Direct-bandgap electroluminescence from tensile-strained Ge/SiGe multiple quantum wells at room temperature*

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(Received 28 February 2014; revised manuscript received 30 May 2014; published online 24 September 2014)

Tensile-strained Ge/SiGe multiple quantum wells (MQWs) were grown on a Ge-on-Si virtual substrate using ultrahigh vacuum chemical vapor deposition on an n^+-Si (001) substrate. Direct-bandgap electroluminescence from the MQWs light emitting diode was observed at room temperature. The quantum confinement effect of the direct-bandgap transitions is in good agreement with the theoretical calculated results. The redshift mechanism of emission wavelength related to the thermal effect is discussed.

Keywords: Ge, multiple quantum wells, tensile strain, electroluminescence

PACS: 61.72.uf, 78.67.De, 78.60.Fi **DOI:** 10.1088/1674-1056/23/11/116103

1. Introduction

Monolithically integrated optical sources on Si have long been considered as one of the most important components, but the biggest challenges for Si-based electronic–photonic integration.[1] In recent years, many efforts have been made to overcome this problem including porous silicon,[2] Si and SiGe nanostructures,[3,4] Er-doped Si based materials,[5] GeSn,[6] and hybrid III–V lasers on Si.[7,8] Ge-on-Si has emerged as a promising candidate because of its high compatibility with the conventional Si CMOS processes, and its pseudo direct bandgap structure. The difference of the direct and indirect bandgap is only 136 meV, and under adequate tensile strain and large n-type doping, we can obtain population inversion in Ge.[9] Based on this theory, the MIT research group made a great breakthrough and achieved lasing from the direct gap transition of tensile-strained n-type Ge-on-Si under optical[10] and electrical pumping.[11]

Compared with bulk Ge materials, Ge/SiGe multiple quantum wells (MQWs) show some unique properties such as a more abrupt band-edge absorption, the presence of excitonic features and the possibility for band structure engineering.[12] The carriers at the gamma valley confined in the Ge wells have been demonstrated to be able to enhance both direct gap absorption and emission, which has been applied in waveguide photo-detectors,[13] Ge/SiGe modulators based on the quantum confined stark effect (QCSE),[14] and waveguide light emitters.[15] While the Ge wells in these works are compressive strained, in which case, the direct bandgap is larger than that of the bulk Ge and the probability of electrons occupying the conduction energy levels is even smaller. In order to increase the internal quantum efficiency, a tensile-strained Ge well is necessary.[16]

In this paper, light emitting diodes with tensile-strained $Ge/Si_{0.15}Ge_{0.85}$ MQWs were grown on n^+-Si (001) substrates by ultrahigh vacuum chemical vapor deposition. The Ge virtual substrate (VS) was annealed *in situ* to increase tensile strain of Ge wells. Electroluminescence measurement was performed at room temperature to examine the emission properties of MQWs.

2. Experimental procedures

First, a 200-nm Ge VS was deposited using the two-step growth process on the n^+-Si(001) wafer. The detailed growth process was described in our previous works.[17,18] Then, the sample was annealed at 800 °C for 2 min *in situ*. Tensile strain was introduced to the Ge VS during cooling processes from the elevated growth temperature to room temperature due to the difference of the thermal expansion coefficient between Ge and Si. After the annealing process, two kinds of MQWs were prepared at 580 °C on the Ge VS: sample 1 with 20 periods of 10-nm Ge/15-nm $Si_{0.15}Ge_{0.85}$ and sample 2 with 11 periods of 14-nm Ge/15-nm $Si_{0.15}Ge_{0.85}$. Finally, a 150-nm-thick Ge cap layer was deposited on the MQWs. The top Ge cap layer was highly P-type-doped by implanting BF^{2+} to form the injection layer and the Ohmic contact layer. After implanting, the sample was thermally activated at 500 °C for 60 s in a N_2 atmosphere. A circular mesa with a diameter of 30 μm was then fabricated by dry etching patterned films down to the n^+-Si (001) substrate using an inductively coupled plasma etcher. After an 800-nm-thick SiO_2 film deposit, metal contacts were formed with a 100-nm nickel adhesion layer and a 700-nm-thick aluminum layer.

