Extended Abstracts of the 2006 International Conference on Solid State Devices and Materials, Yokohama, 2006, pp. 648-649

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Optical constants of beta-$FeSi_2$ film on Si substrate obtained from transmittance and reflectance data and origin of Urbach-tail

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1.Introduction

beta-$FeSi_2$ film has been attracted for the solar cell and infrared diode because it shows the quasi-direct energy band-gap (E_g, 0.85eV) and highly optical absorption coefficient ($\alpha(h\nu)$) ($10^5 cm^{-1}$ at 1.0eV) in previous reports [1-3]. The band transition of beta-$FeSi_2$ film is assumed to be a direct one from experimental $\alpha(h\nu)$ spectrum, however indirect-transition has been reported from band calculation for beta-$FeSi_2$ crystal [2]. It is difficult for judging to direct- or indirect-transition about beta-$FeSi_2$ because strong Urbach-tail has been observed around band-edge in experimental $\alpha(h\nu)$ spectrum [3]. Therefore, solving simultaneous equations (SEs) of reflection ($R(h\nu)$) and transmmission ($T(h\nu)$), we tried to estimate for obtaining the optical constants of beta-$FeSi_2$ film on Si substrate with removing Urbach-tail in order to discuss the origin of Urbach-tail and band-transition of beta-$FeSi_2$ film.

2.Experimental

The Si substrate was selected for Si(100) wafer (1kρcm, P-type, 0.5mm for thickness). The surface treatment of Si(100) substrate was done with a HF and a pure water. The base pressure of growth chamber was kept to 10^{-9}Torr. beta-$FeSi_2$ film was prepared by the molecular beam epitaxy (MBE) method using a Fe molecular beam evaporated by an electron-beam gun [4]. The Si(100) substrate was heated up to 550°C with electron bombardment (EB) from reverse side [5]. The crystallinity of sample was checked by x-ray diffraction (XRD, Rigaku diffractometer RINT2000). The microstructure of sample was observed by the scanning electron microscopy (SEM) for surface morphology and cross-section. The resistivity and mobility of samples were characterized by Hall measurement. The optical properties of sample were measured with a Fourier transport infrared (FTIR) spectrometer (Hitachi U-4000) at room temperature. The FTIR measurement was carried out with $T(h\nu)$ and $R(h\nu)$ configurations. The optical constants, i.e. refractive index ($n(h\nu)$) and extinction coefficient ($\kappa(h\nu)$) of beta-$FeSi_2$ film were calculated by solving the simultaneous equations (SEs) of $R(h\nu)$ and $T(h\nu)$ experimental data using a software (Mathematica, Wolfram Research) [6].

3.Results and Discussion

3.1 Crystallinity of beta-$FeSi_2$ film on Si(100) substrate

Figure 1 shows the XRD pattern and SEM images of sample. The orientation of sample was changed to random one with increasing the film thickness, for example, random oriented pattern is shown in Fig.1(a). The XRD pattern of sample showed partially [100] orientation with (202)/(220) peak [4,5]. The grain size and film thickness of sample were estimated to be about 100nm and 900nm, respectively, from SEM image in Figs.1 (b) and (c).

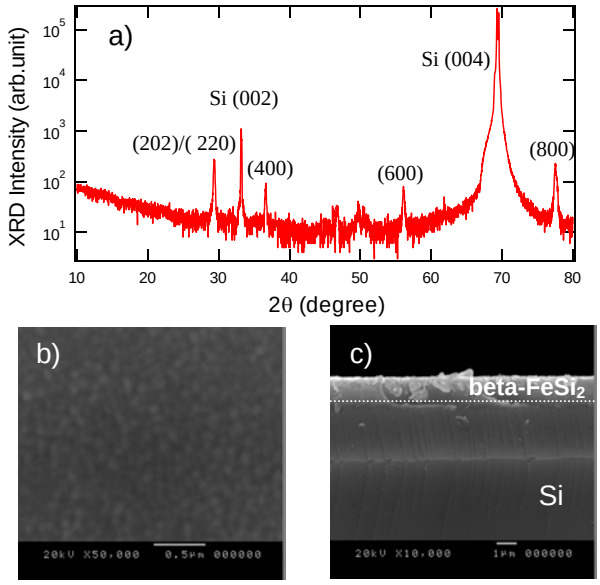

Fig.1 XRD pattern (a) and SEM images (b), (c) of sample.

