Thermoelectric properties of Ga doped SiGe bulk crystal

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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 (SiₓGeₓ) alloy semiconductor is a good material for thermo-electrical power generators at high temperature (from 700 to 1000°C). It is highly challenging to optimize the figure of merit (ZT). Moreover, the thermoelectric properties of the SiₓGeₓ alloy are strongly dependent on the composition of the material. Therefore, it is necessary to grow the SiₓGeₓ crystals with homogeneous composition. After that, the optimum doping conditions are established by adjusting carrier concentration. In the present study, Ga doped (1x10¹⁹ cm⁻³) SiGe crystal was grown by vertical gradient method and its thermoelectric properties were studied.

2. Experimental procedure

Si and Ga doped (1x10¹⁹ cm⁻³) Ge samples were cylindrically polished by using alumina abrasive powder and etched in the acid mixture of HF:HNO₃ (1:1) for Si and HF:H₂O₂ (1:1) for Ga doped Ge to removed oxide layer. The sample was arranged sandwich structure Si(feed)/Ga doped Ge/Si(seed) and covered by BN tube. It was inserted into the quartz ampoule. The ampoule was evacuated about 10⁻⁴ Pa before sealing. The sealed ampoule was vertically fixed into the furnace. Vertical temperature profile of the furnace was carefully 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 homogenous SiₓGeₓ bulk crystal. Ge was completely melted when temperature reached melting point of Ge. The dissolved Si at seed interface was transported into the solution by solutal convection originated from the density difference between Si (2.33 g/cm³) and Ge (5.323 g/cm³). At the same time the dissolved solutes from the feed interface were transported towards the seed interface mainly by diffusion originating from the concentration gradient. With increasing time, solutal convection became weak in the solution and the Si transported from the feed interface to seed interface by diffusion. As a result, the solution near the seed interface got supersaturated which provides the necessary driving force to start the growth of SiGe bulk crystal. After the experiment, the sample was removed from ampoule and composition distribution was measured by EPMA. The rectangular shaped sample was cut for Seebeck coefficient measurement.

3. Results and discussion

The measured compositional distribution of the grown SiGe bulk crystal revealed that the crystal was grown from seed towards feed in the composition range Si₀.₆₆Ge₀.₃₄. The length of grown sample was about 10.6 mm. The composition fluctuation occurred near the feed interface due to solidification of residual solution as shown in Fig. 1. The grown sample was cut with dimensions (10 X 4 X 3 mm³) for Seebeck coefficient measurement. Seebeck coefficient of the sample was measured as a function of temperature from 300 to 633 K. It revealed that Seebeck coefficient of Ga doped sample was positive which showed P-type material. During increased temperature, Seebeck coefficient increased from 409 to 528 μV/K (Fig.2).

![Fig. 1 Vertical composition distribution of SiGe crystal](image1.png)

![Fig. 2 Seebeck coefficient of Ga doped SiGe](image2.png)

Reference