Temperature dependence of electroluminescence from silicon *p-i-n* light-emitting diodes

Cheng Li,[a)] Hongkai Lai, and Songyan Chen
Research Center for Semiconductor Photonics, Department of Physics, Xiamen University, Xiamen, Fujian 361005, People's Republic of China

T. Suemasu and F. Hasegawa
Institute of Applied Physics, University of Tsukuba, Tsukuba, Ibaraki 305-8749, Japan

(Received 27 July 2005; accepted 25 May 2006; published online 19 July 2006)

The temperature dependence of electroluminescence from silicon *p-i-n* light-emitting diodes with a layer of β-$FeSi_2$ particles inserted in intrinsic silicon was investigated. Anomalous blueshift of the peak energy and enhanced electroluminescence intensity of the silicon band-edge emission were observed at temperatures from 50 to 200 K. The electroluminescence intensity was enhanced due to longer diffusion paths of the injected electrons at elevated temperature, as well as thermal escape of the electrons from the β-$FeSi_2$ particles. The low peak energy compared to that from bulk silicon at low temperature is due to the bound electron-hole pairs induced by the strain potential at the interface between silicon and β-$FeSi_2$ particles. The blueshift of the peak is ascribed to the transition of bound electron-hole pairs into free excitons at elevated temperature. Room temperature electroluminescence from such a silicon light-emitting diode can be obtained at a low current density of 0.3 A/cm^2. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2217107]

I. INTRODUCTION

The production of silicon light-emitting diodes for fully silicon-compatible integrated optoelectronic circuits is a big challenge due to the indirect energy band gap of silicon. Because of its importance in technology, numerous efforts have been devoted to get an efficient light emission in the wavelength range from visible to infrared regions of the spectrum from Si-based materials, such as porous Si, Si nanocrystal, dislocation engineered Si, erbium doped Si, SiGe, as well as β-$FeSi_2$.[1–6] Recently, light emission from bulk silicon diodes with dislocation loops[7] or silicon diodes fabricated on silicon-on-insulator substrate and with textured surface[8,9] was demonstrated. The enhancement of light emission at higher temperature was observed in the samples with dislocation loops, which was attributed to the spatial localization of the radiative carrier population decoupled from nonradiative recombination,[7] or to the binding of electron-hole pairs to the boron doping spikes.[10] The enhancement of light emission from other samples was attributed to the reduction of silicon self-absorption.[8,9] In our case, electroluminescence (EL) from the silicon *p-i-n* light-emitting diodes was demonstrated and the anomalous blueshift of the peak energy was observed from 50 to 200 K, which cannot be explained with the above mechanisms.

In this paper, we report on the temperature dependence of luminescence from a silicon *p-i-n* light-emitting diode with a layer of β-$FeSi_2$ particles inserted in the unintentionally doped silicon. In addition to the enhancement of EL intensity, the blueshift of silicon near band-edge emission was observed from 50 to 200 K, which is attributed to the formation of bound electron-hole pairs caused by the local strain in the silicon. Longer diffusion paths of injected electrons and thermal electrons escaping from β-$FeSi_2$ particles at higher temperature were proposed to be responsible for the enhancement of EL intensity.

II. EXPERIMENT

The starting material in our study was 20 μm thick *n*-type epitaxial silicon (resistivity of 0.02 Ω cm)/ Czochralski n^+-silicon (001) wafers. After thermal cleaning, 250 nm unintentionally doped silicon (lightly *p* type, $\sim 5 \times 10^{16}$ cm^{-3}) was grown on the *n*-type epitaxial silicon by molecular beam epitaxy (MBE) at 850 °C. An epitaxial layer of β-$FeSi_2$ 15 nm thick was deposited by reactive deposition epitaxy followed by an approximately 0.4 μm thick, unintentionally doped Si layer and a 0.8 μm thick, boron-doped (5×10^{18} cm^{-3}) silicon cap layer. Finally, samples were annealed at 900 °C in an Ar atmosphere for 14 h, which results in β-$FeSi_2$ particles embedded in Si matrix. Details of the growth procedure have been described elsewhere.[11] For comparison, the other sample with only 250 nm of unintentionally doped silicon was grown on the same type of substrate and annealed under the same conditions.

The device was designed as a mesa structure and 1.5×1.5 mm^2 mesa was made by wet chemical etching, as shown in the inset of Fig. 1. The plan view transmission electron micrograph is also shown in the figure. A finger-type Al contact was made on the *p*-silicon mesa area by standard photolithography and sintered at 450 °C for 20 min. The other contact was AuSb deposited on the backside of silicon substrate.

