Energy band design for p-type tensile strained Si/SiGe multi-quantum well infrared photodetector*

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The band structure of the confined states is calculated for Si/SiGe multi-quantum well infrared photodetector (M-QWIP). The influence of the Ge component in pseudosubstrate on the energy band structure of $Si/Si_{0.54}Ge_{0.46}$ multi-quantum wells (MQWs) is investigated. It is found that the high energy levels in the MQWs move up while the low energy levels move down as the Ge component in pseudosubstrate increases. The influence of the barrier width on the energy band structure of MQWs is also studied based on the 6 × 6 k·p method. The results show that the Si barrier between 5 nm and 10 nm is optimized to enhance the intersubband absorption in the MQWs.

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Multi-quantum well infrared photodetector (M-QWIP) has attracted extensive interests in recent decades[1-7]. Various lasers and photodetectors have been invented based on Ⅲ-Ⅴ materials (such as GaAs). However, the technologies applied in the Ⅲ-Ⅴ devices are incompatible with the mature silicon-based micro-electronics technology. Thus, a new infrared radiation (IR) detector, Si-based Si/SiGe QWIP, which takes advantage of the intersubband transitions among the confined states of multi-quantum wells (MQWs), has been proposed. Compared with the IR detector based on III-V materials, Si-based Si/SiGe QWIP is completely compatible with Si-based micro-electronics technology including on-chip integration of SiGe focal-plane arrays with Si readout circuits. Promisingly, the detector will make a great impact on the development of terahertz detecting devices and will indicate a possible way to integrate active device into silicon-based technology[8].

The design for optimizing energy band structure of MQWs could be feasible by the utilization of SiGe pseudosubstrate with different strains and Si barrier with different thicknesses[8]. Therefore, the strain of pseudosubstrate and the thickness of barrier play important roles in the function of Si-based Si/SiGe QWIP. However, so far there have been few relative reports. In this paper, we investigate the influence of the Ge component in pseudosubstrate and the thickness of barrier layer of MQWs on the band structure of the Si/SiGe QWIP. Here, using 6×6 k·p method, the band structure of 4-period Si/SiGe MQWs grown on $Si_{1-y}Ge_y$ ($y \geqslant 0.5$) pseudosubstrate is calculated by nextnano^3 software. The influence of the thickness of barrier layer in the range of 3−20 nm is also discussed.

Our calculation on valence-subband structure (heavy holes, light holes and spin-orbit subbands) is based on the 6×6 k·p theory[9], and the influence of the conduction band (CB) of MQWs on its valence band (VB) is neglected. The used software is based on the self-consistent calculation of Poisson equation and the 6 × 6 k·p model.

Taking the spin-orbit interaction into account, the VB in the center of Brillouin zone of bulk SiGe is fourfold degenerate[10]. Compared with the previous work[9], we quantitatively investigate the influence of the Ge component in pseudosubstrate on the valence-subband of MQWs by gradually changing the Ge component.

In Fig.1, we calculate the valence-subband structure of 4-period $Si/Si_{0.54}Ge_{0.46}$ MQWs grown on $Si_{1-y}Ge_y$ ($y \geqslant 0.5$) pseudosubstrate. The thicknesses of the well and barrier of MQWs are assumed to be 7 nm and 10 nm, respectively, and the Ge component in $Si_{1-y}Ge_y$ ($y \geqslant 0.5$) pseudosubstrate is

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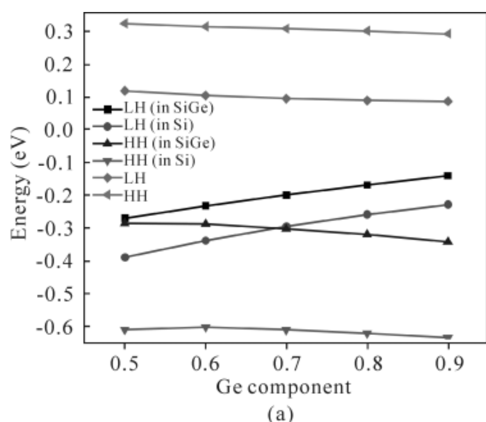
chosen to be 0.5, 0.6, 0.7, 0.8 and 0.9, respectively.

