Numerical Simulations on the Transport Phenomena of the Silicon Melt in Various Size of Crucibles

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Abstract

The momentum, heat and mass transport in the melt of several sizes of crucibles are calculated using a three dimensional numerical simulation technique with and without the k-ε turbulent model. When turbulent model is not used, non-axisymmetric profiles of velocity, temperature and oxygen concentration appear in the melt of all sizes of crucibles. Axisymmetric profiles are obtained when the k-ε model is adopted.

Introduction

One of the main topics of the current Czochralski crystal growth process is the melt flow in the crucible. It has been suggested that the melt flow destroys axisymmetric profiles of temperature and oxygen concentrations and cause fluctuations of these quantities in the melt. Microdepects in the grown crystals are believed to be introduced by those fluctuations of the melt[1].

Measurement of temperature profiles[2] and oxygen concentration[3] show several types of fluctuations occur in the melt. The direct silicon melt observation using X-ray and tracer[4] reveals that several types of non-axisymmetric flow structure appear depending on the wall temperatures and rotation rates of crucible and crystal.

Some numerical simulations reproduced the non-axisymmetric velocity profile and fluctuation behavior of temperature and oxygen in small crucibles[5]. The present study performed numerical simulations on several sizes of crucible with and without the k-ε two equation turbulent model.

Calculation method

The governing equations of the seven variables(u, v, w, k, ε, T, C_O) are represented by a general transportation equation as shown below,

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho u\phi)}{\partial r} + \frac{1}{r}\frac{\partial(\rho v\phi)}{\partial\theta} + \frac{\partial(\rho w\phi)}{\partial z} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\Gamma_\phi\frac{\partial\phi}{\partial r}\right) + \frac{1}{r}\frac{\partial}{\partial\theta}\left(\frac{\Gamma_\phi}{r}\frac{\partial\phi}{\partial\theta}\right) + \frac{\partial}{\partial z}\left(\Gamma_\phi\frac{\partial\phi}{\partial z}\right) + S_\phi \quad (1)$$

where Φ represents variables. ρ is the fluid density. Γ_Φ is the transport constant of each variable as shown below,

Φ	u, v, w,	k	ε	T	Co
Γ_Φ	$\mu+\mu_t$	$\mu+\mu_t/\sigma_k$	$\mu+\mu_t/\sigma_\varepsilon$	k/C_p	ρD

S_Φ is the source term of each variables. For temperature and concentration equations, source term is not so complicated. The term represents heat (or mass) source or heat (or mass) sink in the melt for heat (or mass) equation. On the other hand, the terms for the velocity components are very complicated because of the curvilinear coordinate. S_Φ of the each velocity components are found in other paper[5].

Since pressure gradients are sources of the velocity components, the pressure field also should be solved. This field is calculated from the following continuity equation.

$$\frac{\partial \rho}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}(\rho r v_r)+\frac{1}{r}\frac{\partial}{\partial \theta}(\rho v_\theta)+\frac{\partial}{\partial z}(\rho v_z)=0 \quad (2)$$

Therefore, total 8 differential equations should be solved simultaneously.

Boundary conditions are summarized as belows.

1. Free surface :
   F_r = -dϒ/dT * dT/dr * (Surface Area)/Volume : surface tension force
   F_θ = -dϒ/dT * dT/rdθ * (Surface Area)/Volume : surface tension force
   $q = \varepsilon\sigma(T^4-T_a^4)$: radiation heat loss
   $j = h_O C_O$: evaporation of oxygen
2. Crucible/melt interface :
   velocities, k, ε : non-slip condition on the wall, wall functions
   $T = T_b$(bottom), $T = T_w$(side wall)
   $C_O = 4\times10^5 \exp(-2\times10^4/T)$ ($\times10^{18}$ atoms/cm^3) (equilibrium to the SiO_2)[6]
3. Crystal/melt interface :
   velocities, k, ε : non-slip wall, wall functions
   $T = T_m$ (melting temperature)
   $j = v_p(1-k)C_L$ (v_p : growth rate)

Finite difference method is used to obtain the difference representation of the above differential equations. The grids for the velocities and the scalar variables, such as temperature, pressure and oxygen concentration were staggered to prevent a checkerboard pressure field. Pressure was calculated by the SIMPLE algorithm[7].

For transient calculation, fully implicit scheme is used. Calculations have been done with different crucible rotation rates and different wall (and bottom) temperatures at different sizes of crucibles considering or not considering turbulent effect. Total grid numbers are $40 \times 30 \times 30$. One CPU hour is necessary for calculating 4 seconds time proceeding when time step is 0.1 second on the alpha XL366 machine.

