The intrinsic instabilities of fluid flow occurred in the melt of the Czochralski crystal growth system

Kyung-Woo Yi, Koichi Kakimoto*, Minoru Eguchi* and Taketoshi Hibiya*
School of Materials, Seoul National Univ., Seoul 151-741, Korea
* NEC Corp., 34, Miyukikaoka, Tsukuba, Ibaraki 305, Japan

As one of the cause of the defects in the large diameter Silicon single crystal grown by the Czochralski method, asymmetric flow patterns and temperature profiles in the melt have been studied by many researchers. The idea that the non-symmetric structure of the growing equipment is responsible for the asymmetric profiles is usually accepted at the first time. However further researches revealed that some intrinsic instabilities not related to the non-symmetric equipment structure in the melt could also appear. Ristorcelli[1] had pointed out that there are many possible causes of instabilities in the melt. The instabilities appears because of the coupling effects of fluid flow and temperature profiles in the melt. Among the instabilities, the Bénard type instabilities with no or low crucible rotation rates and rotating instabilities with high crucible rotation rates are analyzed by the visualizing experiments using X-ray radiography[2] and the 3-D numerical simulation[3] in this study.

The velocity profiles in the Silicon melt at different crucible rotation rates were measured using X-ray radiography method using tungsten tracers in the melt. The results showed that there exist two types of fluid flow mode. One is axisymmetric flow, the other is asymmetric flow. In the axisymmetric flow, the trajectory of the tracers show torus pattern. However, more exact measurement of the axisymmetric case shows that this flow field has small non-axisymmetric components of the velocity. When fluid flow is asymmetric, the tracers show random motion from the fixed view point. On the other hand, when the observer rotates to the same velocity of the crucible, the trajectory of the tracers show a rotating motion, the center of the motion is not same the center of the melt.

The temperature of a point in the melt were measured using thermocouples with different rotating rates. Measured temperatures oscillated. Such kind of oscillations are also measured by the other researchers[4]. The behavior of temperature oscillations were quite different between at low rotations and at high rotations.

Above experimental results means that the fluid flow and temperature profiles in the melt is not symmetric, and then the mode of the asymmetric is changed when rotation rates are changed. To compare with these experimental results, the fluid flow and temperature profiles at no rotation and 8 rpm of crucible rotation rates on the same size of crucilbe is calculated using a 3-dimensional numerical simulation. A finite different method is adepted for this simulation. $50 \times 30 \times 30$ grids are used.

The numerical simulation also showed that the velocity and flow profiles are changed when rotation rates change. Futhermore, the flow patterns and temperature profiles of both cases are not axisymmetric even though axisymmetric boundary conditions are used. Several cells appear at no rotation. The cells are formed by the unstable vertical temperature profiles (upper region is colder than lower part) beneath the free surfaces of the melt. When the temperature profile is combined with density difference (Rayleigh-Bénard instability) or surface tension difference (Marangoni-Bénard instability) on temperature, cell structures are naturally formed. Both sources of instabilities are coupled to the cell structures in the melt of the Czochralski process.

With high rotation rates, the shape of the fluid field is changed to another type of asymmetric profile. Because of the velocity profile, isothermal lines on the plane vertical to the centerline change to elliptic. When the velocity profiles are plotted at the rotating view point, two vortices appear at the both sides of centerline. These vortices seem to be the main reason of the tracer behavior shown in the asymmetric velocity experiment. This profile is quite similar to the profiles created by the baroclinic instability on the rotating annulus. The temperature profiles obtained from the numerical calculations and Fourier transforms of it are quite similar to the results of the experiment.

Above results intend that at least two types of intrinsic instabilities can occur in the melt of Czochralski growing systems. Because the instabilities cause temperature fluctuations in the melt and near the crystal-melt interface, some defects may be generated by them. When the crucible size becomes large, the intensity of the instabilities should increase. Therefore, to produce large single crystals with good quality, the behavior of the intrinsic instabilities in the melt as well as the effects of the instabilities on the defects in the ingot should be studied.

