Two dimensional analysis of axial segregation by convection-diffusion model in batchwise and continuous Czochralski process

Jong Hoe Wang and Do Hyun Kim

Dept. of Chem. Eng., KAIST, Taejon, 305-701, KOREA

It is shown theoretically that uniform axial dopant concentration distribution can be made throughout the crystal by continuous Czochralski process. Numerical simulation are performed for the transient two-dimensional convection-diffusion model. A typical value of the growth and system parameters for Czochralski growth of p-type, 4 inches silicon single crystal was used in the numerical calculations. Using this model with proper model parameter, the axial segregation in batchwise Czochralski growth can be described. It is studied by comparing with the experimental data. With this model parameter, the uniform axial concentration distribution of dopant is predicted in continuous Czochralski process.

1. Introduction

Most crystals required for commercial application need to be doped with a deliberately added solute in order to acquire the needed properties. Since Czochralski process is essentially a batch process, segregation of solute at the interface results in a progressive increase in solute concentration in the crystal having a segregation coefficient less than unity. The reverse is true for solutes with the segregation coefficient greater than unity. The device specification will require that the doping level is precisely controlled and that it be uniform throughout the crystal [1]. Much attention has been paid to the radial and the axial dopant distribution and their control in bulk crystal growth [2].

In this work, two dimensional analysis on the segregation in the batchwise Czochralski process was done using the convection-diffusion model. It was shown theoretically that the uniform axial dopant distribution can be obtained with the continuous Czochralski process, such as liquid-feeding Czochralski method.

2. Modelling

Transient two dimensional convection-diffusion model is presented to simulated the segregation phenomena in batchwise Czochralski and to show its control in continuous process. The schematic diagram of the convection-diffusion model for batchwise and continuous Czochralski process is shown in Fig. 1. As shown schematically in Fig. 1, constant crystal radius and flat interfaces are employed to simplify the model. Although Xiao and Derby [3] found the difference of results from bulk-flow model and hydrodynamic thermal capillary model which includes realistic interfacial geometries, an overview of the dopant segregation phenomena in silicon melt considering the free-boundaries was not studied because the very big efforts have to be made to predict the heat, momentum and dopant transport in the melt accurately [4]. As already mentioned, the purpose of this work is to show theoretically the control of axial segregation using continuous Czochralski process.

The dimensionless field equation to describe the concentration distribution of dopant in silicon melt is

$$\frac{\partial c}{\partial \tau}+u\frac{\partial c}{\partial r}+v\frac{\partial c}{\partial z}=\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right)+\frac{\partial^2 c}{\partial z^2},$$

where c is the dimensionless concentration of boron. The definition of dimensionless variables and groups, the meaning of the symbol and the values are summarized in Table 1. The prime represents the dimensional quantity.

The dimensionless melt height, h can be obtained by the macroscopic mass balance of the batchwise Czochralski system. In the continuous Czochralski process, h is assumed to be constant. This is demonstrated by the experiment of Shiraishi *et al* [2].

The solutions of the transient second-order partial differential equation require the initial condition and boundary conditions.

The initial condition is

$$c=0,$$

The boundary condition along the interface is

$$\frac{\partial c}{\partial z}=\mathrm{Pe}(1-k)(1+c),$$

In case of the continuous Czochralski process, another boundary condition is used to consider the addition of the raw material for controlling the concentration of dopant

$$\frac{\partial c}{\partial z}=-f\delta(r_o,h),$$

where f is the dimensionless dilution rate and r_o is the radial position where the raw material is supplied.

Although the flow within the system is a result of the interactions between the effects generated by natural convection, crucible rotation, crystal rotation, surface tension (Marangoni flow) and vertical movements of the crystal and crucible, the flow in the melt is regarded as following stream function.

$$\psi=\psi_o r^2(1-r)\frac{z}{h}\left(1-\frac{z}{h}\right),$$

where ψ_o is the characteristic variable to represent the flow intensity.

