ESTIMATION OF THE COMPOSITION OF Ge RICH $Si_{1-x-y}Ge_xC_y$ LAYERS ON Si FOR PHOTODETECTION AT 1.3 AND 1.55 μms

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ABSTRACT

In this work, we explore the possibility of using ternary $Si_{1-x-y}Ge_xC_y$ layer grown on Si as the material for detection of infrared light of wavelengths 1.3 μm and 1.55 μm. By using an empirical expression for the absorption coefficient α, it is ensured that the ternary alloy exhibits the values of α as high as 5000 cm^{-1} at both these wavelengths. From the corresponding values of the band gap, the compositions of the alloy are then ascertained by using an existing theory of band gap and band offset for ternary SiGeC alloy grown on (001) oriented Si.

INTRODUCTION

Almost all electronic circuits are grown today on a silicon substrate in a monolithically integrated form. If it is possible to grow, in addition to electronic devices, light emitters, amplifiers, photodetectors, passive lightwave circuits and other optoelectronic devices on the same Si chip, a truly monolithic optoelectronic integrated circuit may be realized with the benefit of size and cost reduction, improved reliability, etc. Si based optoelectronics [1,2] has, as a consequence, become an important subject for current research.

Passive lightwave circuits using Si and related materials are well developed and are also in industrial use [3]. Intensive research for the realization of efficient light emitters [1,2] using silicon and its alloys has been going on. A significant amount of success has also been achieved in the development of Si based photodetectors [1,2,4]. Because the cut off wavelength of Si is about 1.1 μm, Si based photodetectors are not useful at the standard telecommunication wavelengths of 1.3 and 1.55 μms. The band structure in Si and its alloy is altered in Si/SiGe heterojunctions and quantum wells due to both strain and quantum confinement leading to an effective band gap corresponding to 1.3 μm [5]. Such photodetectors have been grown and investigated thoroughly.

Films of Ge or Ge-rich SiGe alloys grown on a Si substrate or a SiGe buffer have band gap corresponding to the most important telecommunication wavelength of 1.55 μm. In addition, such layers possess high absorption coefficient needed for efficient photodetection. However, as noted already, the large lattice mismatch between Ge or Ge rich alloy and Si make a practical implementation of the structures quite difficult. Since it is known that introduction of a small amount of C, in approximate proportion Ge:C = 8.8:1, reduces the large lattice mismatch, growth and characterization of SiGeC alloys are receiving increased attention from workers [6]. Growth of almost strain free $Si_{0.11}Ge_{0.88}C_{0.01}$ layer on Si and its absorption spectra have been reported by Orner et al [7]. A theoretical study of SiGeC near infrared photodetector having cut off wavelength of 1.2 μm has been made by Li et al [8]. It seems however that photodetectors at 1.3 and 1.55 μms cannot be realized by Si rich ternary alloys.

In the present work, we explore the possibility of using Ge-rich SiGeC layer as a photodetector material both at 1.3 and 1.55 μms. Our approach is to find out the composition of the alloy using the absorption data given by Orner et al. To find the band gap and band offsets, we have used the well known result that the conduction band minima of $Si_{1-x}Ge_x$ lies at L point for $x > 0.85$. On the other hand, van de Walle and Martin [9] concluded that the minima still lies at Δ point in the strained alloy layer over all values of x. We have calculated the composition using their results also. The band alignment and the method of determination of composition are described below.

BAND ALIGNMENT

We follow the method used by Galdin et al [10] to calculate the band lineup. When two semiconductors are joined at a heterojunction, discontinuities occur in the valence band as well as conduction band. Without strain, that is for a lattice-

matched interface, the band lineup problems simply consist of determining how the band structure of the two materials line up at the interface. If the materials are strained, two additional effects have to be considered on the band structure. One is hydrostatic strain, which produces an additional shift of energy position and the other is uniaxial or biaxial strain which splits degenerate bands. So the total change in a band can be expressed as

$$\Delta E = \Delta E_a + \Delta E_h + \Delta E_s \quad (1)$$

where ΔE_a stands for the material differences and ΔE_h is the shift due to hydrostatic strain and ΔE_s is the possible splitting due to uniaxial strain. For ternary $Si_{1-x-y}Ge_xC_y$ on Si(001) interfaces, all terms in "(1)" depend on both x and y.

