

## Growth and Characterization of Si-Based Light-Emitting Diode with $\beta$ -FeSi<sub>2</sub>-Particles/Si Multilayered Active Region by Molecular Beam Epitaxy

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### 1. Introduction

$\beta$ -FeSi<sub>2</sub> has been attracting much attention as a Si-based light emitter with a wavelength (1.5  $\mu$ m) corresponding to optical fiber communication [1]. In 1997, Leong *et al.* reported the low-temperature electroluminescence (EL) from  $\beta$ -FeSi<sub>2</sub> precipitates embedded in a Si *p-n* junction by ion beam synthesis (IBS) [2]. However, room temperature (RT) EL has been difficult to obtain due to a large number of induced defects. We therefore adopted reactive deposition epitaxy (RDE ; deposition of Fe on a hot Si ) instead of IBS to form  $\beta$ -FeSi<sub>2</sub>, and developed the formation technique of single-crystalline  $\beta$ -FeSi<sub>2</sub> particles embedded in Si by molecular beam epitaxy (MBE), leading to the first RT 1.6 $\mu$ m EL [3,4]. The problem is, however, the fact that active region is not a continuous  $\beta$ -FeSi<sub>2</sub> film but particles. From the viewpoint of carrier injection into  $\beta$ -FeSi<sub>2</sub>, a continuous active layer is favorable. However, the epitaxial  $\beta$ -FeSi<sub>2</sub> film on Si(001) was found to easily aggregate into isolated islands due to the lattice mismatch (1–2 %) between the two materials when it was annealed at high temperature for improving the crystalline quality or embedded by MBE-Si capping layers [5]. We have been trying to enhance EL intensity by increasing the size of  $\beta$ -FeSi<sub>2</sub> particles in Si, but it was found to just increase the defect densities in surrounding Si [6].

In this paper, we have reported that fabrication of multiple  $\beta$ -FeSi<sub>2</sub>-particles/Si layered structure is a very effective way to enhance EL from *p*-Si/ $\beta$ -FeSi<sub>2</sub>-particles/*n*-Si light-emitting diodes (LEDs).

### 2. Experimental

$\beta$ -FeSi<sub>2</sub>-particles/Si multilayered structure was fabricated as follows. First, [100]-oriented  $\beta$ -FeSi<sub>2</sub> epilayers were grown on *n*<sup>+</sup>-Si(001) substrates by RDE at 470°C. The sample was then annealed *in situ* at 850°C for 1 h to improve the crystal quality of the  $\beta$ -FeSi<sub>2</sub>. The  $\beta$ -FeSi<sub>2</sub> film agglomerated into islands during this process, due to the lattice mismatch (1–2 %) between the two materials [5]. Consequently, a 0.3  $\mu$ m-thick undoped Si layer was grown by MBE at 500°C. This process was repeated for double- and triple-layered structures. After embedding  $\beta$ -FeSi<sub>2</sub> in Si, a boron-doped *p*<sup>+</sup>-Si capping layer ( $p1.0 \times 10^{18} \text{ cm}^{-3}$ ) was grown at 700°C. Samples were finally annealed at 900°C in an Ar atmosphere for 14 h to further improve the crystal quality, resulting in  $\beta$ -FeSi<sub>2</sub> particles embedded in Si matrix. The mesa structure of 1.5 $\times$ 1.5 mm<sup>2</sup> was made by wet chemical etching. The EL spectra were measured under 200 Hz pulsed current biasing of 50 % duty cycle. Luminescence was dispersed by a 25cm focal-length grating mono-

chromator, and detected phase sensitively by a liquid nitrogen cooled InP/InGaAs photomultiplier (Hamamatsu Photonics R5509-72).

### 3. Results and Discussion

Cross-sectional SEM images of single-, double- and triple-layered  $\beta$ -FeSi<sub>2</sub>-particles/Si structures without the *p*<sup>+</sup>-Si capping layer were shown in Figs. 1(a), 1(b) and 1(c), respectively. We can see clear layered structure of  $\beta$ -FeSi<sub>2</sub> particles in these samples. It was found from  $\theta$ -2 $\theta$ X-ray diffraction spectra shown in Fig. 2 that only [100]-oriented diffraction peaks of  $\beta$ -FeSi<sub>2</sub> were seen, indicating that the epitaxial relationship between the  $\beta$ -FeSi<sub>2</sub> and Si was preserved even after the aggregation and the Si overgrowth.

