Theoretical Analysis of Direct Transition in SiGeSn/GeSn Strain Balanced QWIP

Mukul K das, Senior Member IEEE
Electronics engineering department
Indian School of Mines
Dhanbad, Jharkhand,India
das_mkdas@yahoo.co.in

Prakash Pareek
Electronics engineering department
Indian School of Mines
Dhanbad, Jharkhand,India
ppareek1@gmail.com

***Abstract*—This work presents a theoretical analysis of direct transition in strain balanced SiGeSn/GeSn quantum well infrared photodetector. Eigen energies for Γ valley conduction band, heavy hole band and light hole band are obtained from the self consistent solution of coupled Schrödinger and Poisson equations by finite difference method. Absorption spectra for direct transition of heavy hole and light hole band to Γ valley is calculated after evaluating Eigen energies and wave functions.**

I. INTRODUCTION

Silicon and Germanium are the front line materials in the micro electronics integration circuits. But they are not suitable for active optoelctronic devices because of their indirect bandgap nature [1]. However, a small energy difference between indirect valley and direct valley in Germanium (Ge) has triggered the idea of Group IV direct band gap semiconductor through bandgap engineering. Researchers had proposed several approaches to modify the band structure of Germanium like heavy n-type doping, biaxial tensile strain in Ge, incorporation of Sn into Ge etc. Substitution of α-Sn into Ge lattice to form the direct band gap semiconducting $Ge_{1-x}Sn_x$ alloy is the most promising route among all above approaches [2]. For modest Sn concentrations (~10%), this alloy is expected to become the first viable group-IV material with a direct band gap, opening up new opportunities for the integration of opto- and micro electronics [2]. By introducing tensile strain in GeSn, the direct band gap can be obtained at lower concentration of Sn (x=0.4-0.8) as compared to relaxed GeSn [2]. Direct band gap can also be obtained by introducing compressive strain in $Ge_{1-x}Sn_x$ alloys for $x > 0.15$ [3]. Compressive strain enables the defect free epitaxial growth and also enables to achieve the amount of Sn incorporation beyond its solid solubility limit of 1% [2].

Accurate physics based modeling for the devices based on compressively strained GeSn alloy is required to analyze their electronic optical properties before their fabrication. In the present work, a theoretical analysis of direct transition in a strain balanced SiGeSn/GeSn quantum well infrared photodetector (QWIP), where the well is made of compressively strained GeSn alloy, is presented. Strain balanced condition is required to reduce the strain energy which reduces the misfit dislocation in QW [4]. Eigen energies for Γ valley conduction band (Γ-CB), heavy hole (HH) band and light hole (LH) band are obtained by solving self consistently both the Schrödinger and Poisson equations with proper boundary conditions. After obtaining these energies, direct interband transition in the QWIP is determined.

II. THEREOTICAL FORMULATION

The device structure considered in our analysis, consists of tensile strained SiGeSn barriers and compressively strained GeSn well which ensures the strain balanced condition for quantum well. A 76Å thick $Ge_{0.83}Sn_{0.17}$layer is sandwiched between two tensile strained $Si_{0.09}Ge_{0.8}Sn_{0.11}$ layers to form a type-I single quantum-well(QW) as shown in Fig.1. A fully relaxed $Ge_{0.872}Sn_{0.128}$ layer is used as a buffer layer. The width of the barrier layer is determined to be 35 Å by using the strain balanced condition for a cubic based multilayer system [4]. P-$Si_{0.08}Ge_{0.78}Sn_{0.14}$ and n-$Si_{0.08}Ge_{0.78}Sn_{0.14}$ layers as shown in figure, serve as contact layers.

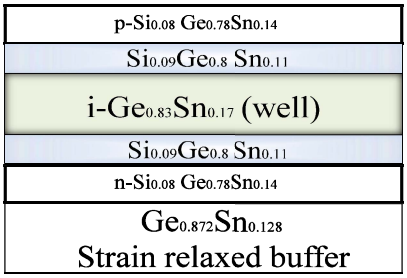


Fig.1 Schematic diagram of strain balanced QWIP

The band profiles for Γ valley conduction band, HH band and LH band were calculated by using Van de Walle's model solid theory [5]. The Schrödinger equation with effective mass approximation, considering the strain effect and electric field F is considered in our analysis and is given as [6]

$$\left(\frac{-\hbar^2}{2} \frac{\partial}{\partial Z} \frac{1}{m_p} \frac{\partial}{\partial Z} + \frac{\hbar^2 K_t^2}{2m_p} + V_p(Z) - qF(z) \right) \psi = E_p \psi \qquad (1)$$

Suffix p stands for type of band e.g., p=c for Γ-CB, p=hh for HH band, p=lh for LH band The equation is solved using Finite Difference Method (FDM) to obtain Eigen energies and wave functions in the well [7]. The whole region of interest is divided into N number of small elements of equal width, Δz and the equation is solved for each of the elements. The

position dependent charge density of carriers in well (electrons in case of CB) is calculated by summing the square of the wave function at each spatial element (Δz) and multiplying this quantity by the number of carriers in each bound state [8]. The obtained charge density is then used in Poisson equation to obtain self consistent potential. Poisson equation relates the potential to the charge density distribution as given in eqn.2

$$\frac{d^2V}{dz^2} = -\frac{q}{\varepsilon}\left(n(z) - p(z) + N_a - N_d\right) \qquad (2)$$

where n(z) and p(z) are the electrons and holes charge density distribution respectively. N_a and N_d are acceptor and doping impurities respectively. Dirichlet and Neumann boundary conditions are considered in solving the Poisson equation. The obtained potential distribution is then again used in Schrödinger equation to obtain Eigen energies and hence, charge density distribution. Let $V_{new}(z)$ be the potential distribution as obtained from the poisson equation and $V_{old}(z)$ be the potential distribution used in the Schrödinger equation. $V_{old}(z)$ is replaced by a new potential, $V_{sc}(z)$, called self consistent potential which is related to $V_{new}(z)$ as follows [9]

