Room-temperature electroluminescence of a Si-based *p-i-n* diode with β-$FeSi_2$ particles embedded in the intrinsic silicon

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A Si-based *p-i-n* light emitting diode for 1.6 μm operation at room temperature has been realized, with β-$FeSi_2$ particles embedded in the unintentionally doped Si prepared by reactive deposition epitaxy. Room-temperature electroluminescence (EL) at 1.6 μm was observed with the diode under a forward bias current density of about 2.0 A/cm^2 and its intensity increased linearly with the current density. The temperature dependence of EL showed that luminescence was due to interband transitions in the β-$FeSi_2$ particles and the loss of electron confinement at *p-p* β-$FeSi_2/Si$ heterojunctions follows a thermally activated process with activation energy of about 0.198 eV, the conduction band offset at β-$FeSi_2/Si$ heterojunction. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1855397]

I. INTRODUCTION

Semiconducting iron disilicide [(β-$FeSi_2$) is a promising material for Si-based optoelectronics, which gives rise to light emission at about 1.55 μm, a minimum absorption window of silica optical fibers.[1–3] Various techniques have been adopted to grow β-$FeSi_2$ on Si substrates and room-temperature electroluminescence (EL) has been observed from β-$FeSi_2$ particles in Si *p-n* junction grown by reactive deposition epitaxy,[4] ion beam synthesis,[5,6] and from β-$FeSi_2$ thin films deposited by magnetron sputtering.[7,8] In all of these light emitting diodes, β-$FeSi_2$ was embedded in relatively heavily doped Si to form *p-n* heterojunctions to obtain high injection of carriers. However, photoluminescence measurement indicated that β-$FeSi_2$ grown on a heavily doped Si substrate would have weak emission. In addition, Suemasu *et al.*[4] attributed the large threshold current density to the defects in the materials system. These results implied that high doping concentration in the surrounding Si of β-$FeSi_2$ would introduce unacceptable nonradiative recombination centers during the β-$FeSi_2$ formation.

In this work, β-$FeSi_2$ particles were introduced in the unintentionally doped Si of a *p-i-n* diode to eliminate the effect of doping in the surrounding Si. Room-temperature EL from such a diode was observed at low current density. With the temperature dependence of the ratio of β-$FeSi_2$ to Si EL intensity, it was indicated that the loss of electron confinement at β-$FeSi_2/Si$ heterojunctions followed a thermally activated process with activation energy of about 0.198 eV, which was thought to be due to the conduction band offset between Si and β-$FeSi_2$.

II. EXPERIMENT

Details of the growth procedure have been described previously.[9,10] Samples were grown using an ion-pumped molecular beam epitaxy system equipped with Si and Fe electron gun evaporation sources. Initially, 250 nm unintentionally doped Si (lightly *p*-type Si) buffer layer was deposited on the *n*-type epitaxial Si(001) substrate, which is thermally cleaned at 850 °C. 4.8 nm of 99.99% Fe was deposited on the unintentionally doped Si buffer layer at 470 °C to form a 15 nm thick β-$FeSi_2$ epitaxial layer. Samples were then annealed *in situ* at 850 °C for 1 h to improve the crystal quality of the β-$FeSi_2$, which agglomerated into islands during this process. Consequently, an $\approx$0.4 μm thick, unintentionally doped Si layer was grown at 500 °C. Finally, a boron-doped Si cap layer with doping concentration of about 5.0×10^{18} cm^{-3} was grown at 700 °C with the growth rate of 4.5 nm/min. Samples were then annealed at 900 °C in an Ar atmosphere for 14 h to further improve the crystal quality, resulting in β-$FeSi_2$ particles embedded in the unintentionally doped Si matrix. The crystal quality was characterized by double crystal x-ray diffraction and only β phase $FeSi_2$ with β-$FeSi_2(100)/Si(001)$ oriented was observed.

