World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:5, No:2, 2011

Photoluminescence Properties of β-$FeSi_2$ on Cu- or Au-coated Si

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***Abstract*—**The photoluminescence (PL) at 1.55 μm from semiconducting β-$FeSi_2$ has attracted a noticeable interest for silicon-based optoelectronic applications. Moreover, its high optical absorption coefficient (higher than 10^5 cm^{-1} above 1.0 eV) allows this semiconducting material to be used as photovoltanics devices.

A clear PL spectrum for β-$FeSi_2$ was observed by Cu or Au coating on Si(001). High-crystal-quality β-$FeSi_2$ with a low-level nonradiative center was formed on a Cu- or Au- reated Si layer. This method of deposition can be applied to other materials requiring high crystal quality.

***Keywords*—**iron silicide, semiconductor, epitaxial, photoluminescence.

I. Introduction

THE photoluminescence (PL) at 1.55 μm from semiconducting β-$FeSi_2$ has attracted a noticeable interest, and has attracted much attention over the past ten years as one of the promising materials for silicon-based optoelectronic applications [1]. It is able to epitaxially grow on Si substrates [2]. Light-emitting diodes using β-$FeSi_2$ active-layer showed the emission efficiency of about 0.1% [3]. It is pointed out that non-radiative recombination centers at hetero-interfaces affect the light emission efficiency.

In this study, we report an improvement in the crystallinity of β-$FeSi_2$ film as well as β-$FeSi_2$/Si hetero-interface and the enhancement of PL intensities by coating Cu or Au layer on Si(100) wafers using metal-organic chemical vapor deposition (MOCVD).

II. Experimental

40-nm-thick Au and 20-nm-thick Cu layers were deposited on n-type floating-zone (FZ) Si(001) wafers at room temperature in vacuum (<5x10e^{-6} Torr) atmosphere. For the Si(001) wafer without metal layer, a 20-nm-thick (100)-oriented β-$FeSi_2$ template was prepared at 743K by the reactive deposition epitaxy (RDE) method. The details of the RDE method were already described in a previous paper [4].

200-nm-thick β-$FeSi_2$ thin films were deposited on the Au-coated Si, Cu-coated Si substrate and on the bare Si substrate by metal-organic chemical vapor deposition (MOCVD) using iron pentacarbonyl [$Fe(CO)_5$] and monosilane (SiH_4). The deposition temperature and rate were 1023K and 1.6 nm/min, respectively.

Crystallographic structure of the films was characterized by x-ray diffraction (XRD, Philips MRD) using a Cu Kα radiation. Thin film specimens for TEM observation were fabricated using a focused ion beam (FIB) machine with a micro-sampling unit. Observations were performed with a JEM-2000EX/T and TECNAI-F20 (STEM-EDS) microscopes.

The PL spectrum was measured using the 514.5 nm line of an argon-ion laser. The average excitation power and the spot diameter of the laser beam were 50 mW and 0.5 mm, respectively. The PL spectrum was collected by aspheric lens group with three groups and three elements (*F/ 1.25*) and analyzed with a 1 m focal length single monochromator (Jobin Yvon THR-1000) and detected with a liquid nitrogen-cooled Ge p-i-n photodiode (Edingburg Instruments) and amplified by the lock-in technique.

III. Results and Discussion

Figure 1 shows the XRD θ-2θ scan profiles for the films on (a) Si(001) with β-$FeSi_2$ template, (b) Cu-coated and (c) Au-coated Si(001) wafers. (100)-oriented β-$FeSi_2$ films were grown on the Si(001) wafers with β-$FeSi_2$ template layer, as shown in Fig. 1(a). This β-$FeSi_2$ films were epitaxially grown on Si(001) [5].

Polycrystalline β-$FeSi_2$ phase preferred to (100)-orientation and a mixture phase of α-$FeSi_2$ and β-$FeSi_2$ were observed on Cu-coated Si and on Au-coated Si(001) wafers, respectively, as shown in Fig. 1(b) and 1(c). Moreover, these α-$FeSi_2$ and β-$FeSi_2$ phases on Au-coated Si(001) wafers were preferred to (001)-orientation and (101)/(110)-orientation, respectively.

Cross-sectional TEM images of β-$FeSi_2$/Si interfaces are shown in Figure 2. The film on the Si(001) with β-$FeSi_2$ template was constituted of crystalline grains growing more than 1 μm in the size, as shown in Fig. 2(a). The striped pattern in the β-$FeSi_2$ grain indicates the existence of the defect, i.e. stacking fault, dislocation.

