Epitaxial Growth of Fe₃Si Thin Films on Si Substrate with MgO Buffer Layer

K. Akiyama, T. Kadowaki, Y. Hirabayashi and S. Kaneko

Kanawaga Industrial Technology Center, 705-1 Shimoimaizumi, Ebina-shi, Kanagawa 243-04, Japan

Fax: 81-46-236-1525, e-mail: akiyama@kanagawa-iri.go.jp,

t-kadowaki@kanagawa-iri.go.jp, hirabaya@kanagawa-iri.go.jp, satoru@kanagawa-iri.go.jp

(100)-oriented epitaxial Fe₃Si films were grown on (100) Si substrates with an epitaxial magnesia (MgO) buffer layer by rf-magnetron sputtering. X-ray pole figure measurements revealed that the Fe₃Si layer is epitaxially grown on MgO buffer layer with an orientation relationship of Fe₃Si(100) // MgO(100) with Fe₃Si[011] // MgO[001]. The coercive forces (H_c) of epitaxial films was approximately 60 Oe, and the saturation magnetizations (M_s) was 750 emu/cm³.

Key words: Fe₃Si, epitaxial thin film, Si, chemical vapor deposition, MgO buffer layer

1. INTRODUCTION

The performance of LSIs must be further improved to realize advanced information systems. However, for high-speed operation with low power consumption, the conventional approach of downsizing metal-oxide-semiconductor field-effect transistors (MOSFETs) is becoming more difficult owing to physical limits. Therefore, a new approach for advanced devices is strongly required. A spin transistor is a promising candidate¹, and the integration of magnetism into semiconductors has been attracting considerable attention. Spin-polarized carrier injection from a ferromagnetic source into a semiconductor or from a ferromagnetic-insulator-semiconductor (MIS) structure is one of the hot topics in this field.

The ferromagnetic iron-silicide (Fe₃Si) is attractive for Si-based spin transistor applications². Because of the similarity of its crystal structure and the lattice constant of $a=5.653\text{\AA}$ ³, Fe₃Si is expected to grow epitaxially on Si substrates. Moreover, from theoretical calculations⁴, it has been shown that DO₃-type Fe₃Si is spin-polarized at the Fermi level, *i.e.*, it is half-metallic.

In this study, we succeeded in carrying out the epitaxial growth of a (100)-oriented Fe₃Si thin film as a ferromagnetic metal on a Si substrate with magnesia (MgO) buffer layer by metal-organic chemical vapor deposition (MOCVD) and achieved MIS structures.

2. EXPERIMENTAL

20-nm-thick MgO buffer layer was epitaxially grown on the (100)Si substrates by rf-magnetron sputtering at 700-750°C using a magnesium target in a mixture of Ar and O₂ ambient. The details of their preparation are described in a previous article⁵. Figure 1 shows the cross sectional and bird's view SEM image of the MgO layer. The average surface roughness of the epitaxial MgO layer was about 2 nm.

Iron (Fe)- silicon (Si) thin films were grown on Si(100) substrates with MgO buffer layers by metal-organic chemical vapor deposition (MOCVD).

Fig.1 (a) Cross-sectional and (b) bird's view SEM images of MgO buffer layer epitaxially grown on (100) Si substrate.

The silicon carbide heater was equipped in the cold-wall-type reactor. Iron pentacarbonyl [Fe(CO)₅] and mono-silane (SiH₄) were used as iron and silicon source, respectively. Fe(CO)₅ was sealed in the vessels and was carried to the reactor by H₂ carrier gas. The deposition rate of the Fe-Si films was 1.6 nm/min at each deposition temperature.

The iron/silicon atomic ratio of the film was

measured by X-ray fluorescence spectrometry (XRF) and Rutherford backscattering spectroscopy (RBS). The crystallographic structure of the films was characterized on the basis of X-ray diffraction (XRD; PaNalytical MRD) patterns using Cu K α radiation. The microstructure and thickness of the films were analyzed by scanning electron microscopy (SEM; FEI Shirion). The room temperature magnetic properties of the films were determined using a vibrating sample magnetometer (VSM; LakeShore 7400).

