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Epitaxial Growth of Ferromagnetic Silicide Fe_3Si on Si (111) Substrate

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1. Introduction

The ferromagnetic silicide Fe_3Si (Tc=840K [1]) is attractive for Si-based spintronics applications. Three phases (A2, B2, DO3) exist for Fe_3Si. The lattice structure of Fe_3Si (DO3) is schematically shown in Fig.1. From the theoretical calculation [2], it is shown that the DO3 phase is completely-spin-polarized at the Fermi level, i.e., half-metallic. Moreover, since the lattice mismatch between Fe_3Si and Si is as small as 4%, epitaxial growth of Fe_3Si on Si is expected to be possible. In the present study, we have examined the possibility of epitaxial growth of Fe_3Si on Si by using the molecular beam deposition (MBD) technique.

2. Experimental Procedure

In the experiment, Fe and Si were co-evaporated on the Si (100) and (111) substrates at 60-400^{o}C by using the solid-source MBD system (base pressure: $5x10^{-11}$Torr, deposition rate: 1.2 (Fe) and 0.4Å/s (Si)), total thickness: 50-100nm). The grown Fe_3Si layers were evaluated by using atomic force microscopy (AFM), Auger electron spectroscopy (AES), x-ray diffraction (XRD), transmission electron microscopy (TEM), and vibrating sample magnetometer (VSM).

3. Results and Discussion

Substrate temperature dependent surface morphology of the samples (thickness: 50nm) deposited on Si (100) and (111) are compared in Fig.2. Grain structures (diameter: 60-100nm) were observed for the samples deposited on Si (100) substrates. On the other hand, band-like structures with flat surfaces were obtained on Si (111) substrates. These band-like structures grew up with increasing substrate temperature.

The XRD spectra of Fe_3Si/Si (100) measured by 2θ and θ-2θ configurations are shown in Figs.3(a) and 3(b), respectively. XRD peaks due to Fe_3Si are observed for the samples deposited at 60-300^{o}C in both the configurations, suggesting formation of poly-Fe_3Si with random orientations. The XRD spectra of Fe_3Si/Si (111) are also shown in Figs.3(c) and 3(d). The peaks due to Fe_3Si (222) are observed for the samples deposited at 60-300^{o}C only in the θ-2θ configuration, which suggests that Fe_3Si (111) layers were epitaxially grown on Si (111) substrates. When the substrate temperature was increased up to 400^{o}C, XRD peaks due to FeSi were observed for samples deposited on Si (100) and (111) substrates. AES results confirmed the concentration ratio of Fe:Si=1:1. These phenomena are attributed to the Si supply from the substrate.

In order to confirm the epitaxial growth of Fe_3Si layers on Si (111) substrates, the cross sectional TEM measurements were performed. The micrographs and the electron diffraction patterns for Fe_3Si deposited at 300^{o}C are shown in Figs.4(a)-4(b) and 4(c)-4(e), respectively. Results indicate that the surface is flat, even though the interface is slightly rough. In addition, identical diffraction patterns (Fig.4(c) and 4(d)) were obtained from the different contrast regions. These patterns have similar symmetrical structures to that of Si along the [112] direction (Fig.4(e)). These results demonstrate that Fe_3Si layers were epitaxially grown on Si (111) substrates. Although the lattice mismatch was same for Si (100) and (111), the epitaxial growth of Fe_3Si was achieved only for Si (111) substrates. The reason for this is now under investigation.

To identify the phase of epitaxially grown Fe_3Si (300^{o}C), XRD measurements (ϕ scan) was performed. The results are shown in Fig.5. The peaks (Fe_3Si (331)) peculiar to the DO3 phase were obtained. In this way, epitaxial growth of Fe_3Si including the DO3 phase was obtained on Si (111) substrates.

