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Control of axial segregation by the modification of crucible geometry

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Abstract We will focus on the horizontal Bridgman growth system to analyze the transport phenomena numerically, because the simple furnace system and the confined growth environment allow for the precise understanding of the transport phenomena in solidification process. In conventional melt growth process, the dopant concentration tends to vary significantly along the crystal. In this work, we propose the modification of crucible geometry for improving the productivity of silicon single-crystal growth by controlling axial specific resistivity distribution. Numerical analysis has been performed to study the transport phenomena of dopant impurities in conventional and proposed Bridgman silicon growth using the finite element method and implicit Euler time integration. It has been demonstrated using mathematical models and by numerical analysis that proposed method is useful for obtaining crystals with superior uniformity along the growth direction at a lower cost than can be obtained by the conventional melt growth process.

Key words Segregation, Bridgman, Silicon, Dopant, Simulation

1. Introduction

At present, silicon is one of the most studied elements in the periodic table, and silicon technology is by far the most advanced among all semiconductor technologies. Growth methods used for the production of semiconductor materials are classified into melt growth, vapor growth, solution growth and solid growth. The melt growth method is generally used for the production of substrate material. Examples of melt growth methods are the Bridgman, the floating zone and the Czochralski method. In melt growth, a known amount of dopant is added to melt to obtain the desired doping concentration in the grown crystal. These dopant impurities play a key role in semiconductor device operation. For silicon, boron and phosphorus are the most common dopants for p- and n-type materials, respectively [1].

Because a crystal is grown from the melt, the doping concentration incorporated into the crystal is usually different from the doping concentration of the melt at the interface. The ratio of these two concentrations is defined as the equilibrium segregation coefficient. Most values for the commonly used dopants for silicon are below 1, which denotes that during growth the dopants are rejected into the melt. Consequently, the melt becomes progressively enriched with the dopant as the crystal grows.

Fig. 1 shows typical resistivity distribution in the growth direction. In actual products, the resistivity (ρ) standard $\rho_{max}/\rho_{min} < 1.3$ is frequently applied. A portion of silicon crystals grown using the conventional melt growth method is available. It is very important to make a large part of crystals useful for products in terms of resistivity specification. Numerous studies have been reported on the control of axial specific resistivity distributions in bulk crystal growth [2-10]. In general, the various method proposed to avoid axial segregation can be classified into two groups. In the first class, the key idea is to ensure that the composition of the liquid in the vicinity of the interface remains constant all through solidification; this can be done using, e.g. the floating crucible [3] or the continuous liquid feeding technique

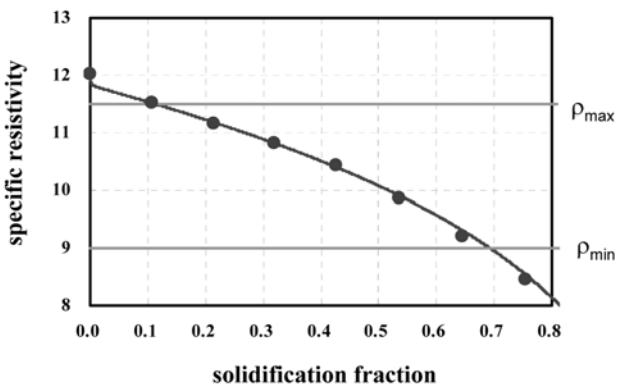

Fig. 1. Axial resistivity distribution as a function of solidified fraction. Experimental data and simulation results are indicated by the filled circles and solid line, respectively.