$$V_{SC}^{\,i}(z) = V_{old}^{i+1}(z) = V_{old}^{i}(z) + f\left[V_{new}^{i}(z) - V_{old}^{i}(z)\right] \qquad (3)$$

where i is the number of iterations and its values are i=0,1,2…etc. V_{old}^{0} is initial value of potential which is nothing but calculated band offset, used to solve Schrödinger equation. A factor 'f' is used to represent mixing fraction of new and old potentials. In this work f is typically set to 0.05. After completion of the i^{th} iteration $V_{sc}^{\,i}(z)$ is compared with $V_{sc}^{\,i+1}(z)$ to obtain a convergence parameter X, which is given as

$$X = \sum_{Z}\left[\frac{V_{SC}^{i+1}(z) - V_{SC}^{i}(z)}{V_0^2}\right] \qquad (4)$$

where, V_0 is the surface potential of QW. If X < 0.001 then self consistent solution is considered to be converged. The same process is also repeated in presence of external electric field F. The plot of obtained Eigen energies and wave functions of Γ-CB, HH band and LH band is shown in Fig. 2. Due to compressive strain in well, HH band shifts upwards and LH band shifts downwards as shown in figure. In Fig.3, plot of Eigen energies in presence of external negative electric field, F, is shown. It is clear from figure that the Γ-CB and HH band are tilted downwards. Due to tilting of the bands, Γ-CB Eigen energy shifted downwards and HH band Eigen energy shifted upwards. After obtaining Eigen energies, absorption coefficient (α) is evaluated for unbiased QW with the help of Fermi's golden rule [6]. The incident light is assumed to be polarized parallel to the plane of the QW layer (TE mode).

α for HH to Γ-CB transition and LH to Γ-CB transition as a function of wavelength is shown in Fig.4. It is clearly observed from the figure that HH to Γ-CB transition observes higher α than that of LH- ΓCB transition. This is due to higher optical matrix element of HH to Γ-CB transition for TE mode, which plays a crucial role in evaluation of α [6]. The significant absorption for HH to Γ-CB transition is observed in infrared range of wavelength, which agrees with the reported result [3]. So, strain balanced GeSn QWIP is a potential candidate for group IV based direct bandgap infrared photo detector.

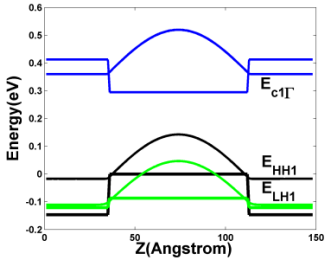
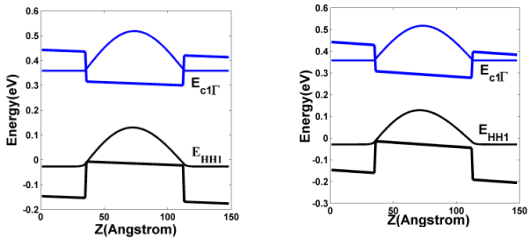


Fig.2 Plot of Eigen energies and wave functions without any electric field



(a) (b)

Fig.3 Plot of Eigen energies in presence of electric field (a) F=2Mv/m, (b) F=4Mv/m

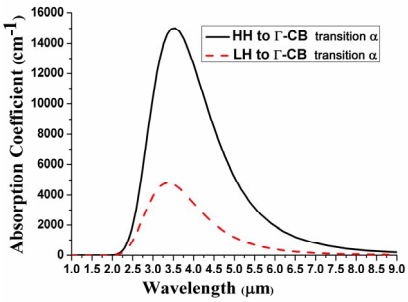


Fig.4 plot of α for HH to Γ-CB and LH to Γ-CB transitions

REFERENCES

[1] Pallab Bhattacharya, Semiconductor optoelectronic devices, *Pearson Education Inc.*, Second ed., New Jersey, 1994.

[2] J. Kouvetakis, J. Menedez, A.V.G. Chizmeshya., "Tin based group IV semiconductors: new platforms for opto and micro electronics and silicon," *Ann. Rev. of Mat. Res.*, Vol.36, pp.497-554, 2006.

[3] N.Yahyaoui et al., "Band engineering and absorption spectra in compressively strained $Ge_{0.92}Sn_{0.08}$/Ge (001) double quantum well for infrared photodetection," *Phys. Status Solidi C.*, doi: 10.1002/pssc.201400054, 2014.

[4] Guo-En Chang, Shu-Wei Chang, Shun-Lien Chuang, "Strain-balanced GezSn1-z-SixGeySn1-x-y multiple-quantum-well lasers," *IEEE Journal of Quantum Electronics*, Vol. 46, pp.1813-1820,2010.

[5] Chris G. Van de Walle, "Band lineups and deformation potentials in the model solid theory," *Phys. Rev. B*, Vol.39, pp.1871-1883, 1989.

[6] Shuan Lien Chuang, Physics of optoelctronic devices, *John Wiley & Sons inc.*, New York, 1995.

[7] Supriyo Dutta, Quantum transport: atom to transisitor, *Cambridge University Press*, New York, 2005.

[8] IH. Tan et al., "A self consistent solution of Schrödinger-Poisson equations using a nonuniform mesh", *JAP*, Vol.68, pp.4071-4076,1990.

[9] Frank Stern, "Iteration methods for calculating self-consistent fields in semiconductor inversion layers," *J. Comp. Physics,* Vol.6, pp.56-67, 1970.