Direct-gap exciton and optical absorption in the Ge/SiGe quantum well system

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Abstract:

The ground-level direct-gap excitons and quantum-confined Stark effect (QCSE) electroabsorption in the Ge/SiGe quantum well structures are studied using the tunneling resonance modeling and the variational method. The exciton radius, transition energy, binding energy, and optical oscillator strength are calculated for various quantum well thicknesses (5-35 nm) and vertical electric fields (0-10^5 V/cm) simultaneously. The relative direct-gap-to-indirect-gap absorption ratios are compared. A quantum well implementation scheme with relatively broad thickness range of ~5-15 nm can provide moderate excitonic absorption and contrast ratio for long wavelength operation. This investigation will improve the QCSE electroabsorption efficiency in the Ge quantum well system.

Main text:

The integration of silicon-based electronic and optoelectronic devices in a monolithic platform can enable optical interconnects for silicon chips, which significantly improves the system performance, especially for high-speed interconnections.[1] A silicon-compatible optical modulator is one of the key components in the optical transmitter end to encode the signals in the laser light. The most efficient optical modulation mechanism is the quantum-confined Stark effect (QCSE),[2,3] which is commonly used for the III-V material system but only available in the SiGe material system until the recent observation of strong QCSE in the Ge/SiGe quantum wells.[4,5] The optical absorption and QCSE in Ge/SiGe quantum wells grown on SiGe virtual substrates on silicon utilize the quantum

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confinement and optical transition associated with the direct-gap electrons (Γ_{7c}) and holes (Γ_{8v}), even though both Ge and Si are indirect band gap materials. The Ge QCSE is comparable to those of III-V materials. The photocurrent, transmission, and photoluminescence measurements had proven the strong quantum confinement for direct-gap carriers in this system.[4-8] The theoretical calculations based on the tunneling resonance simulation,[4,5] k.p modeling,[6,9] and tight-binding method[7,10] had shown agreement with experimental results. This strong electroabsorption effect provides a large absorption coefficient change and enables efficient optical modulators and photodetectors.[11-13] In this letter, we present the investigation of the exciton and optical absorption related to the ground-level electron-to-heavy-hole (e1-hh1) direct-gap transition in the Ge/SiGe quantum well system, which dominates the band-edge absorption and QCSE. The tunneling resonance and variational methods are used to calculate the exciton radius, transition energy, binding energy, and oscillator strength for various quantum well thicknesses and vertical electric fields. The ratios between the direct-gap e1-hh1 and indirect-gap background absorptions are compared for different quantum well thicknesses. A relatively broad quantum well thickness range can possess excitonic absorption enhancement and moderate contrast ratio, which is critical to the optimization of Ge quantum well structure for QCSE applications.

The exciton of a bulk Ge material based on the Bohr model has a radius of ~24 nm (e-hh exciton), but it disappears at high temperature or under high electric field unless a quantum-confinement structure is used to keep the exciton binding. The principle of QCSE in the Ge or III-V quantum well system is based on the strong excitonic absorption and the change of absorption edge (transition energy of excitons in the quantum well) as well as absorption coefficient by varying the electric field in the quantum well. The variational method is used here to study the exciton radius in the Ge quantum well system and its associated absorption behaviors.[3,14-17] A commonly-used Ge/$Si_{0.15}Ge_{0.85}$ single quantum well structure is chosen for theoretical calculation. The structure is assumed to be grown on a Ge-lattice-matched substrate, thus few strain is imposed on the Ge well layer. However, the barrier is still tensile-strained, and the band offsets are calculated

based on Ref. 18. Without strain and strain-induced energy shift occurring on the Ge well, the investigation here can focus on the effects of quantum well thickness and electric field.

