Solid-Phase Growth of $\beta$-FeSi$_2$ on Si Substrates with Different Crystal Orientations

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Solid-Phase Growth of $\beta$-FeSi$_2$ on Si Substrates with Different Crystal Orientations

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Abstract: Orientation dependent solid-phase growth of $\beta$-FeSi$_2$ thin films on (100), (110), and (111) Si substrates has been investigated by using a-Fe(thickness: 20 nm)/c-Si stacked structures. XRD measurements suggested that the substrate orientation dependence of the formation rate of $\beta$-FeSi$_2$ was as follows: (100) > (111) > (110). This dependence can be explained on the basis of the lattice mismatch between $\beta$-FeSi$_2$ and Si substrates, i.e., the lattice mismatch between $\beta$-FeSi$_2$ (100) and Si (100), $\beta$-FeSi$_2$ (110) or (101) and Si (111), and $\beta$-FeSi$_2$ (010) or (001) and Si (110) are 1.4–2.0%, 5.3–5.5%, and 9.2%, respectively. The substrate orientation dependence of solid-phase growth becomes relatively remarkable for very thin films.

Keywords: Semiconductor silicide, $\beta$-FeSi$_2$, Silicidation, Crystal orientation, Lattice mismatch

1. Introduction

Because of its direct energy gap of 1.5μm, $\beta$-FeSi$_2$ attracts technological interests for the optoelectronics application\(^1\). In order to integrate $\beta$-FeSi$_2$ devices on a silicon chip, it is necessary to form $\beta$-FeSi$_2$ thin films with high quality on Si at a low temperature. With decreasing thickness of the films, it is expected that formation kinetics of $\beta$-FeSi$_2$ depend on the orientation of the substrates, owing to the lattice mismatch between $\beta$-FeSi$_2$ and Si.

In the present study, we have investigated the solid-phase growth kinetics of $\beta$-FeSi$_2$ on Si by using the a-Fe/c-Si stacked structures as the starting materials. On the basis of the lattice mismatch between $\beta$-FeSi$_2$ and Si, dependence of the kinetics on orientation of the substrates is discussed.

2. Experimental Procedures

The substrates used were Cz n-type (100), (111), and (110) Si crystals. After a standard cleaning, they were introduced into a deposition chamber, and Fe films were deposited at room temperature by rf-magnetron sputtering. The thickness of the deposited films was 20 nm. Subsequently, the samples were annealed at 700–900°C in a nitrogen ambient.

The phase of the formed silicide was identified by using glancing angle x-ray diffraction (XRD) measurements at an incident angle of 4°. The optical characteristics were performed by using the Fourier-transform infrared spectroscopy (FT-IR).

3. Results and Discussion

Typical results of the XRD measurements for samples with (100), (111), and (110) orientations after annealing at 700–900°C for 30 min are shown in Figs. 1(a), 1(b), and 1(c), respectively. For all orientations, the XRD peaks due to the $\beta$-FeSi$_2$ phase are observed after annealing at 800°C. For samples annealed at 900°C, the peaks due to the $\beta$-FeSi$_2$ phase disappeared, and those due to the $\alpha$-FeSi$_2$ phase appeared. This suggests that the $\beta$-FeSi$_2$ phase was formed at 800°C, and changed into the $\alpha$-FeSi$_2$ phase, which is consistent with the report by other researchers\(^2\). Assuming the same crystallinity, the peak height is a measure of the amount of the material. Comparing the height of peaks corresponding to the $\beta$-FeSi$_2$ phase for samples with various orientations after annealing at 800°C, it is suggested that the amount of $\beta$-FeSi$_2$ is as follows: (100) > (111) > (110).

Next, we investigated more detailed growth characteristics of $\beta$-FeSi$_2$ at 800°C as a function of annealing time. The XRD spectra for samples with (100), (111), and (110) orientations after annealing at 800°C are shown in Figs. 2(a), 2(b), and 2(c), respectively. For annealing time of 1 min, only the XRD peaks due to the FeSi phase are observed. The peaks due to the $\beta$-FeSi$_2$ phase appeared after annealing for 5 min, and became large with increasing annealing time. The annealing time dependence of the amount of $\beta$-FeSi$_2$ evaluated from the XRD peak heights are shown in Fig. 3. The orientation dependence of the formation rate of $\beta$-FeSi$_2$ is
clearly observed, i.e., (100) > (111) > (110).