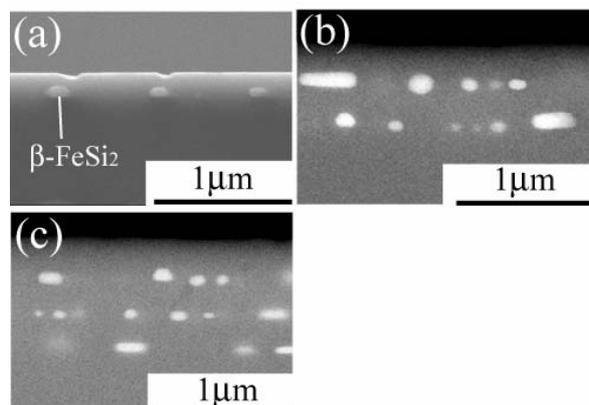


Fig.1 SEM cross sections of (a) single-, (b) double- and (c) triple-layered  $\beta$ -FeSi<sub>2</sub>-particles/Si structures.

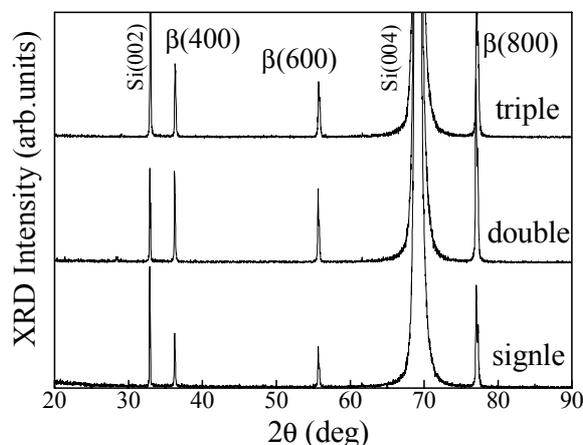


Fig. 2  $\theta$ -2 $\theta$  XRD spectra of single-, double- and triple-layered structures.

Figure 3 shows PL spectra measured at 77 K for these three samples. It was found that the 1.53  $\mu\text{m}$  PL intensity was proportional almost to the number of  $\beta\text{-FeSi}_2$ -particles/Si layered structure. This is attributed to the fact that the number of  $\beta\text{-FeSi}_2$  particles where electron and hole pairs recombine radiatively increased without increasing defect densities.

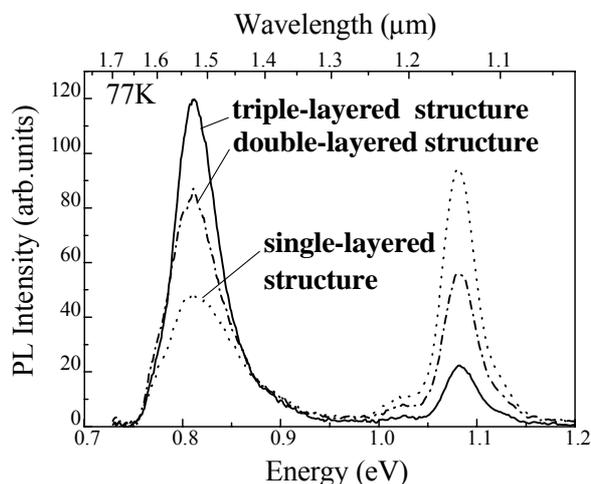


Fig. 3 PL spectra measured at 77 K.

Hereafter we compare the EL properties of a single-layered LED with those of a double-layered one. Both samples showed clear rectifying characteristics of Si  $p$ - $n$  junctions in the current-voltage ( $I$ - $V$ ) characteristics. RT EL spectra as a function of injected current density obtained for single-layered LED were shown in Fig.4 for reference. The 1.6  $\mu\text{m}$  EL was observed for current density above 75  $\text{A}/\text{cm}^2$ , and the EL intensity increased superlinearly with injected current as observed in our previous LEDs, probably due to nonradiative recombination centers in and around the  $\beta\text{-FeSi}_2$  [3,4].

