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Reactive Deposition Epitaxy of $SrGe_2$ Thin Films on Ge (111) and (001) Substrates

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Abstract

Semiconductor $SrGe_2$ is a new material having a large absorption coefficient at near-infrared light. $SrGe_2$ thin films are firstly fabricated by using reactive deposition epitaxy on Ge substrates.

1. Introduction

Alkaline-earth silicides and germanides have useful functions for many technological applications such as solar-cells, thermoelectric, and optoelectronics. However, the study of germanides has not been active compared to that of silicides.

$SrGe_2$ is one of the Alkaline-earth germanides. The theoretical and experimental study of bulk $SrGe_2$ revealed the following properties [1−3]: (i) the $BaSi_2$-type structure (orthorhombic, space group: $D_{2h}^{16} - Pnma$, no. 62, Z = 8), (ii) indirect transition semiconductor with a band gap of approximately 0.82 eV, (iii) absorption coefficient of 7.8×10^5 cm^{-1} at 1.5 eV photon, which is higher than that of Ge (4.5×10^5 cm^{-1} at 1.5 eV photon). These properties mean that $SrGe_2$ is an ideal material for use in the bottom cell of high-efficiency tandem solar cells. Therefore, the fabrication of a $SrGe_2$ thin film on arbitrary substrates realizes thin film tandem solar cells simultaneously achieving high conversion efficiency and low process cost. In this study, we investigate the reactive deposition epitaxy (RDE) of $SrGe_2$ Ge substrates to explore the possibility of the thin film formation of $SrGe_2$.

2. Experimental Procedures

We fabricated high quality $BaSi_2$ thin films on Si(111) and Si(001) substrates using a two-step way: $BaSi_2$ template layer is formed by RDE, which is the Ba deposition with heating Si substrates, followed by molecular beam epitaxy (MBE) [4]. This method will be applicable for $SrGe_2$. Thus, we have tried to form $SrGe_2$ template layers on Ge(111) and Ge(001) substrates using RDE, as shown in Fig. 1. The deposition rate and time of Sr were 1.3 nm/min and 60 min for Ge(111), and 0.7 nm/min and 120 min for Ge(001). The substrate temperature was set at 300−700 °C during the Sr deposition. After that, 5-nm-thick amorphous Si was deposited at room temperature to protect the RDE layer from oxidation because Sr-Ge compounds are easily oxidized by air.

The crystallinity of the sample was evaluated by using reflection high energy electron diffraction (RHEED) and X-ray diffraction (XRD) with Cu Kα radiation. Besides, the surface morphology was observed by scanning electron microscopy (SEM).

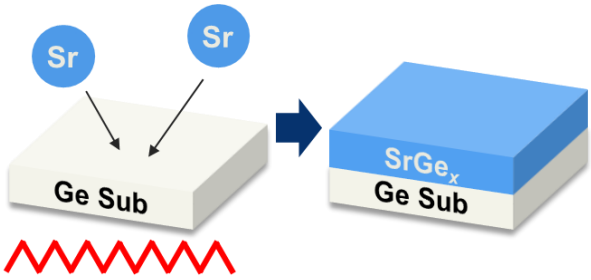

Fig. 1. RDE of a $SrGe_x$ thin film on a Ge substrate.

3. Results and Discussion

For all the samples, streaky RHEED patterns were observed after the Sr deposition, indicating the epitaxial growth of Sr-Ge compounds. For the samples with a Ge(111) substrate, Fig. 2(a) shows that the θ–2θ XRD pattern varies with the substrate temperature. The peaks corresponding to $SrGe_2$ appear for the samples with 500 and 600 °C though the other samples exhibit the peaks corresponding to Sr_2Ge. This behavior is probably related to the balance of the supply rate of Ge atoms from the substrate and the evaporation rates of Sr and Ge atoms from the sample surface. We note that a comparison with the XRD pattern of powder $SrGe_2$ determines that the 600 °C sample is preferentially [111] oriented.

Fig. 2(b) shows the θ–2θ XRD patterns of the samples with a Ge(001) substrate. The 300 °C sample exhibits a peak corresponding to $SrGe_2$(200) in addition to peaks corresponding to Sr_5Ge_3. This result indicates that the $SrGe_2$ thin film is preferentially [100] oriented on a Ge(001) substrate. Because the $SrGe_2$ peak is weak, there is a possibility that the 300 °C sample contains $SrGe_2$ crystals other than [200] orientation. When the substrate temperature is higher than 300 °C, the $SrGe_2$(200) peak is not observed. The optimum temperature for forming $SrGe_2$ is much different between Ge(111) and Ge(001) substrates. This means that the formation energy of $SrGe_2$ significantly varies with the crystal orientation of the substrate.

Fig. 3 shows the SEM images of the sample surfaces. For all the samples, island patterns are observed. When the substrate temperatures are 400−600 °C, we observe the unique patterns reflecting the crystal orientation of the substrates, that is, three-fold symmetry for Ge(111) and two-fold symmetry for Ge(001). These patterns ensure the epitaxial growth of Sr-Ge compounds and account for the streaky RHEED patterns. The 700 °C samples exhibit dot patterns, suggesting that the Sr atoms migrated rapidly or Ge atoms evaporated.

4. Conclusions

We firstly fabricated $SrGe_2$ thin films using RDE on Ge substrates. For a Ge(111) substrate, preferentially [111] oriented $SrGe_2$ thin film was formed at 600 °C. On the other

hand, for a Ge(001) substrate, preferentially [100] oriented $SrGe_2$ thin film was formed at 300 °C together with other Sr-Ge compounds. The detailed crystal quality and surface morphology are discussed in the presentation.