3. Numerical Method

The Galerkin finite element method [3, 5-6] was employed for the solutions of the field equation for the convection-diffusion model. The concentration field is represented in expansions of Lagrangian biquadratic basis functions. The field equation is put into the weak form and boundary conditions are imposed in the normal manner. For the time-dependent calculations, implicit Euler method was used. In the convection-diffusion model for the batchwise Czochralski process, the depth of melt is changed from start to end. In evaluating the time derivative, $\partial c/\partial \tau$, we use the procedure developed by Lynch and Gray [7] to consider the mesh deformation due to the change of the melt depth. Nine- and three-point Gaussian quadrature was applied for the volume and the surface integrals, respectively. The finite element meshes for the computational region in both batchwise and continuous Czochralski process are same with a total of 96 radial elements and 64 axial elements. These meshes contain 24,897 total unknowns. A frontal solution algorithm was employed to solve the entire set of linear equations and minimize the core memory [8].

4. Results and discussions

Transient dopant distribution in the melt phase was obtained by applying the numerical methods to the mathematical model. The axial dopant concentration distribution in batchwise Czochralski process was studied and compared with the experimental data [9]. The growth and system parameters used in the numerical simulation and the experiment are summarized in Table 1. This is a typical value for the growth of p-type, 4 inches silicon single crystal using Czochralski process. The axial dopant distribution concentràtion was studied in continuous Czochralski process.

The numerical analysis of this segregation phenomena at the melt/crystal interface was performed to simulate the axial dopant distribution in batchwise Czochralski process. The results of the experiment and the numerical analysis for the various flow intensity are shown together in Fig. 2. The dimensionless mean concentration along the melt/crystal interface, <c> is defined as

$$\langle c \rangle = \frac{\int_0^{2\pi}\int_0^{R_d} c\, r\, dr\, d\theta}{\int_0^{2\pi}\int_0^{R_d} r\, dr\, d\theta},$$

With the increase of flow intensity, the results of the numerical analysis more correspond with the experimental data. The results above the characteristic value for flow intensity of 10^6 show similar behavior in axial dopant concentration profile. The axial segregation in Czochralski process can be described using the convection-diffusion model with proper model parameter and it was used to show theoretically the control of the axial dopant concentration profile using continuous Czochralski process.

The concentration field in the melt phase during the continuous Czochralski process can be maintained uniformly by continuous Czochralski process. The progressive increase in solute concentration during batchwise Czochralski process was shown in Fig. 2. The axial dopant concentration distribution in continuous Czochralski process is studied in Fig. 3. The uniform axial concentration of dopant can be obtained by the continuous Czochralski process with a proper dilution rate.

It can be concluded that the uniform axial dopant concentration profile can be obtained by continuous Czochralski process with the maintenance of flow structure in batchwise Czochralski process.

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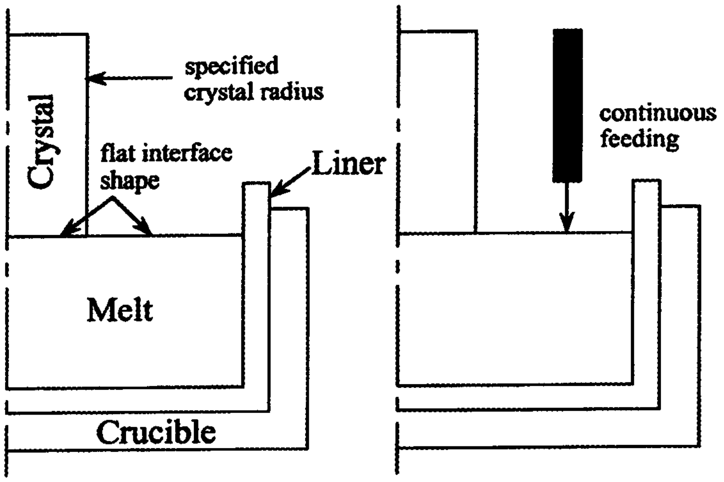
Table 1. The definition of dimensionless variables and groups, the meaning of the symbols and the values used in this study and experiment.

symbol	definition / meaning	value
R_c'	inner radius of crucible	17.78 cm
R_s'	radius of growing crystal	5.30 cm
c	$(c'-c_o')/c_o'$	
u	$R_c'u'/D$	
τ	$Dt'/R_c'^2$	
Pe	$R_c'V_g'/D$	90.55
R_d	R_s/R_c	0.2981
M_o'	mass of start material	25 kg
V_g'	growth rate	5.5 cm/hr
f	dilution rate	- g/cm^2 · sec



(a) (b)

Fig. 1. Schematic diagram of convection-diffusion model for (a) batchwise and (b) continuous Czochralski crystal growth. Computational domain is melt region.

