

## **THE STUDY OF ENERGY BANDGAP AND REFRACTIVE INDEX OF $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ ALLOYS**

N. K. Ali, H. Abu Hassan and M. R. Hashim

*School of Physics  
University Sains Malaysia  
11800 Penang  
MALAYSIA*

*Email: [nalobaidi@hotmail.com](mailto:nalobaidi@hotmail.com)*

### **ABSTRACT**

The addition of C into substitutional sites in  $\text{Si}_{1-x}\text{Ge}_x$  alloys allows one to tailor the strain in the alloys and changes its band structure. This may overcome the critical thickness limitation imposed on  $\text{Si}_{1-x}\text{Ge}_x$  films grown epitaxially on Si [1]. We notice that there are only a few optical studies on strained  $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$  films that examine the band structure of the material. There is no report on the change of the refractive index  $n$  due to the increase of C concentration. Experiments on the individual elements Si, Ge and C reveal an inverse relationship between  $n$  and the indirect bandgap energy  $E_g$ . Therefore, when designing our SiGeC/Si waveguides, we used the guideline  $n(\text{SiGeC}) > n(\text{Si})$  for compositions that have  $E_g(\text{SiGeC}) < E_g(\text{Si})$ . Thus the task of finding  $n$  was replaced by the task of determining  $E_g$  [2]. To calculate the energy bandgap for SiGe alloys we adopted Weber and Alonso [3] expression by adding the exciton binding energy  $E_b(x)$  to the experimentally derived exciton energy gap [4]. The change of energy bandgap of relaxed SiGeC was predicted when the alloys lattice has mismatches of +5%, 0%, -5% with respect to Si [2]. From these studies we carried out three empirical relations for compressive strain, perfect compensation (zero strain) and tensile strain. With the aid of computer programming we can determine the accurate composition of Ge and C content in SiGeC alloy that produce the desired  $n$ . This program facilitates the calculation of SiGeC energy bandgaps and can be used by everyone for the design of waveguide devices. Our results are in agreement with experimental values quoted in literatures.

### **INTRODUCTION**

Although  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  heterostructures have been traditionally used in optoelectronics, for many years due to the availability of heterostructures of both lattice matched and lattice mismatched, it have traditionally faced both fundamental and practical limitations in their application to advanced device technology. These hurdles have been most significantly been the well known critical thickness limitation for pseudomorphic growth and the less known sensitivity of devices to heterojunction process integration. To overcome these hurdles, recently considerable progress has been made in the growth and characterization of  $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$  alloys, which offer greater flexibility, compared to that in the  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ , to control strain and electronic properties in group IV heterostructures. In particular the smaller C atom compensates for the compressive strain present in  $\text{Si}_{1-x}\text{Ge}_x$ , leading to the possibility of

fabricating group IV heterostructures lattice matched to Si substrate [5]. In this paper we will discuss how recent advances in column IV materials such as SiGeC alloys allow us to overcome all of these issues. These issues include critical thickness limitations for dislocation formation, finding the energy bandgap and refractive index of these alloys.

### **Lattice constant and critical thickness**

Although Ge and Si are sharing a common crystal structure, the diamond cubic lattice, they do not have the same lattice constant. The lattice constant of  $\text{Si}_{1-x}\text{Ge}_x$  alloys varies between  $5.431 \text{ \AA}$  for Si ( $x=0$ ) and  $5.657 \text{ \AA}$  for Ge ( $x=1$ ), which can be calculated by the use of Vegard's law. This law expresses the linear interpolation of the lattice constant of alloys as a function of parameter  $x$  defining the Ge content in the alloy. For the binary compound  $\text{Si}_{1-x}\text{Ge}_x$  Vegard's law has the form [6]

$$a(x) = a_{\text{Si}}(1-x) + a_{\text{Ge}}x \quad (1)$$

where  $a(x)$  is the lattice constant of  $\text{Si}_{1-x}\text{Ge}_x$ , for low atomic concentrations ( $x$ ) of Ge. The lattice mismatch between Ge and Si is 4.17%, thus,  $\text{Si}_{1-x}\text{Ge}_x$  alloys cannot be grown epitaxially on Si or Ge substrates without introducing large amounts of strain [7]. There is however, an equilibrium critical thickness ( $h_c$ ) for perfect pseudomorphic growth that depends on the strain in the layer. This thickness is defined as the thickness above which misfit dislocations are generated. It is also depends on the Ge content  $x$ . The critical thickness can be expressed by [8]

