation. The impact of biaxial strain and uniaxial strain on energy band splitting and warping is investigated. The dependency of the valence band structure on the surface electric field and body thickness is also studied in this work.

Keywords—eight-band k·p method; In$_{0.7}$Ga$_{0.3}$As; biaxial strain; uniaxial strain; body thickness

I. INTRODUCTION

III-V compound semiconductors are promising candidates for replacing Si channels beyond the 16-nm node due to its high electron mobility [1]. Recently, high Indium In$_{1-x}$Ga$_x$As has received a lot of attention. Especially, In$_{0.7}$Ga$_{0.3}$As planner thin body MOSFETs, FinFETs or tri-gate, gate-all-around nanowire MOSFETs and Tunneling FETs have been demonstrated experimentally and exhibited outstanding performance for electron transport [2-5]. However, the hole mobility in III-V materials tends to be inferior to strained Si. The large gap between electron and hole mobility for III-V semiconductor becomes an important issue for CMOS application. This necessitates the application of performance boosters such as strain engineer to enhance the hole mobility [6-8]. Furthermore, it is meaningful to select and orient the band structure to yield better properties. Hence in this work, the impact of electric field and body thickness on the valence band structure in In$_{0.7}$Ga$_{0.3}$As devices with (001), (110) and (111) orientation is evaluated. We also study strain effects, including both biaxial strain and uniaxial strain, on valence band structure of In$_{0.7}$Ga$_{0.3}$As devices. The results can be helpful to optimize the design of In$_{0.7}$Ga$_{0.3}$As based devices.

II. SIMULATION METHOD

The valence band structure of strained semiconductor devices under electric field can be calculated by the 8×8 k·p Hamiltonian approach [9], employing a triangular well approximation and assuming an infinite barrier height at both side of the In$_{0.7}$Ga$_{0.3}$As. Considering the quantum confinement, k$_z$ is transformed to −id/dz and coordinate z is perpendicular to the interface. The discretization process of eight-band Hamiltonian is obtained by finite difference method [10]. The space of the in-plane vectors K is discretized by building a mesh in polar coordinates. For calculation of the density of states (DOS), the equi-energy lines corresponding to a given energy are calculated. This can be accomplished by inverting the k·p model in order to obtain an eigenvalue problem for the wave-vector K of rank twice as large as the rank of the original problem. When dealing with different crystal orientation, appropriate rotations of the k space are performed. We take [110] as the channel direction since this is common in PMOS technology. For strained In$_{0.7}$Ga$_{0.3}$As, we consider two cases of technological interest, namely 1) a device under biaxial strain (global strain) due to lattice mismatch and 2) a device stressed by source and drain stressors, inducing uniaxial stress along the channel direction.

Band parameters and deformation potentials for GaAs and InAs are taken from Ref. [11]. All the parameters for In$_{0.7}$Ga$_{0.3}$As are taken as linear interpolation of those of GaAs and InAs except that for the strained energy gap as following [12]:

\[ E_{\text{g}}(\text{In}_{1-x}\text{Ga}_x\text{As}) = 0.324 + 0.7x + 0.4x^2 + (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}). \]

![Fig.1](image-url) (a) The valence band structure for a bulk In$_{0.7}$Ga$_{0.3}$As (biaxial tension) on InP. (b) The valence subband structure for a 9.4 nm thick In$_{0.7}$Ga$_{0.3}$As (lattice matched).

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III. RESULTS AND DISCUSSION

A. Orientation Dependency

Fig.2 (a-c) illustrate the valence subband structure of a 5nm-thick In$_{0.7}$Ga$_{0.3}$As with (001), (110) and (111) orientation. Fig.2 (d-f) present the energy contours in kx-ky plane for the top two subbands (n=1, 2) with corresponding orientation. The strong non-parabolic in-plane energy dispersion is shown for the topmost subband with three orientations. It is clearly seen that (110) orientation has a lower symmetry than (001) and (111) orientation, and the top two subbands maintain their strong anisotropy.

Fig.3 (a)-(c) shows the valence subband structure for In$_{0.7}$Ga$_{0.3}$As under surface electric field $F_S$ of 1MV/cm with (001), (110) and (111) orientations. For ground-state subband (n=1) energy at $\Gamma$ point (k=0), it is observed that $E_0(111) > E_0(110) > E_0(001)$. The surface electric field breaks the inversion symmetry of the zinc-blend crystal and leads to a spin split [14]. In Fig.3 [(d)-(f)], the topmost subband energy shift at $\Gamma$ point versus $F_S$ is plotted for different orientation. With the increase of $F_S$, there is a crossing point where HH2 and LH1 change position for (001) and (111) orientations. The subband energy shift trend with surface electric field is (001)~(110)~(111).

In Fig.4, the topmost three subband energies at $\Gamma$ point versus body thickness are presented for In$_{0.7}$Ga$_{0.3}$As with (001), (110) and (111) orientation. Surface electric field $F_S$ of 1MV/cm (black solid lines) and 0MV/cm (blue dashed lines) are compared. There is a crossing of the HH2 and LH1 for all orientations as $T_{body}$ is decreased.

