A Numerical study on the fluctuation behavior of the oxygen concentration and the temperature in the silicon melt of Czochralski crystal growth system

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Abstract

The momentum, heat and mass transfer phenomena in the silicon melt of the Czochralski crystal growth system are calculated using a three dimensional numerical simulation technique. Even though axisymmetrical boundary conditions are imposed to all calculations in a 3cm diameter crucible, several types of non-axisymmetric profiles of velocities, temperature and oxygen concentration appeared in the melt.

Because of the non-axisymmetric profiles and rotations of fluid induced by the crucible rotation, temperatures and oxygen concentrations in the silicon melt fluctuate. The rotating velocity of the profile is calculated from the phase shift of the data of temperature or oxygen at two different points which have same radius from center but 90 degree angular difference. From this calculation, it is found that the rotating velocity of the oxygen and temperature is different from the crucible rotation rates. Therefore the frequencies of the oscillating temperature and oxygen concentrations are not same to the frequencies of the crucible rotations.

Futhermore, the components of the frequencies of the temperature and oxygen concentration at the same point are not same. The fluctuation behaviors of the temperature or oxygen themselves are also different when the points are different. The calculation show that the temperature and the oxygen concentration near the interface also fluctuate.

The results suggest that the striation pattern found in the grown silicon single crystals may be generated by the oxygen concentration and the temperature oscillations of the melt occurred near the interface.

1. Introduction

In nearly all silicon single crystal ingots, oxygen and dopant concentrations shows microscopic inhomogeneity. This inhomogeneity usually consists of fluctuations of the oxygen and dopant concentration. This is visible as striation patterns of the properly etched and photographed longitudinal or cross sections of the crystals. Because this inhomogeneity cause fluctuations in the electrical resistivity and other properties of the single crystal[1], to grow more homogeneous crystals is one of the important task for the single crystal growers.

The temperature fluctuations in the melt is believed the main cause of the dopant fluctuations. Of course the behavior of the temperature does not directly affect on the behavior of the dopant or oxygen. However, the fluctuation of the temperature can cause the instaneous change of the growth rate at the crystal melt interface. The change of the growth rate affect the segregated dopant concentration. When the distribution coefficient of a dopant is not unity, the dopant concentration in the solid at the interface can be written as below from BPS theory[2],

$$C_S = C_L \cdot k_{eff} = \frac{C_L \cdot k_0}{k_0 + (1-k_0) \cdot \exp(-R \cdot \delta / D)} \tag{1}$$

In which, R, δ, D, C_L, C_S, k_{eff} and k_0 are growth rate, boundary layer thickness, diffusivity in the melt, concentration in the liquid bulk, concentration in the solid at the interface, effective distribution coefficient and distribution coefficient respectively. Equation (1) clearly shows that the change of the growth rate affects the concentration in solid. One can expect similar effect of the growth rate on the solid concentration in the real crystal growing system even though whose conditons near the crystal melt interface should be different from that of the BPS theory.

Many experiments showed that there exist temperature fluctuations in the melt of the Czocharlski system[3] and there exist strong correlations between temperature fluctuations and the segregated dopant profiles in the grown crystals[4].

However, we also consider other possible causes to make the solid concentration fluctate. One of them is the fluctuation of the dopant concentration in the melt. If temperature fluctuations are caused from the instabilities of the melt flow, dopant concentrations also fluctuate because mass is also transfered by the convection of the melt. This idea is the starting point of the present study.

In this study, oxygen concentration is calculated using three dimensional simulation technique. To solve the mass transfer problem, momentum and heat transfer are simulataneously calculated. Because the main topic is to observe the time varing behavior, transient calculation is necessary. The components of the fluctuations and the correlations between temperature and oxygen concentrations are analyzed using discrete data processing technique.

2. Techniques of numerical simulations

Finite volume method is adopted to discretize the transport equations. Because k-ε 2 equations model is used for turbulent behavior, total seven governing equations(u, v, w, k, ε, T, C_O) and one continuity equation are solved simulataneously. For transient calculation, fully implicit scheme is used. The radius and height of the melt is 3 cm. The interface between crystal and melt is assumed flat.

The boundary conditions are as belows:

(1) Bottom and sidewall
  u, v, w, k, ε : turbulent wall function
  T : constant
  C_O : equilibrium to the SiO_2 at the temperature
(2) Centerline
  all variables : symmetry
(3) Free surface
  w, k, ε : symmetry
  u, v : surface driven flow
  T : radiation heat loss
  C_O : evaporation to atmosphere
(4) Solid/Liquid interface
  u, v, w, k, ε : turbulent wall function
  T : melting temperature
  C_O : mass flux ($J=v(1-k)C_LA$)

Total grid numbers are 50×40×40. One hour is necessary for calculating 2 seconds time proceeding when time step is 0.1 second on the alpha XL366 machine.

3. Results of the calculations and discussions

Transport phenomena under low rotation rates (1 and 3 rpm) are calculated with different crucible temperatures(1465℃, 1470℃ and 1475℃). At these conditions, all results show asymmetric profiles of velocity, temperature and oxygen concentration. When crucible rotation rate is 1 rpm, the rotating center of the melt shifts from the center axis of crucible with 1465℃ wall temperature. At the same rotation rate, the velocity profile of 1475℃ wall temperature shows completely disordered structure.