The device was designed as a mesa structure and 1.5×1.5 mm^2 mesa were made by wet chemical etching. An

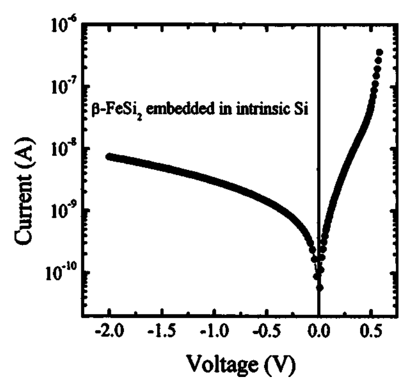

FIG. 1. Current-voltage characteristics of a Si-based *p-i-n* diode with β-$FeSi_2$ particles embedded in the intrinsic Si.

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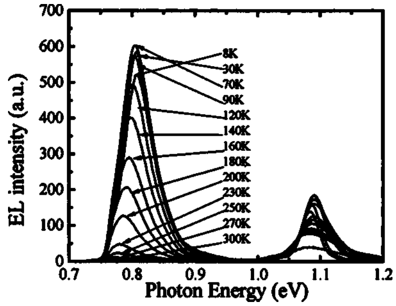

FIG. 2. EL spectra from a Si-based *p-i-n* diode with β-$FeSi_2$ particles embedded in the intrinsic Si from 8 to 300 K. The spectra are recorded under forward bias at a current of 50 mA.

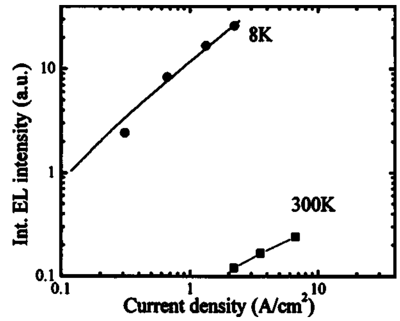

FIG. 4. Intensity of the β-$FeSi_2$ EL at 8 and 300 K as a function of the current density.

aluminum figure-type contact was made on the p^+-Si mesa area by standard photolithography and sintered at 450 °C for 20 min. AuSb was deposited on the backside of Si substrate to form the other contact.

EL spectra of the diode with the β-$FeSi_2$ active region were measured by using a pulse current source with 200 Hz frequency and about 1/2 duty cycle. The device was mounted to a copper holder in a cryostat. Luminescence was analyzed by a 25 cm focal length single monochromator, detected by a liquid nitrogen cooled InP/InGaAs photomultiplier (Hamamatsu Photonics R5509-72) and amplified by the lock-in technique.

III. RESULTS AND DISCUSSION

Figure 1 shows the current-voltage characteristics of the diode at room temperature. The ideal factor *n* and the value of potential barrier are estimated to be 1.4 and 0.72 eV for the *p-i-n* diode with β-$FeSi_2$ particles embedded in the intrinsic Si, respectively. The smaller ideal factor of the *p-i-n* diode with the β-$FeSi_2$ particles embedded in the intrinsic Si implies low density of interface states between the β-$FeSi_2$ particles and Si. In addition, no obvious dislocations are observed near the interface between β-$FeSi_2$ and Si of the samples by transmission electron microscope, as reported in Ref. 11.

Temperature dependent EL spectra from 8 to 300 K are shown in Fig. 2. The forward current peak density used for the EL spectra are 2.2 A/cm^2. EL spectra show two bands from 8 K to room temperature, i.e., the β-$FeSi_2$ luminescence at near 0.8 eV and the Si luminescence at 1.1 eV. The peak energy of EL as a function of temperature is shown in Fig. 3. The experimental dependence of the peak energy on temperature can be well fitted by applying the semiempirical Varshni's law[12] with parameters of $\alpha = 2.3 \times 10^{-4}$ eV/K, $\beta = 230$ K. This result indicates that this emission is originated by a band-to-band recombination of carriers in β-$FeSi_2$.

