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IR Absorption Analysis of Oxidation Behaviors of Nano-Composite Phases with β-$FeSi_2$ Nanocrystals and Si

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We have investigated oxidation behaviors of nano-composite phase with β-$FeSi_2$ nanocrystals (β-NCs) and Si on Si substrates. IR absorption measurements revealed that only oxidation of Si into SiO_2 proceeded in the nano-composite phase. This fact is very important for realization of a novel composite phase with β-NCs and SiO_2, which may contribute to enhancement of light emission and to prevent a large thermal quenching of light emission observed in the composite phase with β-NCs and Si.

1. Introduction

Composite phase consisting of β-$FeSi_2$ nanocrystals (β-NCs) and Si (i.e. nano-composite phase) can be considered to be best for IR light emission at the telecom wavelength because of its strong light emission property. However, pronounced thermal quenching of light emission is an unavoidable problem for realization of light emission at room temperature. This thermal quenching mechanism may be originated from a small band offset in valence bands between β-NCs and Si, so that positive holes generated in β-NCs or holes coming from Si into β-NCs with LO phonon emission can not be confined sufficiently during radiative recombination and radiative efficiency at high temperature may be significantly reduced by thermal activation of holes. In order to make thermal quenching smaller and realize room temperature light emission with enough intensity, large band offsets in conduction and valence bands between β-NCs and Si are required.
In this study, toward realization of the β-NCs/SiO_2/Si nano-composite phase with large conduction and valence band offsets we have investigated oxidation behaviors of the β-NCs/Si nano-composite phase by using FTIR measurements at mid and far IR regions.

2. Experiments

The nano-composite phase with β-NCs and Si was fabricated by ion-beam synthesis (IBS) processes [1]. In the IBS, ion implantation of mass separated $^{56}Fe^+$ into n-type Si(100) with 500 μm 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 2-4 h to form the nano-composite phase in Si(100) substrates. Moreover, the composite phase was oxidized in an electrical furnace at 900 °C in circulating dry air. In this condition, it was confirmed that Si substrates can be oxidized as shown in Fig. 1.
Figure 1 shows that the integrated area of the absorbance (near 460 cm^{-1}) due to Si-O-Si stretching vibrations is proportional to the oxidation duration.
IR absorbance (Abs) spectra at both mid-IR (MIR) and far-IR (FIR) wavelength regions were measured in vacuum in order to prevent pronounced damping of IR source light and large effects of air to the MIR and FIR Abs spectra.

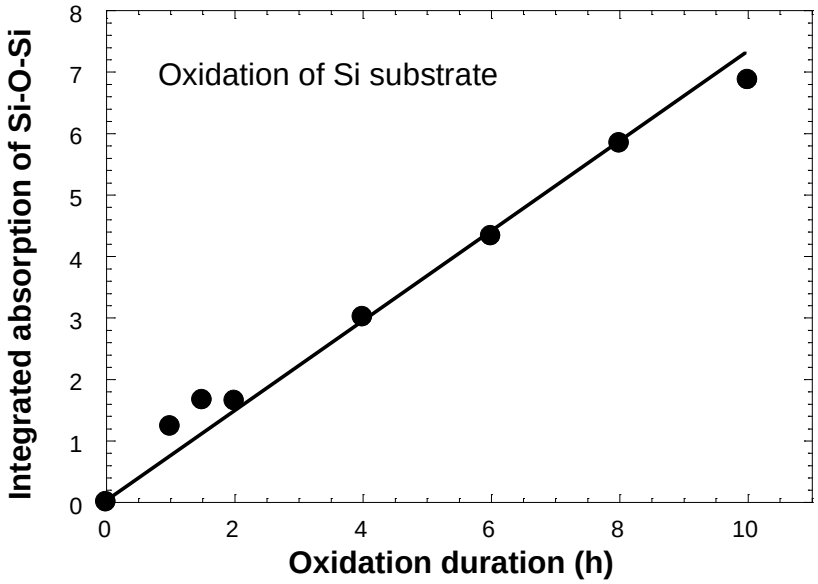

Fig. 1. Integrated area of absorbance due to the Si-O-Si stretching vibration mode of Si substrates as a function of oxidation duration (h) in dry air.

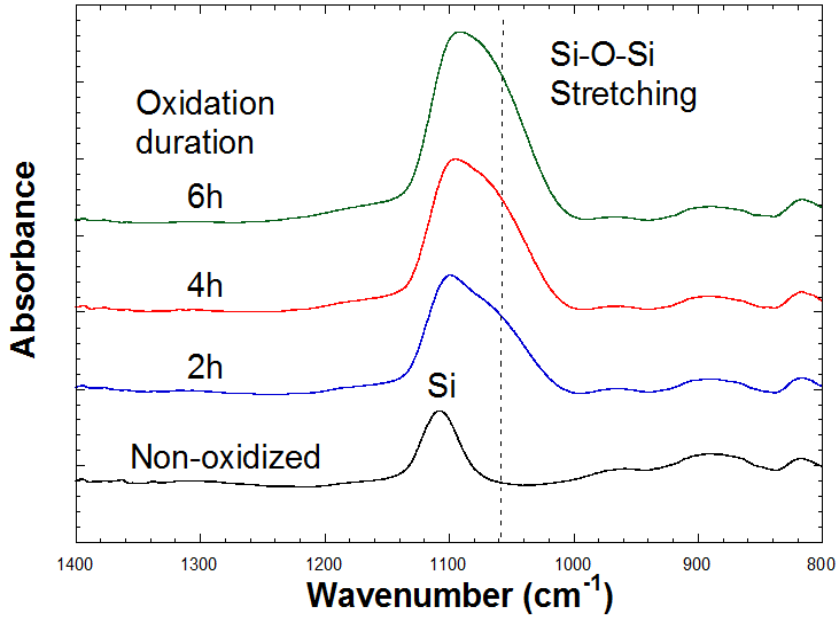

Fig. 2. IR absorption spectra of nano-composite phases oxidized for each times. The dotted line indicates the absorption due to a Si-O-Si stretching vibration mode.

