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Distribution coefficient of boron in Si crystal ingots grown in cusp-magnetic Czochralski process

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Abstract

Silicon single crystals are grown by the Czochralski method with various growing conditions. Effective segregation coefficient of boron is found to depend on the magnetic field in cusp-magnetic Cz method. Effects of zero-Gauss plane (ZGP), ZGP shape and magnetic intensity (MI) on the dopant concentration and its distribution in the crystal are experimentally investigated. The shape of ZGP is not only flat but also parabolic due to the magnetic ratio (MR), which is the ratio of the lower to upper electric-current densities in the configurations of the cusp-magnetic field. Equilibrium distribution coefficient of boron calculated by BPS model is 0.698. With the crystal rotation (w) of 16 rpm and the crucible rotation of -0.5 rpm, the effective distribution coefficient (k_e) is 0.728 in zero magnetic intensity and increases up to 0.8093 in the parabolic ZGP shape. Although the magnetic strength near the crystal–melt interface decreases with increasing MR, it increases in the bulk melt, and hence k_e increases. Flow stability in the bulk melt influences k_e. At the magnetic field and growing conditions, k_e increases with increasing initial charge size of the silicon melt. There is no significant influence of ZGP on the radial distribution of the boron concentration. Simulation results of melt flow in the presence of a parabolic ZGP are outlined, and the segregation results in the experiments are compared with published experimental data.

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1. Introduction

The importance of silicon in the electronic device technology relies on semiconducting properties, which can be controlled by small addition of impurity elements and dopants, such as group III element (e.g., boron) for acceptor and group V elements (e.g., phosphorus) for donor. The degree of dopant segregation during Czochralski (Cz) growth is specified by an effective distribution coefficient. Dopant concentration and its distribution in the crystal are important for predicting device performance. Therefore, there have been a large number of experiments of dopant segregation process in the silicon melt during the Cz crystal growth. A key parameter in obtaining a specified resistivity is the equilibrium distribution coefficient k_0 and, in particular, the effective distribution coefficient k_e. In 1953, Burton, Prim and Slichter (BPS) [1] presented the most extensively used model for steady-state longitudinal segregation during solidification of dilute binary systems. According to the BPS theory, they developed a model for segregation in steady convection flows, which is based on boundary layer in the melt. Most of the studies have focused on the melt convection to investigate dopant segregation during crystal growth. Park et al. [2] reported variations in binding energies and diffusivities of dopant-defect pair under hydrostatic pressure and a pressure-dependent dopant diffusion equation.

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Wang [3] has performed numerical calculation based on the transient two-dimensional mathematical model including rigorous melt convection in horizontal Bridgman silicon growth. The experiment showed that the uniform axial specific resistivity profile is possible using the B–P (boron, phosphorus) co-doping method in the melt-growth process of silicon single crystals.

The effects of growing parameters on dopant concentrations in the crystals are experimentally investigated by Sim et al. [4]. With the very low crystal rotation (w) $\leqslant 3$ rpm, k_e is almost unity. Kodera [5] reported that segregation coefficient of impurities depends on the growth rates and rotation rates.

Effect of magnetic field on k_e was investigated by Hirata and Inoue [6] and Thomas et al. [7] for low k_e dopants. They found that the magnetic field stabilized the melt convection and k_e increased with increasing magnetic strength. These facts were verified in theoretical studies with a simplified model by Hurle and Series [8]. Various types of magnetic field were discussed by Series and Hurle [9].

k_e of the dopant has been found to be nearly equal to the equilibrium value (k_0) when the melt is almost completely stirred by strong thermal convection [10]. On the other hand, if there is no convection in the melt and transport is only accomplished by diffusion, the dopant concentration is theoretically suggested to be constant and equal to the initial concentration in the melt (i.e., $k_e = 1$), except for the initial and terminal transients [11] during crystal growth. Witt et al. [12] used magnetic fields to sufficiently suppress convective mixing in the melt in order to achieve diffusion-controlled segregation. To obtain such levels of quiescence, very large magnetic strengths are generally required. They reported the dramatic increase of the dopant concentration in the axial direction and non-uniform radial distribution in the crystals without gravity, compared with results on earth [13].

Segregation effects were strongly influenced by thermal convection. In a commercial system, melt charge size should increase for large crystal size and mass products. Melt convection in a large amount of the silicon melt is complex and strong because the larger melt makes the natural convection much stronger [14]. To continue the progress in the understanding and ultimate control of these effects, robust experimental conditions, which are established reproducible thermal geometries and controlled thermal symmetry, were required [15]. Thus, in a large amount of the melt, it is difficult to control convection and hence dopant distribution.

In all previous studies [6–9], the effect of the magnetic field on melt flow and dopant distribution has been investigated experimentally and numerically, and the cusp-magnetic field applied to the silicon melt was symmetric to zero-Gauss plane (ZGP), where ZGP is flat (MR = 1 in Fig. 1) due to the same electric-current densities of the upper and lower coils in the configuration of the cusp-magnetic field. Magnetic ratio (MR) is the ratio of the lower to upper current densities in the configurations of the cusp-magnetic field.

In the present study, 200 mm diameter single crystals with various growing conditions are grown in the cusp-magnetic Cz method. The effects of ZGP shape and magnetic intensity (MI) on the melt flow and resistivity profiles are experimentally investigated, and the results are numerically analyzed. The purpose of this research is to study the effect of cusp-magnetic fields on the dopant concentration and its distribution in the boron-doped Cz crystal. In the experiments, ZGP is not flat, and it has various shapes of ZGP (MR > 1 in Fig. 1) due to the ratio of the upper to lower electric-current densities. It is known that the magnetic field gradient in the silicon melt influences the melt flow, and the changed melt flow results in different effective segregation coefficient.

It is found that k_e of the dopant increases as the center of ZGP in the cusp-magnetic field is closer to the melt-free surface from the melt inside, and there is no significant influence of ZGP on the radial distribution of the dopant concentration. The discussion about the new finding is included in the present paper. The experimental results are compared with other experimental and theoretical results.

2. Experiments

Commercial furnace with the cusp-magnetic apparatus is used to grow 200 mm diameter Si single crystals doped with boron. The schematic system is shown in Fig. 1.

The crucible has an inner diameter of 600 mm and is made of quartz. The initial charge size of the silicon melt is in the range of 120–150 kg. Crystal and crucible rotation rates are fixed as 16 and -0.5 rpm, respectively, in the system. Argon flow rate and furnace pressure are constant. The pulling rate of the crystal is changed to keep the crystal diameter constant. The pulling speeds are varied in the range 0.65 ± 0.05 mm/min. k_e did not change with crystal growth [16,17].

The cusp-magnetic field is applied in the melt. There are two coils in the cusp-magnetic configuration, upper and lower coils. MR is defined as the ratio of the lower to upper electric-current densities in the coils, and ZGP is the plane of the magnetic field with zero-vertical magnetic strength in cusp-magnetic field. ZGP with MR = 1 is flat and is located at the mid-position between the upper and lower coils in the cusp-magnetic configuration as shown in Fig. 1. With MR = 1, the cusp-magnetic field is symmetric to ZGP, which means that the upper magnetic distribution is the same as the lower magnetic distribution. The flat ZGP can change into parabolic shapes with MR > 1 in Fig. 1. Magnetic position (MP) is defined as the distance from heater top to mid-position between the upper and lower coils in the cusp-magnetic configuration as shown in Fig. 1. ZGP with MR = 1 is the same as MP. ZGP depends on MR and MP. MI indicates the magnetic field component orthogonal to crucible wall at 260 mm below the heater top, which is the corner position of the crucible as shown in