As is well known, EL at near 0.8 eV is also reported in Si-based diodes with dislocations and porous Si, usually referred to as *D*1 line, which is attributed to the dislocations in Si.[13,14] In this case, although we cannot completely exclude the contribution of *D*1 line, the emission from β-$FeSi_2$ should play a major role, because of the few dislocations observed in the samples, low leakage current, and the small ideal factor of the diode. In fact, the origin of 0.8 eV emission from samples of β-$FeSi_2$ particles embedded in Si has been clarified to be mainly due to β-$FeSi_2$ rather than dislocations.[15,16]

Integrated EL intensity of β-$FeSi_2$ scales linearly with the injected current peak densities at 8 K and room temperature, respectively, as shown in Fig. 4. At room temperature, the current peak density, at which EL signal appears, is about 2.0 A/cm^2. This current peak density is much smaller than that of light emitting diode with β-$FeSi_2$ particles embedded in heavily doped Si at the *p-n* heterojunctions, about 70 A/cm^2, which is attributed to the defect recombination and therefore the superlinear current dependence of EL is observed.[17] Both the linear relationship of EL vs current density and small threshold current density indicate that nonradiative recombination centers are drastically reduced with β-$FeSi_2$ embedded in the unintentionally doped Si. Furthermore, a narrow full width at half maximum (FWHM) of EL

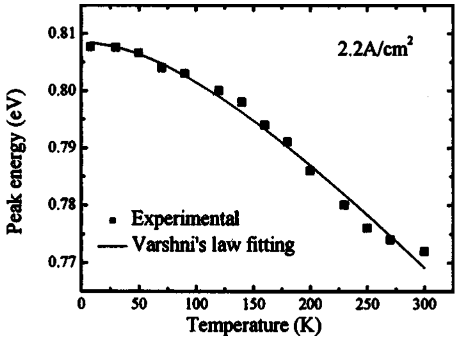

FIG. 3. Peak energy of the β-$FeSi_2$ EL as a function of temperature. The solid line is the fitting by Varshni's law with the parameters: $\alpha = 2.3 \times 10^{-4}$ eV/K, $\beta = 230$ K.

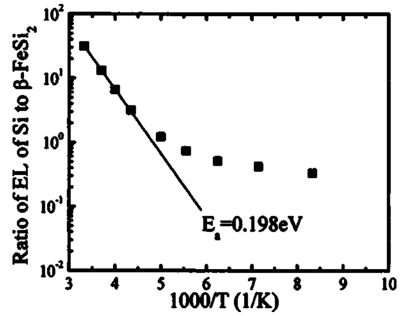

FIG. 5. EL intensity ratio $L_{Si}/L_{\beta\text{-}FeSi_2}$ of the radiation from the Si to that from the β-$FeSi_2$ as a function of temperature follows the thermal radiation model with the activation energy of about 0.198 eV.

spectra is observed to be less than 54 meV in the whole temperature range. It seems that the formation of nonradiative recombination centers due to Fe and dopants interaction in Si are suppressed.

As the temperature increases, electrons surmount the potential barrier at β-$FeSi_2$−Si *p*-*p* heterojunctions to Si region. This behavior increases the EL intensity ratio $L_{Si}/L_{\beta\text{-}FeSi_2}$ of the radiation from the Si to the radiation from the β-$FeSi_2$, as shown in Fig. 5. The temperature dependence of $L_{Si}/L_{\beta\text{-}FeSi_2}$ 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 $L_{Si}/L_{\beta\text{-}FeSi_2} \propto \exp(-E_a/kT)$,[18] with $E_a=0.198$ eV. The activation energy E_a is consistent with the reported conduction band energy discontinuity of 0.23 eV.[19]

IV. CONCLUSION

In conclusion, room-temperature EL from a Si-based *p*-*i*-*n* light emitting diode with β-$FeSi_2$ particles embedded in the intrinsic Si by reactive deposition epitaxy has been observed under a small current density. β-$FeSi_2$ particles grown on the unintentionally doped Si suppress the nonradiative recombination and improve room-temperature emission. Temperature dependent luminescence shows that the band-to-band transition in β-$FeSi_2$ should be responsible for the electroluminescence and the conduction band offset at β-$FeSi_2$−Si heterojunctions of about 0.2 eV has been measured by thermal activation of electrons from β-$FeSi_2$ to Si.

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