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Influence of deep-level concentrations on strong red photoluminescence from nano-porous silicon formed on Fe-contaminated silicon substrate

Dong-Yul Lee, Jong-Won Park, Sang-Soo Choi, Dong-Ho Kim, In-Ho Bae, Jae-Young Leem[1], Jong-Su Kim[2], Se-Kyung Kang[3], Jeong-Sik Son[4], and In-Soo Kim[4]

Department of Physics, Yeungnam University, Gyeongsan 712-749, Korea
E-mail: dongyulee@hanmail.net
[1]School of Nano Engineering, Inje University, Gimhae 621-749, Korea
[2]National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan
[3]Department of Physics, Kyunghee University, Suwon 449-701, Korea
[4]Department of Visual Optics, Kyungwoon University, Gumi 730-850, Korea

1. Introduction

Recently, in order to improve the photoluminescence (PL) efficiency and stability of the luminescent nano-porous silicon (PS), lots of research efforts have been made by using the various formation conditions of PS [1], the HF aqueous solution containing Fe ions [2], the metal passivation of silicon surface such as Au/Si [3] or Pt/Si [4], and the impurity incorporation through a doping [5] or ion implantation [6] on PS layer respectively. But it was very difficult to achieve simultaneously both the high PL efficiency and the invariable PL wavelength in PS layer with the reported process above.

In this work, we report on the strong and thermally stable red PL of PS samples formed on Fe-contaminated Si substrates. PS samples are prepared by a conventional chemical anodization of Si substrates. It is considered that the adoption of PS formed on Fe-contaminated Si substrate is a quite proper and new attempt to improve the PL characteristic because Fe ion such as transition metal can be easily introduced inside of the Si band gap as the deep levels. And then, it is preceded that the correlation is clarified between the PL characteristics and the different deep-level concentrations of PS samples formed on Fe-contaminated Si substrate. Moreover, the steadiness of PL peak position in PS formed on Fe-contaminated Si substrate is inspected with the reference PS.

2. Experiments

Samples were used with a boron-doped p-type Si (100) substrate with the resistivity of 5 - 10 Ω·cm. With using the spin coating method, the front surface of Si substrates was contaminated intentionally by Fe with the concentration of 100, 1,000 and 10,000 ppb. The Fe-contaminated Si substrates have been annealed at 900 °C for 1 hour in a dry N_2 ambient to diffuse Fe ions into the Si substrate, an electrochemical etching was proceeded to form PS layer on the Fe-contaminated Si substrate in the solution of $HF:H_2O:C_2H_5OH$ (1:1:2) under the illumination of halogen lamp with 250 W. The anodization current density was a 60 mA/cm^2 and the etching time was 5 minutes for all Fe-contaminated Si substrates. The reference PS sample was also prepared through the same process except for only the Fe contamination. Following the anodization, the all sample was rinsed in ethanol.

3. Results and discussions

A behavior of trap levels in the Fe-contaminated Si substrates, which is annealed at 900 °C in order to diffuse Fe ions, is observed through DLTS. Figure 1 is DLTS spectra of the reference and Fe-contaminated samples. Two traps, T_1 and T_2, related to Fe are observed. These trap peaks are strongly affected to Fe interstitial (Fe_i) and Fe-O pair [7]. DLTS signal of the Si substrate with Fe contamination of 1,000 ppb is the stronger than the other. This strong signal means that the re-emission of gettered Fe is occurred from the Si substrate with Fe contamination of 1,000 ppb. The drastic decrease of DLTS signal in the Si substrate with Fe contamination of 10,000 ppb is probably caused by an abrupt increase of Fe precipitation. In other words, it means that an excess Fe contamination in Si affects as the defect in Si substrate rather than as the factor of internal gettering.

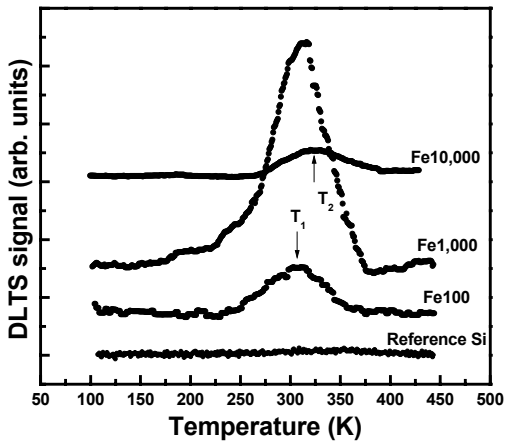

Fig. 1 DLTS spectra of Si substrates with various Fe contaminations.