Samples were set up in a cryostat for EL and photoluminescence (PL) measurements from 8 to 300 K. PL measurements were conducted by exciting the samples with a 442 nm He–Cd laser, while EL spectra were measured by

a)Electronic mail: lich@xmu.edu.cn

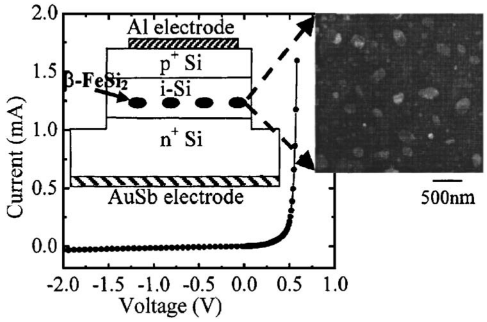

FIG. 1. Current-voltage characteristics of a silicon *p-i-n* light-emitting diode. In the inset is the cross sectional schematic of the device and the image of plan view transmission electron microscopy.

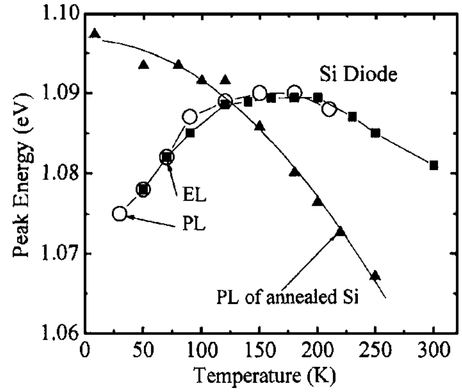

FIG. 3. Temperature dependence of peak energy of EL and PL from the light-emitting diode and PL from an epitaxial silicon sample annealed at the same conditions. The obvious blueshift was observed for both EL and PL from the light-emitting diode.

using a pulsed current source at 200 Hz frequency and about 1/2 duty cycle. Luminescence was analyzed by a 25-cm-focal-length grating monochromator, detected with a liquid nitrogen cooled InP/InGaAs photomultiplier (Hamamatsu Photonics R5509-72) and amplified by the standard lock-in technique.

III. RESULTS AND DISCUSSION

Current-voltage characteristics of the *p-i-n* diode are shown in Fig. 1. Good rectification and low leakage current indicate that the layer of β-$FeSi_2$ particles inserted in the unintentionally doped silicon causes only slight degeneration of the *p-i-n* diode performance. The current-voltage characteristics are typical of *p-i-n* silicon junctions.

The EL spectra of the diode at a forward bias of 50 mA are shown in Fig. 2 from 50 to 300 K. The obvious peak energy shift is indicated with the dashed line in the figure. To demonstrate the unusual evolution of EL and PL spectra, we plotted the EL and PL peak positions as a function of temperature in Fig. 3. For comparison, we also drew the PL peak positions from the annealed samples with only one epitaxial silicon layer in the same figure. For the annealed epitaxial silicon sample, the PL peak energy shifts to low energy with increasing temperature, rigorously following Varshni's law with the parameters for bulk silicon.[12] However, the energy peak positions of the EL and PL for the light-emitting diode are nearly the same, showing clear blueshift from 50 to 200 K. When the temperature is less than 160 K, the peak energy of EL and PL for the light-emitting diode is smaller than those of the annealed silicon samples. When the temperature is higher than 160 K, however, the peak energy is larger than those of the annealed silicon samples. The energy difference is about −18 meV at 50 K and 14 meV at 200 K.

Figure 4 shows the temperature dependence of EL and PL integrated intensities. With increasing temperature, the EL integrated intensity increases until 160 K and then starts to quench slightly, while the PL integrated intensity always quenches in the whole temperature range. In order to clarify the mechanism, the EL and PL intensities at the peak energy near 0.81 eV from β-$FeSi_2$ particles versus temperature is plotted in Fig. 5. The EL intensity from β-$FeSi_2$ increases with increasing temperature until 100 K, while the PL intensity from β-$FeSi_2$ always decreases with increasing temperature. These results indicate that the EL and PL spectra are related to the carrier injection mechanism. For EL, when the temperature increases, the injected electrons diffuse farther in the unintentionally doped silicon and more electrons reach the β-$FeSi_2$ area, which enhances the EL intensity both from the β-$FeSi_2$ and silicon. This indicates that it is the silicon near the β-$FeSi_2$ particles that causes the silicon band-edge luminescence. On the other hand, for PL, the input optical intensity is almost absorbed in the p^+ silicon layer and the carriers are generated mainly in this area. With the increase of temperature, the nonradiative recombination in this area

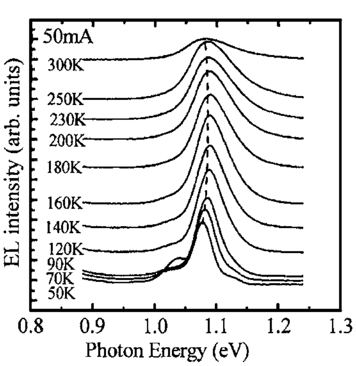

FIG. 2. Temperature dependence of EL spectra of the diode under 50 mA from 50 to 300 K, the dashed line shows the peak energy shift.