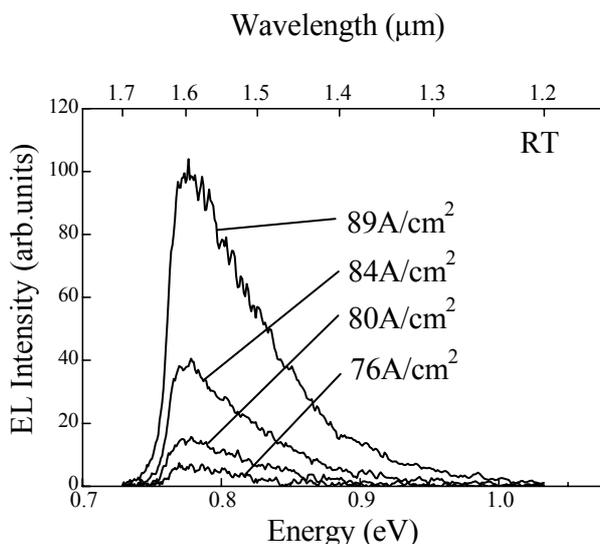


Fig. 4 RT EL spectra as a function of injected current density measured at RT.

Figure 5 shows the temperature dependence of 1.6  $\mu\text{m}$  EL intensity for single- and double-layered LEDs. The EL intensity for the double-layered LED was much stronger than that of the single-layered LED, differently from the results obtained in PL. The reason for this EL enhancement has not yet been clarified, but the densities of electron and hole which recombine radiatively are much higher in the upper  $\beta\text{-FeSi}_2$  particles than in the lower ones. By further optimizing the diode structure and the doping profile, practical Si-based LEDs will be obtained in the near future.

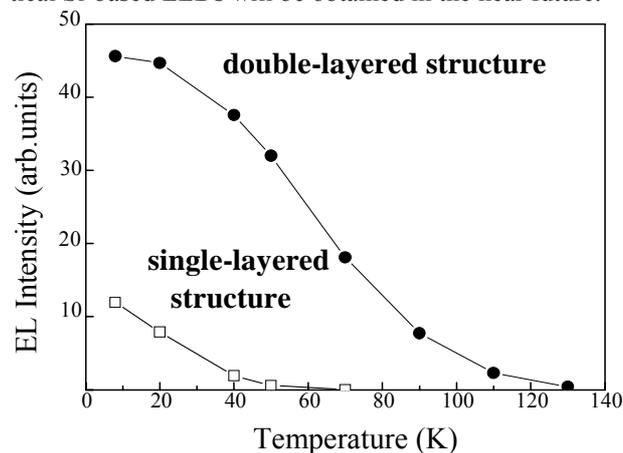


Fig. 5 Temperature dependence of integrated EL intensity.

#### 4. Conclusions

We have fabricated Si-based LEDs with single-, double- and triple-layered  $\beta\text{-FeSi}_2$ -particles/Si active region by RDE for  $\beta\text{-FeSi}_2$  and by MBE for Si. It was found that the multilayered LED structure was very effective to enhance the 1.6  $\mu\text{m}$  EL.

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#### References

- [1] M. C. Bost and J. E. Mahan, J. Appl. Phys. **58** (1985) 2696.
- [2] D. Leong, M. Harry, K. J. Reeson and K. P. Homewood, Nature **387** (1997) 686.
- [3] T. Suemasu, Y. Negishi, K. Takakura and F. Hasegawa, Jpn. J. Appl. Phys. **39** (2000) L1013.
- [4] T. Suemasu, Y. Negishi, K. Takakura, F. Hasegawa and T. Chikyow, Appl. Phys. Lett. **79** (2001) 1804.
- [5] T. Suemasu, M. Tanaka, T. Fujii, S. Hashimoto, Y. Kumagai and F. Hasegawa, Jpn. J. Appl. Phys. **36** (1997) L1225.
- [6] Y. Ozawa, C. Li, T. Suemasu and F. Hasegawa, J. Appl. Phys. **95** (2004) 5483.