Fig.5 Effective quantization mass $m_z^*$ for In$_{0.7}$Ga$_{0.3}$As, which is calculated by fitting energy at $\Gamma$ point to the analytical expression: $E_n = \left( \frac{n}{2m_z^*} \right) \pi^2 / T_{body}$. 

![Fig.2 Valence subband structure of a 5nm thick In$_{0.7}$Ga$_{0.3}$As plotted for (001), (110) and (111) surface orientation (a-c). Equi-energy contours of top two subbands (n=1,2) are plotted for corresponding orientation. The energies are plotted for 25, 50, 75, 100meV below band-edge E(0).](image)

![Fig.3 Valence band structures for 5 nm thick In$_{0.7}$Ga$_{0.3}$As under surface electric field $F_S$=1MV/cm [(a)-(c)]. The subband energy shifts at $\Gamma$ point of top three subband versus electric field $F_S$ with (001), (110) and (111) orientations are plotted in [(d)-(f)].](image)

![Fig.5 Effective quantization mass $m_z^*$ for In$_{0.7}$Ga$_{0.3}$As, which is calculated by fitting energy at $\Gamma$ point to the analytical expression: $E_n = \left( \frac{n}{2m_z^*} \right) \pi^2 / T_{body}$.](image)
B. Strain Effect

Fig 6 (a)-(e) show the valence subband structures for unstressed and 1GPa tensile/compressive stressed In$_{0.7}$Ga$_{0.3}$As with electric field $F_S$ of 1MV/cm respectively. The band structures are plotted along the [110] direction. Strain shifts and warps the valence subband structure. For both biaxial and uniaxial strain, compressive strain pushes the subband upward and warps the band sharply which is beneficial to reduce the hole effective mass and improve hole mobility. Under tensile strain condition, the subbands are shifted downward and become more flat. For biaxial strain, Energy shift and subband warping is strongest for (001) orientation, followed by (111) and (001) orientation. While for uniaxial strain, the trend is (110)>(001)>(111).

Besides, as is illustrated in Fig. 6 (b) and (d), the uniaxial strain induces larger energy shift and more sharp band warping than biaxial strain. To explain this, equi-energy contours are plotted for stressed (001) oriented In$_{0.7}$Ga$_{0.3}$As with $F_S=1$MV/cm in Fig. 7 (a)-(d). Comparing to biaxial strain, the presence of shear component for uniaxial strain contributes to different band warping and results in an in-plane repopulation of the carriers. Uniaxial compression leads to a carrier repopulation from high transport $m^*_h$ regions R2, R4 to low transport $m^*_h$ regions R1, R3.

Fig. 8 shows the density of states (DOS) for (001) oriented In$_{0.7}$Ga$_{0.3}$As. Fig. 8 (a) and (b) are plotted for relaxed In$_{0.7}$Ga$_{0.3}$As with $F_S=0$MV/cm and $F_S=1$MV/cm, and the surface electric field reduces the DOS. Under compressive strain (Fig. 8 (c) and (e)), DOS decreases. On the contrary, compressive strain (Fig. 8 (d) and (f)) increases the DOS.

Fig. 9 (a) and (b) show the top three valence subband energies at $\Gamma$ point versus biaxial and uniaxial stress for (001) oriented In$_{0.7}$Ga$_{0.3}$As with electric field $F_S$ of 0MV/cm and
In biaxial tension case, there are two critical stresses. At first critical stress, the position between the HH2 and LH1 is changed. Beyond the second critical stress, LH1 becomes the ground-state. According to our calculation, strain effects on (110) and (110) orientations have the similar tendency of energy shift as (001) orientation. The critical stress for different orientation is exhibited in TABLE 1.

**TABLE 1 CRITICAL STRESS FOR SUBBAND CROSSING UNDER BIAXIAL TENSION CASE**

<table>
<thead>
<tr>
<th>Orientation</th>
<th>(001)</th>
<th>(110)</th>
<th>(111)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1ˢᵗ crossing(GPa)</td>
<td>0.4</td>
<td>5.2</td>
<td>4.4</td>
</tr>
<tr>
<td>2ⁿᵈ crossing(GPa)</td>
<td>3.6</td>
<td>6.0</td>
<td>6.4</td>
</tr>
</tbody>
</table>

IV. CONCLUSION

The dependency of the valence subband structure on orientation, surface electric field and body thickness in In₀.₇Ga₀.₃As devices is presented. Electric field and body thickness have smallest impact on (110) orientation, due to its large effective quantization mass mₑ, followed by (111) and (001) orientations. For the biaxial strain, the strain effects on the modulation of the band structure: (001)>(110)>(111) orientation. While for the uniaxial strain: (110)>(001)>(111) orientation, resulting from the smallest transport mₑ along [110] direction for (110) orientation. Both biaxial and uniaxial compressive strain is beneficial to reduce the hole effective mass and may be advantageous to improve the hole mobility. Especially, the uniaxial compression leads to not only more band warping than biaxial strain but a carrier repopulation from high transport effective mass region to low transport effective mass region.

**REFERENCES**


