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Ion channeling study of epitaxy of iron based Heusler alloy films on Ge(111)

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ABSTRACT

We have investigated perfection of atomic rows on iron-based Heusler alloy films on Ge(111) planes by using ion channeling technique in order to find the dominant factors for the perfection. Fe_3Si/Ge(111) and Fe_2CoSi/Ge(111) have a high quality of atomic rows at the heterointerface like that of perfect crystals. $Fe_{3-x}Mn_xSi$/Ge(111) ($x = 0.84$, 0.72 and 0.36) interfaces have imperfection of atomic rows which may be controlled by both the lattice mismatch with the Ge substrate and the Mn–Si pairs due to the site disorder in the film with the Mn content $x > 0.75$. Analysis of axial channeling parameters employed in this study is very useful for quantitative evaluation of perfection of atomic rows at the heterointerface.

1. Introduction

Iron based Heusler alloys such as DO_3 ordered Fe_3Si, $L2_1$ ordered ternary alloys such as Fe_2MnSi and Fe_2CoSi, have high spin polarization, some of them have half metallicity [1]. These spintronic properties will be very useful for applications of spin devices. In fact, recently some basic experiments such as spin injection from Fe_3Si electrodes with nonlocal contacts into Si channels [2,3] toward applications of spin polarization have been reported, when high quality epitaxy of the Heusler alloy films on semiconductors has been realized by molecular beam epitaxy (MBE) [2–8]. Perfection of atomic rows at the heterointerface is important for controlling magnetic properties, spin states and spin current transport.

It has been known that the site occupations in the ordered lattice are important to control of magnetic properties and spin polarization states in the Heusler alloys. NMR studies reveal that in DO_3 ordered lattice with four sites (A, B, C, and D) Mn atoms prefer to occupy the B site, while Co atoms prefer to do both the A and B sites. We have already succeeded in epitaxy of $L2_1$ order lattice based on epitaxial growth of the DO_3 Fe_3Si by developing low temperature molecular beam epitaxy, in which film growth is carried out at temperatures below 200 °C [3–5]. In the low temperature MBE, interdiffusion at the interface can be avoided, so small change of concentration can make growth smoothly proceed [6,7].

In this study, we will investigate perfection of atomic rows on iron-based Heusler alloy films on Ge(111) planes by using ion channeling technique in order to find the dominant factors for the perfection. We will compare three Heusler alloy films on Ge(111) planes. They have almost the same lattice constants close to the lattice constant of Ge. Therefore, we can expect some of effects of site preference of each atom on epitaxial perfection of each Heusler alloy film on Ge substrates. First, we will report axial channeling behaviors of iron-based Heusler alloy films on Ge. Second, we will report axial channeling at low temperature to evaluate imperfection from intrinsic displacement due to thermal vibrations and static or extrinsic displacement of atoms along rows. Third, we will make a discussion on what the dominant factors are in each alloy films by borrowing the help of the Debye model and the Barrett–Gemmell model.

2. Experiments

The epitaxial Heusler alloy films with a thickness of ~50 nm were grown by low temperature-molecular beam epitaxy (MBE) on n-type Ge(111) substrates at 200 °C. We used K-cells for Fe, Si and Ge, in addition for Co or Mn solid sources. First we deposited the Ge buffer layer on the clean substrate surface, and then we started deposition of each Heusler alloy films. The essential issue is to keep the growth temperature below 200 °C. The RHEED patterns of Fe_3Si and ternary Fe_2MnSi in Fig.1 showed very clear streak images. This fact brings us expectation of near perfect epitaxial growth of these Heusler alloy films on the Ge buffer layers.

Next we examined the nanostructure of the heterointerface. Fig. 2 shows a TEM image taken at the interface between the Fe_3Si (no Mn content) and Fe_2MnSi film and the Ge buffer layer. The bottom patterns of Fig. 2 are selected area electron diffraction (SAD) patterns. We observed very clear interface with atomically sized flatness. The

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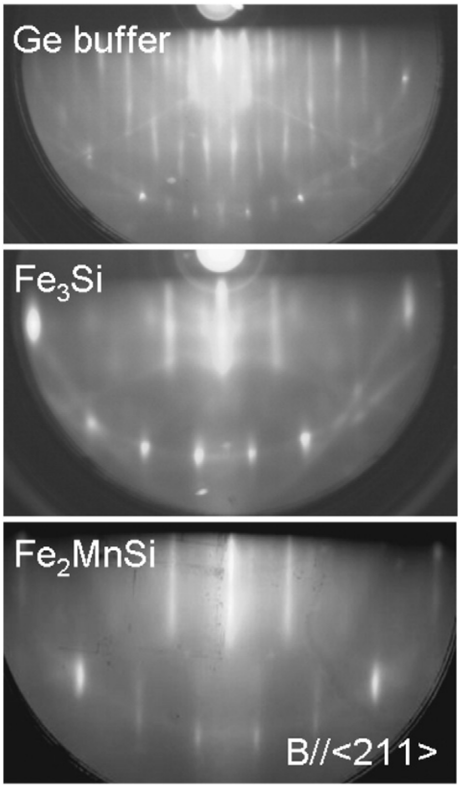

Fig. 1. Reflection high energy electron diffraction (RHEED) patterns of Ge buffer layers, Fe3Si epitaxial films and Fe_2MnSis epitaxial film on Ge(111) planes.