According to the review by Lange\textsuperscript{3)}, the lattice mismatch between $\beta$-FeSi\textsubscript{2} (100) and Si (100), $\beta$-FeSi\textsubscript{2} (110) or (101) and Si (111), and $\beta$-FeSi\textsubscript{2} (010) or (001) and Si (110) are 1.4-2.0\%, 5.3-5.5\%, and 9.2\%, respectively. This trend shows a good agreement with that for the orientation dependence of the growth rate. The XRD measurements with the $\theta$-2$\theta$ configuration showed that the $\beta$-FeSi\textsubscript{2} did not grow epitaxially on the Si substrates. Thus, it can be speculated that the crystal nucleation rate or the initial growth rate of the nuclei are affected by the strain energy induced by the lattice mismatch between $\beta$-FeSi\textsubscript{2} and Si. In order to clarify this,
further studies are needed.

Optical absorption characteristics near the absorption edge for samples annealed at 800°C for 30 min are shown in Figs. 4(a)–4(b). The plots in the higher energy regions could be fitted with straight lines, which suggests the direct transition. By extrapolating the lines to \((a\nu h)^2 = 0\), the energy gap was obtained as about 0.8 eV for all samples. The gradient \(K\) of the lines can be expressed by the next equation:

\[
K = \frac{2e^2(2\mu)^{3/2}}{m^2\hbar}|P_{cv}|E_g^{-3/2},
\]

where \(e\) is an elementary charge, \(m\) the mass of an electron, \(\mu^{-1} = m_{c}^{-1} + m_{v}^{-1}\), \(m_{c}\) and \(m_{v}\) are the effective mass of the conduction band and the valence band, respectively, \(\hbar\) the Plank’s constant, \(P_{cv}\) the transition probability from the valence band to the conduction band, and \(E_g\) the band gap. Since the transition probability becomes larger for the better optical crystallinity, the gradient \(K\) is a good measure for evaluation of the optical crystallinity. From the fitting, the value of \(K\) was obtained as 3.8 \(\times\) 10\(^{12}\), and 3.4 \(\times\) 10\(^{12}\), 2.0 \(\times\) 10\(^{12}\) eV/cm\(^2\) for (100), (111), and (110) substrates, respectively. Thus, it is suggested that the optical crystallinity becomes better as follows: (100) > (111) > (110).

In Fig. 5, the absorption coefficient for \(\beta\)-FeSi\(_2\) is compared with that for GaAs\(^{7}\). The absorption coefficient near the absorption edge for \(\beta\)-FeSi is about 2 order of magnitude larger than that for GaAs. Furthermore, the gradient \(K\) for GaAs is 2.4 \(\times\) 10\(^8\) eV/cm\(^2\), which is 3 order of magnitude smaller than that for \(\beta\)-FeSi\(_2\). These results demonstrate that \(\beta\)-FeSi\(_2\) is a very promising material for the opto-devices at 0.8 eV. Since the optical energy corresponds to the minimum loss energy for the optical quartz fiber, it is expected that \(\beta\)-FeSi\(_2\) can be employed for the optical communication devices.

4. Conclusion

The solid phase growth kinetics of \(\beta\)-FeSi\(_2\) in \(\alpha\)-Fe(thickness: 20 nm)/c-Si structures with (100), (111), and (110) substrates have been investigated. The \(\beta\)-FeSi\(_2\) phase was formed for all samples after
Annealing at 800°C. From the results of the XRD measurements, it is suggested that the growth rate strongly depends on the crystal orientation of the substrates, i.e., (100) > (111) > (110). It was speculated that this trend was due to the different strain energy at the growth front caused by the lattice mismatch between β-FeSi₂ and Si. From the optical measurements, direct band gap with 0.8 eV was obtained for all samples. The absorption coefficient near the band edge is about 2 order of magnitude larger than that for conventional semiconductors, such as GaAs. These results suggest that β-FeSi₂ is a promising material for opto-devices for the fiber communications.

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References