As shown in Fig.1(a), the band edge of light hole subband (LH) in Si is lower than that of heavy hole subband (HH) in SiGe when the Ge component in pseudosubstrate is 0.5. And partial energy overlapping is found between the LH and HH wells of VB. The band edges of HH in SiGe and Si move down, while the band edges of LH in SiGe and Si move up as the Ge component increases. The data also suggests that if we increase the Ge component larger than y = 0.5, the band edge of HH in SiGe drops close to that of LH in SiGe. And then they overlap with each other at y = 0.7. As the Ge component increases further, the band edge of HH in SiGe will cross over that of LH in Si, which means that the overlapping between LH and HH wells disappears. In addition, an obvious decrease of LH and HH offsets can be observed (LH offset: 36 meV; HH offset: 32 meV) when the Ge component increases from 0.5 to 0.9.

In Fig.1(b), the influence of the Ge component in $Si_{1-y}Ge_y$ ($y\geqslant 0.5$) pseudosubstrate on the valence-subband structure and the band edge of LH in MQWs is exhibited. In 4-period Si/SiGe MQWs, one valence-subband will split into four different energy levels due to the interaction between the adjacent QWs. Therefore, there are sixteen eigenenergy levels coming from the four split LH and HH subbands (LH1, LH2, HH1, HH2). We only plot eight energy levels considering the similarity of the sixteen ones. Note that the energy of the two lowest LH drops gradually as the Ge component increases. The energy of the two lowest HH rises rapidly when the Ge component increases from 0.5 to 0.7, and then drops down gradually as the Ge component increases further. From Fig.1(b), two conclusions can be obtained: First, the Ge component at 0.7 is a key point for all curves except for LH1 and LH3, and there are obviously different variation trends on each side of this key point; Second, increasing Ge component will push the high energy levels upwards, and push the low energy levels downwards.

It is worth noticing that HH1 and HH3 do not agree with the second conclusion. As the Ge component of pseudosubstrate increases, the tensile strain increases the difference between the band edges of LH and HH in SiGe, and the two lowest HH states (HH1, HH3) rise rapidly consequently. Because the band edge of HH in SiGe will cross over that of LH in Si when the Ge component is larger than 0.7, the overlapping between two hole wells (LH and HH wells) disappears. Therefore we only need to consider the confinement of HH well for HH1 and HH3, and the variation trend of HH1 and HH3 will be similar to that of LH1 and LH3.



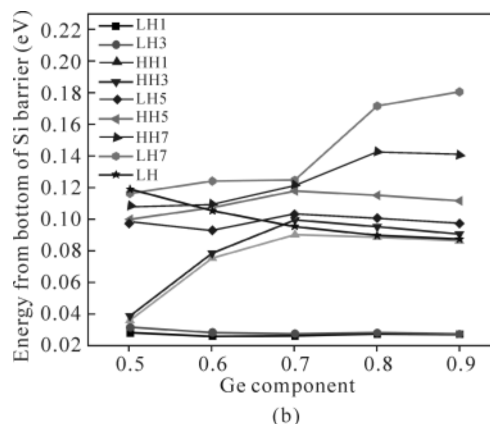


Fig.1(a) LH and HH band edges in Si and $Si_{0.54}Ge_{0.46}$ and their band offsets versus Ge component in $Si_{1-y}Ge_y$($y\geqslant 0.5$) pseudosubstrate (The zero energy is taken at Fermi energy.); (b) LH offset and valence-subband energy levels of tensile strained Si/$Si_{0.54}Ge_{0.46}$ MQWs versus Ge component in $Si_{1-y}Ge_y$($y\geqslant 0.5$) pseudosubstrate (The zero energy is taken at LH band edge in SiGe layer.)

Generally, the tensile strain could push the light hole state upwards to the ground state. But there are still other problems with the tensile strain increasing in SiGe MQWs. For example, excessively high tensile strain will lead to the weakening of the confinement of LH well and the reduction of intersubband transitions between the ground hole state and the quasi-bound hole state. In realistic devices, selecting appropriate Ge component for pseudosubstrate is very important for an infrared photodetector operating at specific wavelength to obtain required band offset and accurate band edge of LH.