The film on the Cu-coated Si substrate contained of small crystalline grains with several hundred nm sizes. The roughness

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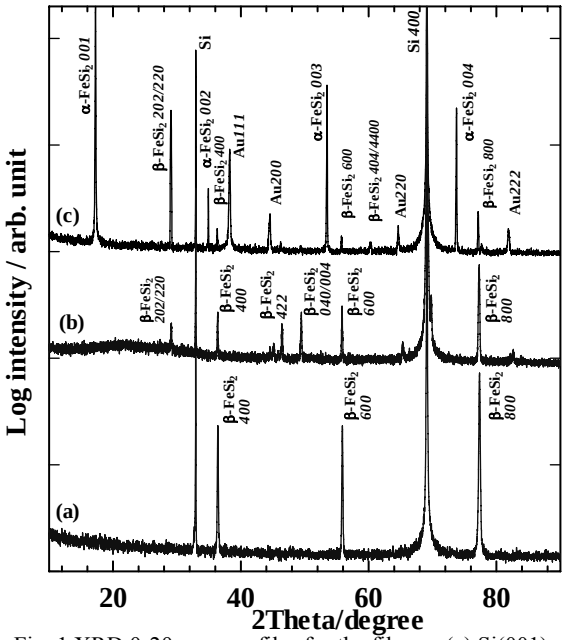

Fig. 1 XRD θ-2θ scan profiles for the film on (a) Si(001) with β-$FeSi_2$ template, (b) 20nm-thick Cu coated Si(001), and (c) 40nm-thick Au-coated Si(001) wafers.

of the interface between the film and the Cu-coated Si substrate increased, and the different facet planes from (100)β-$FeSi_2$/(001)Si was formed (Fig. 2(b)). A slash lines indicating stacking fault grain were observed in β-$FeSi_2$ grains.

As shown in Fig. 2(c), trapezoid β-$FeSi_2$ crystal grains with sizes of several micrometers were observed on the Si surface, for the Au-coated Si(001) wafers. The β-$FeSi_2$ /Si interface was

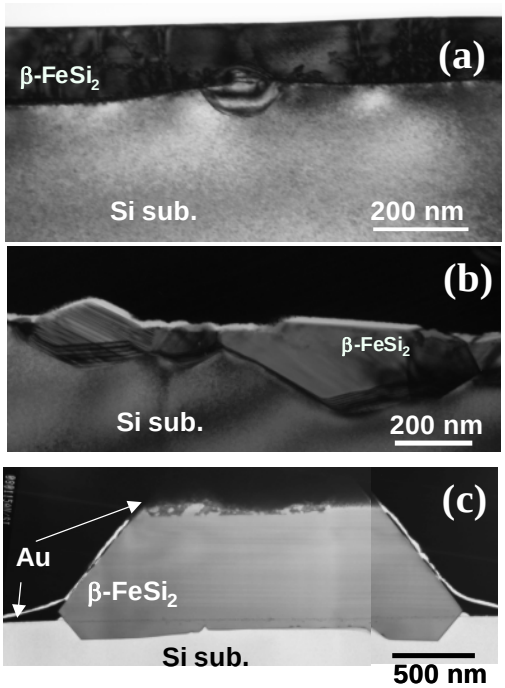

Fig. 2 Cross-sectional TEM images for the film on (a) Si(001) with β-$FeSi_2$ template, (b) 20nm-thick Cu coated Si(001), and (c) 40nm-thick Au-coated Si(001) wafers.

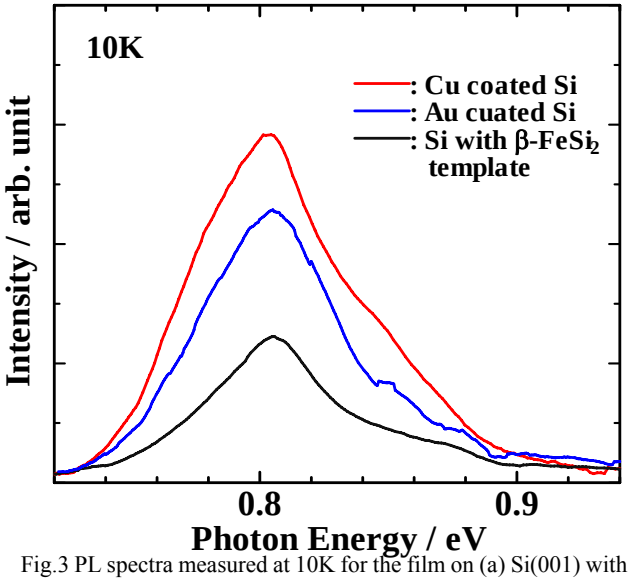

Fig.3 PL spectra measured at 10K for the film on (a) Si(001) with β-$FeSi_2$ template, (b) 20nm-thick Cu coated Si(001), and (c) 40nm-thick Au-coated Si(001) wafers.

formed several hundred nanometers deep in the interior of the Si wafer and formed a steep facet plane. Energy dispersive X-ray spectroscopy (EDX) analysis indicated that Au covered the surface of Si and β-$FeSi_2$ grains. Moreover, boundaries were not observed in the grains.

