Strong quantum-confined Stark effect in a lattice-matched GeSiSn/GeSn multi-quantum-well structure

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Abstract

This paper presents modeling and simulation of a multiple quantum well structure formed with Ge_{0.95}Sn_{0.05} quantum wells separated by Ge_{0.51}Si_{0.35}Sn_{0.14} barriers for the applications. These alloy compositions are chosen to satisfy two conditions simultaneously: type-I band alignment between Ge_{0.95}Sn_{0.05}/Ge_{0.51}Si_{0.35}Sn_{0.14} and a lattice match between wells and barriers. This lattice match ensures that the strain-free structure can be grown upon a relaxed Ge_{0.51}Si_{0.35}Sn_{0.14} buffer on a silicon substrate – a CMOS compatible process.

A electro-absorption modulator with the Ge_{0.95}Sn_{0.05}/Ge_{0.51}Si_{0.35}Sn_{0.14} multiple quantum well structure based on quantum-confined Stark effect (QCSE) is demonstrated in theory. The energy band diagrams of the GeSiSn/GeSn multi-quantum-well structure at 0 and 0.5V bias are calculated, respectively. And the corresponding absorption coefficients as a function of cut-off energy for this multiple quantum well structure at 0 and 0.5V bias are also obtained, respectively. The reduction of cut-off energy is observed with the applying of the external electric field, indicating a strong QCSE in the structure.

1. Introduction

The quantum-confined Stark effect (QCSE) [1] is a strong, electric field dependent change in optical absorption that has been seen in quantum well materials. It is used extensively for high-speed, low power dissipation optical modulators, for example, in telecommunications, and has also been used in large arrays of low power devices [2].

In this paper, we report strong QCSE in Ge_{0.95}Sn_{0.05} quantum wells grown on Si substrates with Ge_{0.51}Si_{0.35}Sn_{0.14} barriers and Ge_{0.51}Si_{0.35}Sn_{0.14} buffer. These observations show clear QCSE whose performance is comparable to, or possibly better than, III–V QCSE effects at similar wavelengths. Here, we give an extended discussion of this work, and the absorption of Ge_{0.95}Sn_{0.05} quantum wells is calculated by using an 8-band k.p solver. The lattice-matched GeSiSn/GeSn multi-quantum-well structure simulated in this paper has emission energy of 0.7eV. It advances applications in chemical and biological sensing, medical therapy, free space communication, spectroscopy-on-a-chip and it aids the development on-chip laser radar transmitters.

2. Band structure and sample design

This section illustrates the sample design in this paper. The design of the lattice-matched
GeSiSn/GeSn multi-quantum-well structure is based on the fact that electric field plays an active role in QCSE, which results in red shift of the cut-off wavelength for absorption spectra.

Fig. 1 shows the basic structure used for our experiments. Ge$_{0.95}$Sn$_{0.05}$ quantum wells with Ge$_{0.51}$Si$_{0.35}$Sn$_{0.14}$ barriers between them are grown on the top of a lattice-matched Ge$_{0.51}$Si$_{0.35}$Sn$_{0.14}$ layer on a Si substrate. The compositions of GeSn and GeSiSn are chosen to provide type-I band alignment at the Γ point as well as lattice matching. The structure would be situated on a relaxed buffer layer of GeSiSn-upon-silicon, a buffer whose lattice parameter is the same as that of the GeSn/GeSiSn structure, hence the entire structure is unstrained. The structure also allows photocurrent to be collected, from which the effective optical absorption coefficient of the quantum well region can be deduced.

![3D schematic of lattice-matched GeSiSn/GeSn multi-quantum-well structure](image)

Since the band offsets between ternary Sn-containing alloys and Si or Ge are not known experimentally, we calculate the conduction-band minima for the lattice-matched heterostructure consisting of Ge$_{1-z}$Sn$_z$ and a ternary Ge$_{1-x-y}$Si$_x$Sn$_y$. We used Jaros' band offset theory [3] which gives results in good agreement with experiment for many heterojunction systems [4]. The major input parameters of GeSn$_{0.05}$ and Ge$_{0.51}$Si$_{0.35}$Sn$_{0.14}$ for the calculations are listed in Table I, lattice constant was evaluated by linear interpolation based on the values of Ge and Sn given in Ref.5.

| Parameter | GeSn$_{0.05}$ | Ge$_{0.51}$Si$_{0.35}$Sn$_{0.14}$ |
|-----------|---------------|-------------------------------|
| Latt. const., $a$ (nm) | 5.688283500 | 5.688283500 |
| Elastic const., $c_{11}$ (GPa) | 125.55 | 133.23 |
| Elastic const., $c_{12}$ (GPa) | 47.31 | 51.09 |
| Elastic const., $c_{44}$ (GPa) | 65.27 | 67.00 |
| $L$ | -31.34 | -34.897 |
| $M$ | -5.90 | -5.689 |
| $N$ | -34.14 | -12.238 |
Fig. 2 shows what we believe to be the form of the line-up of various relevant bands in an unstrained GeSiSn/GeSn multi-quantum-well structure at 0V and 0.5V. We show the conduction band edge at the Γ point, as well as the valence band edges corresponding to the heavy hole, light hole and SO bands. Note that we expect type-I alignment (electron minimum energy and hole maximum energy in the same material) at the zone center, just as in typical III–V quantum well materials used for the QCSE.

3. Calculations of absorption coefficient in GeSiSn/GeSn multi-quantum-well structure

Absorption coefficient $\alpha$ is the most key parameter for determining the electrical and optical performance. In this work, the absorption was calculated by using an 8-band $k.p$ solver. The technique is similar to the envelope function technique derived by Bastard[6] and a full derivation of the absorption coefficient: derivation of the absorption coefficient: derivation of the absorption coefficient: $\alpha(\omega)$ derivation of the absorption coefficient: derivation of the absorption coefficient: $\alpha(\omega)$ as a function of angular frequency, $\omega$ can be found in Ref. 7. The absorption result is from the projection of the susceptibility tensor $\chi_{ij}$ onto the polarization vector $\varepsilon_{j}$ of the incident light to produce[7]

$$\alpha(\omega) = \frac{4\pi\omega}{nc} \varepsilon_{i}^* \chi_{ij}(\omega) \varepsilon_{j}$$

where $n$ is the refractive index and $c$ is the speed of light. The susceptibility is given in Ref.7.

Figure 5 shows the simulated optical absorption spectra for a multiple quantum well structure at 0V and 0.5V. A multiple quantum well structures at 0V and 0.5V demonstrate the cut-off energy of 1.35eV and 1.2eV, respectively. The absorption peak of multiple quantum well structures at 0V and 0.5V are 1.2eV and 0.8eV. Significant red shift of absorption edge is achieved in multiple quantum well structure at 0.5V due to QCSE. The absorption energy can be further decreased to low energy as voltage continues to increase, which will increase the electric field in the structure.
4. Conclusion

In summary, a lattice-matched GeSiSn/GeSn multi-quantum-well structure is investigated by simulation. 8-band k·p method is utilized to calculate the energy band structure and optical transmission properties in the multi-quantum-well structure. The electric field is induced by the voltage that perpendicular to the well, thus resulting in decreased absorption energy. QCSE in a lattice-matched GeSiSn/GeSn multi-quantum-well structure is theoretically studied and the absorption coefficient can be modulated effectively by external electric field.

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