The hydrostatic contribution to the band shifts is given by

$$\Delta E_h = a_{v,c}(\varepsilon_\perp + 2\varepsilon_\parallel), \quad (2)$$

where $a_{v,c}$ stands for the appropriate hydrostatic deformation potential for the valence or conduction band, respectively and $\varepsilon_\parallel$ and $\varepsilon_\perp$ are given as

$$\varepsilon_\parallel = \frac{a_{Si}}{a(x,y)} - 1 \quad \text{and} \quad \varepsilon_\perp = -2(C_{12}/C_{11})\,\varepsilon_\parallel . \quad (3)$$

In "(3)" a(x,y) [$a(x,y) = a_{Si} + x(a_{Ge} - a_{Si}) + y(a_C - a_{Si})$] is the average lattice constant and C_{12} and C_{11} are the elasticity constants.

For the material dependent term ΔE_a, we have to assume additivity, i.e.,

$$\Delta E_a(x,y) = \Delta E_a(x) + \Delta E_a(y), \quad (4)$$

where $\Delta E_a(x)$ and $\Delta E_a(y)$ can be extracted from the binary $Si_{1-x}Ge_x/Si(001)$ and $Si_{1-y}C_y/Si(001)$ cases, respectively.

The hydrostatic contribution for valence band and conduction band can be calculated from "(2)" with the appropriate values for the conduction band and valence band. For valence band, the alloy dependent terms $\Delta E_a^v(x,0)$ and $\Delta E_a^v(0,y)$ are given by

$$\Delta E_a^v(x,0) = 0.6x - 0.07x^2 \text{ [10]} \quad \text{and} \quad \Delta E_a^v(0,y) = -3.14y \text{ [11]}. \quad (5)$$

In our analysis, the Ge content is always more than 30% and carbon concentration is varied between 1% and 3%. So the layer will be always compressively strained and the highest valence band is the heavy-hole (hh) band caused by the splitting ΔE_s^v ($\Delta E_s^v = \frac{\Delta_{layer}}{3} - \frac{\delta E_v}{2}$), where $\delta E_v = 2b\,(\varepsilon_\perp - \varepsilon_\parallel)$, b is the biaxial deformation potential for the valence band, and Δ is the spin orbit splitting.

Therefore, the valence band discontinuity is obtained as

$$\Delta E_v(x,y) = \Delta E_{hh}(x,y) = \Delta E_{h,v}(x,y) + 0.6x - 0.07x^2 - 3.14y + \Delta E_s^v . \quad (6)$$

To calculate the conduction band minima, first we consider the Ge-rich SiGeC neglecting the splitting of bands. For Ge rich alloys, the band structure of the alloys is assumed resembling that of Ge, i.e., the lowest conduction minima has L character. Following the theory of Galdin [10] and Krishnamurthy et al [12] and using "(2)" and "(4)", we get the conduction band discontinuity as

$$\Delta E_c(x,y) = \Delta E_{h,c}(x,y) + 1.432 - 1.147x + 0.26x^2 - 4.85y . \quad (7)$$

So the band gap discontinuity and the original band gap will be

$$\Delta E_G(x,y) = \Delta E_c(x,y) - \Delta E_v(x,y), \quad \text{and} \quad E_G(x,y) = \Delta E_G(x,y) + E_G^{Ge} . \quad (8)$$

According to van de Walle and Martin, the lowest conduction band in the unstrained alloy has Δ character up to 85% Ge, and becomes L like above that, whereas for alloys on Si(001) substrates, the conduction band at L shows no splitting, and the minimum at Δ is lower over the whole range of alloy compositions. For compressively strained layers the lowest conduction band is fourfold degenerate. So the shift will be given by $\Delta E_s^c = \frac{2}{3}\Xi(\varepsilon_\perp - \varepsilon_\parallel)$, where Ξ is the biaxial deformation potential for the conduction band.

For this case, $\Delta E_a(x,0)$ will be given by

$$\Delta E_a(x,0) = 0.44x - 0.093x^2 \quad (9)$$

So the conduction band discontinuity and the original band gap will be given by

$$\Delta E_c(x,y) = \Delta E_{h,c} - 0.093x^2 - 4.85y + \Delta E_s^c . \qquad \Delta E_G(x,y) = \Delta E_G(x,y) + E_G^{Si} . \tag{10}$$

DETERMINATION OF COMPOSITION

Orner et al [7] have given the following expression for the absorption coefficient that fits the measured values for $Si_{0.11}Ge_{0.88}C_{0.01}$ layer grown by them.

$$\alpha = K\left[\left(\hbar\omega - E_G + \hbar\omega_{ph}\right)^2 + \exp\left(\frac{\hbar\omega_{ph}}{kT}\right)\left(\hbar\omega - E_G - \hbar\omega_{ph}\right)\right], \tag{11}$$

where E_G is the band gap, $\hbar\omega$ is the photon energy, $\hbar\omega_{ph}\,(= 25\text{meV})$ is the energy of the phonon involved and K is a fitting parameter. Here we have discussed only the procedure for the wavelength of 1.3 μm. The same process is applicable for 1.55 μm. The curve a in Fig 1 reproduces the absorption spectra for $Si_{0.11}Ge_{0.88}C_{0.01.}$