SAD patterns indicated clear super-lattice reflection spots of (111) and (311) denoted by the circles. Their appearance means that the alloy film has a DO_3 or $L2_1$ type order structure with an evident epitaxial relationship with Ge(111) along the direction of <111> crystal axis. We have also evidence on epitaxial relationships of Fe_3Si and Fe_2MnSi along the same direction:

Fe_3Si\{111\}//Ge\{111\} and Fe_3Si[111]//Ge[111],

Fe_2MnSi\{111\}//Ge\{111\} and Fe_2MnSi[111]//Ge[111].

These TEM and SAD results give us expectation of complete atomic arrangement along the epitaxial crystal orientation. Next we investigated actual situations of the axial atomic row on the epitaxial films by axial ion channeling.

The axial channeling measurement and Rutherford backscattering spectroscopy (RBS) for analysis of composition of alloy films were carried out at either SC1 or MD2 beam lines in TIARA-JAEA. The channeling measurements using 2.0 MeV-$^4He^+$ ions and a backscattering angle of 165° were carried out at 300 K, 110 K and 40 K. The samples were mounted on a cooled holder.

Usually we removed the Ge channel from both spectra by using mathematical treatment. We show both random and aligned spectra of Fe, Mn channels at the left figure. The channeling spectra at the interface could be deduced from a part of the aligned spectrum just at the given axial zone. In measurements of the axial channeling along the <111> zone axis, in this study, we employed the direction between <110> and <211> directions and the tilt range from minus 6° to plus 6° in order to avoid additional plane channeling.

3. Results

3.1. Axial ion channeling behaviors

In this section, we will report the axial channeling behavior of Heusler alloy films epitaxially grown on Ge(111) in order to find each dominant factor for perfection of epitaxy along the Ge <111> direction.

Fig. 3 panels (a) and (d) are important results in our study and show angular yield profiles at the interface of Fe_3Si and $Fe_{3-x}Mn_xSi$ ternary alloys films with the Ge(111) plane. The profiles were deduced from RBS

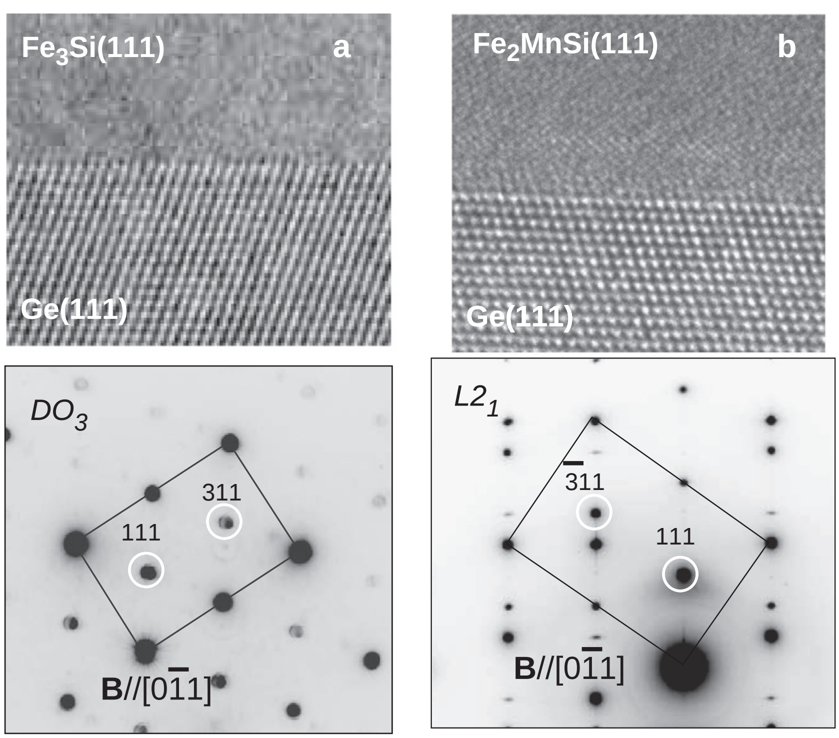

Fig. 2. Cross sectional TEM images of (a) the DO_3–Fe_3Si(111)/Ge(111) and (b) $L2_1$–Fe_2MnSi(111)/Ge(111) interface at the [110] zone axis and the selective area electron diffraction (SAD) pattern. The circles indicate supper lattice diffraction spots of (111) and (311) associated with the DO_3 or $L2_1$ ordered lattice.