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Atomically Controlled Hetero-Epitaxy of DO3-type Fe_3Si on Ge(111) Substrate

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1. Introduction

The ferromagnetic silicide Fe_3Si (Currie temperature: 840 K [1]) is an attractive material for Si-based spin transistor applications. Three types (A2, B2, and DO3) of Fe_3Si exist, where DO3-type is calculated to be spin-polarized at the Fermi level [2]. The lattice structure of DO3-type Fe_3Si is schematically shown in Fig.1. Lattice mismatch between Fe_3Si (lattice constant: 0.564nm) and Ge (lattice constant: 0.565nm) is less than 1%, consequently, good epitaxial growth of Fe_3Si is expected on Ge substrate. By using this epitaxial Fe_3Si/Ge structures as spin injection electrodes, spin transistors, which can be integrated with Si-LSI, will be realized. In line with this, we have been investigating epitaxial growth of Fe_3Si on Ge by using molecular beam epitaxy (MBE) [3]. This paper reports systematically investigated MBE of Fe_3Si/Ge(111). The effects of the Fe/Si ratio and the growth temperature on crystallinity of Fe_3Si will be discussed.

2. Experimental Procedure

In the experiment, *n*-type Ge(111) substrates were used. After cleaning the substrates, they were loaded into an MBE chamber (base pressure: 5×10^{-11} Torr) and heat-treated at 550^{o}C for 20 min. Ge buffer layers (thickness: 30 nm) were grown on the substrates at 400^{o}C. Subsequently, Fe and Si were co-evaporated on the substrates at 60-300^{o}C using Knudsen cells (deposition rate: 0.07-0.12 nm/sec (Fe) and 0.04 nm/sec (Si), total thickness: 50 nm). The Fe_3Si layers grown on Ge(111) substrates were characterized by x-ray diffraction (XRD), transmission electron microscopy (TEM), and Rutherford backscattering spectroscopy (RBS).

3. Results and Discussion

The XRD spectra of Fe_3Si grown on Ge(111) with Fe/Si ratio of Fe:Si=4:1 at 60-300^{o}C were measured under θ-2θ and 2θ configurations. They are shown in Figs.2(a) and (b), respectively. For the samples grown at 60-200^{o}C, XRD peaks identical to the substrate orientations are observed only in the θ-2θ configuration, which indicates epitaxial growth of Fe_3Si(111) on Ge(111). On the other hand, unidentified XRD peaks (36^{o} and 77^{o}) are observed in the θ-2θ configuration for the sample grown at 300^{o}C.

To investigate the crystal quality of Fe_3Si layers quantitatively, RBS measurements were performed. Typical RBS (probe ion: $^4He^+$, incident energy: 2.3MeV, detection angle: 165^{o}) spectra of the Fe_3Si(Fe:Si=4:1) grown on Ge at 60^{o}C are shown in Fig.3. The difference between random and channeling spectra around the channel number of 380 (Fe signal) is large, which suggests good crystallinity of the Fe_3Si layer. The values of χ_{min} of the samples were evaluated from these spectra, where χ_{min} was defined as the ratio of the peak intensity of Fe obtained in the channeling configuration to that in the random configuration. The results for the samples grown at 60-300^{o}C are summarized in Fig.4. In the case of MBE under the non-stoichiometric condition (Fe:Si=4:1), χ_{min} decreases from 7.0 (60^{o}C) to 4.0 (130^{o}C) with increasing growth temperature and then increases up to 50% at 300^{o}C. These results suggest that control of atomic migration at sample surfaces is important to improve the crystal quality.

Results obtained from MBE under the stoichiometric condition (Fe:Si=3:1) are also shown in Fig.4. Very low χ_{min} (2.2%) was obtained in a wide temperature range (60-130^{o}C), even though they gradually increased to 12% at 300^{o}C.

Phenomena observed in high temperature deposition (~300^{o}C) were examined by measuring concentration profiles of Fe and Ge. The results obtained from RBS spectra were shown in Fig.5. It is clear that atomic mixing of Fe and Ge at Fe_3Si/Ge interfaces begins at 300^{o}C. Thus, FeSiGe compound is considered to be formed at 300^{o}C, resulting in the unidentified XRD peaks, as shown in Figs.2(a).

These results clearly indicated that the low temperature MBE growth (<130^{o}C) under the stoichiometric condition (Fe:Si=3:1) is the key factor to achieve high quality Fe_3Si with a sharp interface.

Cross-sectional TEM images of the Fe_3Si/Ge(111) grown at 130^{o}C under stoichiometric condition is shown in Fig.6, together with the electron diffraction (ED) pattern. This result clearly demonstrates that the interface is atomically flat. In addition, diffraction spots due to the ordered superlattice are clearly observed in the ED pattern as indicated with the broken circles in Fig.6(b), which indicates formation of the DO3-type Fe_3Si.

In this way, DO3-type Fe_3Si/Ge structures with atomically flat interfaces were realized by low-temperature MBE.

4. Summary

The effects of the Fe/Si ratio and the deposition temperature on MBE of Fe_3Si on Ge substrates were investigated. By optimumizing substrate temperature (130^{o}C) and Fe/Si ratio (Fe:Si=3:1), atomically controlled epitaxial growth of Fe_3Si was achieved on Ge(111) substrates. In addition, it was confirmed that Fe_3Si was mainly composed of DO3-type. This is an advantage for establishing the Si-based spintronics devices.

