Enhanced Emission of Quantum System in Si-Ge Nanolayer Structure

Zhong-Mei Huang, Wei-Qi Huang, Tai-Ge Dong, Gang Wang and Xue-Ke Wu

Abstract

It is very interesting that the enhanced peaks near 1150 and 1550 nm are observed in the photoluminescence (PL) spectra in the quantum system of Si-Ge nanolayer structure, which have the emission characteristics of a three-level system with quantum dots (QDs) pumping and emission of quasi-direct-gap band, in our experiment. In the preparing process of Si-Ge nanolayer structure by using a pulsed laser deposition method, it is discovered that the nanocrystals of Si and Ge grow in the (100) and (111) directions after annealing or electron beam irradiation. The enhanced PL peaks with multi-longitudinal-mode are measured at room temperature in the super-lattice of Si-Ge nanolayer quantum system on SOI.

Keywords: Quantum system, Si-Ge nanolayer structure, (100) and (111) direction, Super-lattice

Background

Persistent efforts in the hope of extending the reach of silicon technology into a fully integrated optoelectronic circuit have been made to achieve efficient light emission from silicon [1–4], meeting the need for high-bandwidth intra-chip and inter-chip connects. The Si-Ge nanostructures such as quantum wells (2D) and quantum dots (QDs) have aroused huge scientific interest [5–10], which could transfer the indirect bandgap into a direct-gap or quasi-direct-gap band.

In the latter, it is discovered that the nanocrystals of Si-Ge grow in the (100), (110), and (111) directions at the same sample; especially Si-Ge quantum dots form after annealing or electron beam irradiation [11], which results in rising of L valley and X valley of conduction band to form a direct-gap band. In photoluminescence (PL) spectrum, it is interesting that the intensive peaks near 1150 and 1500 nm are measured at room temperature and the characteristic peaks with multi-longitudinal-mode occur in the super-lattice structure of Si-Ge nanolayer quantum system on silicon on insulator (SOI). An emission model with quantum dots (QDs) pumping and quasi-direct-gap band has been provided to explain the experimental results, where the shorter lifetime of QDs is suitable for pumping (the lifetime of QDs is in nanosecond order) and the longer lifetime of the localized states is suitable for inverse of population (microsecond order) [12, 13]. It is a new way to develop Si-Ge laser on a silicon chip.

Methods

As shown in Fig. 1, the silicon wafers of P-type substrate with 10 Ωcm were taken on the sample stage in the fabrication system with pulsed laser depositing (PLD) devices, in which the left picture depicts the PLD process, the mid-picture describes the annealing process on the nanolayers prepared by PLD method with laser and furnace, and the quantum dots (QDs) and the super-lattice structures are built as shown in the right picture. A nanosecond pulsed Nd:YAG laser (wavelength 1064 nm, pulse length 60 ns full width at half maximum (FWHM), repetition rate 1000) and a third harmonic of pulsed Nd:YAG laser at 355 nm are used to deposit the Si-Ge nanolayers and the super-lattice structures in PLD process in an environment of oxygen, nitrogen, or SF₆.

It is interesting that the crystal orientation of (100), (110), and (111) can grow up on the amorphous film prepared by PLD process after annealing, in which the Ge crystal in the (111) direction and its FFT image are shown in Fig. 2. Figure 3a shows the TEM image of Si QDs in the (100) direction and Ge QDs in the (111) direction in the nanolayers prepared by PLD process after annealing or
Fig. 1 Fabrication system with PLD device, in which the Si-Ge layer quantum system and super-lattice structures are prepared after annealing.

Fig. 2 TEM image of Ge crystal in the (111) direction prepared by using PLD method and its FFT pattern.

Fig. 3 a TEM image of Si QDs crystal in the (100) direction and Ge QDs crystal in the (111) direction and their FFT pattern. b Emission peak of QDs in PL spectrum.
electron beam irradiation [11]. And their FFT patterns are shown in the inset of Fig. 3a.

The emission peak of QDs in photoluminescence (PL) spectrum is shown in Fig. 3b, whose average radius is about 4 nm. In the PL system, the power density of excitation laser at 514 nm on the sample is about 1 W/mm² at room temperature. The QD states provide the pumping levels having a shorter lifetime [14] in the three-level quantum system.

It is very interesting that the PL spectra on the Si-Ge nanolayer structure (composition: 2(Si)/1(Ge)) in the (100) direction are measured under the 488 nm excitation in the PL Systems at 17 K, as shown in Fig. 4a, in which the sharper peak at 1154 nm has the emission characteristics of direct-gap band such as the threshold effect (death region: pumping power <0.4W/mm²), the super-linear increasing intensity effect with an increase of pumping power (in the inset of Fig. 4a), and the emission quenching effect with a temperature increase (in Fig. 4b).

