Proc. Asia-Pacific Conf. on Semiconducting Silicides and Related Materials 2016
JJAP Conf. Proc. **5**, 011104 (2017) https://doi.org/10.7567/JJAPCP.5.011104

Ion Channeling Measurements of β-$FeSi_2$ Films Epitaxially Grown on Si(111) and Their Analysis by Multiple Scattering Theory

Masaya Fuchi[1], Mikihiro Arima[1], Kazumasa Narumi[2], Yoshikazu Terai[1] and Yoshihito Maeda[1,2]

[1] *Department of Computer Science and Electronics, Kyushu Institute of Technology, Fukuoka 820-8502, Japan*
[2] *National Institutes for Quantum and Radiological Science and Technology (QST), Gunma 370-1292, Japan*

E-mail: maeda@cse.kyutech.ac.jp

(Received August 3, 2016)

We have evaluated β-$FeSi_2$ (110), (101) planes epitaxially grown on Si(111) by using ion beam analysis. Unexpected large displacements were deduced from analysis based on single ion scattering. We have discussed multiple ion scattering caused inside the film and obtained the comparatively reasonable atomic displacement of Δx=0.04 nm that is close to one sixth of one step height of six domains stacking on the (111) planes. This result suggests that multiple scattering may be attributed to the atomic displacement due to the domain stacking faults.

1. Introduction

Epitaxial growth of crystal planes of β-$FeSi_2$ (110), (101) on Si(111) is one of the most reliable cases in Molecular Beam Epitaxy (MBE), Reactive Deposition Epitaxy (RDE), Metal Organic Chemical Vapor Deposition (MOCVD) or Ion Beam Synthesis (IBS). The orientation relationship, β-$FeSi_2$ [110], [101]//Si[110] with six equivalent domains has been reported [1]. In this heteroepitaxy, the lattice mismatch δ becomes +1.4 to +5.5% in each directions. Ion beam analyses such as Rutherford backscattering spectrometry (RBS) and ion channeling measurements along a given crystal axis of the substrate give element depth profiles and epitaxial quality on specific planes and displacement from atomic rows, so they are very powerful methods to evaluate total feature of epitaxy. However, there are no reports about ion channeling measurements of β-$FeSi_2$/Si heteroepitaxial structures. In this study, using the obtainable high quality MBE films we investigated axial ion channeling measurements of β-$FeSi_2$(110), (101) planes epitaxially grown on Si(111) to evaluate quantitative discussion based on atomic displacements on the atomic rows along the Si<111> direction.

2. Experiments

60 nm-thick β-$FeSi_2$ films were grown on the 20 nm-thick β-$FeSi_2$ template layer formed on Si(111) substrates at 550 ºC by MBE. The template layer was deposited at 670 ºC by RDE. In the MBE growth, a ratio of Si/Fe was hold to be 1.17. Reflection High Energy Electron Diffraction (RHEED) patterns were observed during growth and showed a β-$FeSi_2$ (110) or (101) single plane. Also Raman measurements indicated the single phase of β-$FeSi_2$ in optically detectable depth. 2.0 MeV-$^4He^+$ RBS spectra were measured at the backscattering angle of 165º. Along the axis Si<111>, ion channeling measurements were performed in the β-$FeSi_2$ film with the template layer at each tilt angle of the beam between -2.0 and +2.0 degrees. The tilt direction may be important issue and was employed between [1, -1, 0] and [-1, 0, 1] directions of Si where the minimum yields of Fe and Si channels were obtained. Axial channeling dip curves, which are backscattering yields of Fe and Si atoms as a function of tilt of ion beam incidence angle, were analyzed by the following equation in order to obtain a minimum yield (χ_{min}) and a critical half angle ($\psi_{1/2}$).

$$\chi(\theta) = 1 - (1 - \chi_{min}) exp\left(-ln2\left(\frac{\theta}{\psi_{1/2}}\right)^{p}\right) \tag{1}$$

where p is the order of randomness, in this study we employed p=2 (Gaussian function) for the best curve fitting. Depth profiles of elements concentration were simulated by SIMNRA® code [2].