$$h_c = \left( \frac{1-\nu}{1+\nu} \right) \left( \frac{1}{20\pi\sqrt{2}} \right) \left[ \frac{b^2}{\langle a(x) \rangle} \right] \left[ \frac{1}{f_m^2(x)} \ln \left( \frac{h_c}{b} \right) \right] \quad (2)$$

where  $\nu$  is the Poisson's ratio ( $\nu = 0.28 - 0.02x$ ) [9],  $b$  the Burger's vector modulus [10] ( $b \approx a(x)/\sqrt{2}$ ),  $\langle a(x) \rangle \approx 0.554 \text{ nm}$  is the mean bulk lattice constant of  $\text{Si}_{1-x}\text{Ge}_x$ , and  $f_m(x)$  is the substrate alloy misfit parameter. For thickness larger than that critical thickness plastic strain-relief mechanism takes place by injecting and moving misfit dislocations[11]. These dislocations can have a large influence on the electronic device properties.

Over the past few years, it has been found that the addition of a few atomic percent of C to form  $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$  alloys allows one to overcome all these disadvantages of the  $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$  material system. It is well known [12] that strain in pseudomorphic  $\text{Si}_{1-x}\text{Ge}_x$  epilayers grown by Molecular Beam Epitaxy (MBE) on Si substrates can be adjusted by adding small amounts of carbon to the growing epilayers. Because of the small size of the carbon atom with a covalent radius much smaller than that of silicon and the larger Ge ( $r_{\text{C}} = 0.77 \text{ \AA}$  while,  $r_{\text{Si}} = 1.17 \text{ \AA}$ , and  $r_{\text{Ge}} = 1.22 \text{ \AA}$ ) open the possibility to manipulate the strain. It was shown that it is possible to form an inversely distorted SiGe cell, i.e. a cell that is tetragonally distorted due to tensile stress instead of the usual compressive stress by adding some carbon [13]. Using simple linear relation between the different lattice constants, Vegard's law for ternary system, we can find the effective lattice constant for the  $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$  alloys. Vegard's law has the form

$$a(xy) = (1-x-y) \times a_{\text{Si}} + xa_{\text{Ge}} + ya_{\text{C}} \quad (3)$$

Assuming that Vegard's law is valid, the misfit parameter  $f_m(x)$  for the  $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$  layers grown on Si substrate can be defined as [6]

$$f_m(x) = \frac{(a_{SiGeC} - a_{Si})}{a_{Si}} \tag{4}$$

From this relation we find Ge:C ratio of 8.2 for complete strain compensation (zero misfit), a positive misfit stands for a compressively strained material, and negative misfit indicates tensile strain. The results of such an estimation are shown in Fig.1. An interesting feature in this figure is the line for zero misfit, one may recognize that approximately one percent of carbon is needed to reduce the effective strain of Ge content equal to 10 percent to be zero. To understand the effect of C on the critical thickness  $h_c$  we plotted  $h_c$  versus the misfit Fig. 2. It is clear that  $h_c \approx \infty$  for zero misfit.

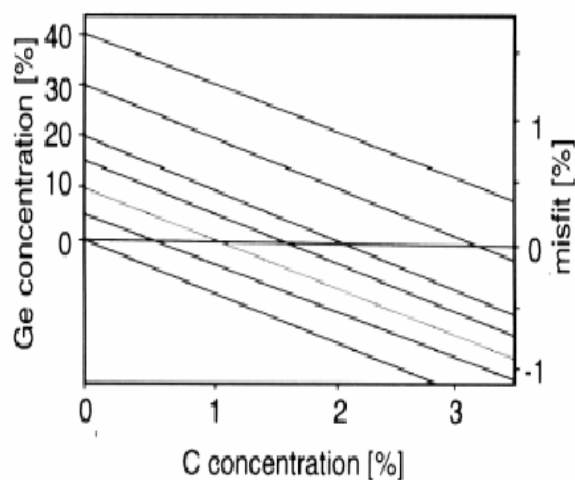


Fig. 1. Estimated misfit reduction in relation to Si for SiGe layers due to the presence of carbon in these layers [6].

