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Growth of Two Inch $Si_{0.5}Ge_{0.5}$ Bulk Single Crystals

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Abstract

Two inch homogeneous $Si_{0.5}Ge_{0.5}$ bulk single crystals were grown by the traveling liquidus-zone (TLZ) method. Concentration variation was less than 1% for the whole area of a disc sliced perpendicular to the growth axis. Axial compositional homogeneity was also excellent and showed good crystallinity.

1. Introduction

The traveling liquidus-zone (TLZ) method is useful for preparing homogeneous mixed crystals [1-6]. We applied the TLZ method to the growth of homogeneous $Si_{0.5}Ge_{0.5}$ crystals because $Si_{0.5}Ge_{0.5}$ is promising as substrates for high mobility electronic devices [7]. We reported 30 mm diameter crystal growth and its crystalline quality [8]. For the process use further increase in crystal diameter is required because two inch-diameter substrate is the minimum size used in the device process. Here, we report two inch $Si_{0.5}Ge_{0.5}$ crystal growth by the TLZ method. We also report crystal quality measured by an electron probe microanalysis (EPMA), electron backscatter diffraction (EBSD) and X-ray diffraction (XRD).

2. Experiments

$Si_{0.5}Ge_{0.5}$ crystals were grown by the TLZ method [1-6]. A 50 mm diameter cylindrical Si seed with 20 mm in length, a Ge zone forming material with the same diameter and 30 mm in length and a Si feed with the same dimensions to a Si seed were inserted into a boron nitride crucible after removing surface contamination. The crucible was then sealed in vacuum at about 10^{-5} Pa in a quartz ampoule. The ampoule was then heated in a gradient heating furnace. The heating temperature was about 1100^{o}C at the freezing interface and temperature gradient was about 7^{o}C/cm. At 1100^{o}C, Ge is melted and Si remains unmelted and a melt zone is formed. The melted Ge dissolves solid Si on both sides and dissolving continues until Si concentration is saturated in the melt zone. Due to the temperature gradient in the zone, concentration difference is created at two ends of the melt zone. According to the Si-Ge phase diagram [9], Ge concentration is higher at the lower temperature side. Such concentration difference causes spontaneous crystal growth. The detail mechanism is described elsewhere [8]. In the one dimensional TLZ growth model, the growth rate is proved to be proportional to the temperature gradient [2]. Therefore, we can calculate the growth rate if we know the temperature gradient in the zone. Compositionally uniform $Si_{0.5}Ge_{0.5}$ crystals can be grown by keeping the freezing interface temperature constant. For this purpose, the growth interface position should be kept at a fixed position relative to the heater zone. This is easy in the TLZ method because the growth rate can be calculated from the given temperature gradient. When the sample device or heater zone is translated at the calculated rate, the growth interface position can be fixed. In the growth, temperature gradient was about 7^{o}C/cm and growth rate was 0.1 mm/h. Orientation of a Si seed was <100>.

Grown crystals were cut parallel or perpendicular to the growth axis and plate like or disk samples were prepared. After mirror polishing of the surface of thus prepared samples, the composition, crystal quality, and so on were evaluated. EPMA for compositional analysis, EBSD for crystal orientation analysis and XRD for crystal quality evaluation were applied.

3. Results and discussion

An example of the outer view of a grown crystal is shown in Fig. 1. A Si seed, a $Si_{0.5}Ge_{0.5}$ crystal, melt region during crystal growth and a Si feed are indicated in the figure.

Compositional profiles along the center line of the grown crystal is shown in Fig. 2. The profiles were measured for a plate cut parallel to the growth axis. Homogeneous composition was obtained for the distance of about 15 mm following the Si seed. It should be noted that the constant Si or Ge concentration started just next to the Si seed. No gradient concentration region exists. This is because the steady state growth began at the start of the crystal growth and this is one merit of the TLZ method. Average Ge concentration is 0.50 plus or minus 0.01 in the crystal, showing excellent compositional uniformity.

Figure 3 shows results of EBSD analysis for a plate cut parallel to the growth axis. Red color indicates <100> orientation and different color indicates different orientation.

It is noted that <100> orientation extends about 5 mm along the growth axis next to the Si seed. After that polycrystallization occurred.