3.2 Theoretical analysis model

Figure 2 shows the SEs analysis model with incidence (I_o), $R(h\nu)$ and $T(h\nu)$ light. The model was defined with the beta-$FeSi_2$ film surface (z=0), boundary between beta-$FeSi_2$ film (d_0=900nm) and Si substrate (d_1=0.5mm) at z=d_0 and reverse side of Si substrate

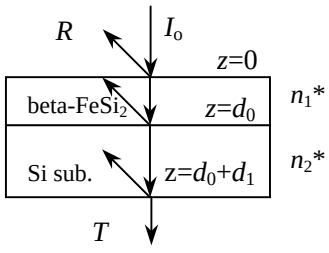

Fig.2 The model for analysis.

at $z=d_0+d_1$. The I_o, $R(h\nu)$ and $T(h\nu)$ light are also defined in Fig.2. The optical constants were also defined to $n_1^*=n_1+i\kappa_1$ for beta-$FeSi_2$ film, $n_2^*=n_2+i\kappa_2$ for Si(100) substrate. From Fig.2, the boundary conditions for electric ($\boldsymbol{E}$) and magnetic ($\boldsymbol{H}$) fields are considered at $z=0$, d_0 and d_0+d_1, as below,

$$\{\boldsymbol{E}_+\exp(ik_+r)+\boldsymbol{E}_-\exp(ik_-r)\}_{\parallel}=\{\boldsymbol{E}_t\exp(ik_tr)\}_{\parallel} \quad (1a)$$

$$n_j^{*2}\{\boldsymbol{E}_+\exp(ik_+r)+\boldsymbol{E}_-\exp(ik_-r)\}_{\perp}=n_{j+1}^{*2}\{\boldsymbol{E}_t\exp(ik_tr)\}_{\perp} \quad (1b)$$

$$\{\boldsymbol{H}_+\exp(ik_+r)+\boldsymbol{H}_-\exp(ik_-r)\}_{\parallel}=\{\boldsymbol{H}_t\exp(ik_tr)\}_{\parallel} \quad (1c)$$

$$\{\boldsymbol{H}_+\exp(ik_+r)+\boldsymbol{H}_-\exp(ik_-r)\}_{\perp}=\{\boldsymbol{H}_t\exp(ik_tr)\}_{\perp}, \quad (1d)$$

where $\parallel$ and $\perp$ indicate the *s*– and *p*–polarized lights to the surface of sample. In this study, I_o was irradiate perpendicular to sample surface as a *s*-polarized light, hence, Eqs.(1a) and (1c) were used for analysis at z=0 (j=0) and z=d_0 (j=1) boundary conditions [6].

3.3 Experimental results and SEs analysis

Figure 3 shows the results of $R(h\nu)$ and $T(h\nu)$ spectra of sample. The onsets of optical absorptions of sample are observed at 1234nm (Si substrate) and 1594nm (beta-$FeSi_2$ film) from $T(h\nu)$.

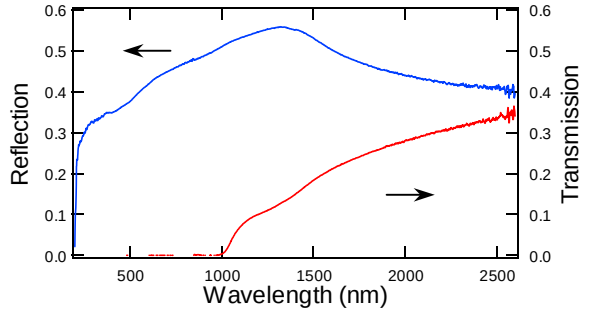

Fig.3 The reflection and transmission spectra of sample.