References

1) J. R. Ristorcelli et al., J. Crystal Growth 116 (1992) 447.
2) M. Watanabe et al., J. Crystal Growth 133 (1993) 326.
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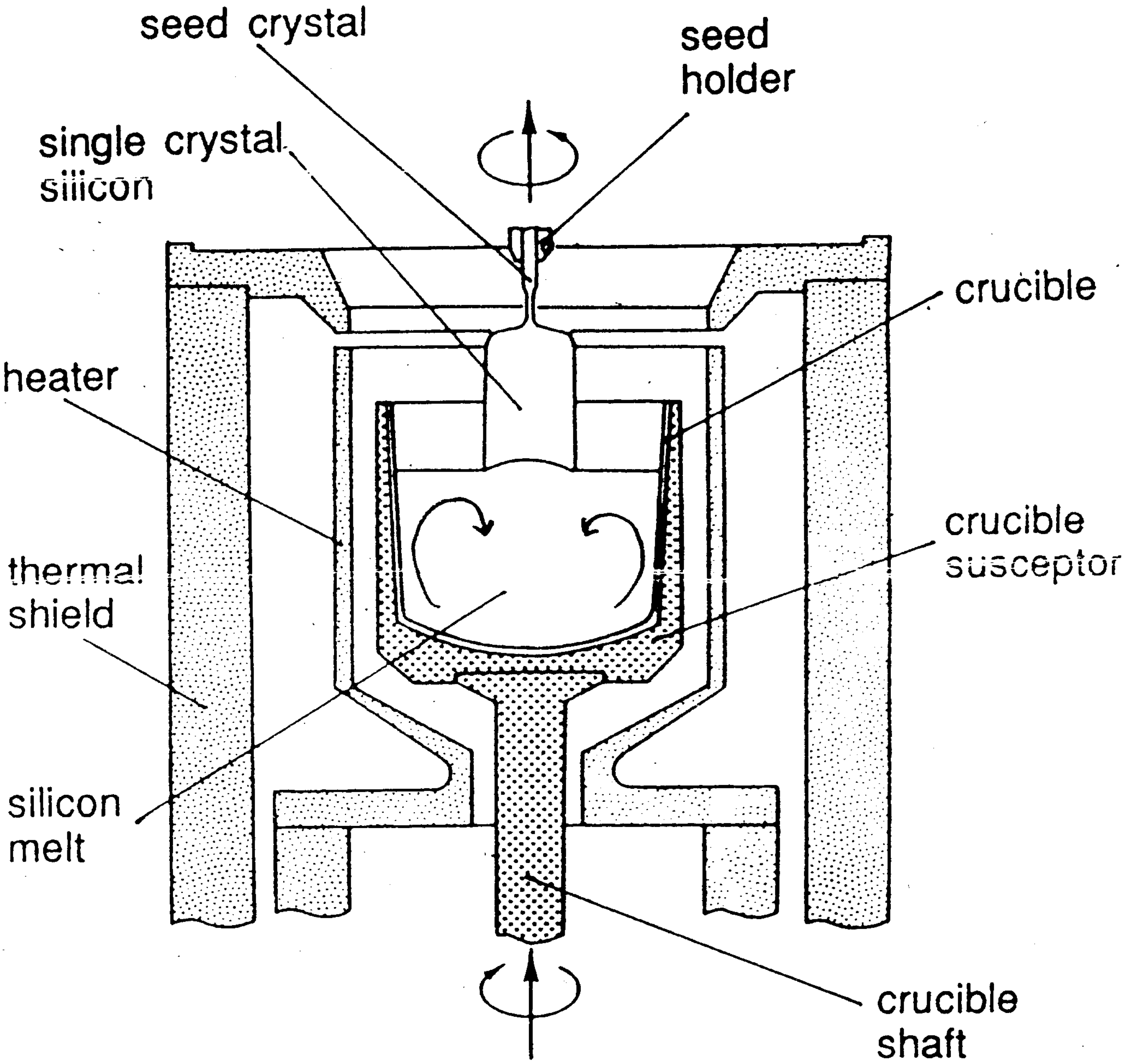


Fig.1 Schematic of the Cz crystal growth apparatus.

Techniques of the study

1. Experiment

   Using X-ray fluid flow is visualized

   Diameter of crucible : 70 mm

   Diameter of crystal : 35 mm

   Melt height : 30 mm

2. Numerical simulation

   Asymmetric profile is analyzed with 3-D FDM model

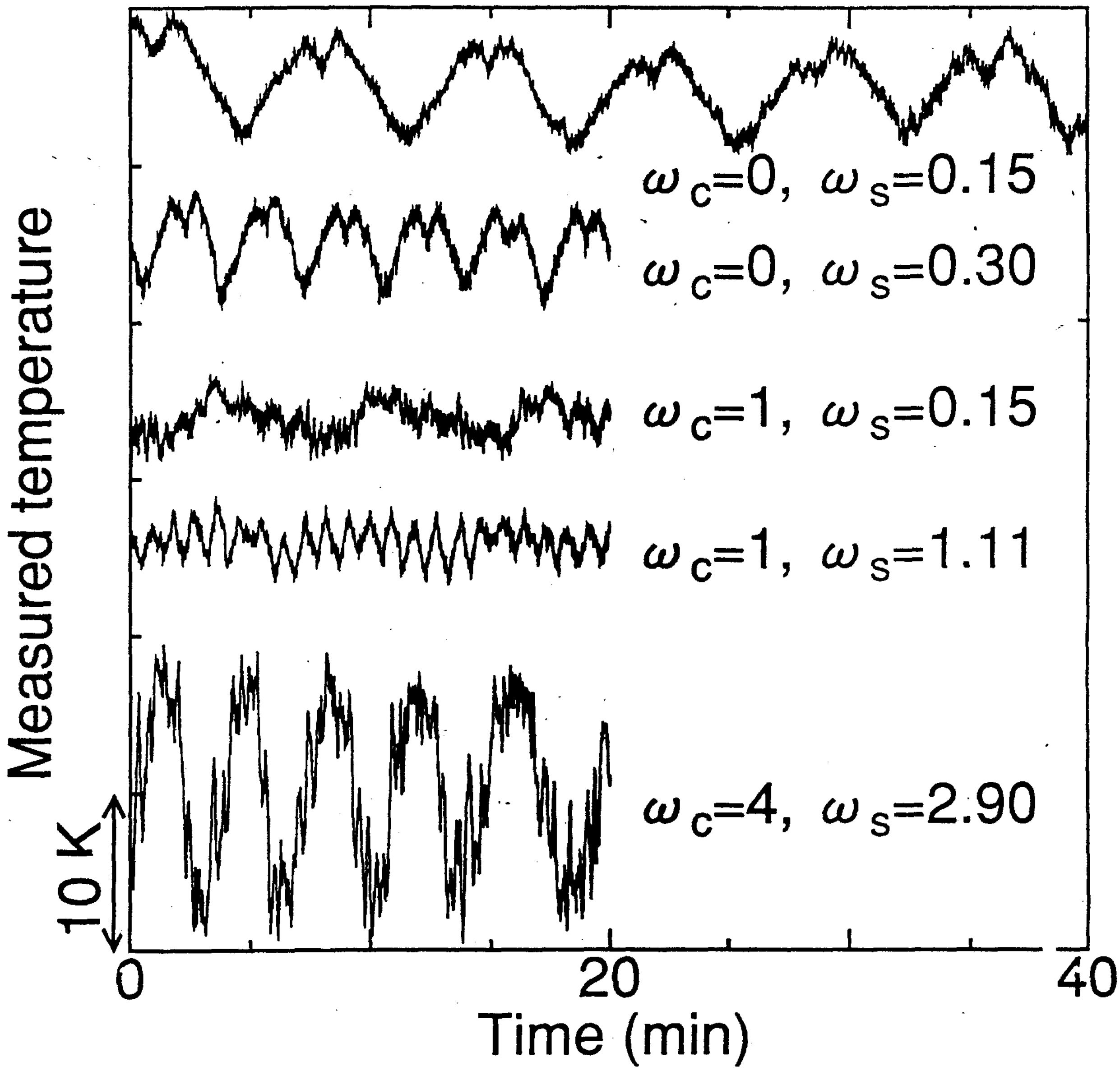
   Number of grid : $50 \times 30 \times 30$

