Extended Abstracts of the 2003 International Conference on Solid State Devices and Materials, Tokyo, 2003, pp. 512-513

P4-11

Formation of Strained β-$FeSi_2$(Ge) by Ge-Segregation Controlled Solid-Phase Growth of [Amorphous Si/FeSiGe]$_n$ Multi-Layered Structure

T. Sadoh, M. Owatari, Y. Murakami, A. Kenjo, T. Yoshitake[1], M. Itakura[1], and M. Miyao
Department of Electronics, Kyushu University, 6-10-1 Hakozaki, Fukuoka 812-8581, Japan
[1]Department of Applied Science for Electronics and Materials, Kyushu University, Kasuga 816-8580, Japan
Phone: +81-92-642-3952, Fax: +81-92-642-3974, E-mail: sadoh@ed.kyushu-u.ac.jp

1. Introduction

The semiconducting silicide β-$FeSi_2$ with a direct energy gap of 1.5μm is attractive for opto-electronics applications. Recently, operation of light emitting diodes with β-$FeSi_2$ was demonstrated [1]. To apply β-$FeSi_2$ to multi-wavelength devices, modulation of the energy gap is necessary. Doping with Ge into β-$FeSi_2$ will realize the energy gap modulation caused by lattice strains, as predicted by a theoretical calculation [2]. For this purpose, precise concentration control of constituent is very important. Our idea to achieve this is controlled diffusion and segregation of Si and Ge by utilizing [a-Si/a-FeSiGe]$_n$ multi-layered structures. In the present study, formation of β-$FeSi_2$(Ge) by segregation controlled solid-phase growth has been investigated.

2. Experimental Procedure

In the experiment, [a-Si/a-$Fe_{0.4}Si_{0.5}Ge_{0.1}$]$_n$ (n=1, 2, 4; total thickness: 500nm) multi-layers were formed on Si (100) substrates by sputtering of Si and FeSiGe targets. The schematics and thickness parameters of samples are shown in Figs. 1(a) and 1(b), respectively, where the thickness ratios correspond to Fe:Si=1:2 after complete mixing. Subsequently, the samples were annealed at 700-900°C for 30min. The concentration profiles for the samples were evaluated by Auger electron spectroscopy (AES). The grown layers were analyzed by the X-ray diffraction (XRD), Raman spectroscopy, and the transmission electron microscopy (TEM).

3. Results and Discussion

The concentration profiles of Fe, Si, and Ge for the samples (n=4) before and after annealing at 700 and 800°C are shown in Figs. 2(a), 2(b), and 2(c), respectively. Before annealing, the [a-Si/a-$Fe_{0.4}Si_{0.5}Ge_{0.1}$]$_4$/c-Si multi-layered structure was clearly observed. After annealing at 700 and 800°C, the profiles changed to [$Si_{0.7}Ge_{0.2}Fe_{0.1}$/ $Fe_{0.25}Si_{0.7}Ge_{0.05}$]$_4$ and [$Si_{0.7}Ge_{0.15}Fe_{0.15}$/$Fe_{0.25}Si_{0.7}Ge_{0.05}$]$_4$, respectively, which was caused by inter diffusion of Fe, Si, and Ge. Moreover, Ge segregation from the a-FeSiGe to the a-Si layers was observed.

The Raman spectra for the samples (n=4) annealed at 700-900°C are shown in Fig. 3. After annealing at 700°C, no peaks were observed. On the other hand, the Raman peaks of Ge-Ge, Si-Ge, and Si-Si bonds in c-$Si_{1-x}Ge_x$ were clearly observed for 800°C. These results show that the $Si_{1-x}Ge_x$ regions were amorphous and crystal after annealing at 700 and 800°C, respectively. From analysis of the peak positions assuming no strains, the Ge concentration was obtained as 30% for samples annealed at 800°C. The value contradicts those obtained by AES, which suggests the heterogeneous island growth of c-$Si_{0.7}Ge_{0.3}$ in the layers.