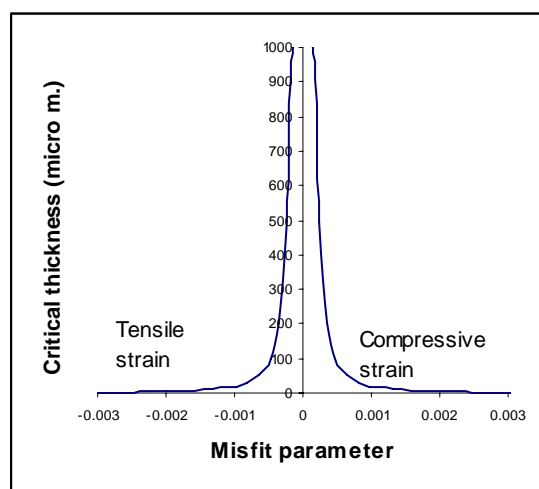


Fig. 2. Critical thickness versus the misfit parameter ( tensile strain and compressive strain ).

### Energy bandgap and refractive index

Germanium and silicon form a continuous series of crystalline materials with gradually varying properties. Refractive indices of both Ge and Si differ by  $\approx 0.6$  in the infrared region. Unfortunately there is a limitation of critical thickness as we discuss above, this limitation prevents the designer to incorporate high Ge concentration, so they proposed C to overcome this hurdles. Now the challenge is how to calculate the refractive indices of these alloys. There is no formula for the change of the refractive index due to the increase of C concentration. Experiments on the individual elements Si, Ge, and C reveal an inverse relationship between  $n$  and the indirect bandgap energy ( $E_g$ ). Thus the task of finding  $n$  was replaced by the task of determining  $E_g$  [2]. These two parameters are the most interesting optical properties of a semiconductor. It is natural that attempts should have been made to find a general relationship between these parameters. Moss (1950) was the first who proposed a general relation based on the concept that in a dielectric energy levels are scaled down by a factor  $1/\epsilon_{opt}^2$ , where  $\epsilon_{opt} = n^2$  is the optical dielectric constant [14]. He proposed

$$E_g(x).n^4 = k \quad \text{with } k = 95 \tag{5}$$

and for particular case of group IV, Moss proposed the relation [15]

$$E_g(x).n^4 = 173 \tag{6}$$

Recently Ravindra et al. [16] have shown that modern experimental data are fitted better if the Moss formula modified to

$$E_g(x).n^4 = 108 \tag{7}$$

Ravindra et al. also proposed an empirical relation but it gives values of  $n$  which are in better agreement with the known values than the Moss relation (5). This relation is given by [17]

$$n = 4.08 - 0.62 E_g(x) \tag{8}$$

This relation was examined by Moss [18] who pointed out that this equation is restricted to energy gaps of less than about 4 eV. and gives unrealistic results for both low and high  $E_g$ .

More recently, Reddy et al. [19] presented a new formula with an exponential behavior quite similar to the Moss relation

$$E_g(x).e^n = 36.3 \tag{9}$$

Soref et al. estimated the index of SiGe alloys with the interpolation formula [20]

$$n(Si_{1-x}Ge_x) = n(Si) + [n(Ge) - n(Si)][E_g(Si) - E_g(x)]/[E_g(Si) - E_g(Ge)] \tag{10}$$

where  $E_g(x)$  is the indirect gap of the  $Si_{1-x}Ge_x$  alloys. We plotted all the relations above in Fig.3. which is the energy bandgap versus the refractive index. It is important to mention that equations(5,6,7,8,9) are estimated for visible light, while, equation (10) calculated for the wavelength  $1.55 \mu m$ .

