Extended X-ray Absorption Find-Structure Investigation of Carbon-Doped β-$FeSi_2$

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Semiconducting iron disilicide β-$FeSi_2$ has recently attracted considerable attention from both scientists and engineers due to its remarkable optical and electrical properties. We fabricated β-$FeSi_2$/Si heterojunctions to be employed near infrared photodiode. Thier hetrojunctions showed typical rectifying actions. However, their current-voltage (I-V) characteristics exhibited large leakage dark current. We believe that the main source of its large leakage current is the high carrier density, of β-$FeSi_2$ epitaxial film. In previous study, we found that C-doping for β-$FeSi_2$ might be an effective for reducing the carrier density somehow. In this study, extended X-ray absorption find-structure (EXAFS) measurement was employed in order to investigate the local-bonding structure of C-doped β-$FeSi_2$ As a first step of the EXAFS evaluation, a change in the EXAFS spectrum for the substrate temperature was studied in order to verify the availability of EXAFS analysis for C-doped β-$FeSi_2$.

C-doped β-$FeSi_2$ films were epitaxially grown on p-type Si (111) substrates with an electrical resistivity of 10 Ω.cm and thickness 260 μm at a substrate temperatures of 500 °C, 540 °C, 560 °C, and 600 °C by Radio Frequency Magnetron sputtering (RFMS). EXAFS measurements were performed in conversion electron yield mode at beam line 6 of Saga Light Source, Kyushu Synchrotron Light Research Center, and the spectra were analyzed using a free software (Athena).

Fourier transform magnitudes of Fe EXAFS, which was transformed from k-weighted EXAFS data, for β-$FeSi_2$ films deposited at different substrate temperatures were shown. K-range was set from 3 to 10 to get the results with minimal noise. The second peak due to the second neighbor coordination shell (Fe-Fe) is gradually strengthened with an increase in the substrate temperature and the peak position obviously approach the bulk value with increasing the substrate temperature. These indicate that atomic ordering in β-$FeSi_2$ lattices is evidently enhanced with increasing substrate temperature. This is well consistent with the results of X-ray diffraction measurements. An enhancement in the atomic ordering in β-$FeSi_2$ lattices with increasing substrate temperature was confirmed by the EXAFS measurement. The availability of EXAFS spectroscopy for evaluating the local bonding structure of β-FeSi2 was experimentally proved. At present, the EXAFS measurement is employed for studying C-incorporation effects on the structure of β-$FeSi_2$ and the result will be reported at the conference.

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ABSTRACT

Semiconducting iron disilicide β-$FeSi_2$ has recently attracted considerable attention from both scientists and engineers due to its remarkable optical and electrical properties. We fabricated β-$FeSi_2$/Si heterojunctions to be employed near infrared photodiode. Thier hetrojunctions showed typical rectifying actions. However, their current-voltage (I-V) characteristics exhibited large leakage dark current. We believe that the main source of its large leakage current is the high carrier density, of β-$FeSi_2$ epitaxial film. In previous study, we found that C-doping for β-$FeSi_2$ might be an effective for reducing the carrier density somehow. In this study, extended X-ray absorption find-structure (EXAFS) measurement was employed in order to investigate the local-bonding structure of C-doped β-$FeSi_2$ As a first step of the EXAFS evaluation, a change in the EXAFS spectrum for the substrate temperature was studied in order to verify the availability of EXAFS analysis for C-doped β-$FeSi_2$.

INTRODUCTION

- β-$FeSi_2$ defined as a ecofriendly semiconductor is regarded as one of the 3-rd generation semiconductors after Si and GaAs.
- β-$FeSi_2$ has a large absorption coefficient, and possesses indirect and direct optical band gaps of 0.74 eV and 0.85 eV, respectively.
- β-$FeSi_2$ can fabricate a variety of devices as energy devices, solar cells and thermoelectric generator can be produced and as optoelectronic devices, photodiodes and light emitting diodes both operating near-infrared (NIR) -up to the wavelength of 1.55 μm- can be made.
- Previously, β-$FeSi_2$ have been epitaxial grown on Si(111)substrates at a substrate temperature 600 °C by facing-targets direct-current sputtering (FTDCS) and radio-frequency magnetron sputtering (RFMS) to form n-type ß-$FeSi_2$/p-Type Si heterojunctions diodes.

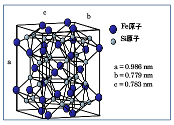

Figure RN Primitive unit cell of orthorhombic β-$FeSi_2$.

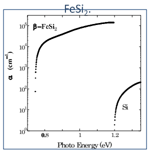

Figure TN Absorption spectrum of β-$FeSi_2$.

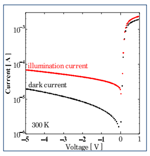

Figure VN I-V characteristics of the n-type β-$FeSi_2$ / p-type Si heterojunction diode.

Research AIM

In this study, we present several β- $FeSi_2$ films formed on Si(111) by RFMS and clarify how growth temperature influence the film quality and the Electrical properties of the n-type **ß-**$FeSi_2$/p-Type Si heterojunctions.

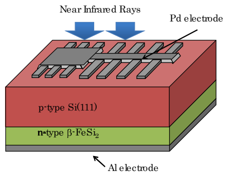

Figure MN Schematic diagram of n-type β-$FeSi_2$/p-type Si heterojunction photodiode.