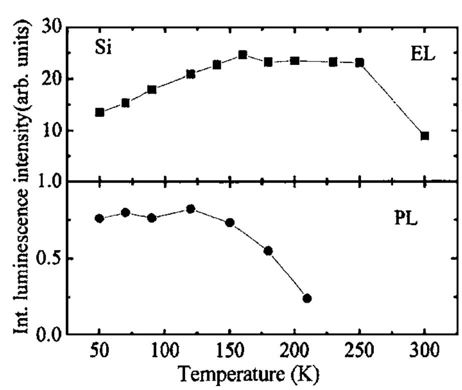

FIG. 4. Temperature dependence of EL and PL integrated intensities. The enhancement was observed for EL, while quenching for PL.

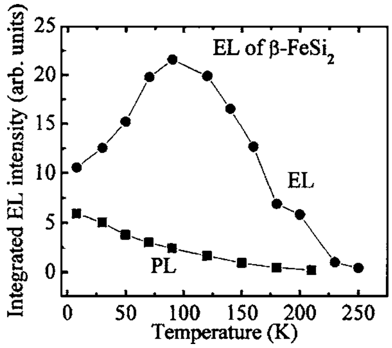

FIG. 5. Temperature dependence of EL and PL integrated intensities from the β-$FeSi_2$ particles (peak energy at about 0.81 eV). The enhancement of EL intensity was also observed with increasing temperature.

consumes a large portion of the electron-hole pairs and only a small number of them contributes to the radiative recombination in and near the area of β-$FeSi_2$ particles.

In order to explain the blueshift of silicon peak energy with increasing temperature, we notice that the β-$FeSi_2$ and surrounding silicon are under strain.[13] The shrinkage of the energy band gap of silicon under compressive strain provides the interface potential for binding electron-hole pairs. This results in the reduction of the peak energy of EL and PL at low temperatures contrasting to that from the bulk silicon. With increasing temperature, the reduction of binding energy gives rise to the blueshift of the peak energy of silicon band-edge luminescence until the start of the transition of bound electron-hole pairs into free excitons.

From 100 to 160 K, the EL intensity at the peak energy near 0.81 eV from β-$FeSi_2$ starts to quench, while the EL intensity of silicon band-edge luminescence continues to increase. To understand the continuous enhancement of silicon band-edge luminescence above 100 K, we plot the temperature dependence of the ratio of the EL radiation intensity from the silicon to that from the β-$FeSi_2$ in Fig. 6. The temperature dependence of $L_{\mathrm{Si}}/L_{\beta\text{-FeSi2}}$ indicates that the loss of electron confinement in β-$FeSi_2$ is consistent with the model of thermal excitation over the heterostructure barrier, which can be fitted as $L_{\mathrm{Si}}/L_{\beta\text{-FeSi2}} \propto \exp(-E_a/\mathrm{kT})$,[11,14] with $E_a \approx 0.2$ eV. The contribution of electrons escaping from β-$FeSi_2$ drives the continuous enhancement of silicon band-edge emission to higher temperature.

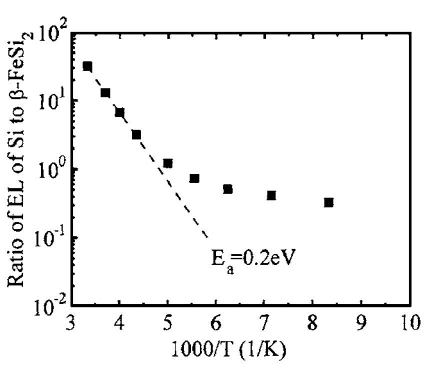

FIG. 6. EL intensity ratio $L_{\mathrm{Si}}/L_{\beta\text{-FeSi2}}$ of the radiation from the intrinsic silicon to the radiation from the β-$FeSi_2$ particles. The carriers thermal escaping from β-$FeSi_2$ was demonstrated.

