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Fabrication of p-Si/β-$FeSi_2$/n-Si Double-Heterostructure Light-Emitting Diode by Molecular Beam Epitaxy

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1. Introduction

Semiconducting iron disilicide (β-$FeSi_2$) has been attracting much attention as a Si-based light emitter with a wavelength (~1.5 μm) corresponding to optical fiber communication [1]. Room temperature (RT) 1.6 μm electroluminescence (EL) has already been realized from β-$FeSi_2$ particles embedded in Si *p-n* diodes formed on Si(001) by ion beam synthesis (IBS) [2-4] and by molecular-beam epitaxy (MBE) methods [5,6]. In an effort to make an efficient light-emitting diode (LED), it is necessary to form a Si/β-$FeSi_2$ film/Si double-hetero (DH) structure by embedding a continuous β-$FeSi_2$ film rather than particles in Si. However, the epitaxial β-$FeSi_2$ film on Si(001) exhibits a strong tendency to form islands when it was annealed at high temperature for improving the crystalline quality or embedded by MBE-Si capping layers for forming a DH structure [7]. Therefore, the β-$FeSi_2$ particles have been used as an active region in LEDs grown by MBE. There have, however been a few reports showing that smooth β-$FeSi_2$ films can be grown on Si(111), even at high temperatures, in spite the large lattice mismatch (~5 %) between the two materials [8,9]. To the best of our knowledge, there have been no reports on the formation of a Si/β-$FeSi_2$/Si DH structure by MBE.

In this work, we report on the realization of EL from *p*-Si/β-$FeSi_2$ film/*n*-Si DH structures formed on Si(111) substrates by MBE for the first time.

2. Experimental

An ion–pumped MBE system equipped with electron-beam evaporation sources for Fe and Si was used. *p*-Si/β-$FeSi_2$/*n*-Si DH structure LEDs were fabricated on an *n*-type epitaxial Si(ρ=0.1–1Ω·cm)/Czochralski n^+- Si(111) (ρ=0.004 Ω·cm) substrate as follows. A 20 nm-thick [110]/[101]-oriented β-$FeSi_2$ epitaxial layer was grown by reactive deposition epitaxy (RDE; Fe deposition on hot Si) at 650ºC as a first step, and this layer was used as a template. Next, a 70 nm-thick [110]/[101]-oriented undoped β-$FeSi_2$ layer was epitaxially grown by MBE at 750ºC, followed by a 0.5 μm-thick undoped MBE-Si overlayer grown at 500ºC. Finally, a 0.2 μm-thick boron-doped p^+-Si capping layer (p~1.0×10^{18} cm^{-3}) was grown at 700ºC. To improve the crystal quality, the wafer was annealed in Ar at 800ºC. The mesa structure of 1.5×1.5 mm^2 was made by wet chemical etching. An Al finger-type contact was formed on the p^+-Si layer and sintered at 450°C for 20 min. The backside contact was made with AuSb. The EL spectra were measured at 77 K and RT under 200 Hz pulsed current biasing of 50 % duty cycle. Luminescence was dispersed by a 25-cm focal-length grating monochromator, and detected phase sensitively by a liquid nitrogen cooled InP/InGaAs photomultiplier (Hamamatsu Photonics R5509-72).

3. Results and Discussion

Figure 1 (a) shows the cross-sectional SEM image of the DH structure formed on the Si(111) substrate. The β-$FeSi_2$ continuous film was successfully embedded in a Si matrix. It was found that both the thickness of the Si overlayer and the annealing temperature were key parameters to forming a Si/β-$FeSi_2$/Si DH structure on Si(111). If the annealing temperature was higher (~900ºC) or the thickness of the Si overlayer was thinner (~0.3 μm), β-$FeSi_2$ was found to aggregate into particles during high temperature annealing as shown in Fig. 1(b). This aggregation is due probably to the lattice mismatch between the two materials. For reference, a typical example of Si/β-$FeSi_2$ particles/Si structure formed on Si(001) is shown in Fig. 1(c) [6].

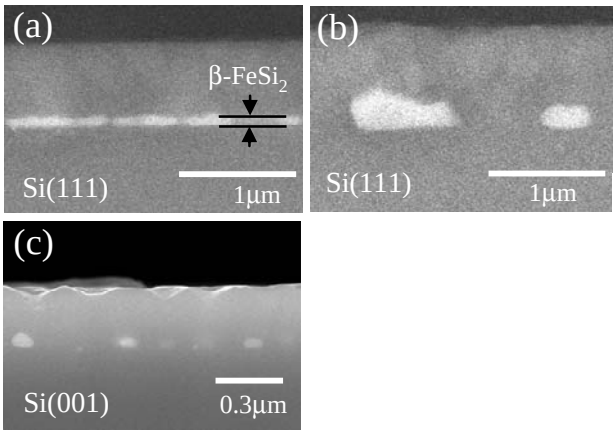

Fig.1 Cross sectional SEM images of Si/β-$FeSi_2$/Si structures on Si(111) obtained after annealing at (a) 800°C and (b) 900°C. (c) is a typical example of Si/β-$FeSi_2$/Si structure formed on Si(001).