3. Results

Figure 1(a) shows a random RBS spectrum and Fig.1(b) shows a depth profile of elements composition (at%) deduced from the random spectrum. The average composition of the film was a little far from the stoichiometric composition, and the template layer and portion near it were Si-rich composition. It was because diffusion of Si atom from the substrate might take place during the film growth at 550 °C.

Figure 2 shows RBS spectra measured when the tilt angle was changed. The spectra indicated a systematic change from the channeling (aligned) spectrum to the random spectrum for both Fe and Si spectra.

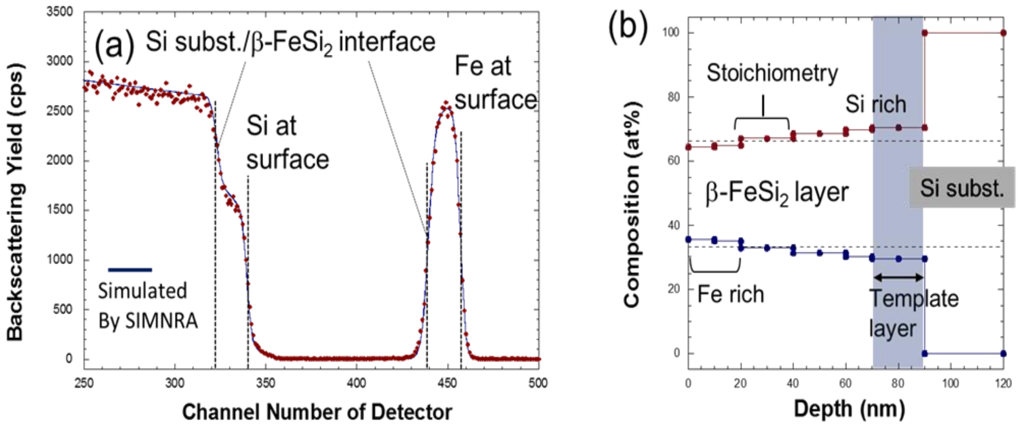

Fig. 1. Random RBS spectrum (a) and a depth profiles of element compositions (b) deduced from the random spectrum (a) by simulation of SIMNRA® code.

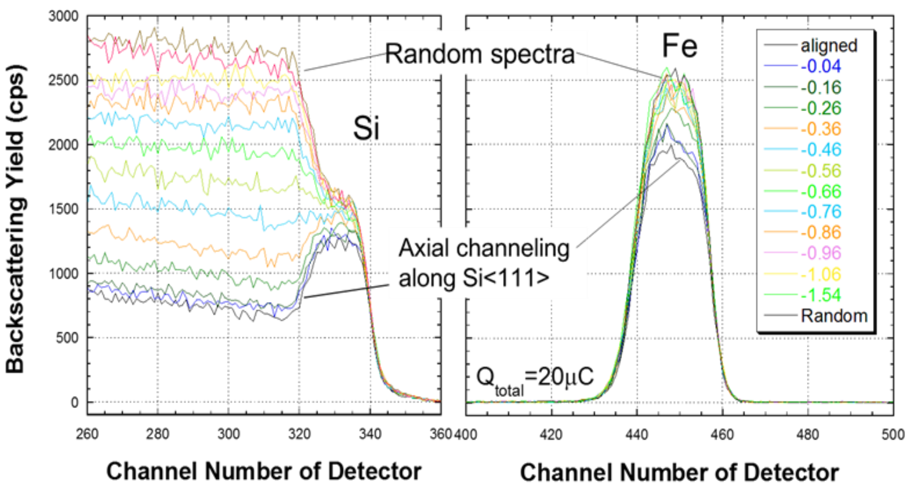

Fig. 2 RBS spectrum-change from the axial channeling (aligned) along a Si<111> direction to the random one at the tilt angle of incident ion beam.