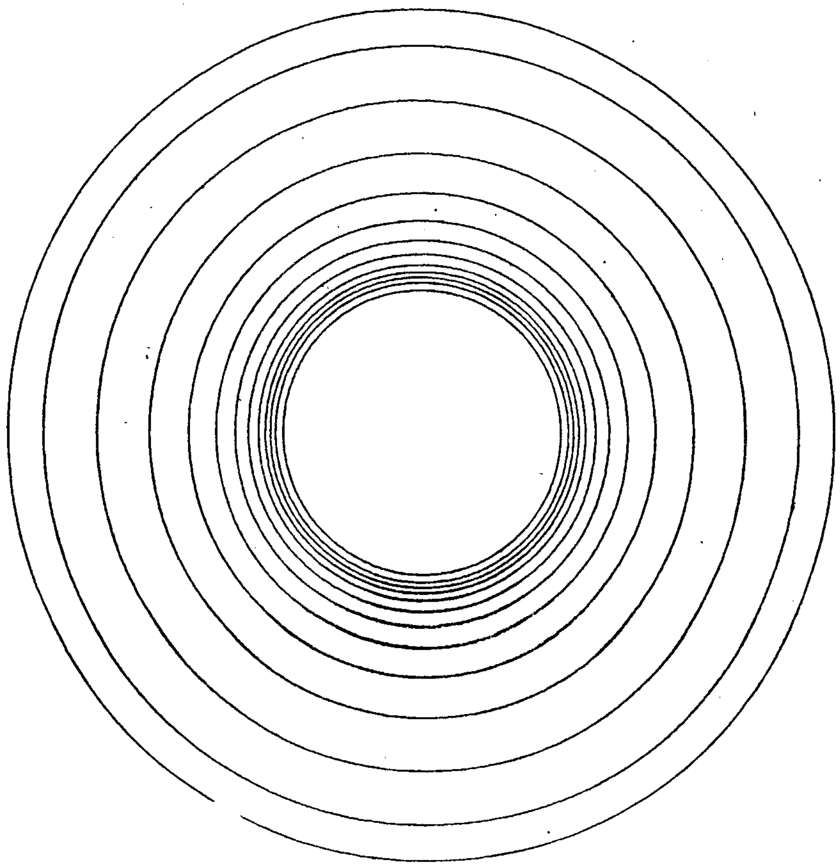
Data for Experiment and Calculation

Crucible diameter	(mm)	75
Crystal diameter	(mm)	35
Density, ρ,	(Kg/m^3)	2530
$\partial\rho/\partial T$	(/K)	-1.4×10^{-4}
Surface tension, γ,	(N/m)	0.72
$\partial\gamma/\partial T$	(N/m·K)	-0.1×10^{-3}