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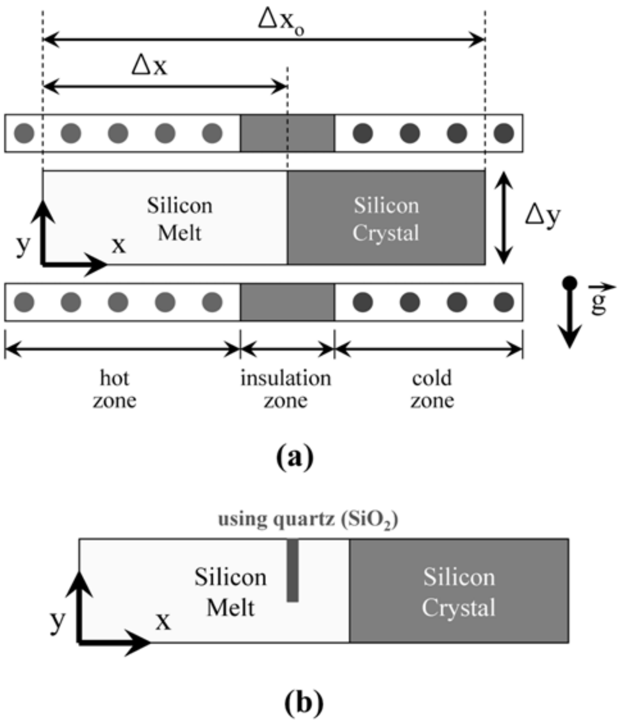

Fig. 2. Schematic diagram of prototypical horizontal Bridgman crystal growth system (a) conventional and (b) proposed configuration.

[4-7]. A second approach consists in adapting the growth conditions to balance the variations in bulk concentration. The most accessible parameter in this respect is the interface velocity; another possibility is to act on convection by means of a magnetic field to change the boundary layer thickness during solidification [8].

In this work, we present the simple modification of crucible geometry for controlling the axial specific resistivity distribution in silicon single crystals. The schematic diagrams of the crucible partition are shown in Fig. 2. The geometric parameters which will affect the melt conditions are the location and size of the blockage. Although not investigated here, the thickness of the partition unless it is very large, is expected to have a small effect. It has been demonstrated by numerical analysis that the axial segregation can be controlled in horizontal Bridgman silicon growth and relatively uniform its profile is feasible by the proposed method.

2. Mathematical Modelling

The Bridgman growth system has been studied intensively, either by theoretical analyses or by experiments, because the simple furnace system and the confined growth environment allows for the precise control of thermal field necessary for solidification. A variant of the vertical Bridgman growth system with horizontal configuration is called the horizontal Bridgman technique. The temperature control is easier using a multi-zone heater in the furnace. We will focus on this simple system to analyze the segregation phenomena in the crystal. The schematic diagrams of growth configuration and the coordinate system used in the numerical computations are shown in Fig. 2.

The model equations for predicting the segregation phenomena are developed. The transient two-dimensional convection-diffusion model for the transport of dopants is constructed as

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D\left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right] \quad (1)$$

where C is the concentrations of dopants. A flat interface is employed to simplify the model. The definition of symbols and growth parameters are summarized in Table 1.

The length of the silicon melt, Δx, can be obtained by the macroscopic mass balance of the Bridgman system

$$\Delta x = \Delta x_o - V_g t \quad (2)$$

Where Δx_o is the initial length of the silicon melt.

The solution of transient second-order partial differential equations requires the initial condition and boundary conditions. The initial condition is $C = Co$. The boundary conditions along the melt/crystal interface is

$$\frac{\partial C}{\partial x} = \frac{V_g}{D}(1 - k)C \quad (3)$$

to account for the injection or incorporation of dopant at the melt/crystal interface.

Although the convective flow in the silicon melt is a combined result of natural convection, Marangoni convection and movement of crucible, the melt flow in the crucible is assumed to be described using the following stream function

Table 1
System and growth parameters

Symbol	Definition/Meaning	Value
Δx	Length of silicon melt	< 5.0 cm
Δy	Height of silicon melt	2.0 cm
D	Diffusion coefficient of dopant in silicon melt	3.0×10^{-4} cm^2/sec
k	Equilibrium distribution coefficient of dopant	0.75
V_g	Crystal growth rate	0.50 mm/min

$$\psi = \psi_o x(\Delta x - x)y(\Delta y - y) \quad (4)$$

where ψ_o is the intensity parameter representing the flow intensity. The flow pattern is easily understood in terms of contours of the stream function. In the two-dimensional rectangular coordinate system, the velocity components are expressed in terms of the Stoke stream function.

