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Optical constants of β-$FeSi_2$ thin film on Si(001) substrate obtained by simultaneous equations from reflectance and transmittance spectra

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Abstract

β-$FeSi_2$ films were prepared on Si(001) substrates by the molecular beam epitaxy method using an Fe source. The crystallinity and crystallographic orientation of β-$FeSi_2$ films on Si(001) substrates were characterized by using X-ray diffraction. Optical constants and the onset of the absorption edge of β-$FeSi_2$ films on Si(001) substrates were evaluated by solving simultaneous equations of reflectance and transmittance data. The extinction coefficient calculated by the simultaneous equation method showed abrupt absorption onset near the band-edge of β-$FeSi_2$.

Keywords: β-$FeSi_2$; Thin film; FTIR; Simultaneous equations; Optical constants

1. Introduction

Fe Si binary compounds are known for a long time since Goss' investigation [1], and nowadays various structural phases, i.e. ε-FeSi, β-$FeSi_2$ and α-Fe_2Si_5 have been found. Particularly, β-$FeSi_2$ and α-Fe_2Si_5 are classified as silicides [2]. β-$FeSi_2$, particularly, β-$FeSi_2$ thin film shows semiconducting properties with a direct energy band gap (E_g) at 0.85 eV in an experimental study. Filonov et al. focused on oscillator strength at Λ point of Brillouin zone in this crystal, and the oscillator strength transition of indirect and direct band to band transition was reported [3].

In recent years, semiconducting silicides have attracted considerable interests because they are expected to present new possibilities for the integration of optoelectronic applications with the currently existing Si technologies.

β-$FeSi_2$ thin film is attractive for the solar cell and infrared diode applications because it has the direct E_g and high optical absorption coefficient ($\alpha(h\nu)$) (10^5 cm^{-1} at 1.0 eV) according to previous reports [3,4]. The band to band transition of β-$FeSi_2$ thin film is assumed to be a direct one from experimental $\alpha(h\nu)$ spectrum, however the presence of indirect-transition has been reported by the band calculations for β-$FeSi_2$ crystal [5]. It is difficult for judging to direct – or indirect – transition about β-$FeSi_2$ because strong Urbach-tail has been observed around the band-edge in the experimental $\alpha(h\nu)$ spectrum. Therefore, solving simultaneous equations (SEs) of reflectance ($R(h\nu)$) and transmittance ($T(h\nu)$), an estimate was attempted by obtaining the optical constants of β-$FeSi_2$ thin film on a Si substrate without Urbach-tail in order to discuss the nature of band transition of β-$FeSi_2$ thin film.

2. Experimental

The Si substrate was selected for un-doped Si(001) wafer (1 kΩ cm, P-type, 0.5 mm thickness). The surface treatment of the Si(001) substrates was carried out using hydrogen fluoride and pure water. The base pressure of the growth chamber was kept at 10^{-9} Torr. β-$FeSi_2$ film was prepared by the molecular beam epitaxy (MBE) method using an Fe molecular beam evaporated by an electron-beam gun. The Si(001) substrate was heated up to 500 °C with electron bombardment during Fe deposition, and samples were subsequently annealed from 0 to 4 h in the growth chamber. Table 1 lists the growth conditions of each sample. The

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Table 1
Growth condition of samples

Sample	Temperature (°C)	Fe deposition time	Annealing	Remarks
A	500 °C	72 min	3 h	Random oriented
B	550 °C	38 min	2 h	Oriented

crystallinity of the sample was checked by X-ray diffraction (XRD, Rigaku X-ray diffractometer, RINT2000).

The optical properties of a randomly oriented sample (Sample A) were measured with a Fourier transport infrared (FTIR) spectrometer (Hitachi U-4000) at room temperature. The FTIR measurement was carried out in transmittance ($T(h\nu)$) and reflectance ($R(h\nu)$) configurations. The optical constants, i.e. refractive index ($n(h\nu)$) and extinction coefficient ($\kappa(h\nu)$): $n(h\nu)+i\kappa(h\nu)$ of β-$FeSi_2$ film were calculated by solving the simultaneous equations (SEs) of $R(h\nu)$ and $T(h\nu)$ experimental data using the software Mathematica (Wolfram Research) [6].

3. Results and discussion

3.1. Structural properties of samples

Fig. 1 shows the log plot of X-ray diffraction patterns of samples. Sample A presented the random orientation. On the other hand, Sample B exhibited an oriented pattern. As shown in Fig. 1(a), Sample A showed a strong (202)/(220) peak at the diffraction angle (2θ)=29.3° with several peaks from 2θ=45° to =55°, and weak (400) and (600) peaks oriented [100] direction were observed. On the other hand, as shown in Fig. 1(b), Sample B also showed a strong (202)/(220) peak, and (400), (600), and (800) peaks, although Si(002) peak disappeared.