Figure 2 shows θ-2θ XRD pattern of the DH structure LED. The β-$FeSi_2$(220) and/or (202) diffraction peak is dominant and there are no other peaks except for the Si and weak β-$FeSi_2$(040) and/or (004), indicating that the highly oriented β-$FeSi_2$ film was embedded in the Si matrix with its epitaxial relationship to the substrate preserved.

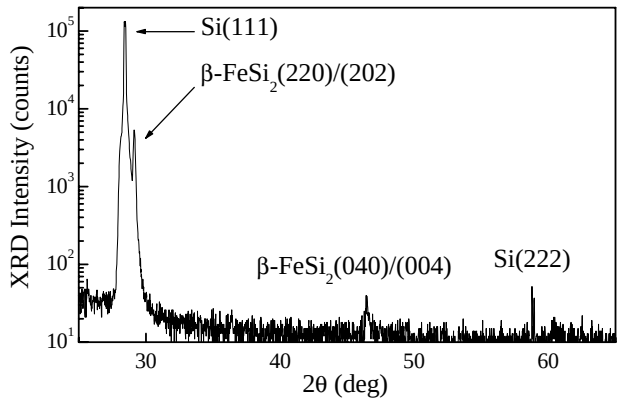

Fig. 2 θ-2θ XRD spectrum of p-Si/β-$FeSi_2$/n-Si DH structure LED.

Figure 3 shows the current-voltage (*I-V*) characteristics of the LED at RT. Clear rectifying characteristics are seen. The solid lines show the slope in the case that an ideality factor η equals to 1 or 2.

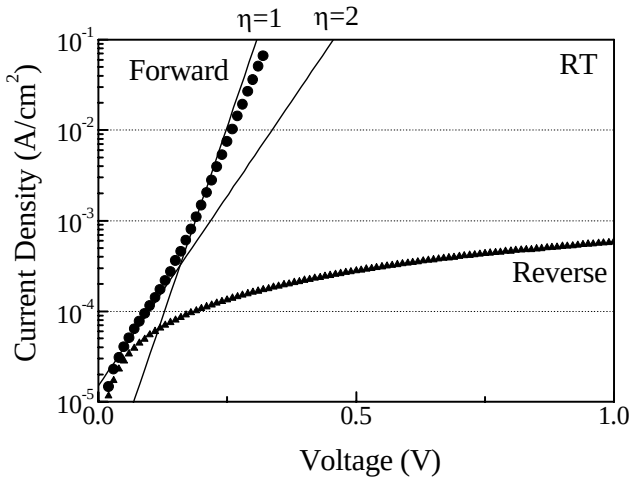

Fig. 3 Current-voltage characteristics of the LED at RT.

Figure 4 shows EL spectra as a function of injected current density at 77K. The EL peak was observed at approximately 1.55 μm at low current injection, but it showed clear blue shift with increasing injected current density. This is due probably to the band-filling effect. When the bias current is large enough, ground states are occupied and injected carriers start to fill the higher energy levels, giving rise to EL with higher peak energy. It was also found that the integrated EL intensity of the LED increased almost linearly with injected current density as shown in the inset of Fig. 4. This result suggests that most of the bias current contributed to the EL from the embedded β-$FeSi_2$ active layer. Our first, non-optimized LED showed weak but observable EL at RT. We therefore suppose that by optimizing the growth condition and the doping profile, practical Si-based LEDs will be obtained in the near future.

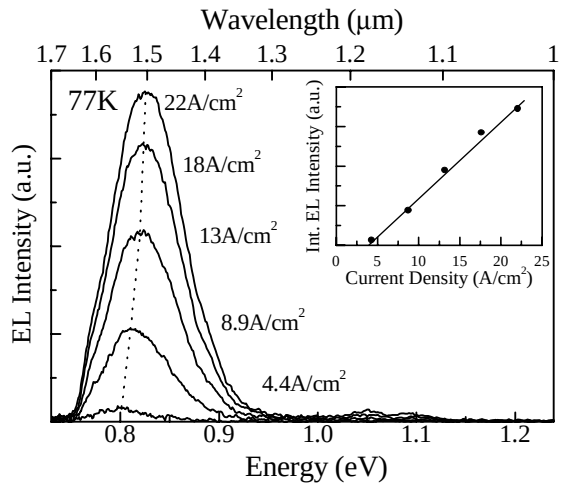

Fig. 4 EL spectra at 77 K. Inset is the current density dependence of integrated EL intensity.

3. Conclusions

We have fabricated *p*-Si/β-$FeSi_2$ film/*n*-Si DH structure LEDs on Si(111) substrate by MBE, and realized 1.5 μm EL. It was found that both the thickness of the Si overlayer and the annealing temperature were key parameters to forming a Si/β-$FeSi_2$/Si DH structure on Si(111) without aggregation of β-$FeSi_2$.

Acknowledgements

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