3. RESULTS AND DISCUSSION

Figure 2 shows XRD θ - 2θ scan profiles of the films deposited from 650°C to 800°C. The thickness of the deposited films was constant at 250 nm and the iron/silicon atomic ratios of the films were ascertained to be almost 3.0 by XRF and RBS. The XRD scan profiles of the films deposited from 650°C to 750°C showed diffraction peaks at $2\theta = 31.55^\circ$, 45.27° and 66.09° , which was almost in agreement with that of the 200, 220 and 400 diffraction peaks of international center for diffraction data (ICDD) card of Fe₃Si; 45-1207, respectively. When the deposition temperature increased from 650°C to 750°C, the Fe₃Si 400 diffraction peaks increased and Fe₃Si 220 diffraction peaks decreased, respectively. This result clearly shows that (100)-preferred orientation of Fe₃Si films was promoted by raising deposition temperature. The diffraction peaks from the α -FeSi₂ and β -FeSi₂ phases were observed instead of the Fe₃Si peak for the films deposited at 800°C, as shown in Fig.2(d). This result of iron-diesilicide formation, irrespective of the iron and silicon supply of a 3:1 atomic ratio, indicates the reaction between the films and Si substrates during deposition. Actually the MgO 200-diffraction peak disappeared after the deposition at 800°C.

The epitaxial growth of these Fe₃Si films on (100) MgO buffer layer was also ascertained from the XRD pole figure measurement, as shown in Figures 3(a) and 3(b). In this figures, the azimuth and the rotation axes perpendicular to the substrate are indicated as ϕ and Φ , respectively. In Fig. 3(a), fourfold symmetry poles of Fe₃Si 220 were located at ϕ of 44.5° and 90° intervals along ϕ axis. By comparing with MgO 220-pole figure as shown in Fig. 3(b), the epitaxial relationship between Fe₃Si and the MgO can be determined, as schematically illustrated in Fig. 3(c), i.e.,

$$\text{Fe}_3\text{Si}(100) // \text{MgO}(100) \text{ with } \text{Fe}_3\text{Si}[011] // \text{MgO}[001]$$

This epitaxial relationship is same as that between Fe₃Si thin film and (100) plane of MgO single crystal⁶. It has been reported that the epitaxial (100) Fe₃Si films grown on the (100) MgO substrates consist of both ordering phase (DO₃) and disordering phase (B2 or A2)⁶. Thus, this epitaxial Fe₃Si film on MgO buffer layer is considered to consist of ordering and disordering phases.

Figure 4 show a cross-sectional SEM image of the epitaxial Fe₃Si film grown on the (100) Si substrate with MgO buffer layer. An interface between the MgO buffer layer and the epitaxial Fe₃Si film was observed and the same clear interface was observed for the film on the (100) Si substrate with MgO buffer layer.

Fig.2 XRD θ - 2θ scan profiles for the films at (a) 650, (b) 700, (c) 750 and (d) 800°C on (100) Si with MgO buffer layer.

Fig.3 X-ray pole figure plots of (a) Fe₃Si 220 and (b) MgO 220 for the films grown on (100) MgO substrates at 750°C, and (c) the schematic growth model of the epitaxial (100)-oriented Fe₃Si film on (100) MgO.

Fig.4 Cross-sectional SEM images of epitaxial Fe_3Si film grown at 750°C on (100)Si with MgO buffer layer.

Fig.5 Room temperature magnetization curves of epitaxial Fe_3Si films grown at 750°C on (100) Si with MgO buffer layer.

Figure 5 shows magnetic field (H) dependence of magnetization (M) for the epitaxial Fe_3Si films grown at 750°C . The value of coercive force (H_c) was approximately 60 Oe, and saturation magnetization (M_s) was 750 emu/cm^3 , which is lower than 980 emu/cm^3 of bulk Fe_3Si ^{3,7}.

4.CONCLUSIONS

We succeeded in growing epitaxial (100)-oriented Fe_3Si films on Si substrates with MgO buffer layer by rf-magnetron sputtering and succeeded in obtaining a MIS structure. The value of coercive force (H_c) was approximately 60 Oe, and saturation magnetization (M_s) was 750 emu/cm^3 , which is slightly lower than 980 emu/cm^3 of bulk Fe_3Si ^{3,7}.

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(Received December 10, 2008 ; Accepted February 2, 2009)