Numerical Analysis on the Flow pattern in the Melt of Cold Model for the Czochralski system

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Abstract : A numerical study was performed on the fluid flow in the melt of the cold model for Czochralski growth system. The fluid flow in the melt of Woods metal with crucible diameter of 20cm was calculated using a three dimensional finite difference method. Since the crucible size is large, fully turbulent model as well as laminar model was used in the calculation. The effects of crucible rotation rate, crystal rotation rate and wall temperature difference on the velocity and temperature distribution were also investigated. For the purpose of verifying the results of calculation, a cold model experiment using Woods metal was also conducted and the velocity distribution in the melt of the model was measured.

1. Introduction

The ever increasing application of semiconductor based electronics creates an enormous demand for high quality semiconductor single crystals. The Czochralski system is usually used to produce silicon single crystals due to its high productivity. Performing experiments in the real system, however, is limited because of the temperature higher than 1420°C and difficulty of variation of process variables. Therefore, cold model study using transparent fluids such as silicon oil and water were mainly performed. But as transparent fluids have transport properties much dissimilar to those of silicon, Woods metal(Bi 50%, Pb 25%, Sn 12.5%, Cd 12.5%, m.p. 70°C) was used as the melt. For the purpose of finding the flow pattern in the melt, a cold model system composed of Woods metal melt, a crucible, a rotating plate, a heater, thermocouple and velocity sensors the principle of which is based on the electromagnetics was constructed and the temperature and velocity variations at various points were measured. As many data must be acquired to analyze the variations of flow velocity and temperature, a plug-in DAQ device was used. To verify the results of experiment, a numerical approach was also made in which three dimensional finite difference method was used to calculate the transport properties with and without the k-ε model and the results of both approach were analyzed and compared.

2. Calculation Method

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

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

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	C_0
Γ_ϕ	$u+u_t$	$u+u_t/\sigma_k$	$u+u_t/\sigma_\varepsilon$	k/C_p	ρD

S_ϕ is the source term of each variables. For the 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 the 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 each velocity components are found in other paper[1]. Since the pressure gradients are sources of the velocity components, the pressure field also should be solved. This field is calculated from the following continuity equation.

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

Therefore, total 8 coupled differential equations should be solved simultaneously.

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 concentration were staggered to prevent a checkerboard pressure field. Pressure was calculated by the SIMPLE algorithm[2]. For transient calculation, fully implicit scheme is used. Calculations have been done with different crucible rotation rates and different wall temperatures at different sizes of crucibles considering or not considering turbulent effect. Total grid numbers are 40*30*30. One CPU hour is necessary for calculating 4 seconds time proceeding when time step is 0.1 second on the alpha XL366 machine.

3. Experimental Procedure

The schematic side view of the cold model system is depicted in Fig. 1. In this figure, the crucible, rotation plate and rotation axis is rotating and the other parts are stationary. The characteristics of rotation devices are the control of rotation rate using an electrical method, which reduces vibration of the rotation axis, and the large deceleration ratio of the gear to support the load of Woods metal. The crucible is made of Aluminum alloy to protect the reaction of Woods metal with the crucible. Cylindrical band-shaped heater was used to maintain the crucible wall temperature nearly constant and the power to this heater was PID controlled. The most important part of this cold model system is the velocity sensor called incorporated magnet probe. The use of flow visualization methods(interferometer) is excluded in this study on account of the opacity of the Wood's metal. Various sensors, such as the Pitot-Prandtl tubes[3], with a working principle founded on pressure difference measurements, are ineffective due to metal solidification within the manometric tubes. The incorporated magnet probe, developed by C. Vives is based on the fundamental study of a liquid metal flow around a permanent magnet of cylindrical shape[4]. This probe relies on the principle that a conductor moving within a magnetic field will generate an electric field. With this velocity probe and the K-type thermocouple, the velocity and temperature variation at various points within the melt with the passage of time were measured. The temperature and velocity data were acquired using a DAQ card and were analyzed using PC.