Many theoretical and experimental investigations have demonstrated that Si/SiGe single QW could not produce large enough photocurrent for the actual application due to its low absorption coefficient[11]. In order to improve the absorption coefficient, more multi-periodic Si/SiGe QWs should be manufactured. MQWs can extend the absorbing region effectively, and can also improve the coupling efficiency by selecting the appropriate barrier width.

Hence, we calculate the band structure of Si/$Si_{0.54}Ge_{0.46}$ MQWs grown on the $Si_{0.5}Ge_{0.5}$ pseudosubstrate. The well width and the period are chosen to be 7 nm and 4 respectively,

and the barrier width is set to be 3, 5, 8, 15 and 20 nm, respectively.

Fig.2(a) shows the relationship between the barrier width and the light and heavy hole band edges (LH(in SiGe), LH (in Si), HH(in SiGe), HH(in Si)) as well as the band offsets (LH, HH) of Si and SiGe alloys. Fig.2(b) displays the influence of the barrier width on the energy levels in the MQWs. When the barrier width of MQWs is less than 5 nm, an obvious change of energy levels in LH well can be observed as barrier width increases. The low energy levels (such as LH1 and HH1) move up while the high energy levels (such as LH7) move down when the barrier width increasing[12]. With the barrier width increasing from 5 nm to 10 nm, the energy of LH1 and HH1 remains flat, while the energy of LH7 decreases. When the barrier width is larger than 10 nm, all hole states are unaffected by the change of barrier width.

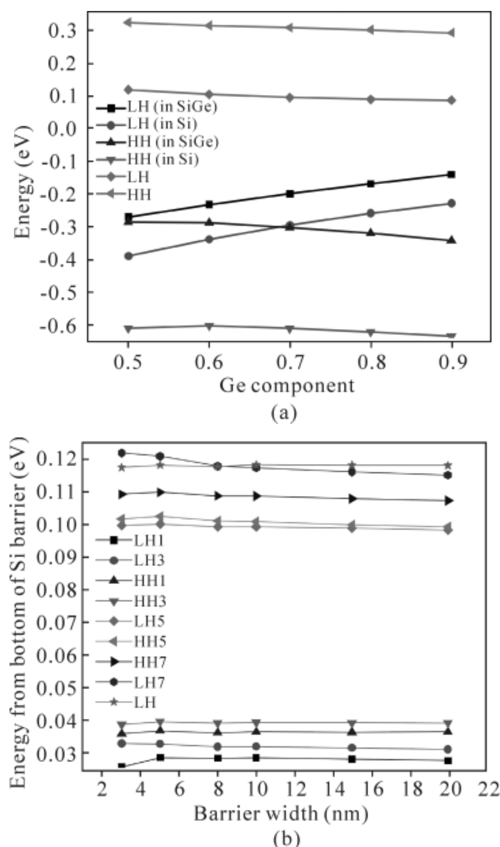


Fig.2(a) LH and HH band edges and their offsets versus the barrier width (The zero energy is taken at Fermi energy.); (b) Energy levels in quantum well versus the barrier width (The zero energy is taken at LH band edge in SiGe layer.)

Based on the above analysis, the selection of barrier width plays an important role in enhancing the absorption of valence-subband in Si/SiGe MQWs. Too thick barrier may suppress the formation of hole subbands, and will reduce the proportion of effective absorption region in the MQWs structure, and therefore results in lower quantum efficiency. Because the QWIP should operate under a fixed negative bias, if the barrier is too thin, the reverse electric field will push the hole tunneling through the barrier and directly affects the function of infrared photodetector. Therefore, there is only a narrow range of barrier width that we can choose for a specific M-QWIP structure.

In conclusion, the valence-subband structure of Si/SiGe MQWs is calculated in order to optimize the energy band design of Si/SiGe M-QWIP. We investigate the influence of the Ge component in pseudosubstrate and barrier width on the valence-subband structure of $Si/Si_{0.54}Ge_{0.46}$ MQWs. Our calculation suggests that the Ge component at 0.7 is a key point for all curves except for LH1 and LH3. On each side of Ge component 0.7, there are obviously different variation trends for different energy levels. In addition, we find that the Si barrier in the range from 5 nm to10 nm could be optimized to enhance the absorption of the inter-subband transitions in the p-type Si/SiGe MQWs.

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