The emission peaks near 1400 nm in the PL spectra are measured in Si-Ge nanostructure (composition: 1(Si)/2(Ge)) in the (111) direction at 20 K, as shown in Fig. 5a, in which the PL intensity evolution with excitation power is observed. Figure 5b shows the PL

**Fig. 4** a PL spectra on the Si-Ge nanolayers (composition: 2(Si)/1(Ge)) in the (100) direction measured under the 488-nm excitation by using PL Systems at 17 K, in which the intensity of emission peak near 1150 nm super-linearly increases with pumping power; as shown in the inset, the evolution curve of the emission intensity at 1154 nm is increasing with pumping power super-linearly. b Evolution of PL peaks at different temperature with pumping power of 1 W.

**Fig. 5** a PL spectra on the Si-Ge nanolayers (composition: 1(Si)/2(Ge)) in the (111) direction measured under the 488-nm excitation by using PL Systems at 17 K, in which the intensity of emission peak near 1400 nm increases with pumping power; as shown in the inset, the evolution curve of the emission intensity at 1154 nm is increasing with pumping power super-linearly. b Evolution of PL peaks at different temperature with pumping power of 1 W.
peak near 1550 nm measured in Si-Ge nanostructure (composition: 1(Si)/2(Ge)) in the (111) direction at room temperature. The peak red-shift at room temperature attributes to the impurities states and the phonons effect.

It is very interesting that the splitting structure of states occur in the super-lattice with much more Si-Ge nanolayers as shown in Fig. 6a. Their more emission peaks with multi-longitudinal-mode appear in the PL spectra as shown in Fig. 6b (composition: 2(Si)/1(Ge) in the (100) direction) measured in room temperature, and in Fig. 6c (composition: 1(Si)/2(Ge) in the (111) direction) measured with various excitation power in 20 K.

Results and discussion
Some models have been chosen to simulate the experimental process. In the work, the electronic behavior is investigated by an ab initio non-relativistic quantum mechanical analysis. The DFT calculation was carried out by using the local density approximation (LDA) and non-local gradient-corrected exchange-correlation functional (GGA) for the self-consistent total energy calculation.

In the simulating calculation, Fig. 7 shows the Ge-Si layer model (a) and its energy band structure (b), in which the valley of conduction band of germanium at L point rises to be higher than the valley of conduction band at $\Gamma$ point originated from the tensile strain of Ge-Si layers due to annealing to form a direct-gap band structure. The tensile strain of Ge-Si layers is measured in the peak shift of Raman spectra in the experiment, as shown in Fig. 7c [15, 16], in which the tensile strain in germanium is obtained by the mismatch between the thermal expansion coefficients of Si and Ge and the hindered relaxation of the Ge layer upon cooling. Here, the tensile strain of Ge-Si layers builds the direct-gap band structure for emission levels.
A physical model of quasi-direct-gap emission with a three-level system is built in the Si-Ge nanolayer structure, as shown in Fig. 8a, in which it is clear that the rise of X valley in nanosilicon and L valley in nanogermanium forms the pumping levels, and the Γ valley of Ge direct-gap band or the localized state near Si edge band becomes emission level with inverse population. Figure 8b shows the structure of three levels in the Si-Ge layer quantum system, in which the states of Si-Ge QDs are higher to become pumping levels for forming the population inversion in the Γ valley of Ge.

Conclusions
In summary, the Si-Ge nanolayer quantum system in the (100) and (111) directions were fabricated by using PLD process, on which the PL emission of quasi-direct-gap was measured at room temperature and 20 K. It is interesting that the sharper intensive peaks with multi-longitudinal-mode near 1150 nm and near 1500 nm were observed at room temperature and 20 K on the super-lattice structure of Si-Ge nanolayer quantum system, which have the characteristics of direct-gap band material with the bandgap energy useful for technological application. We have built the physical model of quasi-direct-gap emission with a three-level quantum system to explain the simulation and experimental results. It is a new road to obtain a new direct-gap band emission in four-group materials and to develop Si-Ge laser on a silicon chip.

Abbreviations
FWHM: Full width at half maximum; nm: Nanometer; ns: Nanosecond; PL: Photoluminescence; PLD: Pulsed laser depositing; QDs: Quantum dots; SOI: Silicon on insulator; TEM: Transmission electron microscopy

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Competing interests
The authors declare that they have no competing interests.

Authors’ contributions
2MH is the main writer and researcher in the experimental work, who prepared Figs. 4, 5, and 6, and took part in the measurement of the PL and the EL spectra on the samples. WQH is the main writer and researcher who wrote the main manuscript text, prepared Figs. 1, 2, 3, and 7, provided new ideas and design investigation plan in the research, is the main researcher in the experimental work, took part in the preparation process of the samples, and made the measurement of the PL and the EL spectra on the samples. TGD is the main researcher in the experimental work, who prepared Figs. 5 and 6, took part in the preparing process of the samples, and made the optical measurement on the samples. GW is the main researcher in the experimental work, who prepared Figs. 2 and 3, and took part in the PL and optical measurement on the samples. XKW is the main researcher in the experimental work, who prepared Figs. 1 and 7, and took part in the preparation process of the samples.
researcher in the experimental work, who prepared Fig. 6, and took part in the PL and the EL spectra measurement on the samples. All authors reviewed the manuscript.

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