We have changed the band gap in such a manner that the values of α become 2000 and 5000 cm^{-1} at photon energy E_λ=0.9538 eV corresponding to λ=1.3 μm. The curves b and c shown in Fig 1 are the absorption spectra giving α_1=2000 cm^{-1} and α_2=5000 cm^{-1} respectively at E_λ. From "(11)" the band gap energies yielding the values α_1 and α_2 at E_λ are respectively E_{G1}=880.76 meV and E_{G2}=841.085 meV.

The next step is to determine the composition of the ternary alloy corresponding to the values of E_G's estimated from the absorption curves and "(11)". As an illustration of the determination of x and y, we have indicated the two band gaps corresponding to α = 2000 and 5000 cm^{-1} as two horizontal lines in Fig. 2. We have then plotted the variation of band gap as a function of x with y as a parameter. In the figure, three values of y (0.01, 0.02, 0.03) as the parameters are shown. The points of intersection of the curves and the horizontal lines give the required values of x for fixed values of y. The values of x and y, so obtained, are given in the tables 2-4. It is seen from the results that the required band gaps corresponding to 1.3 μm and 1.55 μm are obtained with lower concentration of Ge when the theory of van de Walle and Martin is applied.

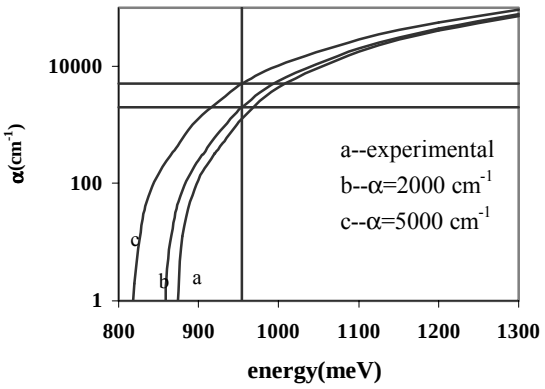

Fig 1. Absorption spectra of $Si_{0.11}Ge_{0.88}C_{0.01.}$

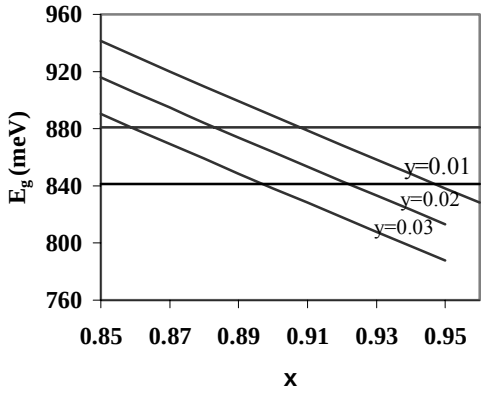

Fig 2. Graphical determination of composition for two band gaps

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Table 1: Values of the parameters used in calculation

Parameter	Si	Ge	C
a(Å)	5.43	5.657	3.567
C_{11}	165.8	128.5	
C_{12}	63.9	48.3	
a_v(eV)	2.46	1.24	
a_c^L (eV)	-0.66	-1.54	
a_c^Δ (eV)	4.18	2.55	
Δ (eV)	0.04	0.3	
b (eV)	-2.35	-2.55	
Ξ (eV)	9.16	9.42	

Table 2: Compositions and band gap for 1.3 μm corresponding to different α [10].

α at 1.3 μm	Band gap (meV)	Compositions of x for		
		y=0.01	y=0.02	y=0.03
2000 cm^{-1}	880.76	0.908	0.883	0.859
5000 cm^{-1}	841.09	0.947	0.922	0.897

Table 3: Compositions and band gap for 1.3 μm corresponding to different α [9].

α at 1.3 μm	Band gap (meV)	Compositions of x for		
		y=0.01	y=0.02	y=0.03
2000 cm^{-1}	880.76	0.426	0.465	0.511
5000 cm^{-1}	841.08	0.478	0.519	0.563

Table 4: Compositions and band gap for 1.55 μm corresponding to different α [9].

α at 1.55 μm	Band gap (meV)	Compositions of x for		
		y=0.01	y=0.02	y=0.03
2000 cm^{-1}	726.96	0.637	0.675	0.72
5000 cm^{-1}	687.29	0.69	0.73	0.78