3. Results and Discussion

Figure 2 shows absorbance spectra of nano-composite phase on Si(100) in the mid IR region (800-1400 cm^{-1}) as a function of oxidation duration 2~6 h. The MIR absorbance due to a Si-O-Si stretching TO and LO (anti-symmetric) mode can be observed around 1100 cm^{-1} in the presence of SiO_2.

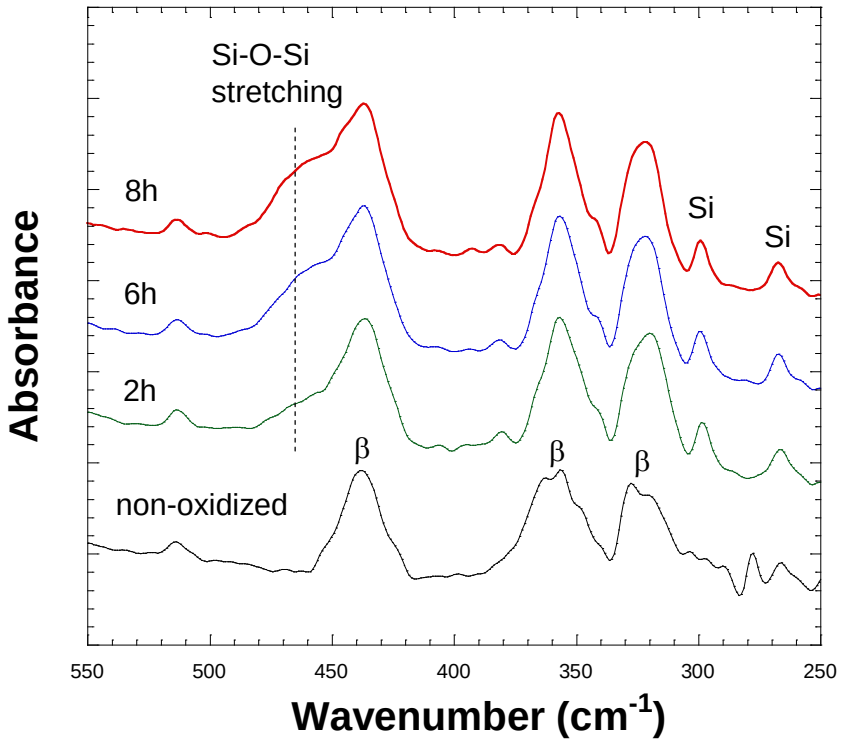

Fig. 3. Absorbance spectra of nano-composite phase oxidized for each times. The dotted line indicates a position of the absorbance due to the stretching vibration of Si-O-Si. The bottom spectrum corresponds to the non-oxidized composite phase, three absorption peaks due to localized phonons in the β-NCs can be observed near 330, 360 and 440 cm^{-1}.

The non-oxidized composite phase (the bottom spectrum) also indicated clear absorbance at 1060 cm^{-1} as a shoulder of the absorbance peaks which come from the Si-O-Si stretching vibration [2]. In fact, there is no appearance of it in the non-oxidized composite phase. It was observed that the absorbance at 1060 cm^{-1} increased as oxidation duration increased. This increase of absorbance intensity corresponds to the volume increase of SiO_2 in the composite phase. However, there is a remaining question if the oxidation takes place in both β-NCs and Si. So, we investigated oxidation behavior for both β-NCs and Si by using far IR absorption measurements.

Figure 3 shows absorbance spectra of the nano-composite phase on Si(100) in the far IR region (250-550 cm^{-1}) as a function of oxidation duration 2-8 h. In the spectra of non-oxidized composite phase, three typical absorptions due to localized phonons in β-NCs were observed near 330, 360 and 440 cm^{-1} [3].

In this FIR region, the absorbance peak due to symmetric stretch-stretching TO and LO modes should be also observed around 465 cm^{-1} (shown by the dotted line in Fig. 3) [2]. In fact, we observed a clear shoulder of absorbance in the peak at 465 cm^{-1} and its increase with increasing the oxidation duration.

On the other hand, intensities of three independent absorbance peaks due to β-NCs showed no change with increasing the oxidation duration. These observation results indicate very important facts that in the nano-composite phase oxidation takes place only in the Si phase. The chemical bond of (Fe-Si-O-Si) formed at the heterointerface may give large band offsets enough to confine electrons and holes inside β-NCs during a radiative recombination of the electron-hole pair.

4. Conclusion

We have investigated oxidation behaviors of nano-composite phase with β-NCs and Si on Si substrates. IR absorption measurements reveal that only oxidation of Si into SiO_2 proceeds in the nano-composite phase. This fact is very important for realization of a novel composite phase with β-NCs and SiO_2, which may contribute to enhancement of light emission [4] and to prevent a large thermal quenching of light emission observed in the composite phase with β-NCs and Si.

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