The dependence of the magnetic hysteresis loop of Fe_3Si (50nm thick)/Si (111) deposited at 300^{o}C was measured as a function of the in-plane angle of the magnetic field. The result is shown in Fig.6(a). The values of the saturated magnetization (~1000emu/cc) are almost the same as that for the bulk Fe_3Si [3]. Figure 6(b) shows the coercive force as a function of the angle, which shows a magnetic anisotropy with a period of 180^o. Since the coercive force for the samples deposited on Si (100) substrates did not depend on the angle, the angle dependence was due to epitaxial growth of Fe_3Si. The mechanism for the 180^o period is now under investigation.

This technique for epitaxial growth of Fe_3Si on Si substrates is expected to be employed to realize Si-based spintronics devices.

4. Summary

Epitaxial growth of Fe_3Si on Si substrates was investigated by using the MBD technique. Fe_3Si (111) layers were successfully epitaxially grown on Si (111) substrates at 60-300^{o}C. The formed layers contained the half-metallic phase (DO3). This is an advantage for realization of Si-based spintronics devices.

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References

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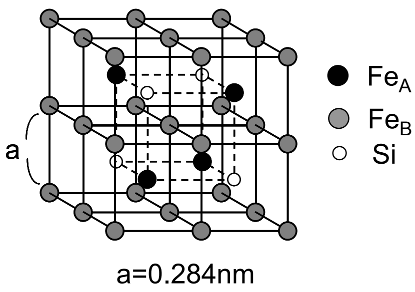

Fig.1 Lattice structure of Fe_3Si (DO3).

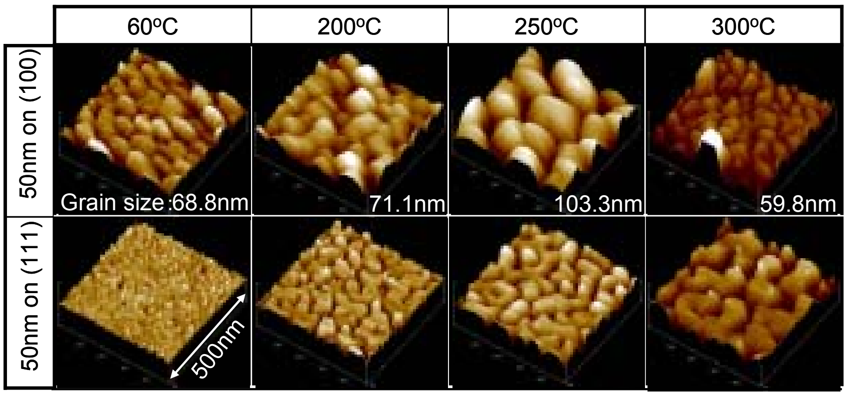

Fig.2 AFM images for samples grown on Si (100) and Si (111).