Figure 2 is red PL spectra of the PS samples formed on Si substrates with various concentrations of Fe contamination. The reference PS sample shows a broad PL centered at around 1.65 eV and this red PL has the origin from the localized exciton at the interface region between nanocrystalline Si and SiO_2 layer of surface [8]. This

indicates the efficient localization of charge carriers into the surface-localized states of nanocrystalline Si, even though no intended confining layer for carriers was introduced. All Fe-contaminated PS samples exhibit a strong PL intensity but the reference PS sample shows a weak PL signal at the peak position of 1.65 eV. The PL intensity of PS sample with the Fe contamination of 1,000 ppb is the stronger than the others and it is decreased when the concentration of Fe contamination is exceeded too much until 10,000 ppb. From the results of Fig. 1 and Fig. 2, it is certain that the enhancement of this red PL is closely related to trap concentrations produced by Fe contaminations of Si substrate. In particular, the PS sample with Fe contamination of 1,000 ppb shows almost a ten times stronger red PL intensity, compared to the reference PS sample without any Fe contamination. And also, it is noticeable that the PL peak position is nearly fixed at about 1.65 eV regardless of various concentrations of Fe contamination. This means that there is no significant effect such as a size distribution of nanocrystalline Si in PS layer on Fe-contaminated Si substrate.

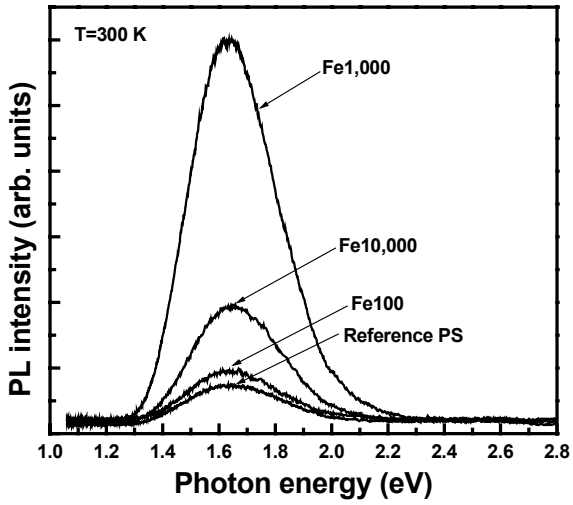

Fig. 2 300 K PL spectra of the reference PS and PS samples prepared by Si substrate with various Fe contaminations.

Figure 3 shows the direct correlations between the red PL intensities of PS samples and the trap concentrations of Si substrates with different concentrations of Fe contaminations. This correlations indicate that the distinct increase of PL efficiency can be attributed to the increase of trap concentrations produced by the Fe contaminations, and it seems that the remarkable enhancement of PL intensity is due to the increase of carrier localization in the PS surface via trap levels induced by the incorporation of Fe into Si crystalline phase. For Si substrate and PS sample with the same Fe contamination of 10,000 ppb, the decrease of both trap concentration and PL intensity must be due to a generation of crystallographic defects as non-radiative recombination center in Si caused by an abrupt increase of Fe precipitation.

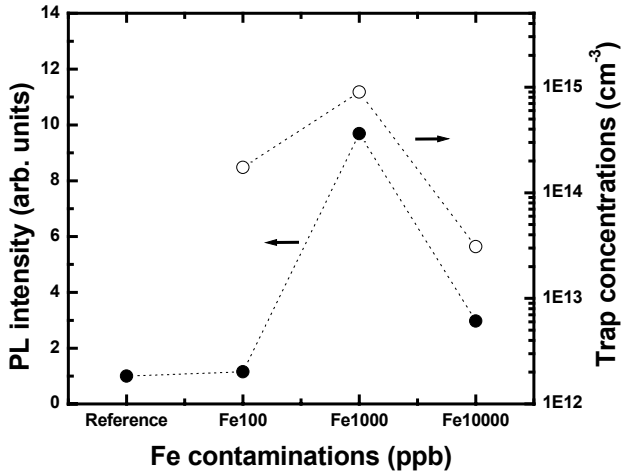

Fig. 3 Trap concentrations of Si substrate obtained from DLTS results and the PL intensity of PS layers prepared by Si substrate with various Fe contaminations.

4. Conclusions

PS sample with Fe contamination of 1,000 ppb exhibits strong and thermally stable red PL characteristics than the reference PS. Regardless of Fe contamination concentrations, all the PS samples are exhibited with the same PL peak position of 1.65 eV at 300 K. Especially, the PS sample with Fe contamination of 1,000 ppb showed a ten times stronger red PL than the reference sample, and also showed the thermal stability of PL characteristic definitely as compared with the reference PS sample. The enhancement of the red PL is closely related to trap concentrations produced by Fe contaminations of Si substrate.

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