Extended Abstracts of the 2012 International Conference on Solid State Devices and Materials, Kyoto, 2012, pp1041-1042

Increase of $Si_{0.5}Ge_{0.5}$ Bulk Single Crystal Size as Substrates for Strained Ge Epitaxial Layers

Kyoichi Kinoshita[1], Osamu Nakatsuka[2], Yasutomo Arai[1], Keisuke Taguchi[3], Hiroshi Tomioka[3], Ryota Tanaka[3] and Shinichi Yoda[1]

[1] [1]Institute of Space and Astronautical Science, JAXA
2-1-1, Sengen, Tsukuba, 305-8505, Japan
Phone: +81-50-3362-2760 E-mail: kinoshita.kyoichi@jaxa.jp
[2] Graduate School of Engineering, Nagoya University
Furo-cho, Chikusa-ku, Nagoya, Aichi 464-8603, Japan
[3]Advanced Engineering Services Co. Ltd.
Takezono, Tsukuba, 305-0032, Japan

1. Introduction

$Si_{0.5}Ge_{0.5}$ bulk single crystals are promising as substrates for stressors for both Ge and Si epitaxial layers on them. However, growth of compositionally uniform $Si_{0.5}Ge_{0.5}$ bulk crystals is extremely difficult. This is because liquidus and solidus lines are widely separated in the Si-Ge phase diagram. Segregation at the freezing interface and convective mixing in a melt increases Ge concentration in a melt according as crystal growth proceeds and this leads to the gradual increase of Ge concentration in the direction of growth axis. Therefore, many researchers tried to grow homogeneous bulk $Si_{0.5}Ge_{0.5}$ single crystals but none of them were successful. In order to overcome this difficulty, we invented a new crystal growth method named as a traveling liquidus-zone (abbreviated as TLZ) method [1-3]. We applied the TLZ method to the growth of $Si_{0.5}Ge_{0.5}$ crystals and homogeneous crystals with 2 to 10 mm in diameter were successfully grown [4-6]. For substrate use increase of crystal diameter is required and we tried 30 mm diameter $Si_{0.5}Ge_{0.5}$ crystal growth. Here, we report results of growth experiments of 30 mm diameter bulk crystals.

2. Experiments

$Si_{0.5}Ge_{0.5}$ crystals were grown by the TLZ method [1-8]. A 30 mm diameter cylindrical Si seed with 10 mm in length, a Ge zone forming material with the same diameter and 20 mm in length and a Si feed with same dimensions as the Ge zone forming material were inserted into a boron nitride crucible after removing surface contamination and an oxide layer by etching. 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. When the heating temperature is higher than the melting point of Ge and lower than that of Si, 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. If temperature gradient is applied to the melt zone, concentration difference is created due to the solubility dependence on temperature and Ge gets richer at a lower temperature side. Such concentration difference causes spontaneous crystal growth. The mechanism is as follows; diffusion occurs due to concentration difference, and richer Ge is transported away to a poor side (high temperature side). When Ge is transported away, Si is supersaturated and crystal growth occurs at a lower temperature side. Upon crystallization, Ge is segregated and the segregated Ge is transported away by diffusion and the transported Ge dissolves Si at a higher temperature side and thus crystal growth continues (the melt zone proceeds to the higher temperature side). The growth rate is proved to be proportional to the temperature gradient [3]. Therefore, we can calculate the growth rate if we know the temperature gradient. Compositionally uniform $Si_{0.5}Ge_{0.5}$ crystals can be grown by keeping the freezing interface at a fixed position (keeping the freezing interface temperature constant). This is easy because the growth rate can be calculated from the given temperature gradient. In the growth, temperature gradient was about 7^{o}C/cm and growth rate was 0.1 mm/h. This relation between the temperature gradient and growth rate agreed well with our one-dimensional TLZ growth model equation [3]. 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. Electron probe microanalysis (EPMA) for compositional analysis, electron back scattering patterns (EBSP) for crystal orientation analysis and X-ray diffraction (XRD) for crystal quality evaluation were applied.

3. Results and discussion

An example of the outer view of grown crystals is shown in Fig. 1. The growth length of a SiGe crystal was about 5 mm. In the case of 10 mm diameter crystal growth, the single crystal region length is limited to about 5 mm [5, 6]. Increase of crystal diameter to 30 mm increased convective flow velocity in a melt and made single crystal growth more difficult [5]. However, convection in a melt was suppressed to some extent by small temperature gradients like 7^{o}C/cm and single crystals up to 5 mm in length were grown by the TLZ method. A Si seed, melt region during crystal growth and a Si feed are indicated in the figure.

Figure 2 shows results of EBSP analysis for a disk cut perpendicular to the growth axis. Red color indicates <100> orientation and it is noted that <100> orientation extends whole of the disk, showing single crystal growth.

