BAND STRUCTURES AND OPTICAL GAIN OF DIRECT-BANDGAP TENSILE STRAINED GE/$GE_{1-X-Y}SI_XSN_Y$ TYPE I QUANTUM WELLS

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Introduction

Recently, Ge/GeSiSn has been received great attention due to its potential applications in silicon photonics [1]. Menendez *et. al*. theoretically predict that the fully tensile strained Ge layers grown on relaxed GeSiSn alloys can have a direct fundamental band gap and the Ge/GeSiSn heterostructures have type I band lineup [2]. Chang *et. al*. report the optical gain calculation of $Ge/Ge_{0.75}Si_{0.05}Sn_{0.2}$ quantum well lasers using 4-band k.p method under the axial approximation. [3]. However, they have to estimate the band gap of GeSiSn using interpolation among those of Ge, Si, and Sn due to lack of material parameters of GeSiSn. Yin *et. al*. calculate the bowing factors of GeSn alloys using the first-principle method [4] and V. R. D'Costa et. al. use ellipsometric data to extract the bowing factors of GeSn, GeSi and SiSn [5-6]. They find that the bowing factors of SnGe, SiSn are very large, b_{SnGe}=2.55 eV [4] and b_{SnGe}=3.05 eV [5], which can influence the band gap significantly. Therefore, it is meaningful to investigate the band structures and optical gain of Ge/GeSiSn quantum wells (QWs) considering the bowing factors. In this paper, the band structure and optical gain of the direct-bandgap tensile strained $Ge/Ge_{1-x-y}Si_xSn_y$ type I quantum well are investigated by using a 6-band k.p method without the axial approximation.

Method

The 6-band Hamiltonian from Ref [7] is adopted. The band gap of $Ge_{1-x-y}Si_xSn_y$ is

$$Eg^{\Gamma}(alloy)=Eg_{Ge}(1-x-y)+Eg_{Si}x+Eg_{Sn}y -b_{GeSi}(1-x-y)x-b_{GeSn}(1-x-y)y-b_{SiSn}xy \quad (1)$$

The bowing factor b_{GeSi}=0.14 from Ref [5], b_{GeSn}=2.55 from Ref [4], b_{SiSn}=3.05 from Ref [5]. Other parameters used in the calculation are listed in Table I.

Table I. The band parameters at 300K for bulk α-Sn, Ge, and Si.

Parameter	Sn	Ge	Si
a (Å)	6.4892	5.6573	5.4307
m_c (m_0) -0.058	0.038	0.528	
γ_1	-15	13.38	4.22
γ_2	-11.45	4.24	0.39
γ_3	-8.55	5.69	1.44
E_p (eV)	24.0	26.3	21.6
E_g^{Γ} (eV)	-0.413	0.7985	4.185
Eg^L (eV)	0.092	0.664	1.65
Δ (eV)	0.8	0.29	0.044
a_c (eV)	-5.33	-8.24	1.98
a_v (eV)	1.55	1.24	2.46
a_L (eV)	?	-1.54	-0.66
b (eV)	-2.7	-2.9	-2.1
C_{11} (10 GPa)	6.9	12.853	16.577
C_{12} (10 GPa)	2.9	4.826	6.393
n_r	4.90	4.02	3.45

Results and Discussion

The band lineups of three Ge/GeSiSn are calculated by model solid theory and shown is Fig. 1. With increasing Sn composition from 0.2 to 0.3, the tensile strain in Ge layer increases and band gap of Ge decrease. The band lineup for the strained Ge on relaxed GeSiSn is type I. The E-K curves of Ge/GeSiSn QWs with well width of 80 Å and barrier width of 200 Å are obtained and shown in Fig2. The Si composition is fixed at 0.15. Sn composition is changed from 0.2 to 0.3. We take hole energy positive. The

origin is at the top of valence band after hydrostatic strain.

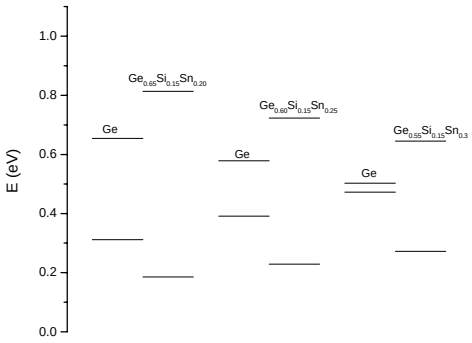

Fig. 1. The band lineups of Ge/GeSiSn.

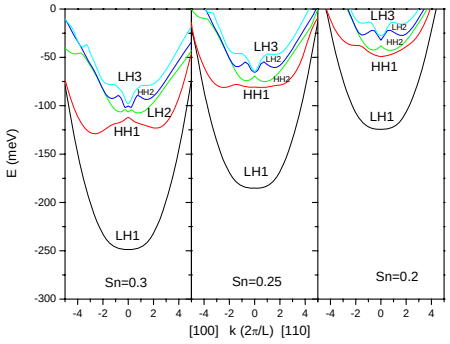

Fig. 2. The hole energy dispersion curves of 80 Å/200 Å Ge/GeSiSn QWs.

When the Sn composition increases from 0.2 to 0.3, the tensile strain in Ge well will increase from 0.0234 to 0.0381, which causes the light hole band moves down (move to conduction band). For Sn composition y=0.3 case, the larger tensile strain results in the third hole energy level LH2 not HH2 like the other two cases. The TM mode optical gain spectra are calculated for 80 Å/200 Å Ge/GeSiSn QWs at n=6x10^{18} cm^{-3}, see Fig. 2. TE mode gain is very small, not shown in Fig. 2. When y increases from 0.2 to 0.3, the gain peak position is decrease from 490 meV to 175 meV, and the gain is increase from 5529 cm^{-1} to 18240 cm^{-1}. The tensile strain increase causes the Ge well bandgap decrease. When y increases, the band offset of valence band the hole increases, see Fig. 1. Therefore, the light hole confinement is enhanced. So, the peak gain increases when y increases. Note that the peak gain will be greatly reduced if the L conduction subbands is included [3]. However, the trend of the peak gain increase with y is unchanged.

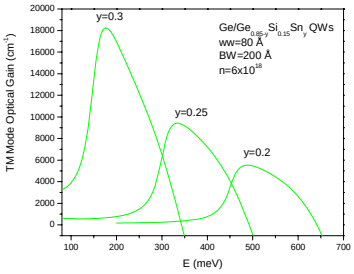

Fig. 3. TM mode optical gain spectra of 80 Å/200 Å Ge/GeSiSn QWs at n=6x10^{18} cm^{-3}.

Conclusion

The band structures and optical gain of tensile strained 80 Å/200 Å Ge/GeSiSn QWs with different Sn composition are investigated. When Sn increases, the bandgap decreases, the Ge becomes direct band gap material, the QWs are type I. Optical gain will crease and the peak position will decreases when increasing Sn composition.

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