	ß-$FeSi_2$	Al	Pd
Substrate temperature	600°C - 500°C (20°C step)	R.T.	R.T.
Pressure	2.66×10^{-1} Pa	6.65×10^{-1} Pa	2.66×10^{-1} Pa
Electric power	20 W	100 W	50 W
Film thickness	300 nm	250 nm	250 nm
Ar gas flow rate	15sccm	5sccm	5sccm

Table 1. Conditions of sputtering for the film, and electrodes.

Evaluate

XAFS measurement used by Kyushu university beamline(BL6) at SAGA-LS

Measurement methods: Conversion Electron Yield (CEY)

Measurement data's analyze using Athena and Artemis software

RESULTS and DISCUSSION

XRD measurements

- To investigate the epitaxial growth and crystallinity of the deposited films, they were characterized by XRD (Rigaku, RINT2000/PC) using 2θ-θ, θ, and pole figure measurement techniques.

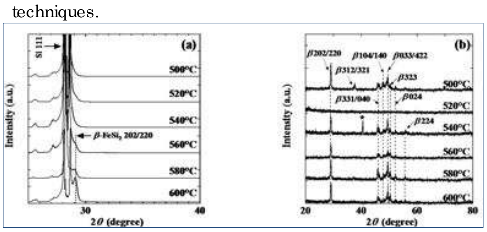

Figure Q (a) 2θ-θ XRD pattern of ß-$FeSi_2$ thin film epitaxially grown on Si(111) substrate with different temperatures, and (b) 2θ XRD pattern of ß-$FeSi_2$ thin film epitaxially grown on Si(111) substrate as a function of temperature

- The 202/220 peak of β-$FeSi_2$ was observed at 29 ° until 560 °C.
- For 2θ method, Except β-$FeSi_2$ film of 520 ° C, the diffraction peaks were observed at all substrate temperatures.

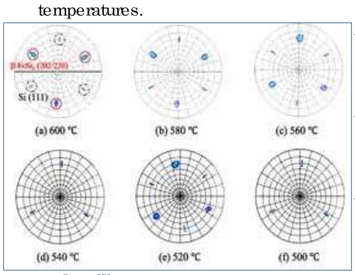

Figure W Pole figure patterns of β-$FeSi_2$ thin films deposited on different substrate temperature.

- At 600 °C, the 202/220 peak of β-$FeSi_2$ was observed.
- For the 580 °C and 560 °C state patterns the peaks are not separated.
- The peak of the β-$FeSi_2$ was not observed 500 °C and 540 °C substrate temperature.

J-V measurement

- We confirm that the rectifying action is exist at 600 ~ 540 °C substrate temperature.
- With reducing the temperature than 540 °C the rectifying action is dramatically decrease, that it showed an ohmic behavior at 500 °C substrate temperature. Which we believe it's because of the degradation in the crystallinity with reducing the temperature.

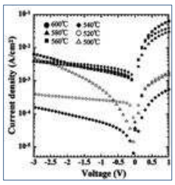

Figure Y *J-V* characteristics, which measured in the dark at 300 K, of n-type β-$FeSi_2$ deposited on Si (111) Substrate with different temperature.

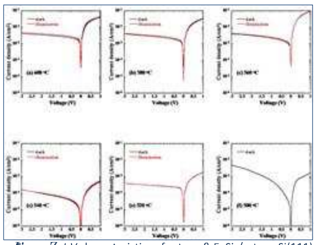

Figure Z *J-V* characteristics of n-type β-$FeSi_2$/p-type Si(111) Substrate, with different Temperatures, heterojunction diode in the dark and illumination states.

- The β-$FeSi_2$ deposited on Si (111) Substrate with Temp. 560 °C heterojunctions showed a significant improvement in leakage current and high response under illumination of 1.3 μm light.

XAFS measurement

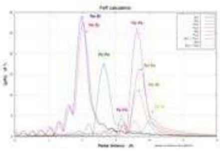

Figure ^. FeSi2 distance between neighboring atoms simulated by Artemis

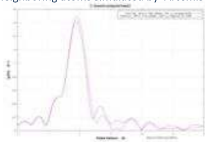

Figure R_. The distance between the absorbing and scattering (Un-doped & 0.5%at C-doped β-$FeSi_2$ at 500C)

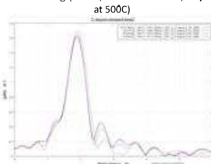

Figure RR The distance between the absorbing and scattering. (0.5%at C-doped β-$FeSi_2$ at different tempentures)

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- β-$FeSi_2$ /Si heterojunctions were fabricated by RFMS at different temperatures.
- The film was formed at 600 ~ 560 °C substrate temperature, but β-$FeSi_2$ film included multi-crystalline component.
- Due to the defects, lattice mismatch, and Fe atoms diffusion in the Si substrate we found low directivity, and high leakage current which showed high improvement for 560 °C deposition temperature. Depend on the above results 560 °C deposition temperature is confirmed as an optimum deposition temperature for β-$FeSi_2$ /Si heterojunctions for the ongoing research.
- As a result of changing the conditions of thin films, there is a change in the portion of the vibration on Fe-Fe.

Acknowledgement

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