# Photoluminescence Enhancement in β-FeSi<sub>2</sub> by Annealing in Oxygen

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## 1. Introduction

Semiconducting  $\beta$ -FeSi<sub>2</sub> shows photoluminescence (PL) and photoresponse near 1.54 µm, which is a wavelength for fiber optics communications. This material has been regarded as a candidate for application to monolithic integrated circuits of optoelectronics devices because of the compatibility with the Si-process technology [1]. However, detailed mechanism of optical processes in  $\beta$ -FeSi<sub>2</sub> has not been well understood. In order to obtain more intense 1.5 µm-emission, a technology for improvement is required. Recently, we reported that the doping of Al atoms into  $\beta$ -FeSi<sub>2</sub> induces the significant enhancement of PL intensity, and pointed out that the Si vacancies play a role of nonradiative center in  $\beta$ -FeSi<sub>2</sub> [2].

In this study, we examined the effects of annealing ambient on the PL intensity. We found that the PL intensity was much enhanced when  $\beta$ -FeSi<sub>2</sub> was annealed in oxygen.

### 2. Experiments

Samples of on Si(100) were prepared by an ion beam synthesis (IBS) methods [3]. After the implantation of <sup>56</sup>Fe<sup>+</sup> ions into Si(100), the substrates were annealed at 800°C for 2-16 h by a rapid thermal anneal (RTA) in order to form  $\beta$ -FeSi<sub>2</sub> and to remove implantation damages. We performed the sample annealing in a vacuum, Ar, N<sub>2</sub>, or air(O<sub>2</sub>+N<sub>2</sub>). The cross-section images of scanning electron microscope (SEM) show the formation of  $\beta$ -FeSi<sub>2</sub> precipitates near the surface. PL was investigated at 10-300 K with an Ar<sup>+</sup> ion laser of the 514.5 nm line, a 32 cm focal length single monochromator and a liquid nitrogen-cooled Ge pin photodiode. In X-ray photoelectron spectroscopy (XPS), the depth profiles from the surface were examined by the XPS intensity of O 1s, Si 2p and Fe 2p.

### 3. Results and Discussion

Figure 1 shows the PL spectra from  $\beta$ -FeSi<sub>2</sub> samples annealed at 800°C for 8 h in the vacuum, air (O<sub>2</sub>+N<sub>2</sub>) or N<sub>2</sub>. It should be noted that the sample annealed in the air shows much larger PL intensity than others. The result reveals that the annealing in the air is a technique to enhance the PL intensity of  $\beta$ -FeSi<sub>2</sub>.

From the analysis of the temperature dependence of the PL intensity, we obtained the activation energy  $(E_a)$  for non-radiative recombination processes. Figure 2 shows the annealing time dependence of  $E_a$ .  $E_a$  of the sample annealed in the air are much larger than that annealed in the vacuum. Therefore, the annealing in the air is considered to reduce the non-radiative centers in  $\beta$ -FeSi<sub>2</sub> and make it possible to obtain the intense PL by the short time annealing.

In XPS spectra of the samples annealed in the air, we found that thick oxides were formed at the surface. Figure 3 shows the dependence of the oxide thickness on the annealing time in the air. The thickness of the surface oxide shows an increase with the annealing time in the air. While, the depth profile of Fe 2p spectra does not change with the annealing time. Hence, during the annealing in the air, the distribution of  $\beta$ -FeSi<sub>2</sub> is almost constant while the surface oxide becomes thick. These results suggest that the PL intensity becomes much larger when the sample surface is covered with the thickness of the surface oxide is about 1-2 nm and has no dependence on the annealing time.

As described before, the Si vacancy producing dangling bonds of Fe has a possibility to act as the non-radiative recombination centers that cause quenching the PL. During a post-annealing at 800°C in a vacuum, the diffusion of Si atoms from the silicon matrix into  $\beta$ -FeSi<sub>2</sub> precipitates takes place. In fact, Si atoms are the dominant moving species in the diffusion of  $\beta$ -FeSi<sub>2</sub> [4]. As a result, the number of Si vacancies in  $\beta$ -FeSi<sub>2</sub> decreases with increase of the annealing time and then the non-radiative transition is suppressed. The increase of  $E_a$  in the sample annealed with the vacuum is due to the effect of the long time annealing (in Fig. 2).

In this study, we found that both the PL intensity and  $E_a$ are much lager in the sample annealed in the air than in that annealed in the vacuum after the same annealing time. Assuming that the Si vacancies in the  $\beta$ -FeSi<sub>2</sub> play an important role for the PL intensity, our results can be explained as follows. During the post-annealing in a vacuum, SiO gases evaporate from the thin SiO<sub>2</sub> surface because the O<sub>2</sub> pressure is too low to form SiO<sub>2</sub>. The SiO evaporation and the decomposition of SiO<sub>2</sub> were found to be maintained for a while even after the oxide growth [5]. The SiO evaporation induces number of Si vacancies in B-FeSi2 and consequently suppresses the PL enhancement after the long time annealing. During the annealing in the air, the very thick SiO<sub>2</sub> layer is easily formed at the surface. The SiO<sub>2</sub> capping layer prevents the evaporation of SiO gases. We speculate that enhancement of the PL intensity and increase of  $E_a$  in the sample annealed in the air originates from the suppression of the Si vacancies due to SiO evaporation.

#### 4. Conclusions

We confirmed that the post-annealing with oxygen is a technique to enhance the 1.5  $\mu$ m PL emission of  $\beta$ -FeSi<sub>2</sub>.

#### References

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Fig. 1 PL spectra from  $\beta$ -FeSi<sub>2</sub> precipitates after annealing in a vacuum, the air and N<sub>2</sub> gas.



Fig. 2 Annealing time dependence of the activation energy for a non-radiative recombination process.



Fig. 3 Annealing time dependence of SiO<sub>2</sub> thickness at the surface.