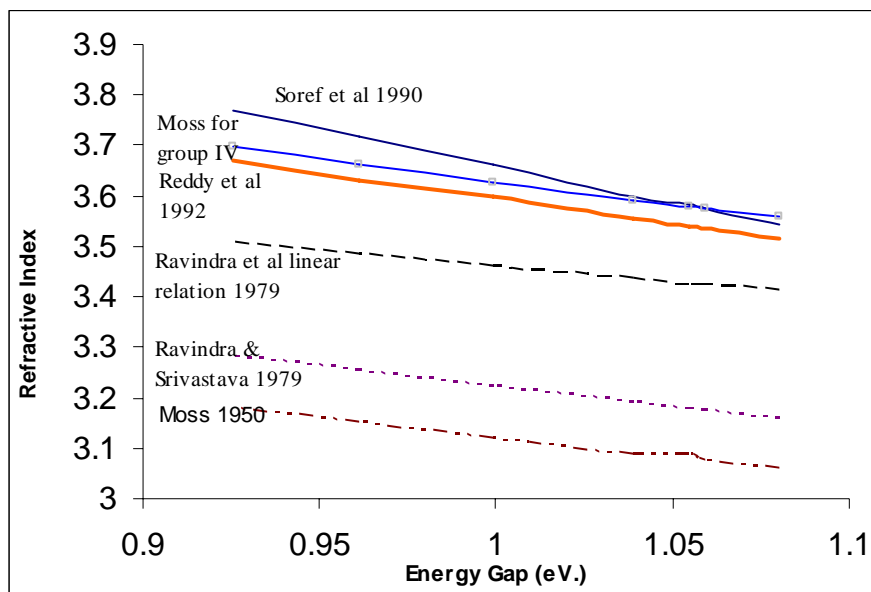


Fig. 3. Energy gap of SiGe alloy versus refractive index for different relations.

To calculate the refractive index of  $Si_{1-x}Ge_x$  alloys we must know the energy gaps which depend on the Ge concentration  $x$ . According to Persall [21], the composition dependence of the strained layer bandgap is given by the analytic relation

$$E_g(x) = 1.1 - 1.02 x + 0.52 x^2 \tag{11}$$

while Levinshtien et al. [9] suggest the relation

$$E_g = 1.12 - 0.41 x + 0.008 x^2 \tag{12}$$

and the systematic study by Weber and Alonso [22] give the following expression for the exciton energy gap in cubic alloys

$$E_{\chi}^c(x) = 1.155 - 0.43x + 0.206x^2 \quad \text{for } x < 0.25 \quad (13)$$

The energy bandgap can be calculated by adding the exciton binding energy  $E_b(x)$  to the experimentally derived exciton energy gap. The energy  $E_b^c$  for  $\text{Si}_{1-x}\text{Ge}_x$  has been calculated between the parameter values for Si and Ge, which can be fitted by a quadratic relation

$$E_b^c(x) = 0.0145 - 0.022x + 0.02x^2 \quad (14)$$

therefore  $E_g^c(x) = E_{\chi}^c(x) + E_b^c(x)$

$$\text{thus } E_g^c(x) = 1.1695 - 0.452x + 0.226x^2 \quad \text{for } x < 0.25 \quad (15)$$

For strained alloy Robbins et al.[23] measurements of exciton energy  $E_{\chi}^s$  where performed with  $x < 0.24$  in the form

$$E_{\chi}^s(x) = 1.155 - 0.874x + 0.376x^2 \quad (16)$$

adding  $E_b^c$  to the measured exciton energy yields

$$E_g^s = 1.1695 - 0.896x + 0.396x^2 \quad (17)$$

In Fig. 4. we plotted the energy bandgap versus the Ge content and compare these relations with the fundamental indirect bandgap of unstrained SiGe alloys given by R. Braunstein [24], and the calculated curves for heavy hole and light hole from R. People [25] and Van de et al. [26] for strained alloys. In this study we adopted relation (15) and relation (17) for unstrained and strained alloys respectively due to their fit with the experimental results as shown in Fig. 4.

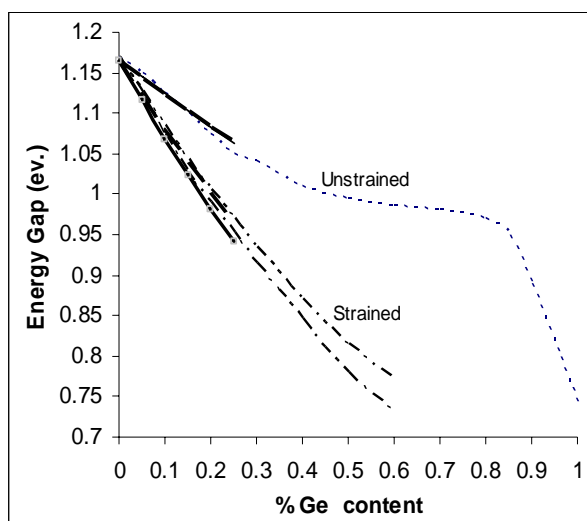


Fig. 4. The dependence of the fundamental indirect bandgap versus Ge content of pseudomorphic SiGe alloys on Si substrate.