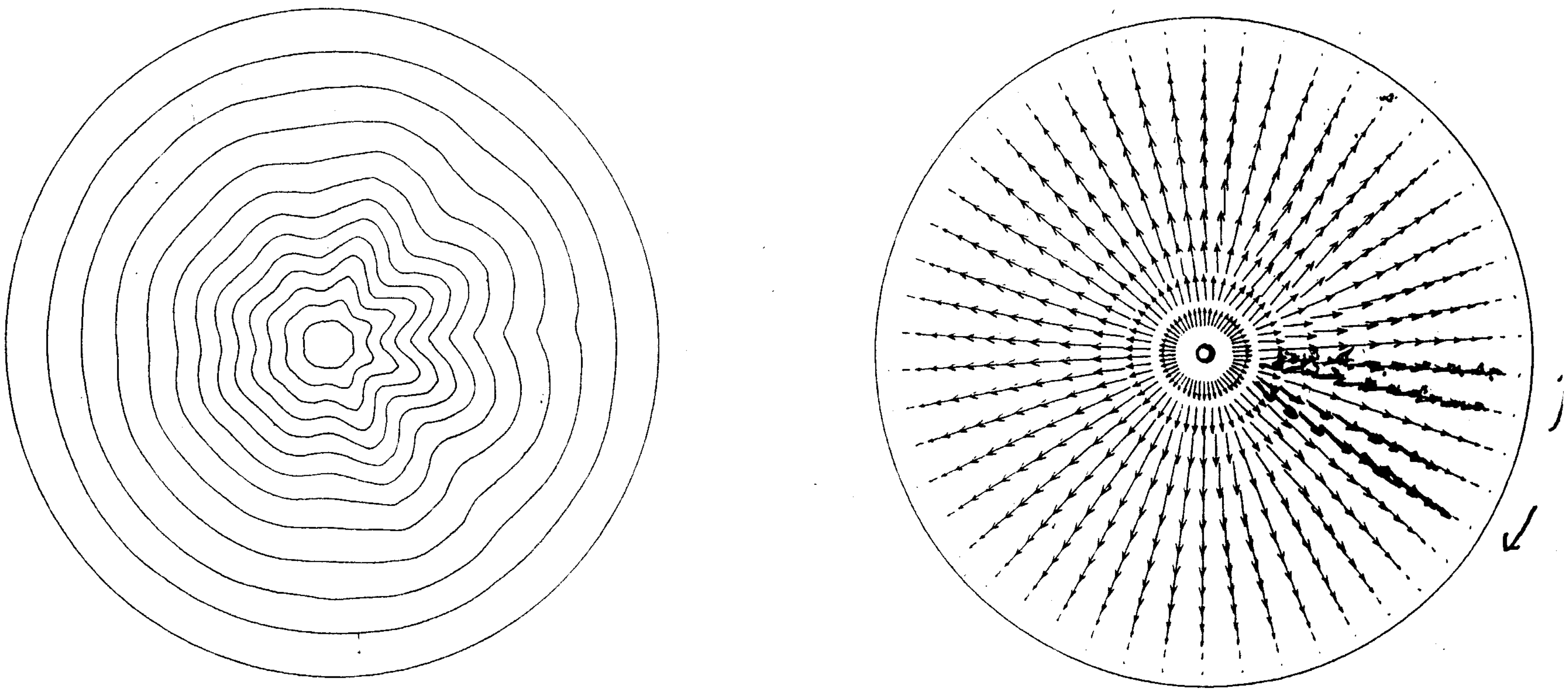
0.05 ~ 0.28
0.3

Temperature fluctuations in the Si melt for different rotation rates of crucible

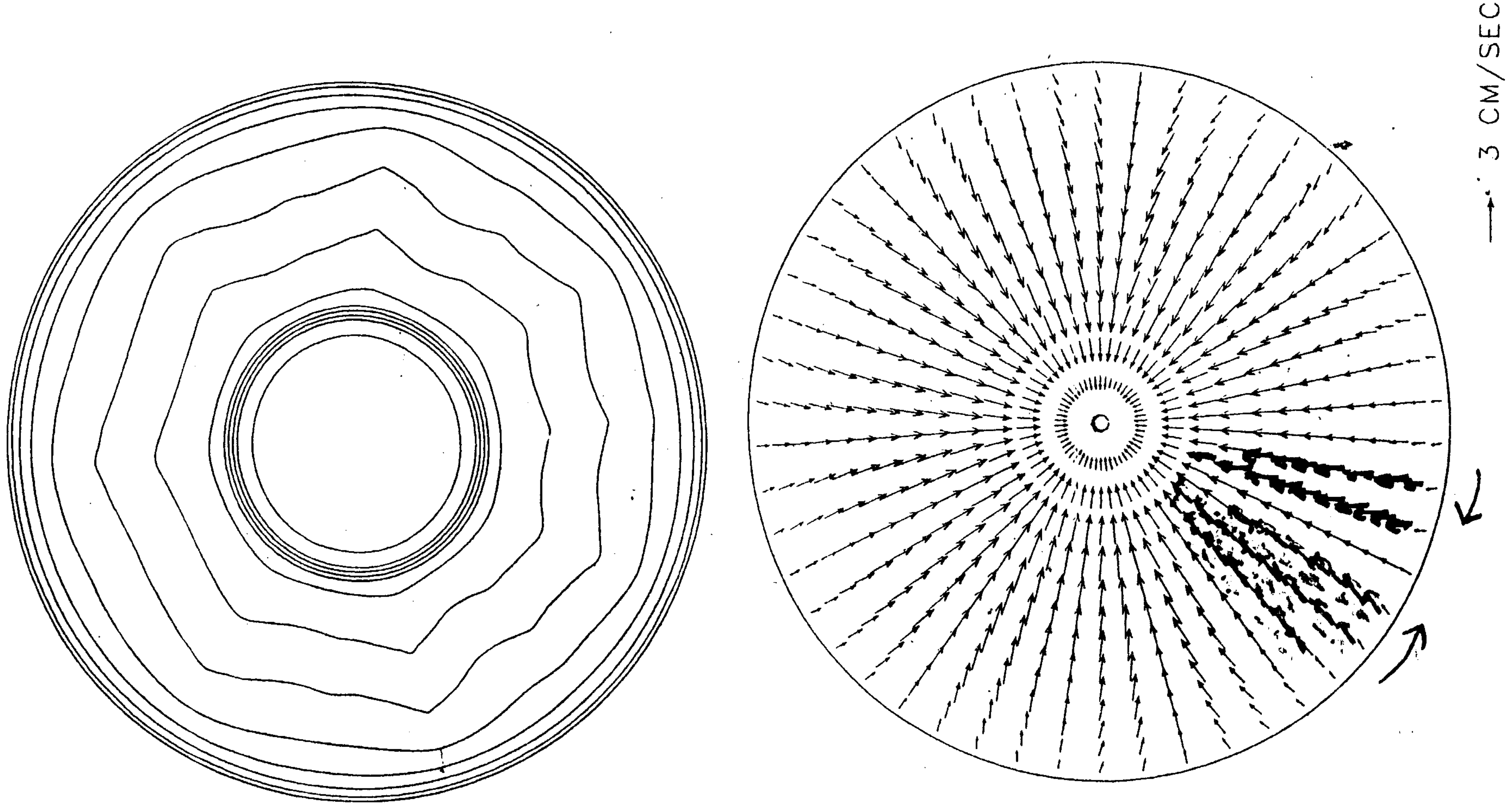