*Project supported by the National Basic Research Program of China (Grant No. 2013CB632103), the National Natural Science Foundation of China (Grant Nos. 61036003, 61176013, and 61177038), and the High Technology Research and Development Program of China (Grant No. 2011AA010302).

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X-ray diffraction (XRD) measurements along the (004) direction were performed using the Cu $K_{\alpha 1}$ ($\lambda = 0.15406$ nm) X-ray source to evaluate the strain status and crystal quality of the Ge/$Si_{0.15}Ge_{0.85}$ MQWs. The electroluminescence of the Ge/$Si_{0.15}Ge_{0.85}$ MQWs was measured using LabRam HR 800 Raman instrumentation at room temperature with an InGaAs detector array within the range 0.775–1.24 eV cooled by liquid nitrogen.

3. Results and discussion

Figure 1(a) shows the XRD curve of Ge film annealed *in situ* at 800 °C for 2 min and un-annealed Ge film as a reference signal. The Ge peak separation of the two samples can be clearly distinguished. The peak distance between the Ge and the Si substrate of an un-annealed sample is 5533 arc sec and an annealed sample is 5483 arc sec. The tensile strain is 0.12% and 0.17%, respectively. This result demonstrates that annealing *in situ* at high temperature can increase the tensile strain in Ge epilayers.

Figures 1(b) and 1(c) show the XRD curves of samples 1 and 2 along the (004) direction. A series of satellite peaks and the peaks originating from the Si substrate and the Ge VS can be clearly observed, which indicates the high crystal quality of the Ge/$Si_{0.15}Ge_{0.85}$ MQWs. According to the XRD curves, the tensile strain in Ge VS of sample 1 is calculated to be 0.07%, while sample 2 is 0.12%. The large difference of tensile strain between the two samples is mainly due to the different total thicknesses of MQWs. For a pseudomorphic interface, the in-plain constant $a_{\parallel}$ is determined by both the substrate and epitaxial layer[19]

$$a_{\parallel} = \frac{a_{\rm sub}G_{\rm sub}h_{\rm sub} + a_{\rm epi}G_{\rm epi}h_{\rm epi}}{G_{\rm sub}h_{\rm sub} + G_{\rm epi}h_{\rm epi}}, \tag{1}$$

where a, G, and h denote the lattice constant, the shear modulus and the thickness, respectively. The subscript sub and epi indicate the substrate and epitaxial layer, respectively. As per this formula, when the epitaxial MQWs become thicker, the in-plain constant of Ge VS decreases, i.e. the tensile strain decreases. Consequently, the tensile strain of sample 1 with 20 periods of MQWs is less than that of sample 2. From the perspective of obtaining large strain, fewer periods of QWs are favorable. However, to optimize the device performance, more QWs are appropriate.

The current–voltage (I–V) characteristic of the device was obtained by using a Keithley 4200 semiconductor characterization system. The typical I–V characteristics of the Ge/$Si_{0.15}Ge_{0.85}$ MQWs light emitting diode are shown in Fig. 2. The device exhibits a good rectifying behavior with a small leakage current of 300 nA at a −1 V reverse bias and large current under a forward bias.