Results and Conclusions

Top views of the temperature profiles on the middle plane of the small sizes (radius and height of the melt are 3 cm) of crucibles shown in fig. 1(a). This results are obtained from laminar calculation. Even axisymmetric boundary conditions are adopted during the calculation, asymmetric temperature profiles are obtained. The oxygen also shows not axisymmetric profiles as shown in fig. 1(b). Time series data of this calculation shows fluctuations reported from the experimental studies. These profiles are caused by the non- axisymmetric velocity profiles(fig. 1(c)). The calculation results (figures 1(d~f)) on the same size and boundary conditions with k-ε turbulent model are different from the previous results.

Similar difference between the calculation results of two types is shown on larger size of crucibles. Therefore, laminar model should be adopted when we want to reproduce the fluctuation behavior measured in the experiments. However, because the Ra numbers of the silicon melts in large crucibles whose radius and height are greater than 20 cm are as large as 10^8, it is usual to assume turbulent flow occurs. To overcome this contradiction, precise measurement of the melt behavior and numerical simulations with other low Reynolds turbulent model are necessary.

Appendices

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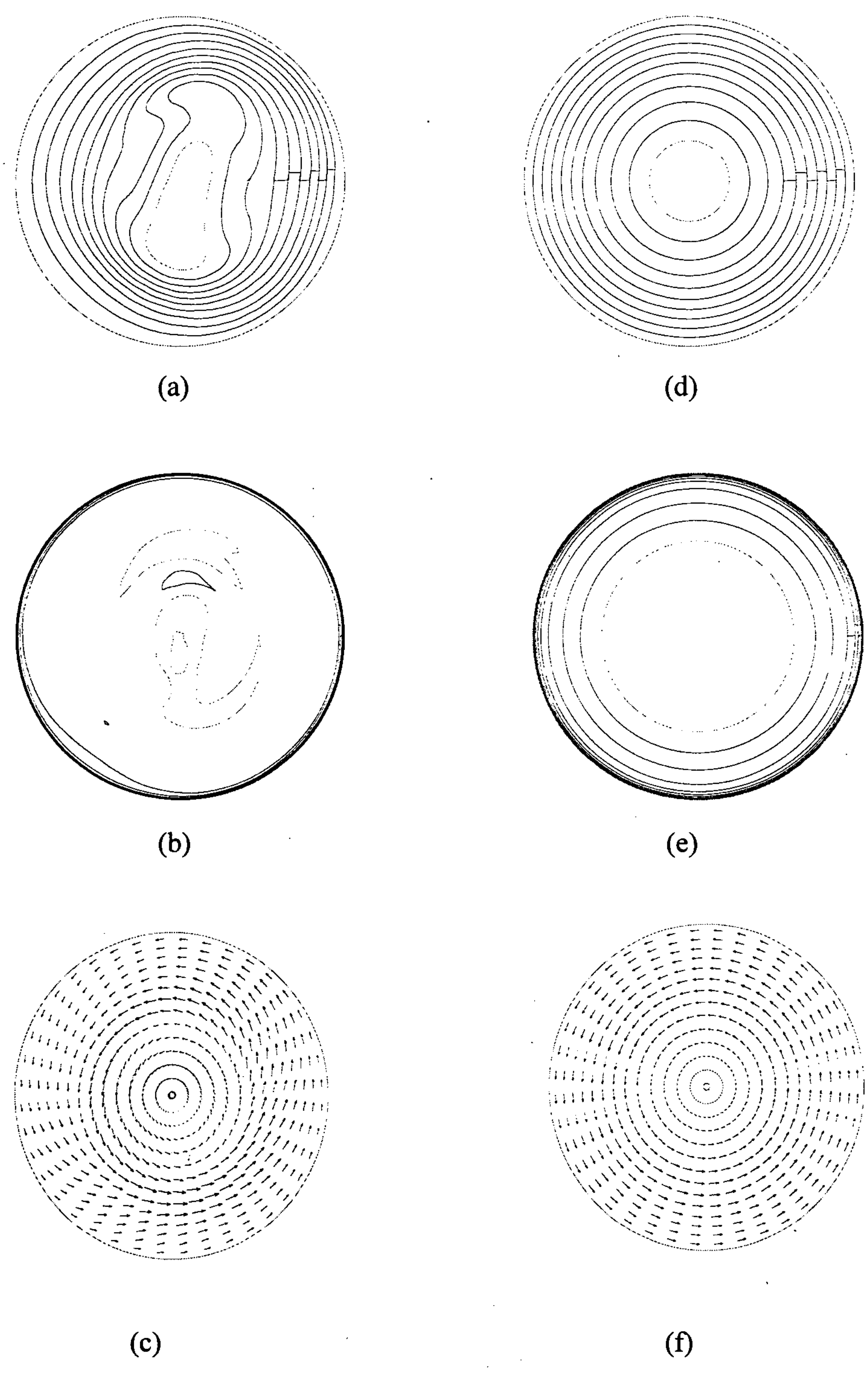

Fig. 1 Profiles on the middle plane of the crucible. Laminar calculation (a~c) and turbulent calculation (d~e). Temperature profiles (a, d). Oxygen concentration (b,, e) Velocity profiles (c, f)