Because of the asymmetric velocity profiles, the temperature and the oxygen distributions in the melt becomes non-axisymmetric. Figures 1 and 2 shows the iso-thermal and iso-concnetration lines on a plane with 1rpm and 1465℃. The oxygen distribution is more complex. Because the diffusivity of oxygen is much less than the thermal diffusivity, the effect of the velocity fluctuation on the oxygen concentration is stronger than on the temperature. Temperature and concentration change at some selected points are shown in figs. 3 and 4. Points A, C, D, E and F locate on the same meridional plane with different radius. Point B locates on a plane which have 90° behind to the previous plane. Points E and F locate just below the solid/liquid interface. Temperature and oxgen show different behavior. From the Fourier analysis results of both data of point A (fig.5 and 6), more peaks exist at high frequency range in the oxygen data.

The oxygen concentration data near the interface fluctuate as shown by the lines E and F of fig. 4. Because these points locate about 0.5 mm below the interface, the fluctuation of these position can change the segregation concentration of the solid. Even though more microscopic study is necessary to confirm this fluctuation of oxygen affects on the solid concentration, these results suggest that the striation can be caused by the oxygen concentration in the melt.

4. Conclusions

Oxygen concentration in the silicon melt of Czochralski crystal growth system fluctuates with frequencies different from those of the temperature. Because the temperature and the oxygen concentration fluctuate near the interface, both can be the origin of the striation in the grown single crystal.

5. References

[1] G. Müller, Crsytal Growth from the melt, Springer-Verlag, Berlin (1988).
[2] J. A. Burton et al., J. Chem. Phys. 21, 1987 (1953).
[3] K. Kakimoto et al., J. Crystal Growth 126, 435 (1993).
[4] A. Murgai et al., J. Electrochem. Soc. 126, 2240 (1979).

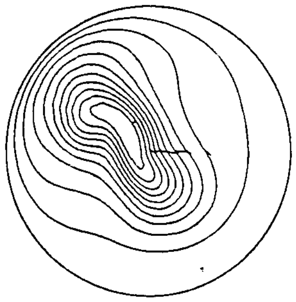

Fig. 1 Temperature profile

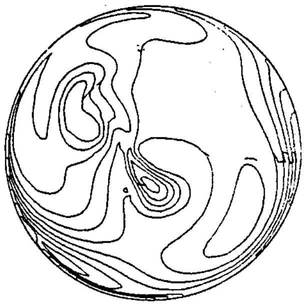

Fig. 2 Oxygen profile

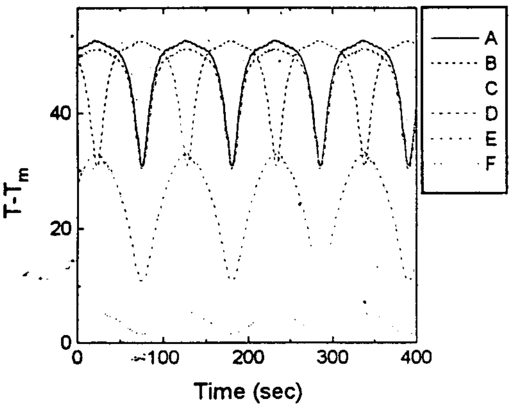

Fig. 3 Temperature fluctuations

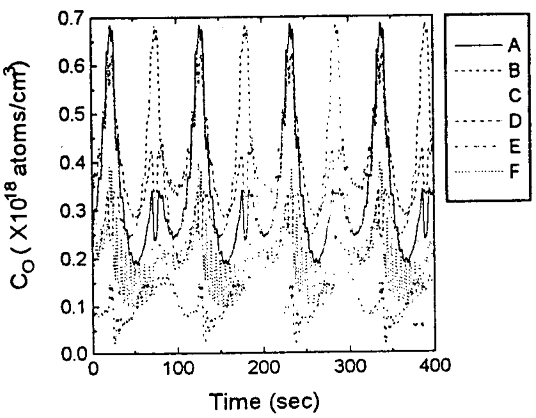

Fig. 4 Oxygen concentration fluctuations

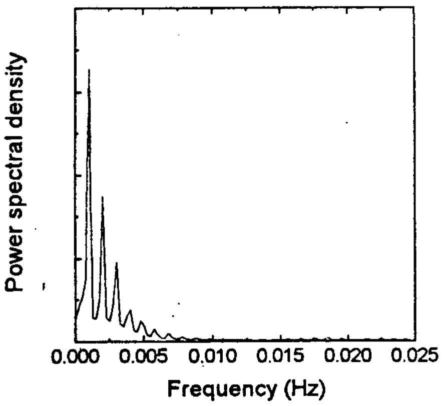

Fig. 5 PSD of temperature at A

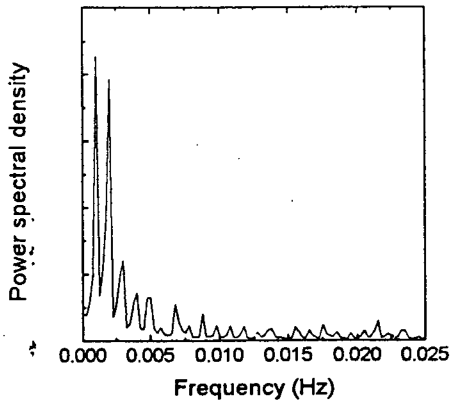

Fig. 6 PSD of oxygen concentration at A