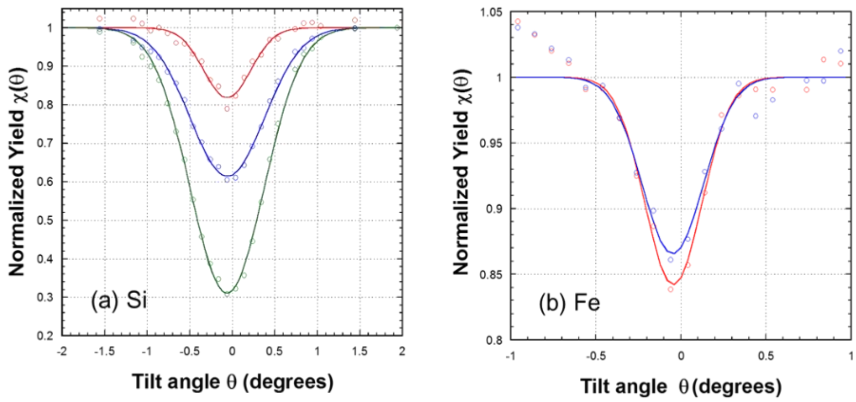

Fig. 3 Axial channeling dip curves for Si (a) and Fe (b) atoms in β-$FeSi_2$ along a Si<111> direction. The vertical axes are normalized by random scattering yields. The green curve is for interface with the Si substrate, the blue one is for the template layer and the red one is for the β-$FeSi_2$ film.

Using these spectra, we can draw the axial channeling dip curves as shown in Fig.3 (a) and (b) and determine channeling parameters (χ_{min} and $\psi_{1/2}$) after fitting by eq.(1) with p=2. Unexpectedly we obtained the larger χ_{min} and the smaller $\psi_{1/2}$ than those predicted usually in epitaxially grown films. This result suggests directly that both Fe and Si atomic rows on β-$FeSi_2$ (101), (110) planes are much disordered along Si<111> axial directions. As shown in Fig.3(a), both χ_{min} and $\psi_{1/2}$ are dependent upon the location where ions are scattered. When thinking the Fe dip curves in Fig.3(b) together, in inside of the film we obtain the χ_{min} values of 0.8-0.85. In the 20 nm-thick templated layer, the χ_{min} of Si and Fe atomic rows were 0.6 and 0.86, respectively. At the interface with the Si substrate, the χ_{min} of Si was 0.31. As shown in Fig.3(b) there was not large difference between the χ_{min} in the template layer and that in the film.

4. Discussion

4.1 Analysis using single ion scattering condition

We discuss the reason of such a large value of χ_{min} for Si and Fe atomic rows in β-$FeSi_2$ films along Si<111> directions. First, degradation of epitaxy during the film growth on the template layer can be considered. We have computed static displacements of Si and Fe atoms along the atomic rows $\langle u_s \rangle$, which may reflect some defects, stacking faults, defaults etc., form the channeling parameters by using Maeda theory combined with Barret-Gemmel theory and Debye thermal vibration theory [3-5]. We obtained $\langle u_s \rangle$ of 0.095 nm and 0.11 nm for Si and Fe atoms, respectively. If these large displacements amounting each 40% and 30% of atomic spacing along the rows takes place in the lattice, the lattice with covalent bonds cannot be maintained and may become amorphous phase. However, the β-$FeSi_2$ films employed in this study were confirmed to be a high quality single crystal by XRD and Raman measurements. These analysis results are inconsistent to such experimental results.