As we mention above, in order to reduce the strain and thus increase the critical thickness, C was incorporated to  $\text{Si}_{1-x}\text{Ge}_x$  alloys. This actually will affect the band structure and the energy gap as well as the band offsets significantly. The current knowledge about the band structure

of  $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$  alloys is still limited. Osten [27] proposed an estimation for the band offsets and the fundamental bandgap for  $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$  alloys tensile or compressive strained on Si. This estimation considers both the band lineup at the interface of two different materials as well as the strain effects. Figure (5) and (6) summarize the results for the valance and conduction bands offsets of strained  $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$  on Si respectively, for a layer with 10 % Ge. The carbon concentration was varied between 0 and 3 %, changing the strain from compressive to tensile. In Fig. 5, the change in valence band versus the effective lattice mismatch, several trends become visible. For compressively strained layers the highest valence band is the heavy hole (hh) band. A light hole (lh) band forms the highest valence band for tensile strained materials. The hh band decreases linearly with increasing C concentration for a given Ge concentration. Opposite to that, the dependence of the lh band on C concentration is very weak. Fig. 6. shows the change in the conduction band versus the effective lattice mismatch. For compressively strained layers the lowest conduction band is the four fold degenerated  $\Delta(4)$  band. Opposite the two fold degenerated  $\Delta(2)$  band forms the lowest conduction band for tensile strained materials. Both bands are linear function of the lattice mismatch. The conduction band offsets between tensile strained layers and Si is generally larger than that at the compressive strained layers and Si interface [27].

The bandgap discontinuity  $\Delta E_g$  depends on the strain type. For compressive strained the lowest conduction bands and the highest valence band are  $\Delta(4)$  bands and the hh band, respectively.

$$\Delta E_g = \Delta E_{\Delta(4)} - \Delta E_{hh} \quad (18)$$

while for tensile strained alloys the lowest conduction bands and the highest valence band are  $\Delta(2)$  bands and the lh band, respectively, therefore

$$\Delta E_g = \Delta E_{\Delta(2)} - \Delta E_{lh} \quad (19)$$

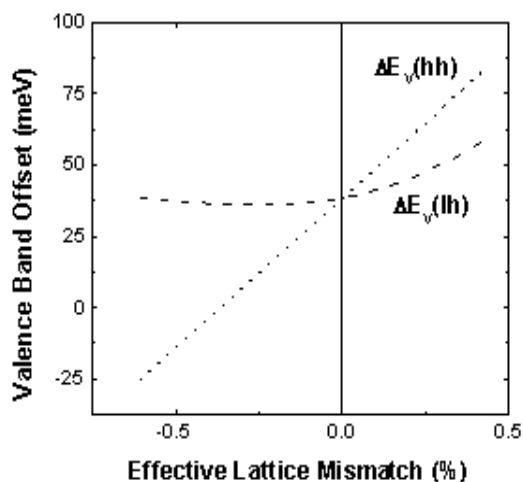


Fig. 5. Valance band offsets for SiGeC layer on Si with 10 % Ge as a function of effective lattice mismatch [27].

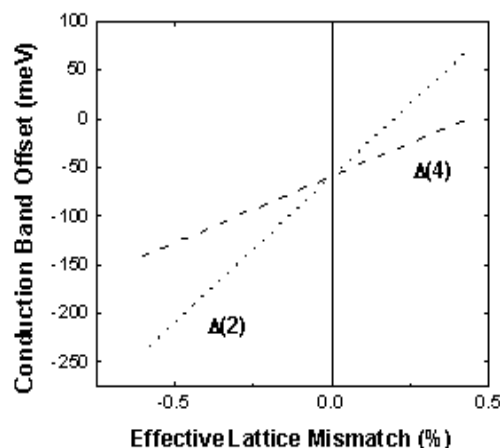


Fig. 6. Conduction band offsets for SiGeC layer on Si with 10 % Ge as a function of effective lattice mismatch [27].