Firstly, the wave functions, $\Psi_e(z_e)$ and $\Psi_h(z_h)$, of ground-level direct-gap electrons and holes under a vertical electric field (along the well growth direction, z-axis) are calculated separately using the tunneling resonance method. z_e and z_h are the positions of electron and hole, respectively, in the z axis while r is the relative in-plane (x-y) distance between electron and hole. The effective masses at the Γ point are linearly interpolated between those of Si and Ge, using m_e=0.156m_o, m_{hhz}=0.291m_o, m_{hhxy}=0.216m_o for Si and m_e=0.041m_o, m_{hhz}=0.21m_o, m_{hhxy}=0.057m_o for Ge,[5] neglecting the nonparabolicity effect for these ground-level states here. Then a trial wave function,[14-17]

$$\phi(r,z_e,z_h)=\psi_e(z_e)\psi_h(z_h)\exp\left(-\frac{\sqrt{r^2+\eta(z_e-z_h)^2}}{\lambda}\right) \quad (1)$$

where the last exponential term represents the exciton binding, is used to model the exciton effect. The variational parameters λ and η give the exciton radius and dimensionality when the system energy is minimized. Here η is set to 1, which has no significant difference in the exciton radius and oscillator strength as compared to the case of actual η.[14,16] Figure 1 shows the exciton radius λ for

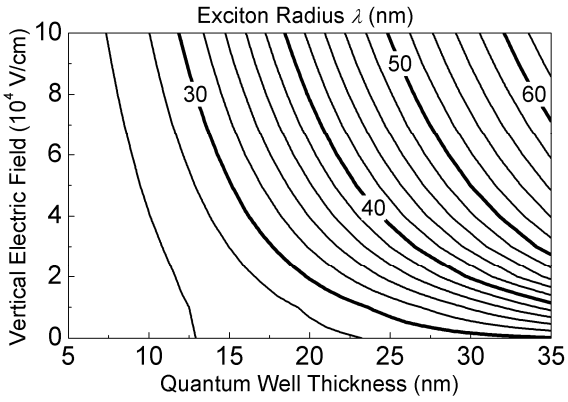

FIG. 1. Contour plot of the exciton radius (variational parameter λ) in a single finite Ge/Si0.15Ge0.85 quantum well for various well thicknesses and vertical electric fields.

various quantum well thicknesses (5-35 nm) and vertical electric fields (0-10^5 V/cm). The exciton

radius has small difference (~5 nm) for various well thicknesses at zero field. With a high electric field, the electron and hole are separated in the vertical direction against the well confinement. This

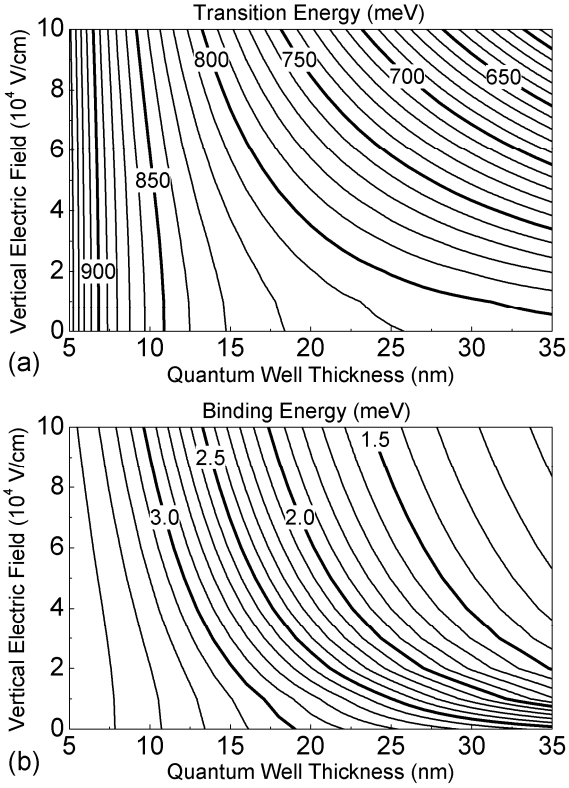

FIG. 2. Contour plots of (a) transition energy and (b) exciton binding energy in the Ge/SiGe quantum well system for the direct-gap e1-hh1 exciton. The shift is mainly dominated by the electric-field-dependent quantum well energy.