Figure 4(a) shows XRD spectra for the samples (n=4) annealed at 700-900°C. After annealing at 700°C, XRD peaks of β-$FeSi_2$ were observed. The lattice strains evaluated from the peak positions for the samples (n=1-4) annealed at 700°C are summarized in Fig. 4(b), where the zero level corresponds to unstrained β-$FeSi_2$. For the sample with n=1, compressive and expansive strains of 0.4-0.5% were induced along the a-axis, and b and c-axis, respectively. These results indicate that strained β-$FeSi_2$(Ge) was successfully realized by the introduction of Ge into the β-$FeSi_2$ lattice. This is the first report of strained β-$FeSi_2$(Ge). Further study is needed to clarify the position of Ge atoms in the lattice. The strains became small with increasing n, i.e., with thinning layer, which was probably due to Ge sweeping out from the β-$FeSi_2$ lattice. These results suggest that the Ge concentration more than 5% is necessary to induce strain, as suggested from Fig. 2(b).

As shown in Fig. 4(a), the XRD peak height of β-$FeSi_2$ increased, and that of c-$Si_{0.7}Ge_{0.3}$ appeared after annealing at 800°C. The β-$FeSi_2$ phase was transformed into α-$FeSi_2$ after annealing at 900°C. The formation of c-$Si_{0.7}Ge_{0.3}$ at 800°C was consistent with the Raman results. The strains in β-$FeSi_2$ were fully relaxed after annealing at 800°C, as shown in Fig. 4(b). To investigate the reason for the strain relaxation, the crystal structure was observed by TEM. The cross sectional image for the sample annealed at 800°C is shown in Fig. 5(a), where the bright and dark regions correspond to c-$Si_{0.7}Ge_{0.3}$ and β-$FeSi_2$, respectively. The electron diffraction pattern indicated that Ge atoms were completely swept out from the β-$FeSi_2$ lattice. It is found that the grown regions were composed of c-$Si_{0.7}Ge_{0.3}$ and β-$FeSi_2$ nanocrystals (diameter: 20-100nm). These results suggest that the strains in β-$FeSi_2$(Ge) were relaxed by complete sweeping out of Ge from the β-$FeSi_2$ lattice to form c-$Si_{0.7}Ge_{0.3}$ at 800°C. In addition, it is found that the fractions of c-$Si_{0.7}Ge_{0.3}$ and β-$FeSi_2$ seem larger in the regions corresponding to the first ($Si_{0.7}Ge_{0.15}Fe_{0.15}$) and the second ($Fe_{0.25}Si_{0.7}Ge_{0.05}$) layers, respectively. These demonstrate that the c-$Si_{0.7}Ge_{0.3}$/β-$FeSi_2$ superstructures as shown schematically in Fig. 5(b) were formed. Such formation of nanocrystals by Ge segregation should be used for fabrication of new optically and electrically functional materials.

4. Summary

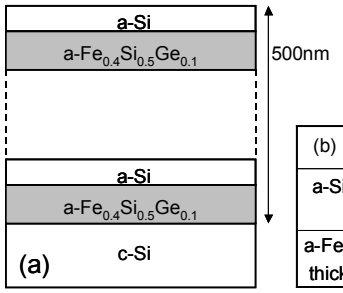
Solid-phase growth of [a-Si/a-$Fe_{0.4}Si_{0.5}Ge_{0.1}$]$_n$ multi-layered structures has been investigated. After annealing at 700°C, β-$FeSi_2$(Ge) strained by 0.4-0.5% was successfully formed. In addition, superstructures consisting of β-$FeSi_2$ and c-$Si_{0.7}Ge_{0.3}$ nanocrystals were obtained by Ge segregation after annealing at 800°C. These new structures are useful for formation of opto-electrical devices.

A part of this work was supported by CREST of Japan Science and Technology Corporation.

References

[1] D. Leong, et al., Nature **387**, 686 (1997).

[2] L. Miglio and V. Meregalli, J. Vac. Sci. Technol. B **16**, 1604 (1998).



(b)	n=1	n=2	n=4
a-Si thickness (nm)	160	80	40
a-$Fe_{0.4}Si_{0.5}Ge_{0.1}$ thickness (nm)	340	170	85

Fig.1 Schematic structure (a) and thickness parameters of samples (b).