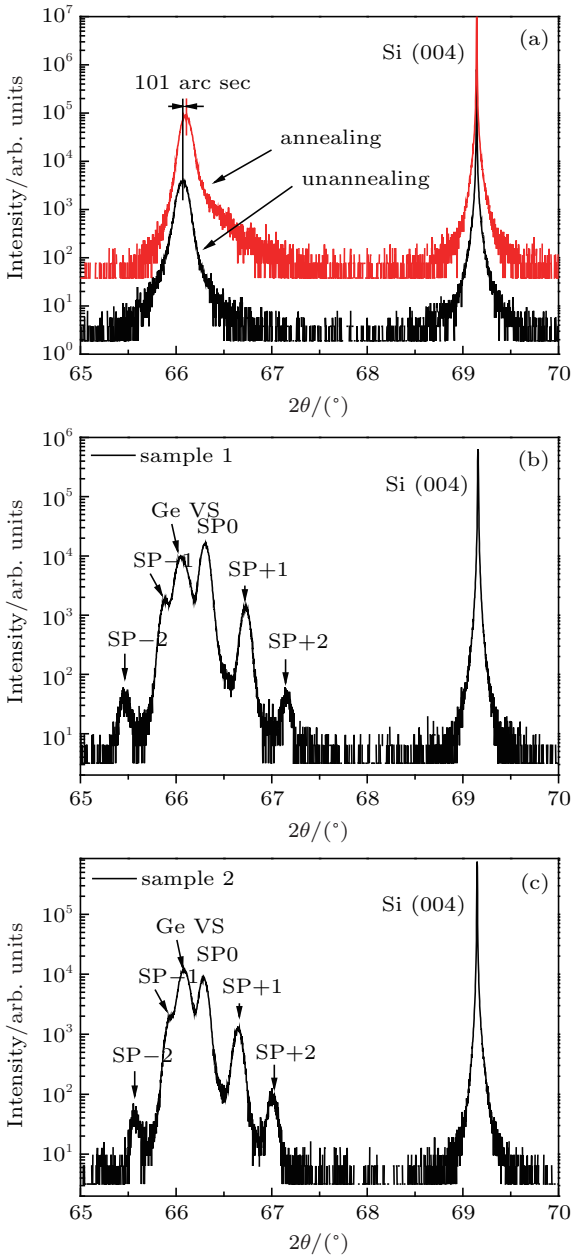


Fig. 1. (color online) XRD curves of Ge VS after being annealed *in situ* at 800 °C and an un-annealed sample as a comparison in panel (a), sample 1 and sample 2 in panels (b) and (c).

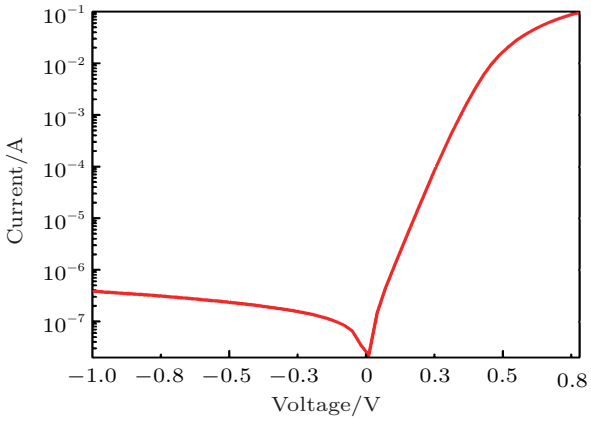


Fig. 2. (color online) The typical I–V characteristic of the device.

Figure 3(a) shows the electroluminescence spectra from sample 1 with 20 periods of Ge/$Si_{0.15}Ge_{0.85}$ MQWs at room temperature. As a comparison, the EL of a Ge film grown at the same condition with the Ge VS is also shown in Fig. 3(a). As depicted in the figure, the shape of EL spectra of the sample and the Ge film is different. The Ge film has only one luminescence peak at about 1580 nm, while the Ge/$Si_{0.15}Ge_{0.85}$ MQWs sample has two luminescence peaks. The fitting result is shown in Fig. 3(b). The peak at the longer wavelength of about 1580 nm originates from the Ge VS under MQWs in the diode, and the peak at the shorter wavelength of about 1500 nm is from the tensile-strained Ge MQWs.