field-ionization of excitons weakens the binding and also leads to broader exciton radius, especially for thicker quantum wells. Figure 2(a) shows the e1-hh1 transition energy, consisting of the direct gap energy (at room temperature) and quantum well energy minus the exciton binding energy in Fig. 2(b). The dramatic transition energy reduction under high applied electric field causes the red shift of the absorption edge for QCSE. The shift is mainly dominated by the quantum well energy while the exciton binding energy of ~1-3.5 meV slightly modifies the absorption edge by ~3-6 nm. For the C-band operation (~1530-1565 nm) with ~0.8 eV transition energy, it is obvious that a wide well design is preferred here. However, the well can be thinner if the electroabsorption device is operated at a higher temperature or under tensile strain.

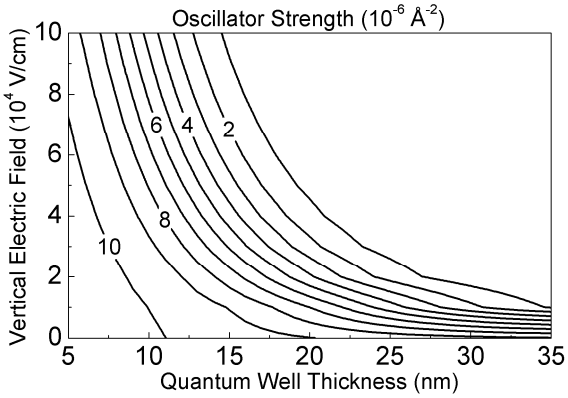

FIG. 3. Contour plot of the optical oscillator strength for the direct-gap e1-hh1 transition in the Ge/SiGe quantum well system. It represents the absorption capability in a quantum well for QCSE electroabsorption modulation. The strength reduces with thicker well and higher vertical electric field.

Figure 3 shows the relative oscillator strength of direct-gap e1-hh1 excitonic transition, which is proportional to the square of normalized overlap integral of the electron and hole wave functions: [16,17]

$$I \propto \frac{\langle \psi_e | \psi_h \rangle^2}{\langle \phi | \phi \rangle} . \qquad (2)$$

The overlap is mainly dominated by the exciton radius in the horizontal plane and by the separate wave functions in the vertical direction; however, the exciton radius broadening in the vertical direction starts to affect the strength when the quantum well becomes wider. The oscillator strength at zero field reduces by only ~24% when the well thickness increases from 5 to 35 nm. After a biasing field is applied, a wider well and higher electric field can reduce the coupling probability of electron and hole and lower the oscillator strength. The oscillator strength reduction between electric fields of 0 and 5×10^4 V/cm is around 10%, 55%, and 90% for the 5-, 10-, and 15-nm well, respectively. The strength contours in Fig. 3 clearly indicate that the oscillator strength increases monotonically with thinner well design, but the effect of well thickness on the background absorption should also be taken into consideration for this indirect-gap system. Since the absorption associated with the weakly-confined electrons of the indirect conduction band would not have

pronounced change with applied field, it becomes background absorption and deteriorates the modulation contrast ratio.