Figure 3 shows results of compositional analysis. The composition was almost $Si_{0.55}Ge_{0.45}$. This composition does not coincide with $Si_{0.5}Ge_{0.5}$ but compositional uniformity is excellent. The Si concentration 0.55 plus or minus 0.01 is realized for the whole area of the disk. Such excellent compositional uniformity was realized for the first time. This shows the applicability of the TLZ method to SiGe homogeneous crystal growth as well as InGaAs homogeneous crystal growth [1-3, 7, 8]. According to the Si-Ge phase diagram, $Si_{0.5}Ge_{0.5}$ crystal will be grown at 25^{o}C lower freezing temperature and it is very easy to reduce the growth temperature in the TLZ method because Si is almost saturated in the melt zone and merely lowering set temperatures or changing relative position between a sample and heater zones enables us to reduce the freezing temperature.

The crystal quality was evaluated by measuring X-ray rocking curves 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 $Si_{0.55}Ge_{0.45}$ crystal.

Ge epitaxial layers on the $Si_{0.55}Ge_{0.45}$ substrate is now being prepared. Details will be published elsewhere.

4. Conclusions

30 mm diameter $Si_{0.55}Ge_{0.45}$ 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 SiGe crystals as substrates for strained Ge or Si epitaxial layers.

Acknowledgements

This work was supported by the New Energy and Industrial Technology Development Organization (NEDO).

References

[1] K. Kinoshita, H. Kato, M. Iwai, T. Tsuru, Y. Muramatsu and S. Yoda, J. Crystal Growth, **225** (2001) 59.

[2] K. Kinoshita, Y. Hanaue, H. Nakamura, S. Yoda, M. Iwai, T. Tsuru, and Y. Muramatsu, J. Crystal Growth, **237-239** (2002) 1859.

[3] H. Nakamura, Y. Hanaue, H. Kato, K. Kinoshita and S. Yoda, J. Crystal Growth, **258** (2003) 49.

[4] H. Miyata, S. Adachi, Y. Ogata, T. Tsuru, Y. Muramatsu, K. Kinoshita, O. Odawara, and S. Yoda, J. Crystal Growth, **303** (2007) 607.

[5] K. Kinoshita, O. Nakatsuka, S. Yoda and S. Zaima, Thin Solid Films, **520** (2012) 3279.

[6] K. Kinoshita, H. Miyata, R. Tanaka, T. Ueda, Y. Arai and S. Yoda, J. Crystal Growth, **349** (2012) 50.

[7] K. Kinoshita and S. Yoda, J. Crystal Growth, **318** (2011) 1026.

[8] K. Kinoshita and S. Yoda, *Modern aspects of bulk crystal and thin film preparation*, Chapter 8, (InTech, 2012).

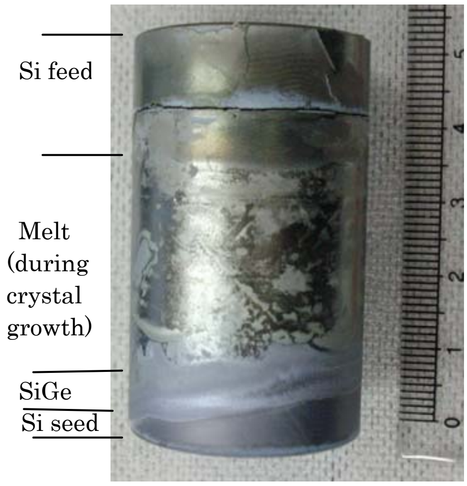

Fig. 1 Outer view of a grown SiGe crystal.

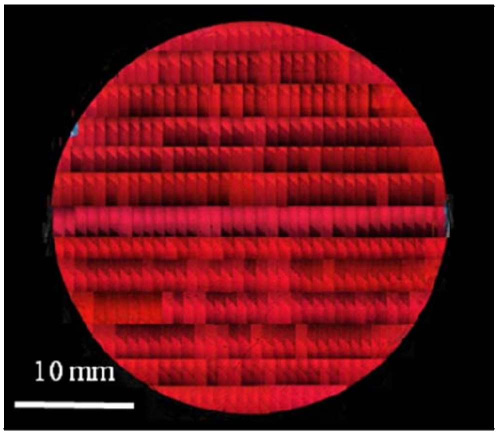

Fig. 2 Crystal orientation of a SiGe disk cut perpendicular to the growth axis.

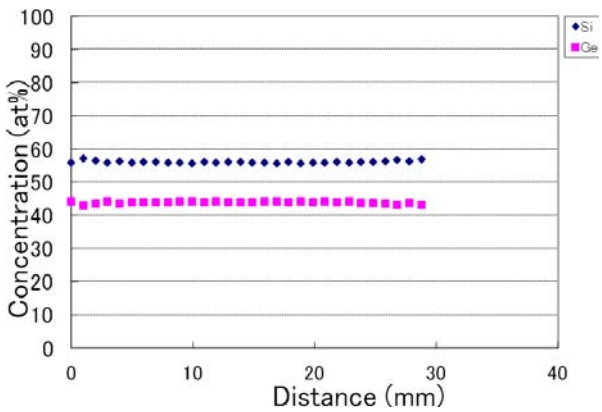

Fig. 3 Radial compositional profiles of a grown crystal. Upper marks show Si concentration and lower ones show Ge concentration.