Measurements of Carrier Confinement at β-$FeSi_2$-Si Heterojunction by Electroluminescence *

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Abstract : A Si p-π-n diode with β-$FeSi_2$ particles embedded in the unintentionally doped Si (p^--type) was designed for determining the band offset at β-$FeSi_2$-Si heterojunction. When the diode is under forward bias ,the electrons injected via the Si n-p^- junction diffuse to and are confined in the β-$FeSi_2$ particles due to the band offset. The storage charge at the β-$FeSi_2$-Si heterojunction inversely hamper the further diffusion of electrons ,giving rise to the localization of electrons in the p^--Si near the Si junction ,which prevents them from nonradiative recombination channels. This results in electroluminescence (EL) intensity from both Si and β-$FeSi_2$ quenching slowly up to room temperature. The temperature dependent ratio of EL intensity of β-$FeSi_2$ to Si indicates the loss of electron confinement following thermal excitation model. The conduction band offset between Si and β-$FeSi_2$ is determined to be about 0.2eV.

Key words : β-$FeSi_2$-Si heterojunction ; electroluminescence ; band offset ; carrier confinement
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1 Introduction

Semiconducting iron disilicide (β-$FeSi_2$) has been widely investigated as one of the promising materials for Si-based optoelectronic components ,especially for Si-based light emitters at about 1.5μm[1,2]. So far , room temperature electroluminescence (EL) has been observed for β-$FeSi_2$ embedded in silicon matrix grown by ion-beam synthesis (IBS) ,reactive deposition epitaxy (RDE) ,and magnetron-sputtering deposition[3~7] ,respectively. However ,the band offset between β-$FeSi_2$ and Si ,which has great effect on the hetero-junction diode performance ,has not been made clearly. The experimental band gap energy of β-$FeSi_2$ obtained from EL and PL as well as absorption spectra varies in a wide range from 0.8 to 0.9eV and the conduction band offset between Si and β-$FeSi_2$ varies from 0.1 to 0.26eV[1,5,8~11]. These different values may be due to the introduction of defects in β-$FeSi_2$ or its interface ,as well as the effect of doping in the Si substrate during various growth processes. In order to eliminate the extrinsic effect ,a sample with β-$FeSi_2$ surrounded by intrinsic Si was prepared.

In this work ,a Si p-π-n diode with β-$FeSi_2$ particles embedded in the intrinsic Si (lightly p type) was investigated. The β-$FeSi_2$ particles were grown on the unintentionally doped Si to eliminate the effect of doping in the Si substrate. The injected electrons are mainly distributed in β-$FeSi_2$ and unintentionally doped Si region near the junction due to the band offset at Si/β-$FeSi_2$ heterojunction ,which improves the

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EL intensity from both the β-$FeSi_2$ and Si. The temperature dependent ratio of EL intensity from β-$FeSi_2$ to Si indicates the loss of electron confinement in the β-$FeSi_2$ following thermal excitation model and the conduction of band offset is inferred.

2 Experiment

Samples were grown using an ion-pumped MBE system equipped with Si and Fe electron gun evaporation sources. Initially, 250nm unintentionally doped silicon buffer layer was deposited on the thermally cleaned n-type epitaxial Si(001) substrate at 850 ℃. A 10nm-thick β-$FeSi_2$ epitaxial layer was deposited on the unintentionally doped Si buffer layer at 470 ℃ by reactive deposition epitaxy. Samples were then annealed in situ at 850 ℃ for 1h to improve the crystal quality of β-$FeSi_2$, which agglomerated into islands during this process. Consequently, an approximately 0.4μm-thick, unintentionally doped Si layer was grown at 500 ℃. Finally, a boron-doped Si cap layer with doping concentration of about 10^{18} cm^{-3} was grown at 700 ℃ with the growth rate of 4.5nm/min. The samples were then annealed at 900 ℃ in Ar atmosphere for 14h to further improve the crystal quality, resulting in β-$FeSi_2$ particles embedded in unintentionally doped Si matrix[12]. The crystal quality was characterized by double crystal X-ray diffraction and only β phase $FeSi_2$ with β-$FeSi_2$(100)/Si(001) orientation was observed.

The device was designed as a mesa type diode with about 1.5mm × 1.5mm mesa area made by wet chemical etching. An Al figure-type contact was made on the p^+-Si mesa by standard photolithography and sintered at 450 ℃ for 20min. AuSb was deposited on the backside of Si substrate to form the other contact.

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

3 Results and discussion

The cross sectional schematic of the device structure is shown in Fig. 1. The unintentionally doped Si grown in the chamber shows p-type with the doping concentration of about $10^{16}$$cm^{-3}$ and the β-$FeSi_2$ is intrinsic p-type, which consists of p-p heterojunction between β-$FeSi_2$ and Si. Temperature dependent EL spectra from 8 to 300K are shown in Fig. 2. The forward current used for the EL spectra is 50mA. EL spectra show two bands, i.e. the β-$FeSi_2$ luminescence at near 0.8eV and silicon band edge luminescence at 1.1eV. The peak energy of EL from β-$FeSi_2$ as a function of temperature is shown in Fig. 3. The dependence of peak energy on temperature can be well fitted by applying the semiempirical Varshni's law[13] with parameters of $\alpha = 2.3 \times 10^{-4}$ eV/K, $\beta = 230$ K and the peak energy is about 0.808eV at 0K. This result indicates that the emission could be assigned as being due to the recombination of electron-hole pairs associated with the conduction and valence bands of β-$FeSi_2$.