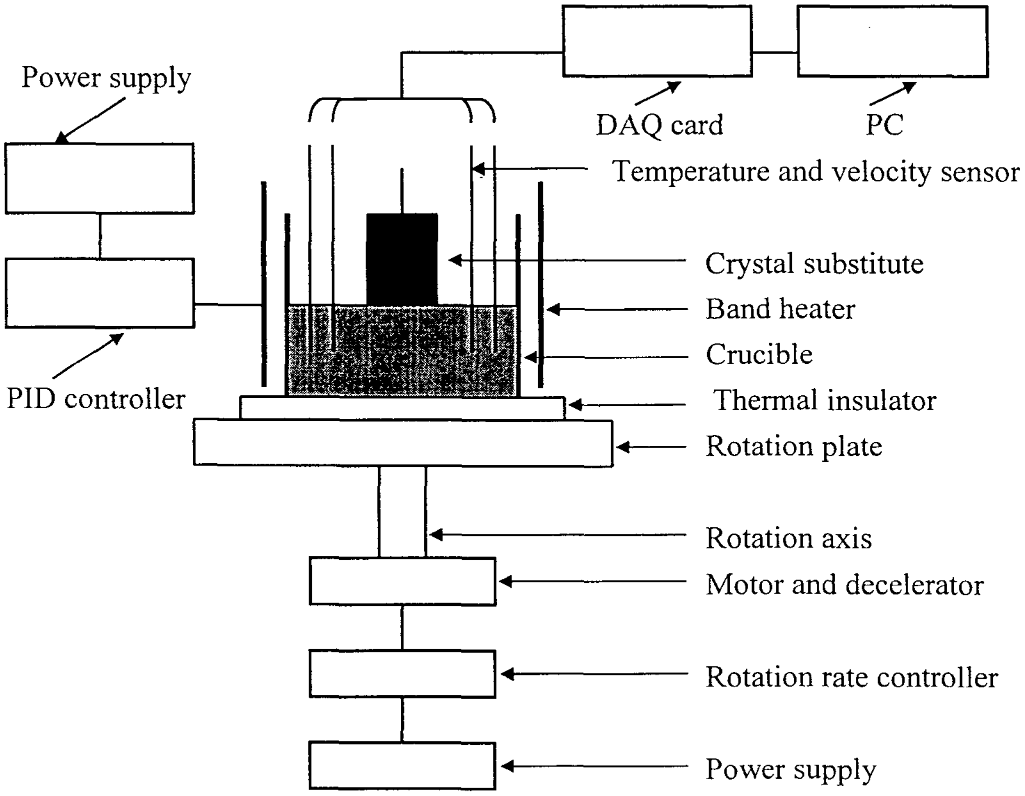

Fig. 1. Schematic diagram of the cold model system.

4. Results and Conclusions

The experimental and numerical results are shown in Fig. 2 and Fig. 3, respectively. The velocity profile is nearly axisymmetric in Fig. 2. In the calculation, the velocity profile was different from that of experiment when laminar flow was assumed and was similar to that of experiment when the k-ε model was used. The difference of magnitude of average velocity in the calculation and experiment was small. When laminar flow was assumed, the velocity and temperature profile were non-axisymmetric behavior as shown in Fig. 4 and Fig. 5.

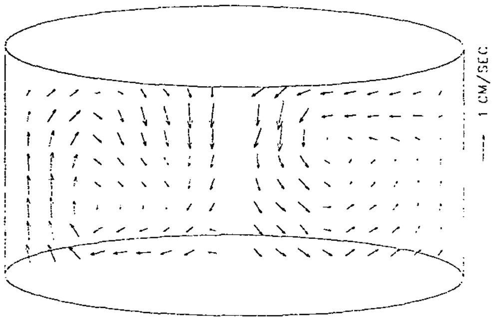

Fig. 2 Experimental velocity distribution

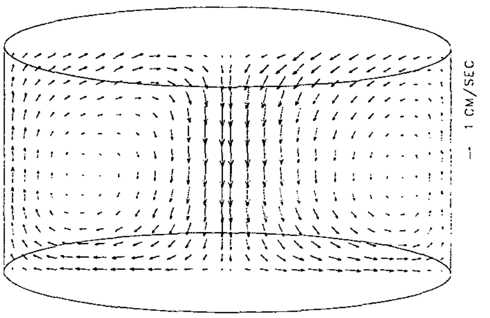

Fig. 3 Calculation result (k-ε model used)

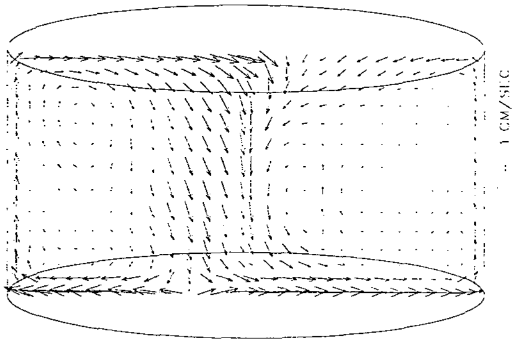

Fig. 4 Calculation result (laminar flow assumed)

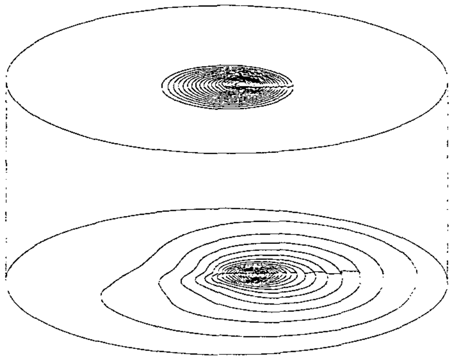

Fig. 5 Temperature contour (calculation)

5. Acknowledgments

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6. References

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