Isothermal lines on **top** plane, $\Delta T=10$ K

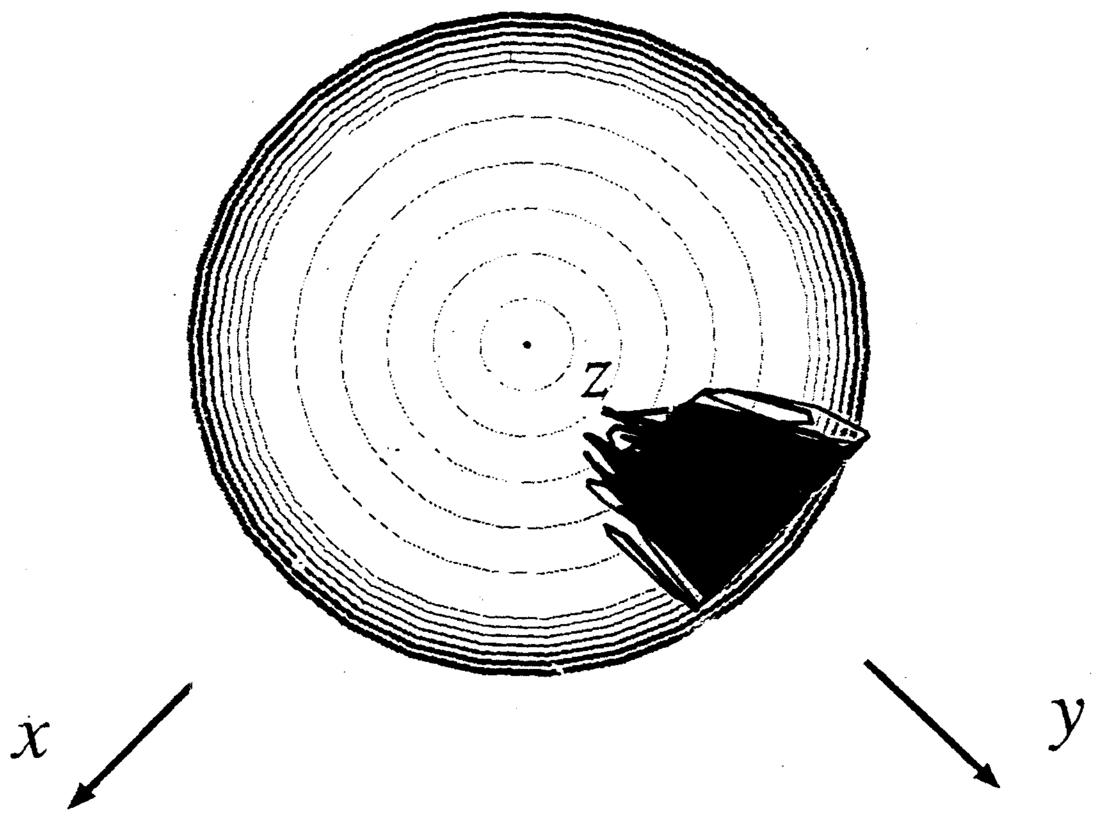


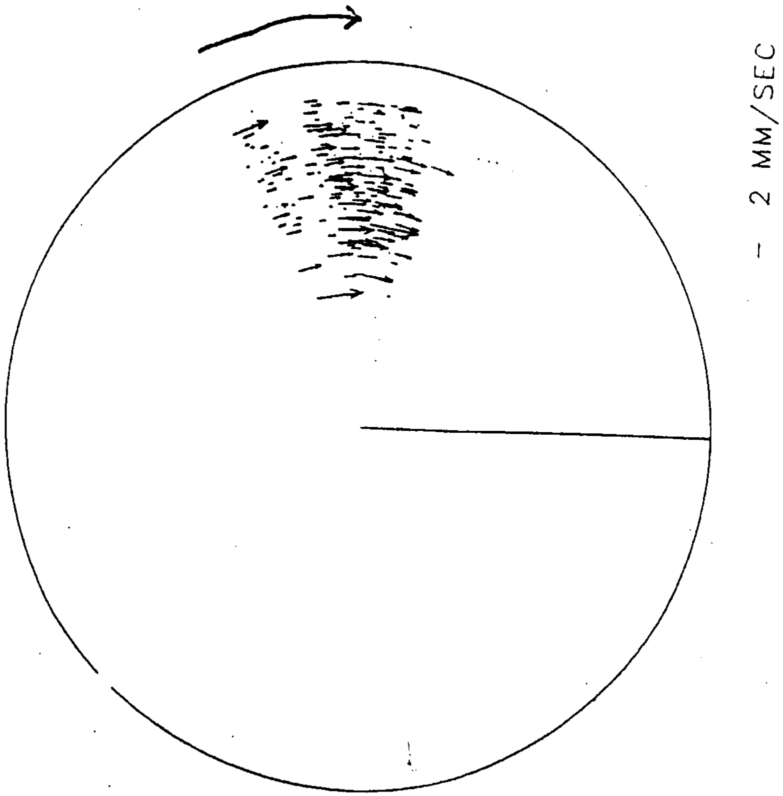