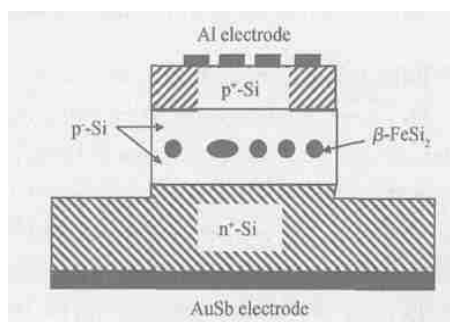

Fig. 1 Cross sectional schematic of Si p-π-n diode with β-$FeSi_2$ particles embedded in the unintentionally doped Si

When the diode is under forward bias, electrons injected via the Si n-p^- junction to p- Si diffuse to β-$FeSi_2$ particles and are confined in them due to the large conduction band offset. The charge storage in the β-$FeSi_2$ inversely hampers electrons further diffusion, which localizes the electrons in the p^--Si, preventing electrons from nonradiative recombination channels. Furthermore, β-$FeSi_2$ being grown on the

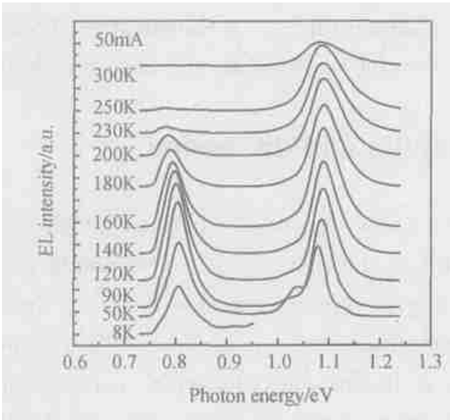

Fig. 2 EL spectra of the Si p-π-n diode with β-$FeSi_2$ particles embedded in the intrinsic Si at a current of 50mA

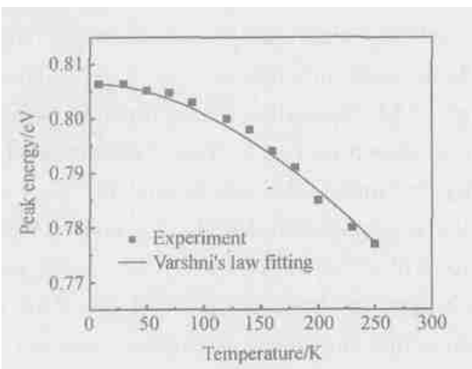

Fig. 3 Peak energy as a function of temperature The well fitting by Varshni's law shows that the emission should be related to the interband transition of β-$FeSi_2$.

unintentionally doped Si buffer layer is deposited at higher temperature, thus the formation of non-radiative recombination centers possible due to Fe and dopants interaction in Si is oppressed. Strong EL intensity both from β-$FeSi_2$ and Si is observed and the quenching rate becomes slow.

As the temperature increases, the confinement of electrons by the p-p β-$FeSi_2$/Si heterojunction becomes weak. The electrons surmount the potential barrier to contribute to Si radiation. This behavior increases the EL intensity ratio $L_{Si}/L_{β\text{-}FeSi_2}$ of the radiation from Si to the radiation from β-$FeSi_2$, as shown in Fig. 4. The data can be fitted to an expression such as $L_{Si}/L_{β\text{-}FeSi_2} \propto \exp(-E_a/kT)$, with $E_a = 0.2$eV. The temperature dependence of $L_{Si}/L_{β\text{-}FeSi_2}$ indicates the loss of electron confinement in β-$FeSi_2$ is consistent with the model of thermal excitation over the heterostructure barrier. The conduction band offset at β-$FeSi_2$-Si heterojunction of 0.2eV is inferred.

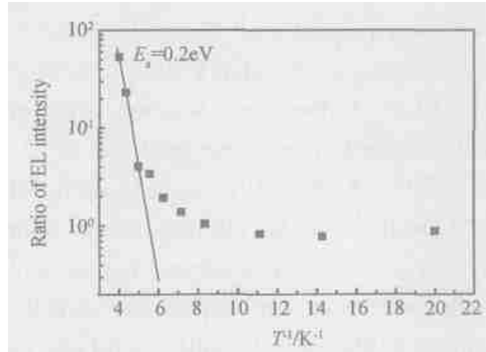

Fig. 4 EL intensity ratio $L_{Si}/L_{β\text{-}FeSi_2}$ as a function of temperature

4 Conclusion

With a Si p-π-n diode with β-$FeSi_2$ particles embedded in the unintentionally doped Si, EL intensity from both Si and β-$FeSi_2$ is improved due to the carrier localization. The conduction band offset at β-$FeSi_2$-Si heterojunction is measured to be 0.2eV using the temperature dependence of EL intensity ratio of the radiation from Si to the radiation from β-$FeSi_2$.

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电致发光谱测量β-$FeSi_2$-Si 异质结载流子限制*

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摘要：设计了一种将β-$FeSi_2$ 颗粒埋入非故意掺杂 Si 中的 Si p-π-n 二极管来确定β-$FeSi_2$-Si 异质结的能隙差. 当二极管处于正向偏置时，通过 Si n-p^- 结注入的电子扩散到β-$FeSi_2$ 并由于 Si 与β-$FeSi_2$ 之间的能隙差而受到限制，电荷在异质结的积累反过来阻挡了电子的继续扩散，将电子局域化在靠近 Si n-p^- 结的 p^--Si 区. 少子的局域化减少了非辐射复合的途径，Si 和β-$FeSi_2$ 的发光增强，淬灭速率变慢，在室温低电流下仍可得到 Si 和β-$FeSi_2$ 电致发光. Si 和β-$FeSi_2$ 发光强度的比率对温度的依存性表明同型异质结对电子限制能力的减弱符合热发射模型，由此确定出 Si 和β-$FeSi_2$ 异质结导带带阶差为 0.2eV.

关键词：β-$FeSi_2$-Si 异质结；电致发光；带阶；载流子限制

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