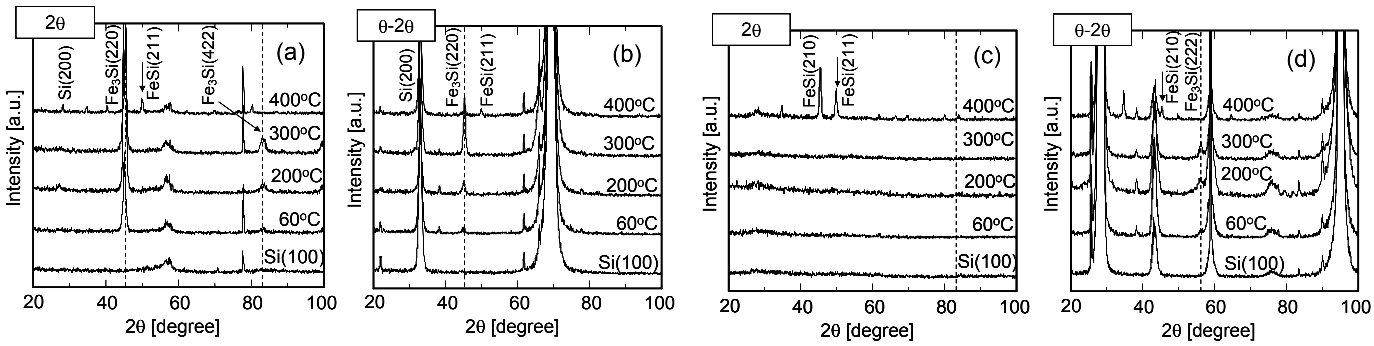

Fig.3 XRD spectra for samples deposited on Si (100) ((a) and (b)) and Si (111) substrates ((c) and (d)). The measurements were performed in 2θ ((a) and (c)) and θ-2θ configurations ((b) and (d)). The film thickness was 50 and 100nm for samples deposited at 60 and 400, and 200 and 300°C, respectively.

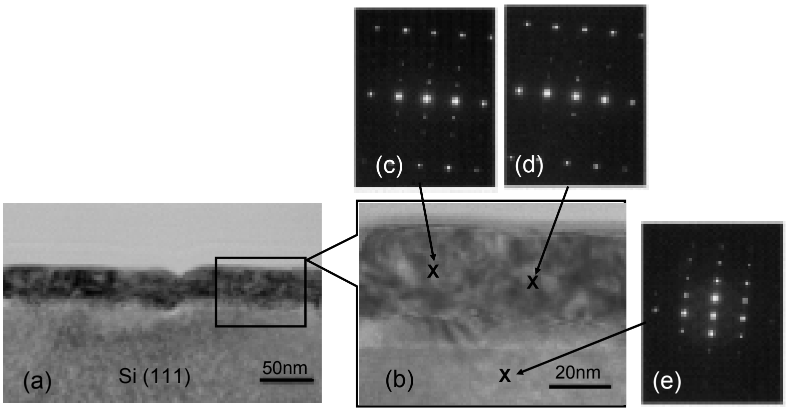

Fig.4 Cross sectional TEM images ((a)-(b)) and electron diffraction patterns ((c)-(e)) for sample (thickness: 50nm) deposited on Si(100) at 300°C.

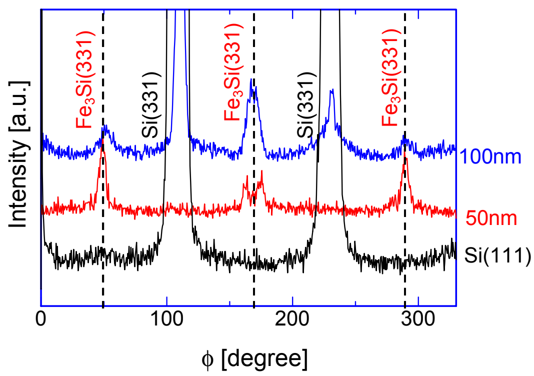

Fig.5 XRD spectra (ϕ-scan) for samples deposited on Si (111) at 300°C.

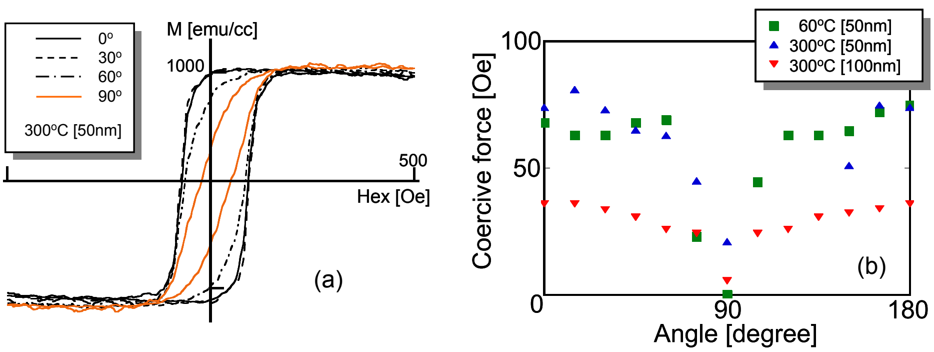

Fig.6 Magnetic hysteresis loop (a) and coercive force (b) as a function of in-plane angle of magnetic field for samples deposited on Si (111) substrates.