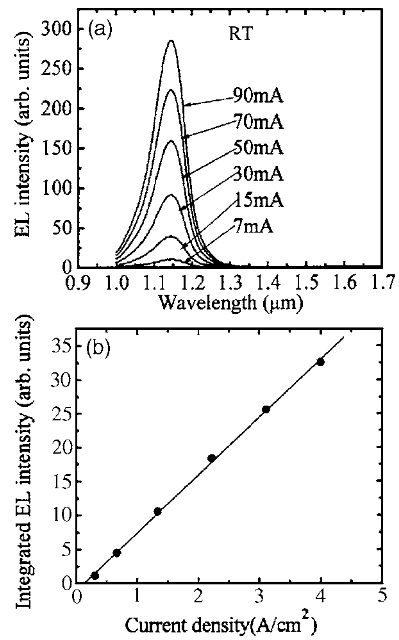

FIG. 7. EL spectra of a forward biased diode from 7 to 90 mA at room temperature (a) and the integrated EL intensity as a function of current density (b).

Figure 7(a) presents EL spectra of a forward-biased diode at room temperature. In the range of current from 7 to 90 mA, the strong silicon band-edge luminescence is observed with a full width at half maximum (FWHM) of about 100 nm. The integrated EL intensity as a function of the forward-bias current density is shown in Fig. 7(b). The band-edge emission of the silicon increases linearly with current density from 0.3 to 4 A/cm^2 and no saturation was observed.

IV. SUMMARY

Temperature dependence of EL was measured for the silicon *p-i-n* light-emitting diodes with a layer of β-$FeSi_2$ particles inserted in the unintentionally doped silicon. In contrast to the EL from boron-doped silicon diodes,[7,10] the blueshift of the peak energy in a large range of temperature was observed. The enhancement of silicon band-edge emission was demonstrated and attributed to the carriers that diffuse farther and to the carriers escaping from β-$FeSi_2$ at elevated temperature. The blueshift of the peak energy was proposed to be due to the reduction of the binding energy of electron-hole pairs at the interface between silicon and β-$FeSi_2$ particles with increasing temperature. Strain at the interface between silicon and β-$FeSi_2$ particles should play a major role in this structure. Room temperature EL from such a silicon light-emitting diode was realized at the low current density of less than 0.3 A/cm^2. Finally, we would like to mention that this device strategy was compatible with Si technology and could be used for other Si-based material.

ACKNOWLEDGMENTS

This work was partially supported by Innovation Projects of Fujian Province for Young Scientific Researchers (Contract No. 2004J021) and State Key Laboratory on Integrated Optoelectronics (Institute of Semiconductors, Chinese Academy of Sciences) and National Natural Science Foundation of China (Contract No. 60336010). One of the authors (C.L.) would like to thank editor Steven J. Rothman and the author's colleagues for their careful English proof reading.

[1]K. D. Hirschman, L. Tysbekov, S. P. Duttagupta, and P. M. Fauchet, Nature (London) **384**, 338 (1996).
[2]L. Pavesi, L. Dal Negro, C. Mazzoleni, G. Franzò, and F. Priolo, Nature (London) **408**, 440 (2000).
[3]M. Lourenco, M. Siddiqui, R. Gwilliam, G. Shao, and K. Homewood, Physica E (Amsterdam) **16**, 376 (2003).
[4]B. Zheng, J. Michel, F. Y. G. Ren, L. C. Kimerling, D. C. Jacobson, and J. M. Poate, Appl. Phys. Lett. **64**, 2842 (1994).
[5]L. Vescan and T. Stoica, J. Lumin. **80**, 485 (1999).
[6]D. Leong, M. Harry, K. J. Reeson, and K. P. Homewood, Nature (London) **387**, 686 (1997).
[7]W. L. Ng, M. Lourenco, R. Gwilliam, S. Ledain, G. Shao, and K. Homewood, Nature (London) **410**, 192 (2001).
[8]M. A. Green, J. Zhao, A. Wang, P. J. Reece, and M. Gal, Nature (London) **412**, 805 (2001).
[9]J. Zhao, G. Zhang, T. Trupke, A. Wang, F. Hudert, and M. A. Green, Appl. Phys. Lett. **85**, 2830 (2004).
[10]J. Sun, T. Dekorsy, W. Skorupa, B. Schmidt, A. Mucklich, and M. Helm, Phys. Rev. B **70**, 155316 (2004).
[11]C. Li, T. Suemasu, and F. Hasegawa, J. Appl. Phys. **97**, 043529 (2005).
[12]S. M. Sze, *Physics of Semiconductor Devices*, 2nd ed. (Wiley, New York, 1981), Chap. 1, p. 7.
[13]T. Suemasu, Y. Negishi, K. Takakura, F. Hasegawa, and T. Chikyow, Appl. Phys. Lett. **79**, 1804 (2001).
[14]H. Kressel, H. F. Lockwood, and J. K. Butler, J. Appl. Phys. **44**, 4095 (1973).