Isothermal lines and velocity vectors on **bottom** plane, $\Delta T = 25$ K



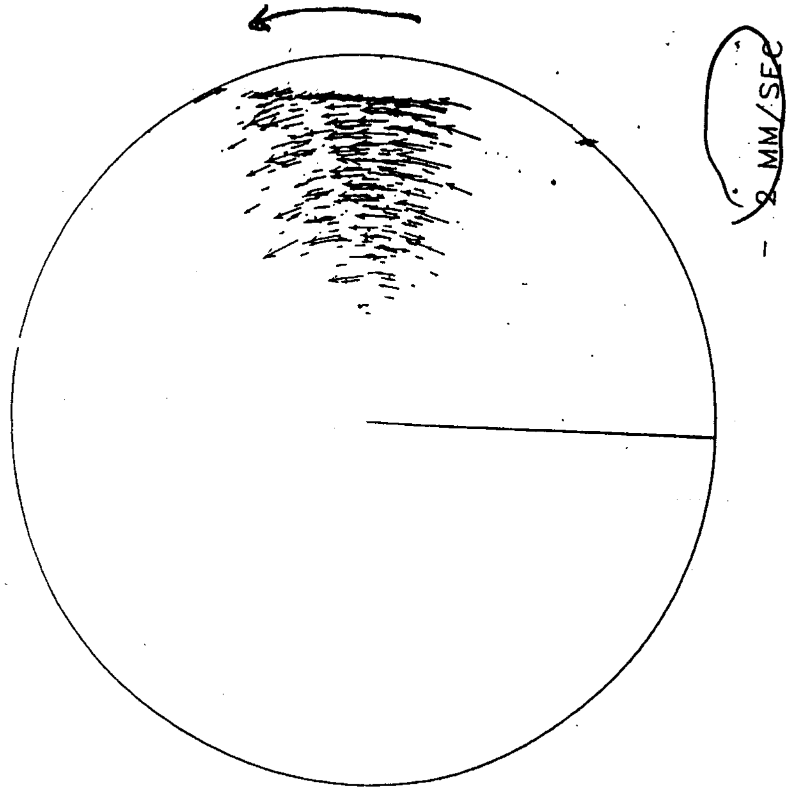
Isothermal lines and velocity vectors on **top** plane, $\Delta T = 25$ K