### RESULTS AND DISCUSSION

In this study we adopted the predicted bandgap proposed by Soref [28] for relaxed SiGeC when the alloy's lattice has mismatches of +0.5%, 0.0%, -0.5% with respect to Si, as illustrated in Fig. 7. which was obtained by drawing constant lattice constant lines for the three cases. In this figure the SiGeC gap is less than the Si gap when the C concentration is less than 9 %. However, the change in  $E_g(x,y)$  is not only due to the increase in C concentration (y) but also due to the increase of Ge content (x) which is necessary for constant lattice constant. We determine the Ge content using Vegard's law equation (3) and finding the energy bandgap  $E_g(x)$  for each point in the three lines from equation (15). By subtracting  $E_g(x)$  from  $E_g(x,y)$  we find  $\Delta E_g$ , the effect of C on the energy bandgap of SiGeC alloy. We plotted  $\Delta E_g$  versus C concentration and carried out three empirical relations. For compressive strain ( $y < x/8.2$ ) is

$$\Delta E_g = 263.34 y^2 - 7.527 y \tag{20}$$

while for perfect compensation ( zero strain,  $y = x/8.2$  )

$$\Delta E_g = 84.8 y^2 - 5.312 y \tag{21}$$

and for tensile strain ( $y > x/8.2$  )

$$\Delta E_g = 114.26 y^2 - 7.628 y + 0.022 \tag{22}$$

With the aid of computer programming, we facilitates the calculation of SiGeC energy bandgaps. Opposite to that we can determine the accurate composition of the alloy for the desire n with knowledge of critical thickness. Our results illustrated in Fig. 8, which is the energy bandgap versus C concentration for different Ge content. An interesting feature in this figure is the drop of energy bandgap with the change of strain from compressive to tensile. Table 1. shows the composition of the predicted values of energy gap done by Soref et al. [29] with our calculated results.

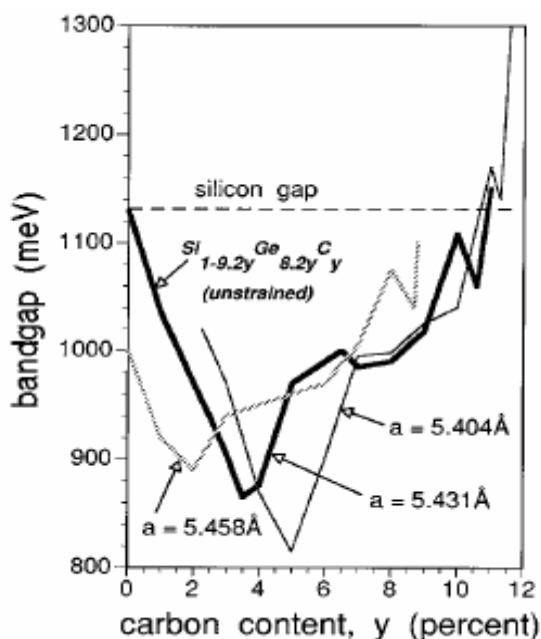


Fig. 7. Bandgap of SiGeC lattice matched, or nearly matched to Si substrate [28].

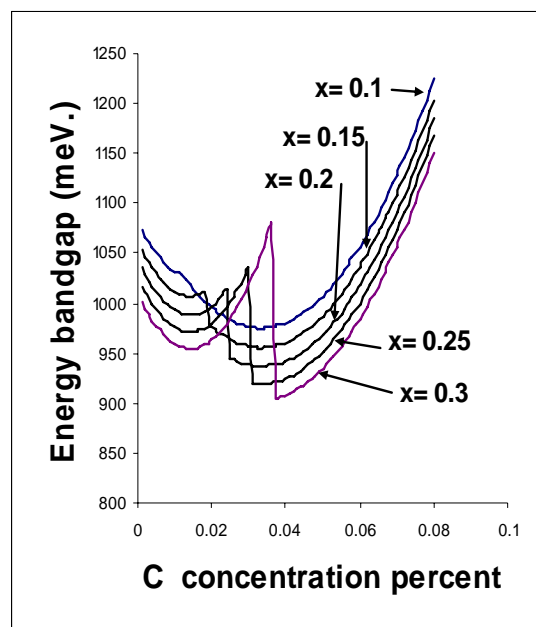


Fig. 8. Bandgap of SiGeC versus carbon percent for different Ge content (x).

Table 1. The dependence of the unstrained alloy bandgap energy  $E_g(x,y)$  on C concentration.

$Si_{1-x-y}Ge_xC_y$ Composition	$E_g$ meV. Soref [29]	$E_g$ meV. Our study
$Si_{.82}Ge_{.16}C_{.02}$	960	971
$Si_{.82}Ge_{.17}C_{.01}$	990	1004
$Si_{.785}Ge_{.205}C_{.01}$	950	991
$Si_{.77}Ge_{.21}C_{.02}$	930	993

## CONCLUSION

Fundamental issues which have limited the development of optoelectronics in the SiGe material system have been discussed. These issues include the critical thickness, the effect of C on the energy bandgap and the most important parameter  $n$  of SiGeC alloys. Knowledge of  $n$  was replaced by finding the energy bandgap. Three empirical relations were carried out for compressive strain, perfect compensation (zero strain) and tensile strain. With the aid of computer programming we can determine the accurate composition of Ge and C content in SiGeC alloy that produce the desired  $n$ . Our results are in agreement with experimental values quoted in literatures.

