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Crystal Growth and Photoresponse of Al-doped β-$FeSi_2$ /Si Heterojunctions

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1. Introduction

Orthorhombic $FeSi_2$ (β-$FeSi_2$) shows clear light emission and photoresponse near 1.55 μm in wavelength and a high refractive index (>5.8) [1]. The monolithic fabrication of 1.55 μm-light emitting diodes and IR-photodetectors connected effectively with Si waveguides can be made possibly by conventional fine ion beam synthesis (IBS) procedures of β-$FeSi_2$. However, photoelectrical responses of β-$FeSi_2$ were reported to be much less sensitive than that of InGaAs systems [2-5]. Further study is required to enhance the photoresponse of β-$FeSi_2$. Doping of some elements is a promising method for improvement. In fact, pronounced photoluminescence enhancement induced by doping Al atoms into β-$FeSi_2$ was recently reported [6].

In this study, we examined effects of the Al-doping into β-$FeSi_2$/Si heterojunctions on the crystal growth and the photovoltaic properties.

2. Experiments

Samples of β-$FeSi_2$ on FZ-Si(001) were prepared by an ion-beam synthesis (IBS) method [3,4]. Al-doping was also performed by ion implantation [5]. Then, all the samples were annealed at 800 ^{o}C by a rapid thermal anneal in order to form β–$FeSi_2$ and to remove the implantation damage. Structural analyses were examined by Raman spectroscopy (RAMAN), Rutherford backscattering spectroscopy (RBS), and transmission electron microscopy (TEM). The spectral photoelectrical response was investigated at 300 K with a monochromatic light, PbS and Si photodetectors and a high sensitive voltmeter.

3. Results and Discussion

Raman peaks of A_g-modes corresponding to movements of Fe atoms revealed that doped Al atoms cannot replace at the Fe site but at the Si site. After the Al-doping β-$FeSi_2$ was p-type and the hole concentration increased from 10^{18} to $4x10^{18}$ cm^{-3}. This shows acceptor actions of doped Al.

The difference in the interface structure between non- or Al-doped β-$FeSi_2$ was investigated by RBS. The RBS results showed that enhancement of crystalline growth by Al-doping takes place near the heterojunction between β-$FeSi_2$ and Si. This feature is preferable for fabricating clear interfaces of p-n junctions. So we observed directly the interface of heterojunction by TEM.

Figure 1 shows XTEM images of (a) the Al-doped and (b) the non-doped samples. The defective regions including stacking faults (SF) and dislocation loops (DL) were observed in both samples. The stacking faults in the Al-doped sample showed a coherent feature along Si[111] caused by relaxation during solid phase epitaxial growth, while the SF showed very defective and incoherent features. High resolution TEM and electron diffraction pattern near the interface in Fig.2 confirmed one of typical epitaxial relationships:β-$FeSi_2$[010](101),[001](110)//Si[110](111) with the lattice mismatch δ=-1.45 or -2.0% [1].

Figure 3 shows photoresponse spectra at 300 K for (a) the Al-doped sample and (b) the non-doped sample. The photovoltaic response for the Al-doped sample showed a clear and pronounced increase from Φ_0=0.75 eV (threshold energy) and the maximum at 0.96 eV. The band off-sets (ΔE_c) at conduction bands and the ΔE_v at valence bands of

β-$FeSi_2$ and Si were estimated to be 0.32 eV and ~0.02 eV at 300 K [1-3]. It was reported that photoemissions at the minimum threshold energies of Φ_1=0.64 eV and Φ_2=0.96 eV correspond respectively to the optical transition from the trap level (E_t) to the conduction band ($E_c(\beta)$) of β-$FeSi_2$, and the transition from the E_t to the top of the bent conduction band of Si at the junction [2,3]. By taking these photoemission data into account and assuming that the ΔE_c is less than 0.12 eV, we can explain that the photoelectrical responses observed in 0.75-0.95 eV probably correspond to the optical transitions from the bottom of the conduction band or the acceptor level (Al) to the E_t or valence bands of β-$FeSi_2$. The lowering of ΔE_c probably caused by pining of the conduction band of β-$FeSi_2$ at the interface level.

We speculate the enhancement mechanism. The effects of the Al-doping on epitaxial growth of β-$FeSi_2$ on Si and on formation of less defective β-$FeSi_2$ and interfaces as confirmed in Figs. 1 and 2 can contribute to separation of photo-injected electrons-holes at the depletion and their transport through p-type β-$FeSi_2$.

4. Conclusions

We confirmed that the Al-doping is much effective on the typical epitaxial growth and on improvement of the photovoltaic efficiency near the band-gap of β-$FeSi_2$.

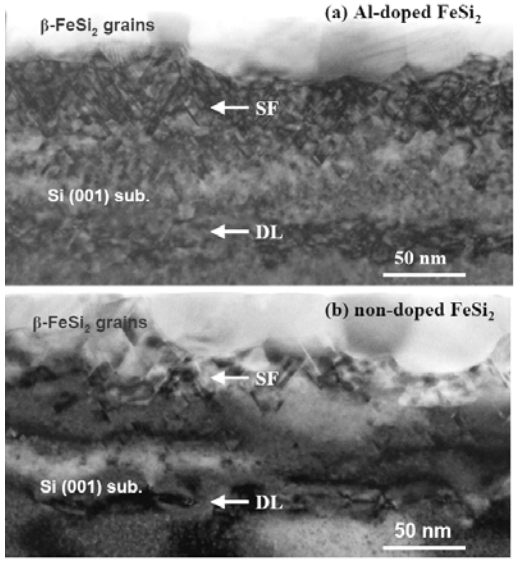

Fig. 1 XTEM images for (a) Al-doped and (b) non-doped sample interfaces.

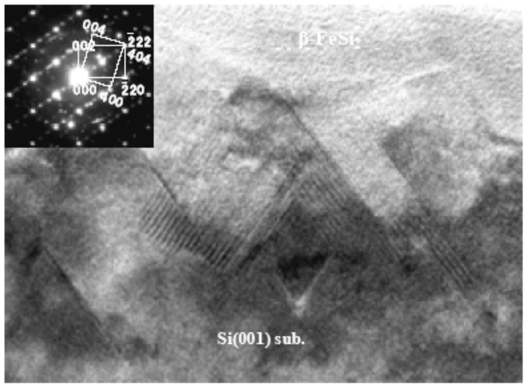

Fig. 2 High resolution TEM image near the interface between Al-doped β-$FeSi_2$ and Si(001).

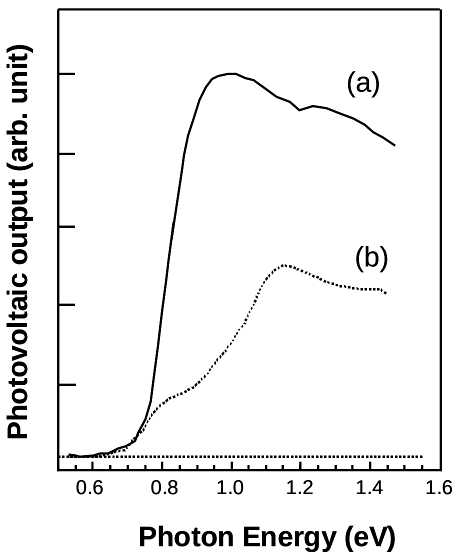

Fig. 3 Photoresponse spectra at 300 K for (a) the Al-doped and (b) non-doped samples.

Acknowledgement

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