Fig. Tracer tajectory at no rotation



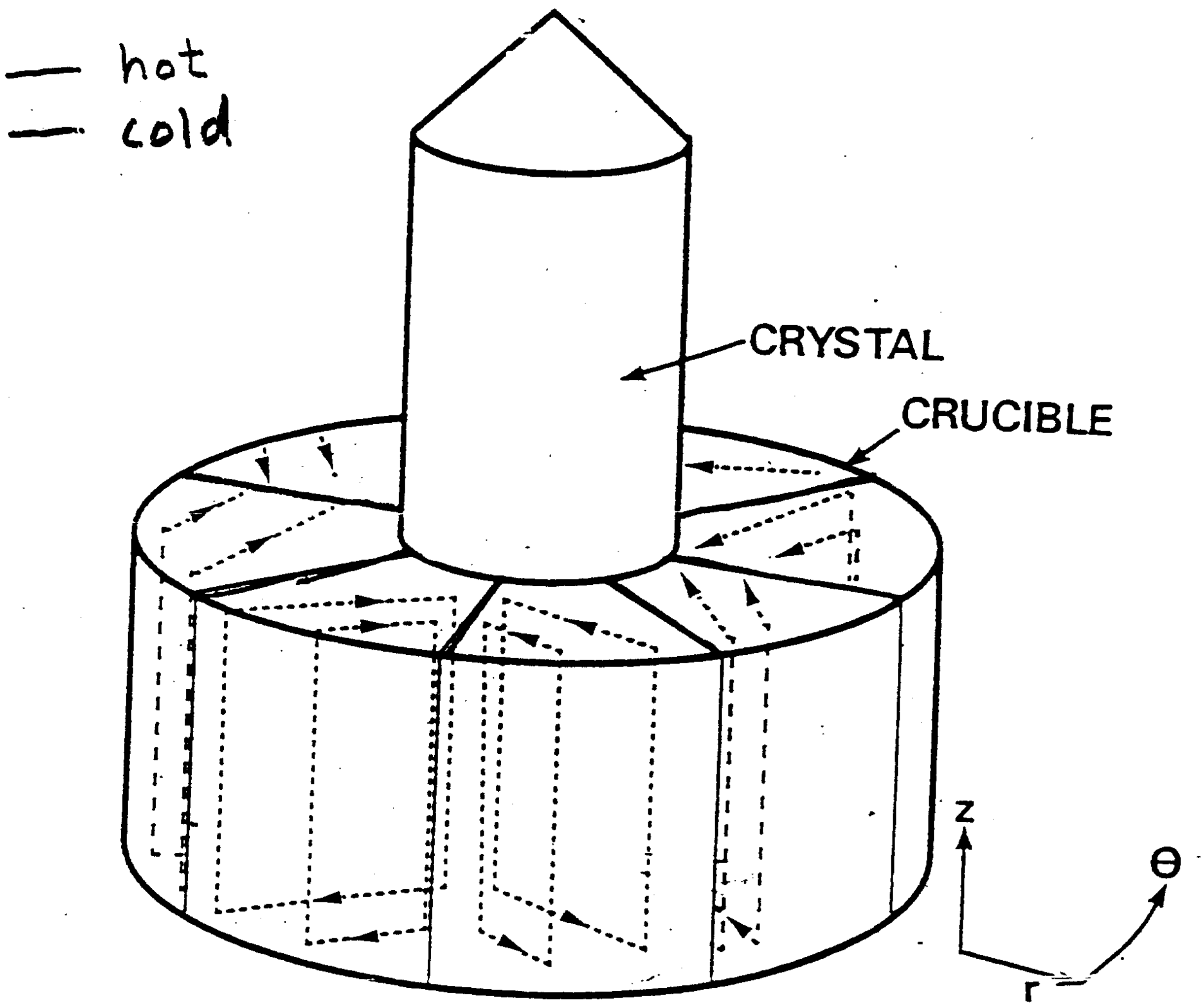


Near the top



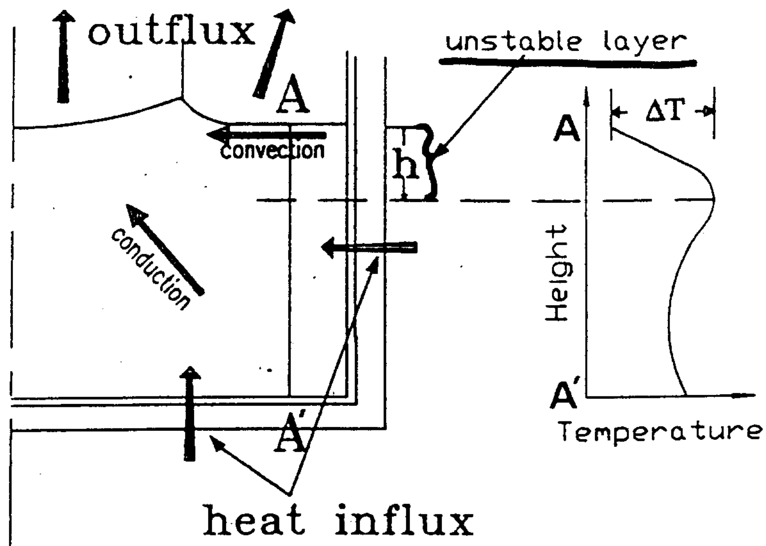
Near the bottom

Azimuthal velocity of the tracer

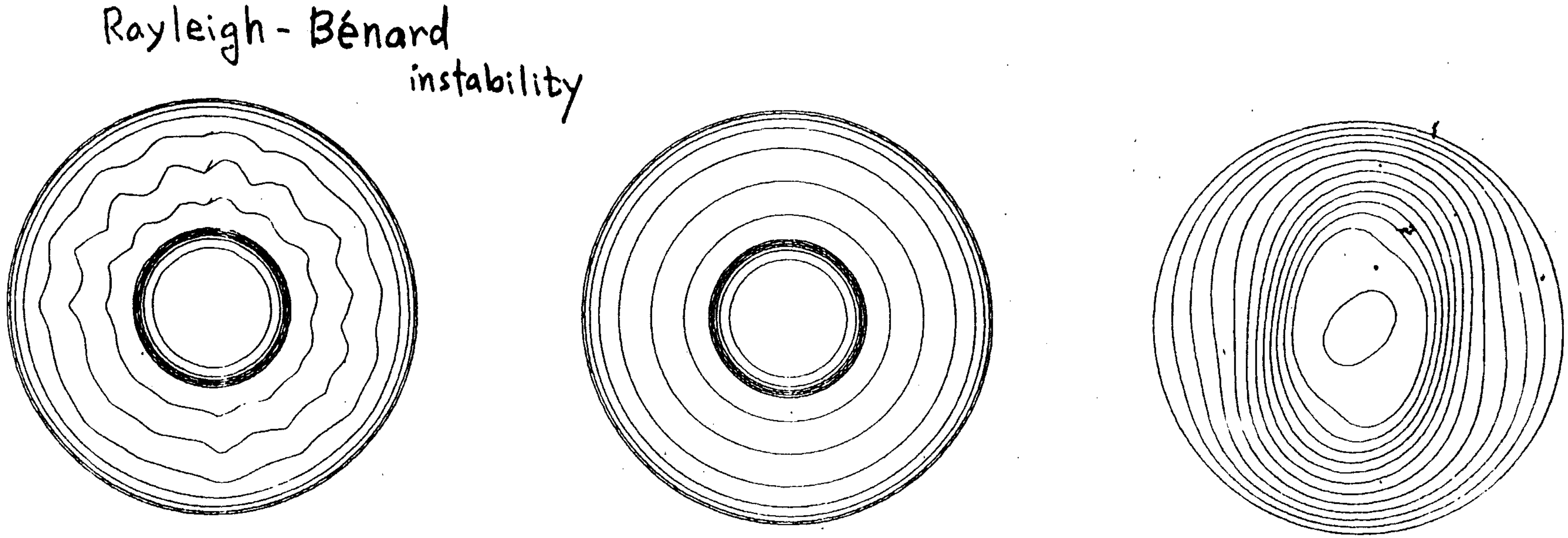


Schematic structure of the fluid flow