From Fig. 1(a) and (b), the crystallographic orientations were changed as the functions of Fe deposition time and subsequent annealing time as listed in Table 1. The orientation ratio (p_o) is defined as $p_o = \sum_h I(h00)/\sum_{hkl} I(hkl)$, where $I(h00)$ is the XRD intensity of ($h00$) peaks, and $I(hkl)$ is the XRD intensity of (hkl) peaks. From measured 2θ=10° to 80° in Fig. 1(a) and (b), the p_o of Sample A was estimated to be 0.144, indicating random orientation, and p_o of Sample B was estimated to be 0.705, indicating 71% oriented.

The crystal structure of β-$FeSi_2$ has been investigated by Dusausoy et al. [7]. Normally, p_o for a-axis orientation of β-$FeSi_2$ crystal has a low value because β-$FeSi_2$ has a preferred orientation in the [101]/[110] direction, but a high orientation was realized in this study by means of film formation [8–10].

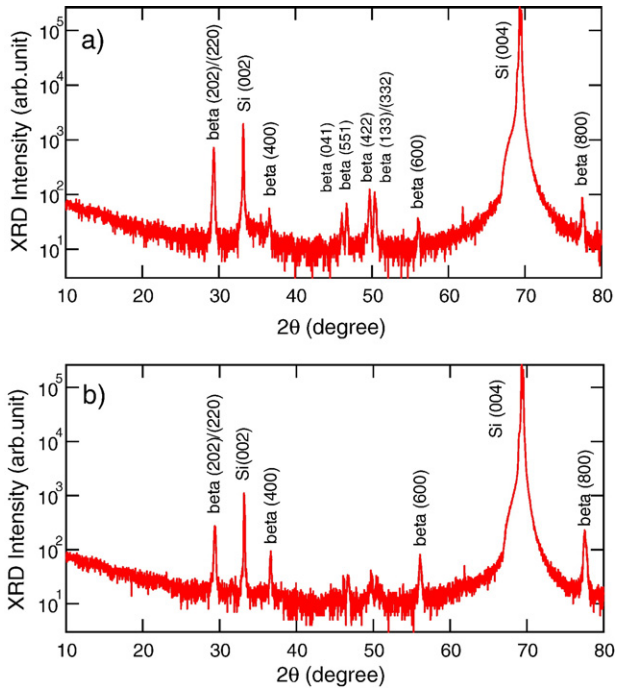

Fig. 1. The X-ray diffraction patterns of (a) Sample A: random orientation and (b) Sample B: oriented.

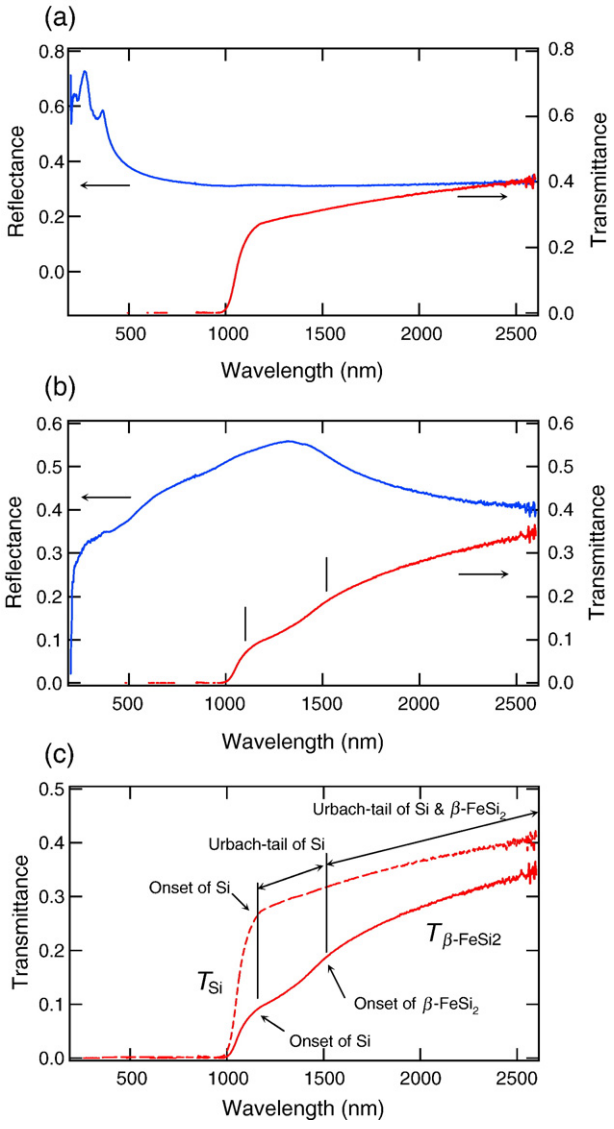

Fig. 2. The reflectance and transmittance spectra of (a) Si(001) substrate, (b) β-$FeSi_2$/Si(001) substrate (Sample A) measured by FT-IR at room temperature, and (c) image of transmittance spectra of Si(001) substrate and β-$FeSi_2$ film, and their Urbach-tails.