18p-PB10-1

Growth of compositionally homogeneous P-type Si_{1-x}Ge_x bulk crystal for thermoelectric application

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1. Introduction

Thermoelectric energy conversion is one of the promising ways to convert the electric energy from waste heat [1]. Silicon-germanium $(Si_{1-x}Ge_x)$ alloy semiconductor is a good material for thermo-electrical power generators at high temperature. The thermoelectric properties of the $Si_{1-x}Ge_x$ alloy are strongly dependent on the composition of the material. Therefore, it is necessary to grow the $Si_{1-x}Ge_x$ crystals with homogeneous composition. In present study Ga-doped compositionally homogeneous $Si_{0.68}Ge_{0.32}$ bulk crystals were grown by vertical gradient temperature method under mild temperature gradient (0.57 °C/mm) with dopant concentration (7 x 10^{18} cm⁻³) and (1.1 x 10^{19} cm⁻³) and its thermoelectric properties were studied.

2. Experimental procedure

The cylindrically shaped samples were arranged as sandwich structure of Si(feed)/Ga-doped Ge/Si(seed) and covered by BN crucible. It was inserted into the quartz ampoule. The ampoule was evacuated upto 10^{-4} Pa before sealing. The sealed ampoule was vertically fixed into the furnace. Vertical temperature profile of the furnace was measured by R-type thermocouple. The sandwich sample was placed inside the furnace under mild temperature gradient position (0.57 °C/mm). The furnace temperature was kept constant for 300 h for growth of homogeneous Si_{1-x}Ge_x bulk crystal and cooling rate was 0.6 °C/h. After the experiment, the sample was removed from ampoule and polished sample surface. The Si composition distribution was measured by EPMA. The grown sample was cut with dimensions (10 X 3 X 2 mm³) for Seebeck coefficient and electrical resistivity measurement. Seebeck coefficient and electrical resistivity of the sample was measured as a function of temperature.

3. Results and discussion

Fig. 1 shows the Si composition distribution of Ga-doped (7 x 10^{18} cm⁻³ and 1.1 x 10¹⁹ cm⁻³) SiGe bulk crystals along growth direction measured by EPMA. It revealed that in both samples the crystals were grown from seed towards feed and the corresponding Si composition of both samples were Si_{0.68}Ge_{0.32} (±0.09), respectively. It corresponded to the growth temperature of 1195 °C. Resistivity of both samples were increased with temperature from 325 to 892 K which indicates the degenerate semiconducting nature as shown in Fig. 2. The mobility of Ga (7 x 10^{18} cm⁻³) doped Si_{0.68}Ge_{0.32} bulk crystal (23.4 cm²/V.s) was slightly higher than the Ga (1.1 x 10^{19} cm⁻³) doped Si_{0.68}Ge_{0.32} bulk crystal (17.16 cm²/V.s). The Seebeck coefficients of Ga-doped $(7 \text{ x } 10^{18} \text{ cm}^{-3} \text{ and } 1.1 \text{ x } 10^{19} \text{ cm}^{-3}) \text{ Si}_{0.68}\text{Ge}_{0.32}$ were positive which showed P-type material. The Seebeck coefficients of Ga-doped (7 x 10¹⁸ cm^{-3} and 1.1 x 10¹⁹ cm⁻³) Si_{0.68}Ge_{0.32} were 346 and 371µV/K at room temperature as shown in Fig. 3. The variation of Seebeck coefficients due to changes in carrier concentration and mobility of the samples. It revealed that Seebeck coefficient was increased with carrier concentration at room temperature. The maximum value of Seebeck coefficient of both samples were 465 µV/K at 844 K. Above 844 K, Seebeck coefficients were decreased because of charge carrier scattering at high temperature [2]. The Seebeck coefficient of both samples reached higher value (346, and 371 μ V/K) compared to reported value $(274 \mu V/K)$ of Ga-doped Si_{0.81}Ge_{0.19} at room temperature [3].

References

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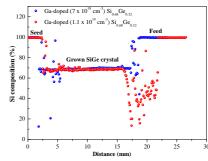


Fig. 1 Si composition distribution of Ga-doped (7 x 10^{18} cm⁻³ and 1.1 x 10^{19} cm⁻³) Si_{0.68}Ge_{0.32} bulk crystal

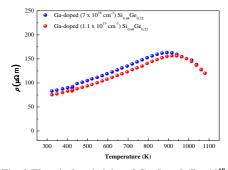


Fig. 2 Electrical resistivity of Ga-doped (7 x 10^{18} cm⁻³ and 1.1 x 10^{19} cm⁻³) Si_{0.68}Ge_{0.32} as a function of temperature

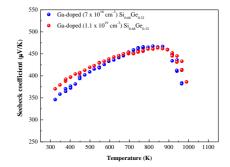


Fig. 3 Seebeck coefficient of Ga-doped (7 x $10^{18}\ cm^{-3}$ and 1.1 x $10^{19}\ cm^{-3})\ Si_{0.68}Ge_{0.32}$ as a function of temperature