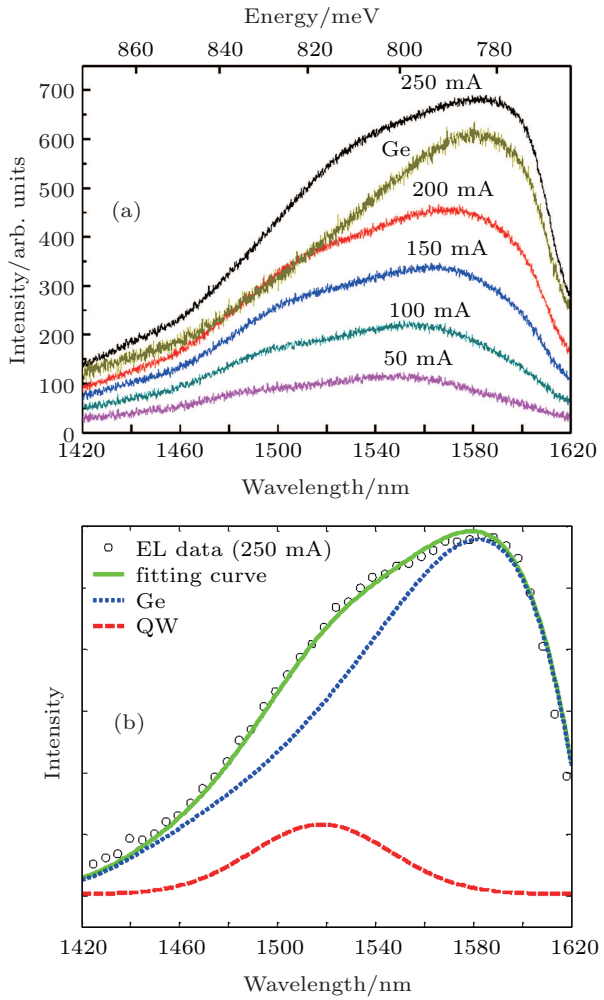


Fig. 3. (color online) (a) The room-temperature EL spectra of the device under various injection currents. The EL of the Ge film is also given as a comparison. (b) A luminescence spectra fitted by the direct transition of Ge VS and Ge QW.

To interpret the experimental results, the electronic states and energy band structures were calculated. Considering the 0.07% tensile strain in the Ge VS, and the Ge wells of 10 nm and the $Si_{0.15}Ge_{0.85}$ barriers were coherently grown on the Ge VS, the strain of the Ge wells and $Si_{0.15}Ge_{0.85}$ barriers of the MQWs were estimated to be 0.07% and 0.67%, respectively. The band edge diagram of the sample was calculated using the deformation potentials theory. The deformation potentials and direct bandgap of $Si_{0.15}Ge_{0.85}$ were linearly interpolated by Si and Ge.[20,21] The quantized energy of the quantum well was calculated using the finite potential well model with the parameter ($m_e = 0.041m_0 + 0.115(1-x)m_0$, $m_h = 0.28m_0 + 0.21(1-x)m_0$, where m_0 is free electron mass, and x is the fraction of Ge), as described in Ref. [16]. The calculated band discontinuities of the light hole (LH), heavy hole (HH), and electron at the Γ point are 72 meV, 131 meV, and 226 meV, respectively. The direct bandgap of the Ge well is $E_{g\Gamma} = 788$ meV under the certain tensile strain. The ground energy state of electron $E_{\Gamma 0}$ is 35 meV, and the heavy hole E_{HH0} is 8 meV. The results are shown in Fig. 4. Considering the LH–HH spitting energy of 6 meV, the calculated transition energy of the Ge well is about 837 meV, and the corresponding wavelength is about 1481 nm, which is in good agreement with the EL results.

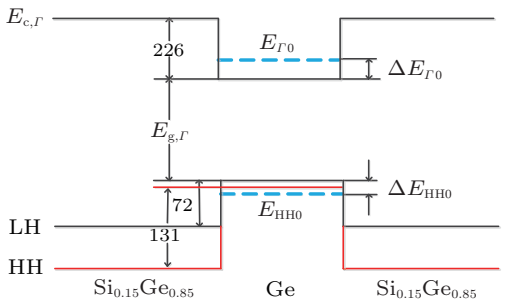


Fig. 4. (color online) The energy band edge diagram of the sample, $E_{c,\Gamma}$ is the conduction band minima at the Γ point. LH and HH are the valence band maxima of the light hole and the heavy hole, respectively, $E_{\Gamma 0}$ and E_{HH0} are the ground states of electrons and heavy holes at the Γ point, respectively.