4.2 Analysis using multiple ion scattering condition

Next we discuss effect of multiple ion scattering caused in the surface layer on the channeling measurements. In usual condition for channeling measurements and computation of some parameters, we assume single ion channeling of direct collimated beam, however, possible multiple scattering of beam deflected by a random and effectively thick surface layer should be taken into account. Here, we determine the value of m of the initial reduced film thickness: $m=\pi a_{TF}^2 Nt$, where a_{TF} is the Thomas-Fermi screening radius, Nt is the number of atoms in cm^2. If m<0.2, the single scattering approximation holds [6]. We calculated the m values for β-$FeSi_2$, then obtained ~ 20 nm for the critical thickness t_c. This result suggests that the actual thickness ~89 nm is too thick to hold the single scattering approximation. When taking into account this condition, we need to analyze the channeling data by using the multiple ion scattering theory [6, 7]. The minimum yield χ_{min} is given by

$$\chi_{\min} = P(\widetilde{\theta_c}, m), \quad \widetilde{\theta_c} = \frac{a_{TF}E}{2Z_1Z_2e^2}\Psi_{1/2}$$

where $\widetilde{\theta_c}$ is a reduced critical angle for small angle scattering, e^2=1.44 eV nm, Z_1 and Z_2 are atomic numbers of incident ion ($^4He^+$: Z_1=2) with an energy E (=2 MeV) and target atoms, respectively. The fraction $P(\widetilde{\theta_c}, m)$of particle scattered outside the reduced critical angle $\widetilde{\theta_c}$ is given by

$$P(\widetilde{\theta_c}) = \int_{\widetilde{\theta_c}}^{\infty} f_1(m, \tilde{\theta})\, 2\pi\tilde{\theta} \cdot d\tilde{\theta},$$

where the function $f_1(m, \tilde{\theta}) = \int_0^{\infty} e^{-m\Delta(\epsilon)} J_0(\tilde{\theta}z)zdz$, the phase $\Delta(z) = \frac{1}{4}\int_0^{\infty} f(y)\left\{1 - J_0\left[z\left(\frac{1}{2}y\right)\right]\right\}dy$, J_0 is the zeroth-order Bessel function of the first kind [7]. Using the apparent $\chi_{\min}$=0.31 for the Si substrate due to small angle scattering of incident ion beam in the β-$FeSi_2$ film, we get m=14.2. The reduced thickness including average atomic displacements in atomic rows can be extended by $m = \pi(a_{TF}^2 + \Delta x^2)(N_\beta \cdot t_\beta)$. When using the values m =14.2, $N_\beta = 2.60 \times 10^{22}$ atoms/cm^3, t_β=89 nm, $a_{TF} =$ 0.0182 nm, we can get Δx=0.04 nm that is 13% of atomic spacing in the row. It has been observed that the epitaxial β-$FeSi_2$(111) planes may consist of random distributing six equivalent (111) domains and the one step height is 0.31 nm [1]. This six equivalent staking domains along β<111> directions can be regarded as some kinds of stacking faults because they have slightly different atomic spacing in each domains. If the film employed in this study has six different domains, the average atomic displacement due to the staking fault is 0.31/6=0.05 nm that is close to Δx=0.04 nm within range of total error. From above discussion, we think that multiple scattering due to small angle scattering of incident ions may be attributed to the stacking fault of domains in β-$FeSi_2$(111) planes.

5. Conclusions

We have investigated axial channeling measurements along Si<111> direction using β-$FeSi_2$ (110), (101) planes epitaxially grown on Si(111). Unexpected large static displacements were computed by analysis based on single ion scattering. We have discussed multiple ion scattering in the film and obtained atomic displacement Δx=0.04 nm (that is 13% of the atomic spacing) being close to 0.05 nm that is one sixth of one step of six domains stacking on the (111) planes. This result suggests that multiple scattering may be attributed to atomic displacement due to the domain stacking faults. If ion scattering is attributed to the stacking fault formed in the film, a dechanneling factor σ_D is equal to the minimum yield $\chi_{\min}$ and ideally independent upon the energy of incident ion beam [6]. We are going to measure energy dependence of the $\chi_{\min}$.

Acknowledgment

This work has been supported by the joint research program between Kyutech and QST.

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