Figure 4 shows $n(h\nu)$ and $\kappa(h\nu)$ spectra of beta-$FeSi_2$ film obtained by the SEs analysis using Eqs.(1a)-(1d) (open circles with dashed lines), and $\kappa(h\nu)$ spectrum of beta-$FeSi_2$ film directly calculated result from experimental data (Exp.): $(\lambda/4\pi)[-(1/d_1)\ln(T_{beta}(h\nu)/T_{si\ sub}(h\nu))]$ (solid line). The SEs analysis was carried out with inputting the result of SEs analysis for Si substrate (about $n_{Si}(h\nu)$=3.6). In Fig.4, $\kappa(h\nu)$ obtained from SEs analysis is exhibited the abrupt onset of absorption at 0.85eV in comparison with Exp.

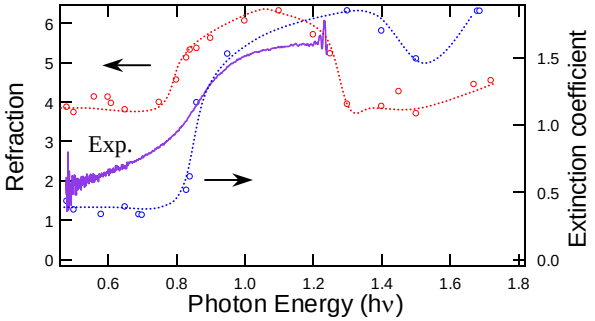

Fig.4 Refraction and extinction coefficient spectra of sample obtained by simultaneous equations analysis with comparison of directly calculated result from experimental data.

From Fig.4, the model in Fig.2 and SEs analysis are useful to obtain optical constants of beta-$FeSi_2$ film itself with removing the effect of interface between beta-$FeSi_2$ film and Si substrate, and its results can be discuss about origin of Urbach-tail and band-transition [7]. The origin of Urbach-tail was caused from shallow impurity level and defect. Particularly, defect is caused from crystallinity of sample. As shown in Fig.1(c), the interface of sample is not sharp one, and the defect is assumed to be caused from local inclusion of Fe or Si atoms at interface between beta-$FeSi_2$ film and Si substrate [3].

4.Conclusion

beta-$FeSi_2$ film was formed by molecular beam epitaxiy method by a Fe deposition using electron beam. The crystallinity of sample was measured with x-ray diffraction, and the orientation of sample was changed as a function of film thickness. The reflection and transmission of sample was measured by a Fourier transformed infrared spectroscopy. The analysis of simultaneous equations using obtained reflection and transmission data was carried out, optical constant of beta-$FeSi_2$ film was exhibited. From obtained optical constants, the origin of band -transition can be investigated in future study.

Acknowledgments

The study was supported by Sumitomo foundation for basic science, Venture Business Laboratory foundation (Tokyo Tech.) and Nippon Sheet Glass foundation for materials science and engineering.

References

[1] C.A.Dimitriadis, J.H.Werner, S.Logothetidis, M.Stutzmann, J.Weber and R.Nesper, J. Appl. Phys. **68** (1990) 1726.

[2] A.B.Filonov, D.B.Migas, V.L.Shaposhnikow, N.N.Dorozhkin, G.V.Petrov, V.E.Borisenko, W.Henrion and H.Lange, J. Appl. Phys. **79** (1996) 7708.

[3] C.H.Olk, S.M.Yalisove and G.L.Doll, Phys. Rev **B52** (1995) 1962.

[4] N.Hiroi, T.Suemasu, K.Takakura, N.Seki and F.Hasegawa, Jpn. J. Appl. Phys. **40** (2000) L1008.

[5] H.Kakemoto, Y.Makita, A.Obara, Y.Tsai, S.Sakuragi, S.Ando and T.Tsukamoto, Mat. Res. Soc. Sympo. Proc. **478** (1997) 273.

[6] L.H.Palmer and M.Tinkham, Phys. Rev. **108** (1957) 108.

[7] M.Ueta, H.Kanzaki, K.Kobayashi, Y.Toyozawa, and E.Hanamura, *"Excitonic Processes in Solids", Solid State Sciences 60, Springer Verlag (1984).*