Figure 5(a) shows the variation of the directbandgap transition energy of the Ge wells as a function of the current density. The variation of the directbandgap transition energy exhibits a sublinear relationship with the current. The redshift of emission peaks is mainly due to the Joule heat induced by the injection current. According to the vanish law, the bandgap variation has a linear relationship with the temperature.[22] The temperature dependence of the direct gap energy of Ge is expressed by

$$\frac{\Delta E_{g,\Gamma}}{\Delta T} = -6.842 \times 10^{-4}\left[1 - \frac{398}{(398+T)^2}\right] \text{(eV/K)}, \quad (2)$$

where $\Delta E_{g,\Gamma}$ is the variation of direct band gap transition energy of the Ge well when the temperature changes from T to $T + \Delta T$. However, when considering that the specific heat increases with increasing temperature,[23] the change of temperature decreases under larger current. Consequently, the direct-bandgap transition energy changes sublinearly with the current density. In our experiments, $\Delta E \propto J^{0.42}$. It is worth noting that under an injecting current of 250 mA, the variation of the direct-bandgap transition energy of the Ge well is 21 meV

while that of Ge VS is 15 meV. One of the main reasons causing this difference is probably the big difference of resistivity between Si and Ge, resulting in a large part of the voltage being on the MQWs. Another reason may be the quantum confinement stark effect (QCSE).

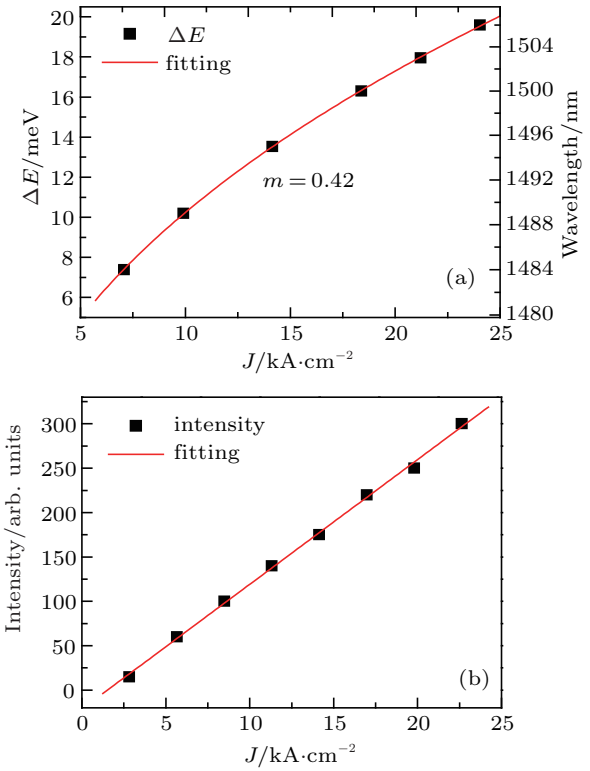


Fig. 5. (color online) (a) The current dependent of the variation of direct bandgap transition energy, ΔE is the energy difference between the theory value at zero bias and the measured value under current injection. (b) The relationship between the integrated EL intensity and the injection current.

Figure 5(b) shows the relationship between the intensity of emission and the injection current. The intensity exhibits a roughly linear relationship with the current. The dependence is characterized by $P \propto J^{\mathrm{m}}$, where P is the integrated EL intensity. The injected carrier concentration dependent of power is $P \propto \Delta n(p_0 + \Delta p)$, so the intensity is proportional to the square of the current as the injected carrier concentrations Δn and Δp are proportional to the injection current.[24] While when taking into account the ion implantation induced damages on the top p^+ layer, for example the acceptor diffusion and forming a p^--Ge region near the p^+-Ge/*i*-Ge interface in the *i*-Ge layer, $(p_0 + \Delta p)$ changes little under different current. As a consequence, the intensity changes only with Δn i.e., linearly with current.

4. Conclusions

In summary, we have observed the direct-bandgap electroluminescence from a tensile-strained Ge/$Si_{0.15}Ge_{0.85}$ MQWs light emitting diode at room temperature. The blue shift of the direct bandgap transition of Ge induced by the quantum confinement effect agrees well with the calculated results. The redshift mechanism of the emission peak induced by the thermal effect under injection current is explained. The quantum confinement effect of the tensile-strained Ge/SiGe MQWs is expected to be applied in Si-based optoelectronic devices.

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