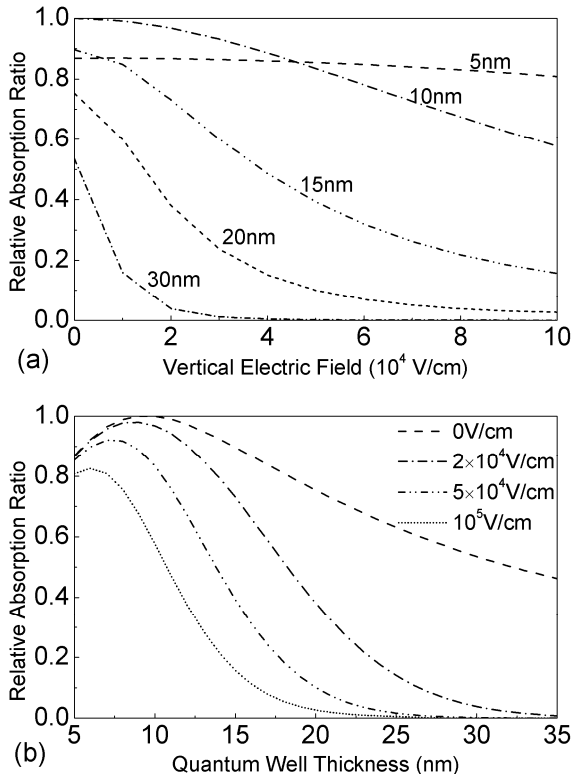

FIG. 4. Relative ratio of the direct-gap e1-hh1 absorption to the background absorption as a function of (a) vertical electric field and (b) well thickness. The background absorption is the indirect-gap absorption coefficient of Ge at the wavelength corresponding to the direct-gap transition energy. The ratio of 10-nm quantum well under zero field is normalized to 1. For the region where the direct-gap transition energy is lower than the indirect-gap energy, the background absorption issue does not exist.

Recent experimental works of the Ge/SiGe quantum well system had demonstrated the QCSE in the well of thickness ranging from 10 to 24 nm.[4,19] As compared to the thin well case, a wider well indeed results in a weaker excitonic absorption, but it is still (or even more) suitable to implement the waveguide-type modulators. Furthermore, its lower quantum confinement energy reduces the direct-gap photon transition energy and moves the absorption edge to longer wavelength end. Hence the background absorption caused by the indirect-gap transition is lower, so

the contrast ratio of a wide well is also comparable to that of thin quantum well case. Apparently the optimal quantum well thickness would not only depend on the enhancement of the oscillator strength through the excitonic effect but also on the improvement of the ratio between direct-gap and indirect-gap absorptions.

For a QCSE modulator design, the output light intensity is usually high without bias, thus the indirect-gap absorption at zero field is considered as the background absorption here. Figure 4 shows the relative optical absorption ratios of the direct-gap excitonic absorption[20] under various fields to the background absorption. The ratio of 10 nm well under zero field is set to unity as a reference. The indirect-gap absorption coefficient is based on the bulk Ge[21] for the ease of calculation, which is close to the combination of stepwise absorption curves from all quantized levels of holes and indirect electrons. Fig. 4(a) shows that a high field can reduce the ratio, especially for thick well, but the reduction is less than 40% in a field of 10^5 V/cm when the well is thinner than 10 nm. The optimal well thickness in Fig. 4(b) is ~10 nm (and ~7 nm) in a field of 0 V/cm (and 5×10^4 V/cm). The relative ratio is higher than 0.4 for the well thickness ranging from 5 to 15 nm under a moderate bias field of 5×10^4 V/cm or less. It should also be noted that if comparing the performance of different quantum well designs under the same applied voltage instead of the same electric field, a thicker well would possess even better performance. Besides, if a SiGe substrate is used or the total thickness of the quantum well structure is comparable to the substrate (or virtual-substrate buffer), the Ge well would become compressively-strained. This strain has negligible effects in the quantum well energy and exciton behaviors (radius, binding energy, and oscillator strength), but it can increase the transition energy in Fig. 2(a) and also reduce the direct-gap-to-indirect-gap absorption ratio.

In summary, we have studied the behavior of e1-hh1 excitons in the Ge quantum well structures of different well thicknesses under various vertical electric fields. The exciton radius, transition energy, binding energy, and oscillator strength are numerically calculated. A high electric field can ionize the exciton and reduce its oscillator strength dramatically, especially for thick wells.

The ratios between direct-gap and indirect-gap absorptions in different well thickness designs are compared, indicating a relatively broad design range can provide moderate excitonic absorption and low background absorption. The investigation provides an efficient evaluation of the excitonic absorption and QCSE efficiency for the Ge quantum well design.

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