Acknowledgements

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References

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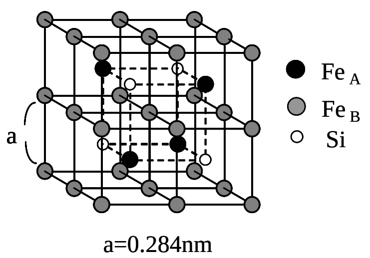

Fig.1 Lattice structure of Fe_3Si (DO3-type).

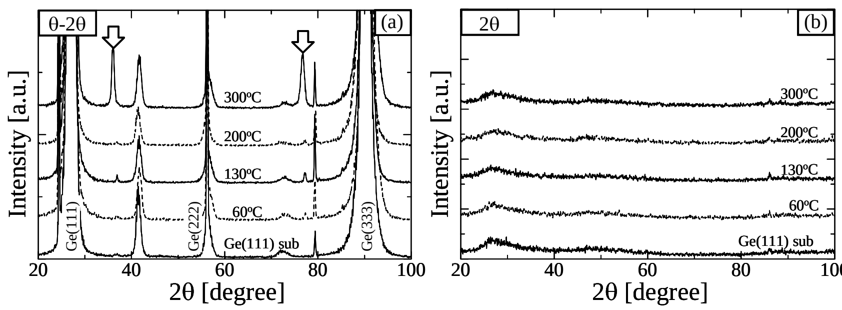

Fig.2 XRD spectra for Fe_3Si grown on Ge(111) obtained under θ-2θ (a) and 2θ (b) configurations. Fe_3Si thickness, growth temperature, and Fe/Si ratio were 50nm, 60-300°C, and 4/1, respectively.

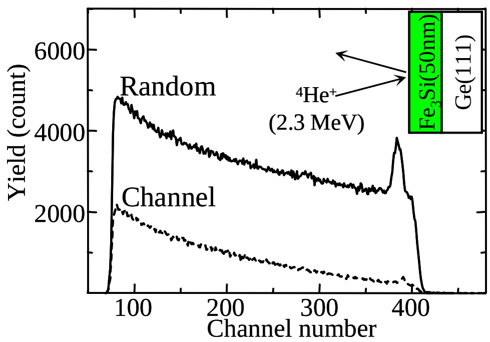

Fig.3 RBS spectra for Fe_3Si (Fe:Si=4:1) deposited on Ge(111) substrate at 60°C, and cross sectional view of sample structure.

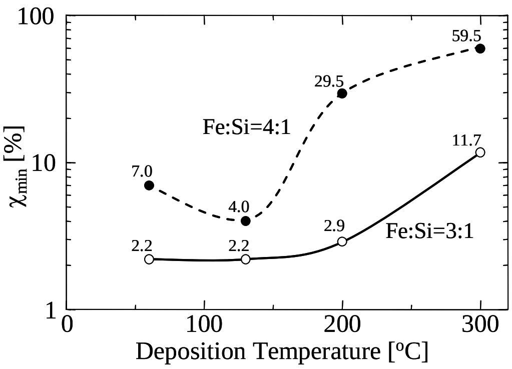

Fig.4 χ_{min} evaluated from RBS spectra of Fe_3Si deposited at 60-300°C. Results obtained under non-stoichiometric and stoichiometric conditions are compared.

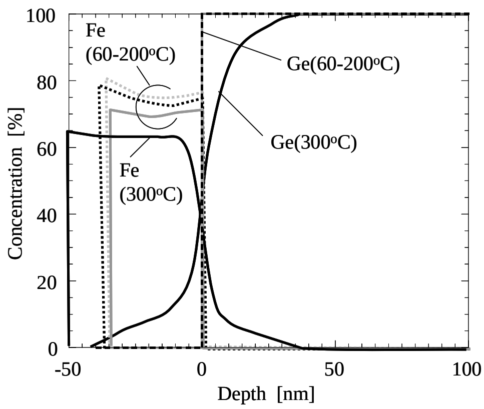

Fig.5 Fe and Ge concentration profile evaluated from RBS measurements in the Fe_3Si/Ge structures as a function of growth temperature.

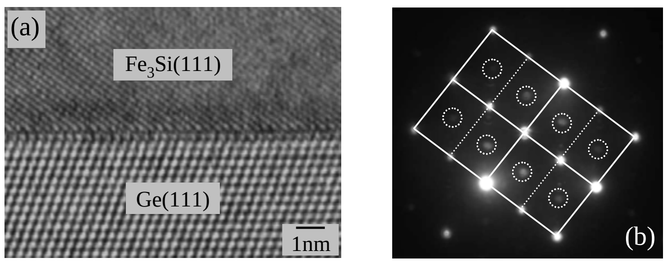

Fig.6 TEM lattice image of Fe_3Si/Ge(111) interface, which was formed at 130°C under stoichiometric condition (a), and electron diffraction pattern of Fe_3Si layer (b). The broken circles in (b) indicate diffraction spots due to the ordered superlattice of DO3-type Fe_3Si.