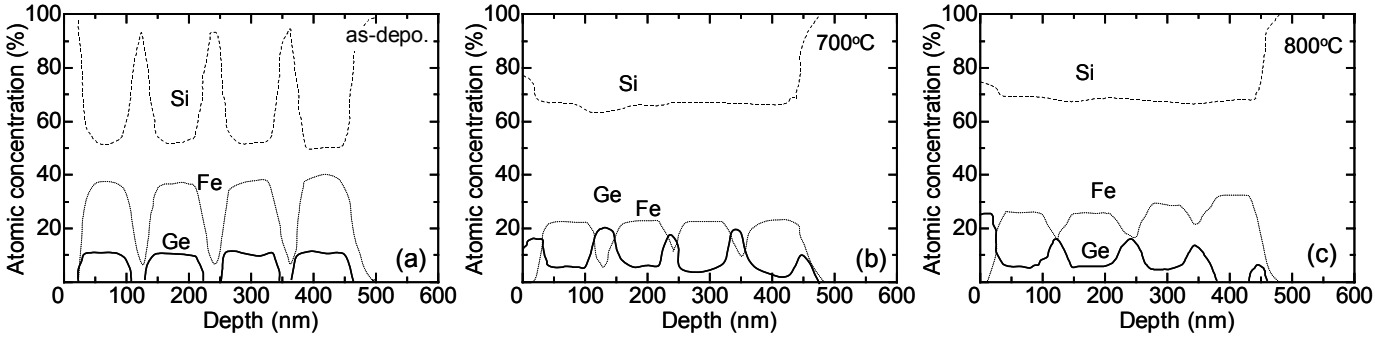


Fig.2 Concentration profiles of Fe, Si, and Ge for samples (n=4) before (a) and after annealing at 700 (b) and 800°C (c) for 30min.

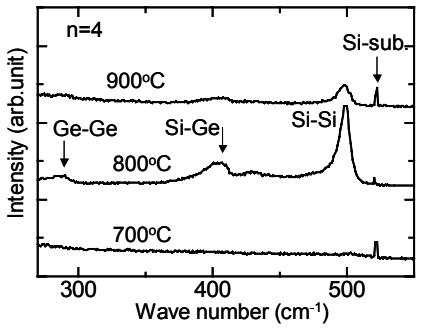


Fig.3 Raman spectra for samples (n=4) annealed at 700, 800, and 900°C for 30min.

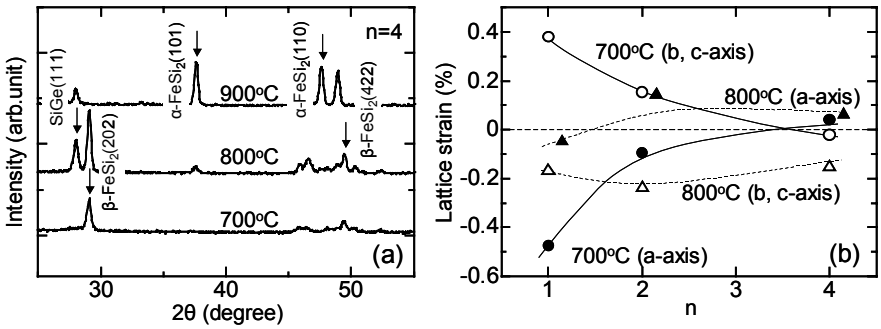
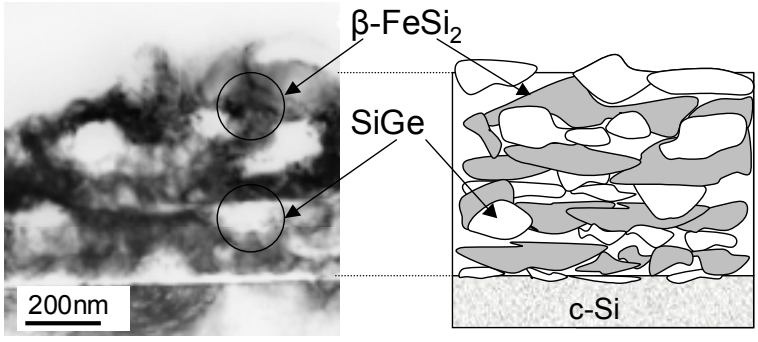


Fig.4 XRD spectra for samples (n=4) annealed at 700, 800, and 900°C for 30min (a), and lattice strain of β-$FeSi_2$(Ge) as a function of n (b). In analysis of strains, b=c was assumed.



(a) (b)

Fig.5 TEM image (a) and its schematics (b) for sample (n=4) annealed at 800°C for 30min.