Figure 3 shows PL spectra for the β-$FeSi_2$ on Si(001) with β-$FeSi_2$ template, Cu-coated and Au-coated Si(001) wafers, which were annealed at 1173K for 30 min in Argon atmosphere. Even after post-annealing for 30 min, the initial mixture phase of α-$FeSi_2$ and β-$FeSi_2$ phases remained in the sample on Au-coated Si(001).

The PL spectra for any samples showed clear peaks at 0.806 eV. While the apparent shapes of the PL spectra appear to be structured with few luminescence bands, the peak energy corresponded to that of β-$FeSi_2$, reported by Hunt et al. [6] and Martinelli et al. [7]. The peak intensity for the β-$FeSi_2$ grain on Cu- and Au-coated Si(001) was approximately twice as large as that for the epitaxial β-$FeSi_2$ film on Si(001) with β-$FeSi_2$ template.

Figure 4 shows the dependence of PL peak intensity on temperature for the β-$FeSi_2$ grain on Cu- and Au-coated Si(001), together with those for epitaxial β-$FeSi_2$ films on Si(001) with the template, which were annealed at 1173K for 30 min. The PL spectra with varied temperature showed almost same shape. The peak intensities for the β-$FeSi_2$ grain on Cu- and Au-coated Si(001), remained higher than that for epitaxial films even though the temperature was elevated. However, the peak intensity for the β-$FeSi_2$ grain on Au-coated Si(001) was higher than that for films on Cu-coated Si(001) above 50K.

PL quenching at elevated temperatures is generally attributed to the escape of carriers to nonradiative recombination paths [8]. These results convinced us that the

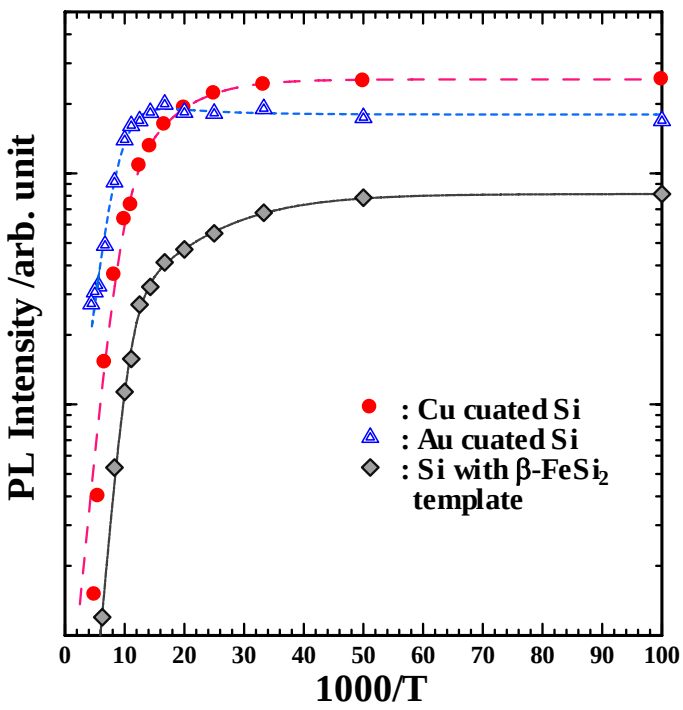

Fig. 4 PL peak intensities as a function of temperature for the film on (a) Si(001) with β-$FeSi_2$ template, (b) 20nm-thick Cu coated Si(001), and (c) 40nm-thick Au-coated Si(001) wafers.

density of the nonradiative recombination center in β-$FeSi_2$ grain on Cu- and Au-coated Si(001) is lower than that in epitaxial β-$FeSi_2$ films. Moreover, the density of the nonradiative recombination center in β-$FeSi_2$ grain on Au-coated Si(001) is lower than that in β-$FeSi_2$ grain on Au-coated Si(001). These results agreed with the result of TEM observation.

IV. Summary

A clear PL spectrum for β-$FeSi_2$ was observed by Cu or Au coating on Si(001). High-crystal-quality β-$FeSi_2$ with a low-level nonradiative center was formed on a Cu- or Au-reacted Si layer. This method of deposition can be applied to other materials requiring high crystal quality. The TEM observation of β-$FeSi_2$/Si interface showed the formation of clear facet planes and suggested this speculation.

Acknowledgment

The authors would like to thank Yoshitsugu Sato at Kanagawa Industrial Technology Center for technical support. This research was supported in part by Grants-in-Aid for Scientific Research, Japan Society for the Promotion of Science.

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