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Photoluminescence Property of Nano-Composite Phases of $\beta$-FeSi$_2$ Nanocrystals Embedded in SiO$_2$

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We have investigated photoluminescence (PL) behaviors of nano-composite phase of $\beta$-NCs embedded in SiO$_2$ ($\beta$-NCs/SiO$_2$). The inhomogeneous spectra consisting of the A, B and C emission bands were observed. PL enhancement also was confirmed in comparison with $\beta$-NCs/Si. Under high pumping rate, we observed PL spectra near room temperatures (~270 K). This fact means that oxidation of the nano-composite phase can contribute to reduction of thermal quenching, which may come from increase of band offsets around $\beta$-NCs.

1. Introduction

Nano-Composite phases of $\beta$-FeSi$_2$ nanocrystals ($\beta$-NCs) embedded in Si may be best IR light emitters because of their strong intrinsic band (A band) emission. However, in the nano-composite of $\beta$-NCs/Si, pronounced thermal quenching of emission, that means large damping of emission intensity as temperature increases, like a stone wall for realization of light emission at room temperature. It was reported that surface oxidation of $\beta$-FeSi$_2$ was effective to reduction of surface recombination adapting to thermal relaxation and to enhancement of light emission [1]. Ion beam analysis revealed that the surface of $\beta$-FeSi$_2$ was covered with Si rich layers. Therefore, the surface oxidation creates SiO$_2$ surface layers on $\beta$-FeSi$_2$ [2]. From an electronic view point, the formation of SiO$_2$ at the surface is very important to make the radiative recombination between electrons and holes larger, because SiO$_2$ has a larger band-gap and can make larger band offsets ($\Delta E_c$, $\Delta E_v$) with $\beta$-FeSi$_2$ than Si. FTIR study of oxidation of nano-composite phase revealed that only Si phase can be oxidized into SiO$_2$ and promising nano-composite of $\beta$-NCs embedded in SiO$_2$ [3]. In this study, photoluminescence property of nano-composite of $\beta$-NCs embedded in SiO$_2$ ($\beta$-NCs/SiO$_2$) was investigated toward possible light emission near room temperature.

2. Experiments

The nano-composite phase with $\beta$-NCs and Si was fabricated by ion-beam synthesis (IBS) processes [4]. In the IBS, ion implantation of mass separated $^{56}$Fe$^+$ into n-type Si(100) with 500 mm thickness was carried out at 200 keV. The ion dose was $10^{17}$ ions/cm$^2$. After the implantation, the sample was annealed at 800 °C for 2 h to make the nano-composite phase on Si(100) substrates. Moreover, the composite phase was oxidized in an electrical furnace at 900 °C in circulating dry air. Photoluminescence (PL) of nano-composite phase was excited with a 641 nm wavelength laser diode (LD) and the PL spectrum detected with a monochromator (Jobin-Yvon HR 320) and a Ge PIN photodiode (Edinburgh Instrument). Photocarrier-injection PL (PCI-PL) was excited when sample back-side (Si substrate) was irradiated with the LD. In the PCI-PL measurements, we measured the intensity and phase shift from the
reference signal of irradiated laser in order to get information of minority carrier transport and injection into β-NCs which may play as a radiative well for a radiative recombination of electrons and holes.

3. Results and Discussion

Figure 1 shows PL spectrum of nano-composite phase oxidized for 6 h. The PL spectrum of non-oxidized NCs is also shown in their comparison. The broad PL spectrum with intrinsic A band at 0.803 eV, extrinsic B band near 0.87 eV and C band at 0.77 eV was observed in Fig.1. It was found that both intensities of B and C bands were specially enhanced. The C band emission is originated from a radiative recombination transition between impurity (donor or acceptor) levels and a valence or conduction band in β-FeSi$_2$. However, the origin of the B band emission has not been clarified, which may be an impurity or defect related emission band.

![PL Spectrum](image)

**Fig. 1.** PL spectrum of nano-composite phase of β-NCs embedded in SiO$_2$ after oxidation for 6 h.

Figure 2 shows temperature dependence of whole PL spectra. The A, B and C bands have absolutely different temperature dependences each other, so that the apparent shape of PL spectrum showed inhomogeneous change at each temperature can be expressed by Varshni empirical formula (thermodynamic model), however, the energy of the C band can be expressed by a transition function (two levels model) [5]. We confirmed that the same situation was consistent also in the nano-composite phase of β-NCs embedded in SiO$_2$. This fact means that oxidation does not bring any different mechanisms to initial radiative processes in β-NCs.
Fig. 2. Temperature dependence of PL spectra observed in non-composite phases oxidized at 900 °C for 6 h.

Fig. 3. PL spectra near room temperatures observed in non-composite phases oxidized at 900 °C for 6 h.
Next we investigated thermal quenching of the PL of oxidized nano-composite phases. The PL spectra were excited by the same pumping rate (the same excitation laser power density), so that the PL spectra near room temperature showed large intensity damping. The PL spectra above 250 K excited under high pumping rate (\(P_{ex}\)=40 mW) were shown in Fig.3. Systematic change of the PL spectrum was firstly observed in nano-composite phase. Therefore, we can confirm that oxidation of nano-composite phases can contribute to reduce thermal quenching of radiative emission. We will discuss radiative process of oxidized nano-composite phases using results of PCI-PL measurements which may be helpful to understand electronic structures around \(\beta\)-NCs through a minority (holes) carrier injection process into \(\beta\)-NCs.

4. Conclusion

Photoluminescence behaviors of nano-composite phase of \(\beta\)-NCs embedded in SiO\(_2\) (\(\beta\)-NCs/SiO\(_2\) heterostructures) have been investigated. The inhomogeneous PL spectra consisting of the A, B and C emission bands and their enhancement also are observed in the \(\beta\)-NCs/SiO\(_2\) heterostructure. Under high pumping rate, we can observe PL spectra near room temperatures (\(~270\) K). This fact means that oxidation of the nano-composite phase can contribute to reduction of thermal quenching, which may come from increase of band offsets around \(\beta\)-NCs.

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