Figure 4 shows results of EBSD analysis for a half disc cut perpendicular to the growth axis. No polycrystallization occurs for the whole of the disc. Ge concentration was measured on this half disc along a cut edge of the half disc and in a direction perpendicular to the cut edge. In both directions, Ge concentration 0.50 plus or minus 0.01 was measured, showing the excellent compositional uniformity. Excellent uniformity for such large area was realized for the first time. This shows the applicability of the TLZ method to large bulk SiGe crystal growth [4, 5, 8].

The crystal quality was evaluated by measuring an X-ray rocking curve for 004 reflection. The full width at half maximum (FWHM) of the reflection was less than 0.02 degree (72 arcsec) and showed good crystalline nature of a grown $Si_{0.5}Ge_{0.5}$ crystal. Increased convective flow in a melt decreased concentration gradient in the melt and might decrease the growth rate since the concentration gradient is a driving force in the TLZ method. However, convection in a melt may increase the compositional homogeneity of grown crystals due to minimizing concentration variation in a melt and might contribute to the increase in compositional uniformity of TLZ grown crystals and to high crystal quality.

Ge epitaxial layers on the $Si_{0.5}Ge_{0.5}$ substrate was tried. Evaluation of both $Si_{0.5}Ge_{0.5}$ substrates and Ge epitaxial layers were published elsewhere [10].

4. Conclusions

50 mm diameter $Si_{0.5}Ge_{0.5}$ single crystals were grown by the TLZ method. The compositional uniformity and crystal quality were excellent for the whole of the disk cut perpendicular to the growth axis. Results showed applicability of the TLZ method to the growth of large homogeneous SiGe crystals as substrates for strained Ge or Si epitaxial layers.

Acknowledgements

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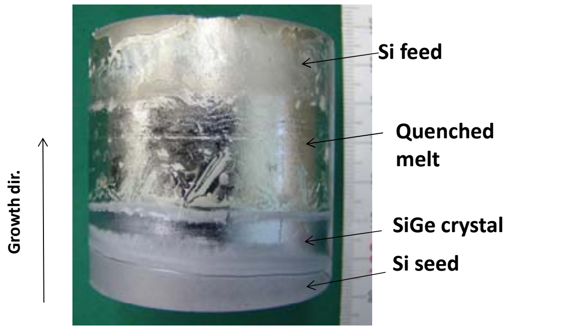

Fig. 1. Outer view of a SiGe crystal.

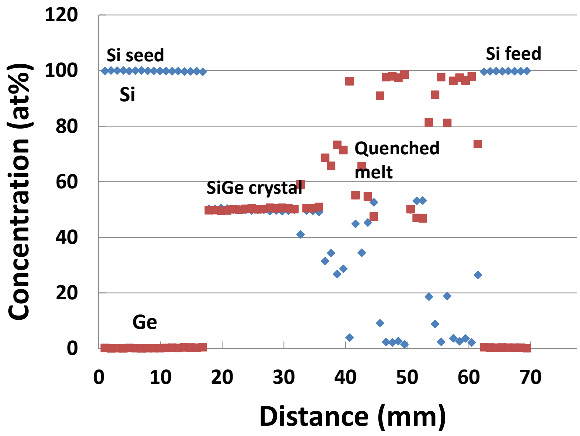

Fig. 2. Axial compositional profiles along a center line.

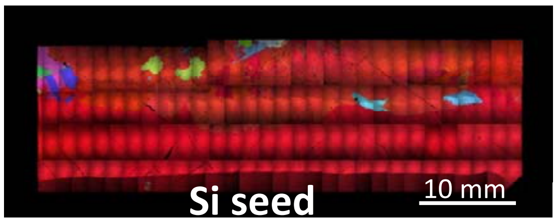

Fig. 3. Crystal orientation next to a Si seed.

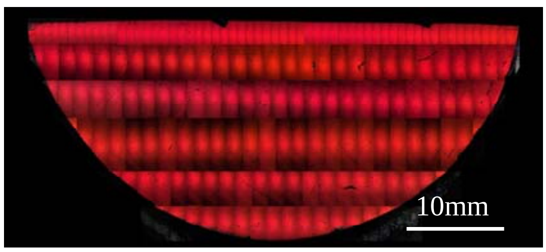

Fig. 4. Crystal orientation for a half disc cut perpendicular to the growth axis.