## ACKNOWLEDGEMENTS

The authors are grateful to School of Physics, USM under an IRPA RMK-8 Strategic Research Grant for supporting this work.

## REFERENCES

- [1] Grimmeiss HG, Olajos J. Phys. Scr. T69, PP.52 (1997).
- [2] R. A. Soref, J. Vac. Sci. Technol. A14(3), PP. 913(1996).
- [3] J. Weber and M. I. Alonso, Phys. Rev. B40, PP. 5683(1989).
- [4] D. J. Robbins, L. T. Canham, S. J. Barnett, A. D. Pitt, and P. Calcott, J. Appl. Phys. 71(3), PP. 1407(1992).
- [5] R. A. Soref, J. Appl. Phys. 70, PP. 2470 (1991).
- [6] M. A. Herman, Crys. Res. Technol. 34, PP. 583 (1999).
- [7] S. C. Jain, Germanium-Silicon strained layers and heterostructures (Academic press, Boston 1994).
- [8] R. People, IEEE J. Quant. Electron. 22, PP. 1696 (1986).
- [9] M. E. Levinshtein, S. L. Rumyantsev, Ms. Shur. Properties of advanced semiconductor materials. (A Wiley- Interscience publication 2001 ).
- [10] Rudiger Lange, S. S. Iyer, A. P. Powell, K. Eberl, J. Appl. Phys. 80 (8), PP. 4578 (1996).
- [11] E. Kasper and H. Jorke, J. Vac. Sci. Technol. A 10, PP. 11927 (1992).
- [12] Osten, H. J., Dietrich, B. , Rucker, H. , Methfesse, M. J. Cryst. Growth, 150. PP. 931 (1995).



- [13] H. J. Osten, E. Bugiel, and P. Zahdmseil, *Appl. Phys. Lett.* 64, PP. 3440 (1994).
- [14] P. Herve and L. K. J. Vandamme, *Infrared Phys. Technol.* V.35, No. 4, PP.609 (1994).
- [15] T. S. Moss, (*Photoconductivity in the elements*,(Academic Press 1952).
- [16] N. M. Ravindra and V. K. Srivstava, *Infrared Phys.* 19, PP. 603 (1979).
- [17] N. M. Ravindra, Sushil, and V. K. Srivastava, *Phys. Stat. Sol. (b)* 93, K 155 (1979).
- [18] T. S. Moss, *Physica Status Solidi (b)*, 131, PP. 415 (1985).
- [19] R. R. Reddy and S. Anjaneyulu, *Phys. Stat. Sol. (b)* 174, K 91 (1992).
- [20] R. A. Soref, R. D. Lareau. *IEEE. Electronics Lett.* Vol. 26, 20, PP. 1633 (1990).
- [21] Persall, T. P. , *CRC Critical review in solid state and materials science*, 15, PP551 (1989).
- [22] J. Weber and M. I. Alonso, *Phys. Rev. B.*Vol. 40, PP.5683 (1989).
- [23] D. J. Robbins, L. T. Canham, S. J. Barnett, A. D. Pitt, P. Calcott, *J. Appl. Phys.* Vol. 71, PP. 1407 (1992).
- [24] R. Braunstein, A. R. Moor, and F. Herman. *Phys. Rev.* 109, PP. 695 (1958).
- [25] R. People, *IEEE. J. of Quant. Electron.* Vol. 22, PP. 1696 (1986).
- [26] Van de Walle, R. M. Martin, *Phys. Rev. B.* Vol. 34, PP. 5621 (1986).
- [27] H. Jorg Osten, *J. of Appl. Phys.* Vol. 84, No. 5, PP. 2716 (1998).
- [28] R. A. Soref, *J. Vac. Sci. Technol. A* 14 (3), PP. 913 (1996).
- [29] R. A. Soref, Z. Atzman, F. Shaapur, Mc D. Robinson, and R. Westhoff, *Optics Letters*, Vol. 21, No. 5, PP.345 (1996).