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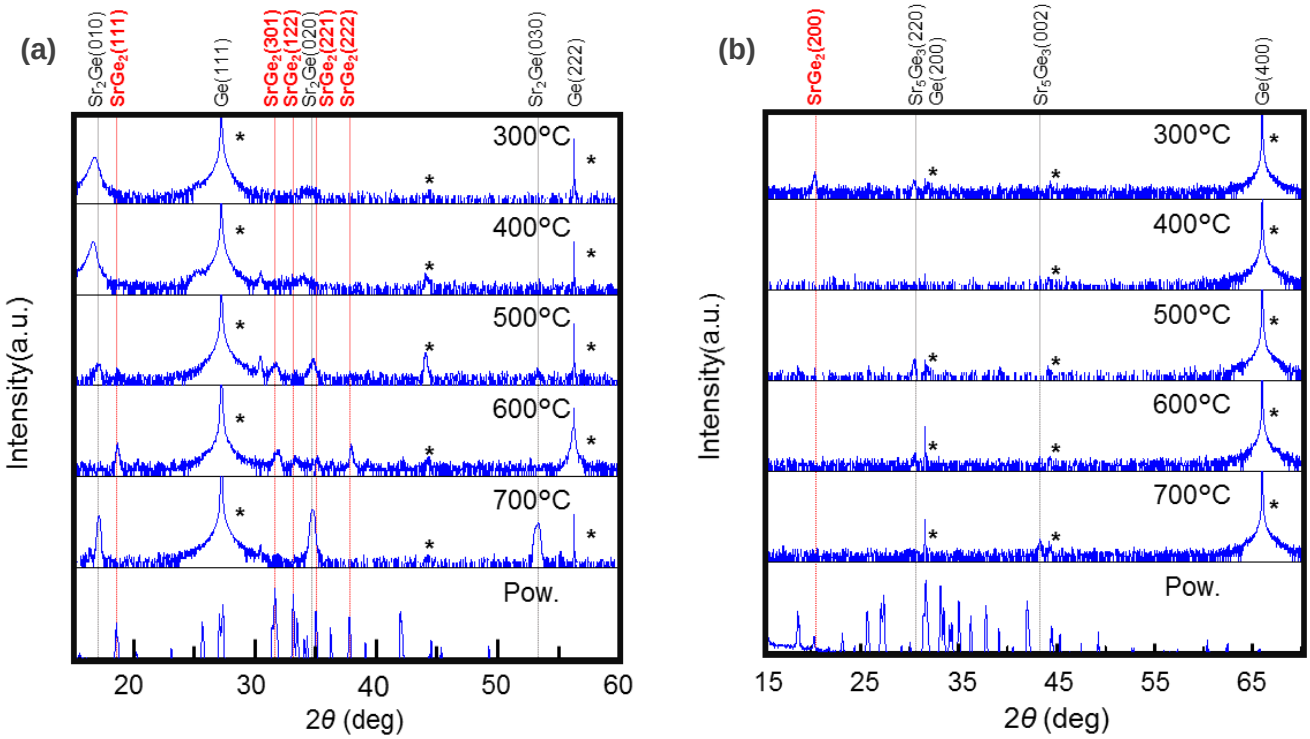

Fig. 2. θ–2θ XRD patterns of the samples with (a) Ge(111) and (b) Ge(100) substrates where the substrate temperatures are 300-700 °C. The powder diffraction of $SrGe_2$ is shown for comparison.

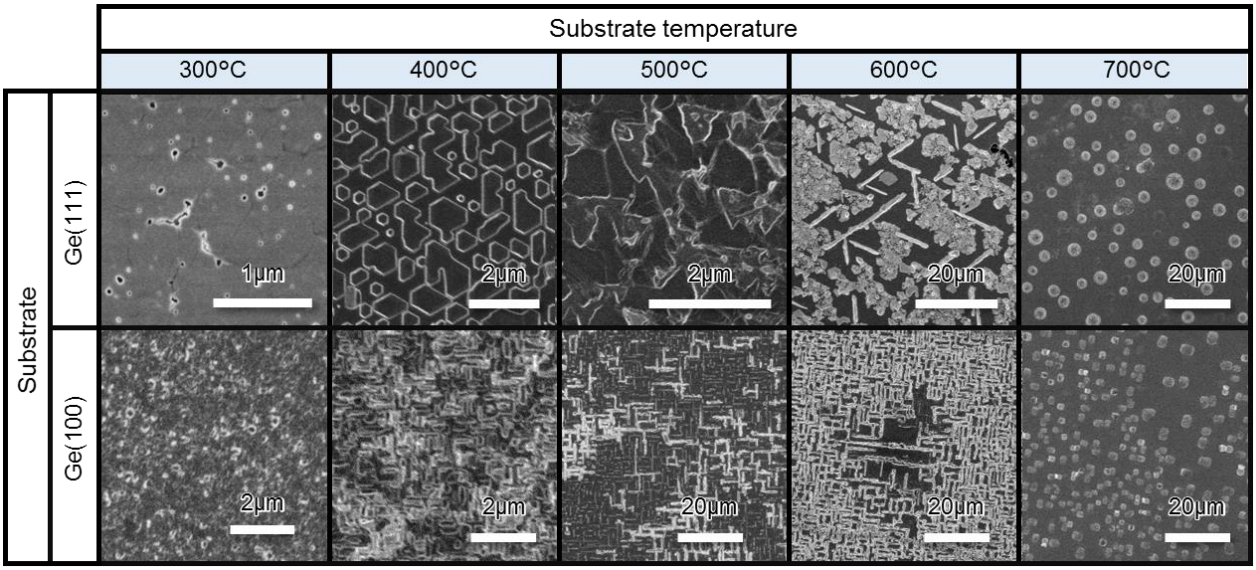

Fig. 3. SEM images of the surfaces of the samples.