3. Numerical Analysis

The Galerkin finite element method is used for the discretization of the complete set of the mathematical model. The concentration fields are represented in expansions of Lagrangian biquadratic basis functions. A mesh is formed of quadrilateral elements which span the computational domains corresponding to the silicon melt phase. The field equations are put into the weak form and boundary conditions are imposed in the normal manner [2, 9].

Numerical nine-point Gaussian quadrature for volume integrals and three-point Gaussian quadrature for surface integrals are used for calculating the residual equations and Jacobian matrix. A frontal solution algorithm is employed to solve the entire set of linear equations and minimize the core memory [10].

For the time-dependent calculations, the implicit Euler method is used. The Bridgman silicon growth process is batch-type and the length of the silicon melt is altered throughout the process. In evaluating the time derivative, we use the procedure developed by Lynch and Gray to consider the mesh deformation due to the change in computational domain [11].

4. Results and Discussion

Boron-doped silicon single crystal was grown in melt-growth configuration. The specific resistivity of the grown crystal is indicated by filled circles in Fig. 1. The x-axis indicates the solidified fraction and the y-axis shows the resistivity on the center axis measured by the probe method after a donor-killing heat treatment. The line shows the predicted resistivity curve for a silicon crystal grown by the conventional Bridgman method. As shown in Fig. 1, the concentration of boron in the crystal increases gradually as the solidification fraction is increased with the growth of silicon crystal. The results of the numerical analysis approach the experimental data. The result

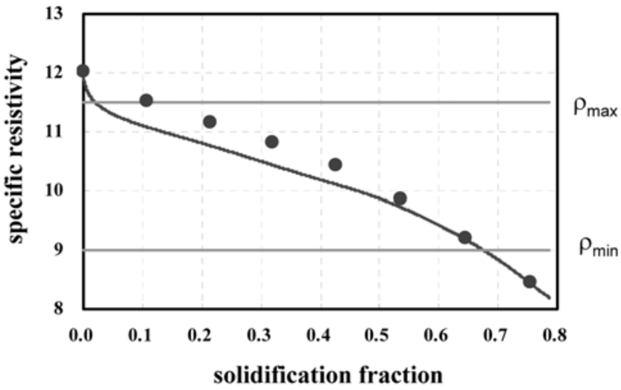

Fig. 3. Axial resistivity distribution as a function of solidified fraction. Experimental data and simulation results for the modification of crucible geometry are indicated by the filled circles and solid line, respectively.

with ψ_o of 1.44×10^{-7} describes the experimental axial dopant concentration profile successfully.

The mean concentration in the crystal phase along the melt/crystal interface, $\langle C_s \rangle$ is defined as

$$\langle C_s \rangle \equiv \int_0^{\Delta y} kC dy / \int_0^{\Delta y} dy \quad (5)$$

The specific resistivity is calculated using the mean concentration.

In the present study, an attempt was made to control dopant segregation in Bridgman growth, using the modification of crucible geometry, i.e. crucible partition, as shown schematically in Fig. 2(b). The relative position between melt/crystal interface and quartz is kept constant to control the axial distribution of dopant concentration. As shown in Fig. 3, the resistivity distribution is controlled by the modification of crucible geometry and almost 8% of grown silicon single crystal comes useful for products in the specification of specific resistivity by the proposed method. The production yield is calculated using reference resistivity specification shown in Fig. 1 and Fig. 3.

5. Conclusions

In this work, we performed numerical calculations based on the transient two-dimensional convection-diffusion model in Bridgman silicon growth which has been developed to describe the dopant distribution in the conventional and the modification of crucible geometry. It is demonstrated by numerical simulation that the axial segregation phenomena can be controlled in horizontal Bridgman method and relatively uniform its profile is feasible by the proposed modification method.

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