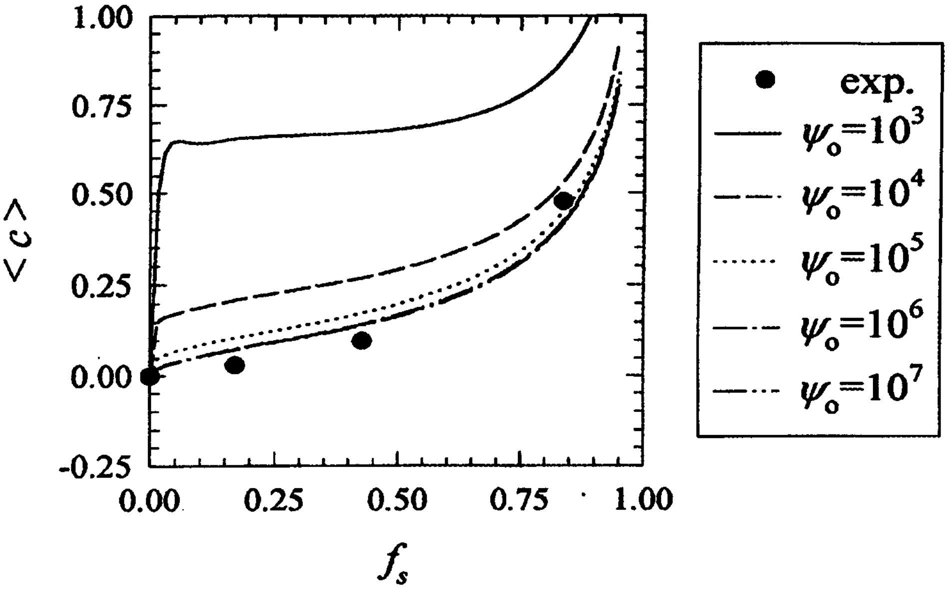


Fig. 2. The axial dopant concentration profile as a function of fraction solidified in batchwise Czochralski process. The fraction solidification is defined as $f_s \equiv 1-V_m/V_{mo}$, where V_m is melt volume and V_{mo} is initial melt volume. The experiment data (•) and the simulation results for the various flow intensity is shown together.

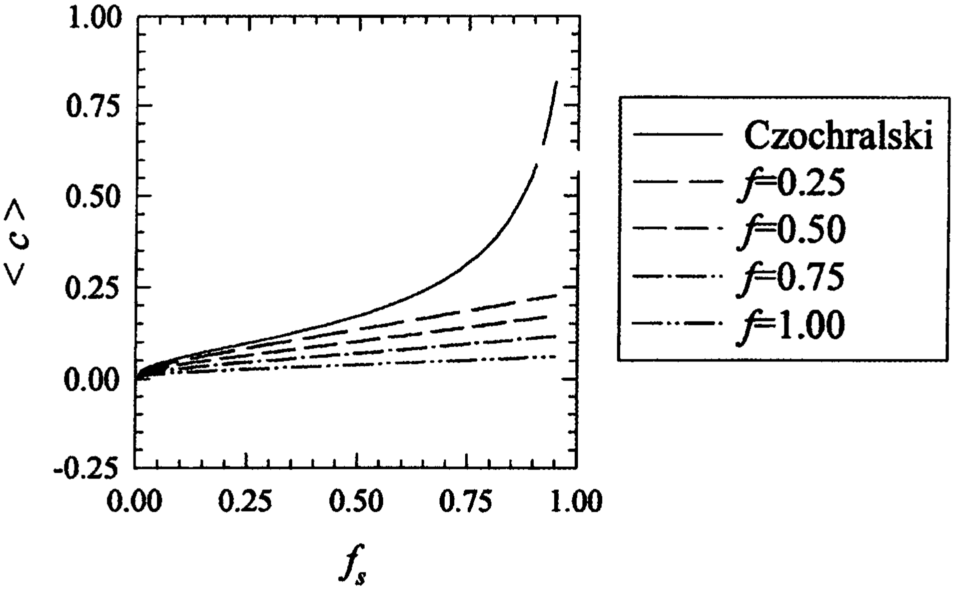


Fig. 3. The axial dopant concentration profile as a function of fraction solidified for various dilution rate in continuous Czochralski process ($\psi_o=10^6$).