Unstable layer in the Si melt



(a) (b)

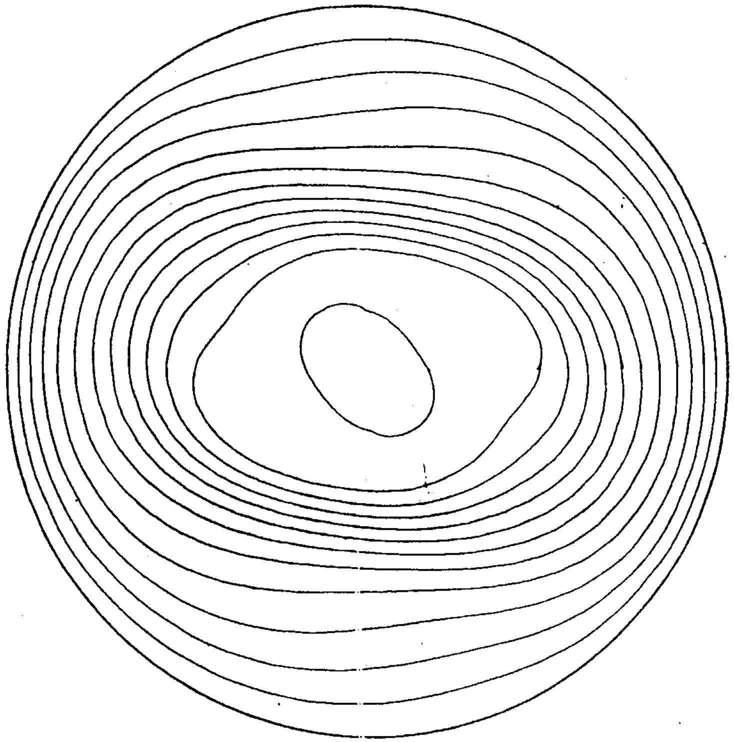


(a) 0 rpm (b) 0.5 rpm (c) 8 rpm

Fig. Isothermal lines on the top plane

H = 3.3 cm
R = 3.5 cm
Position = 1/3 H

Crystal = 0 rpm
Crucible = 8 rpm
Rotational view point



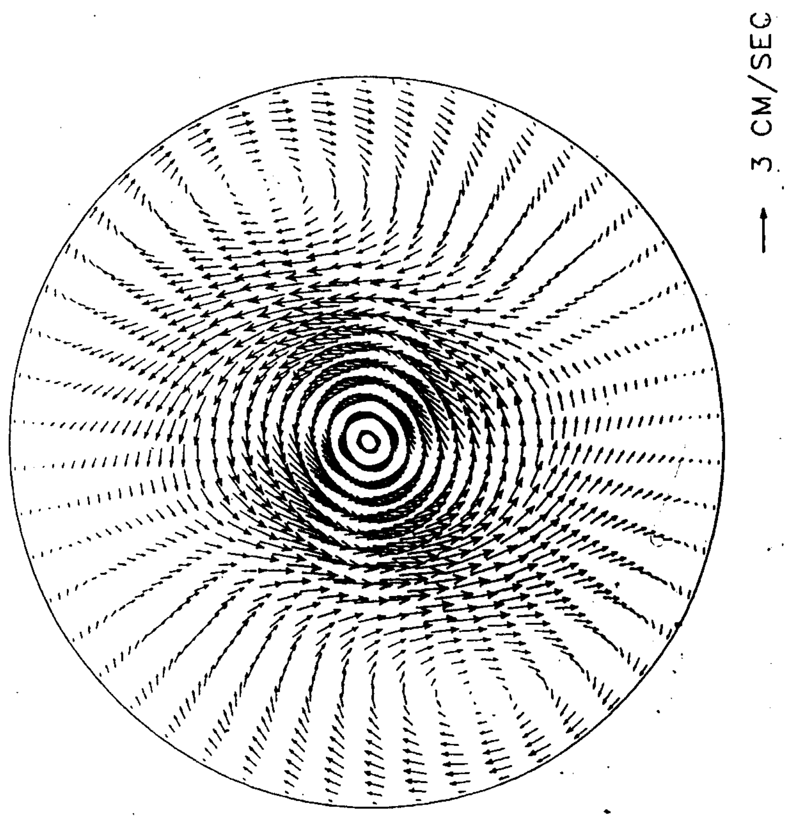
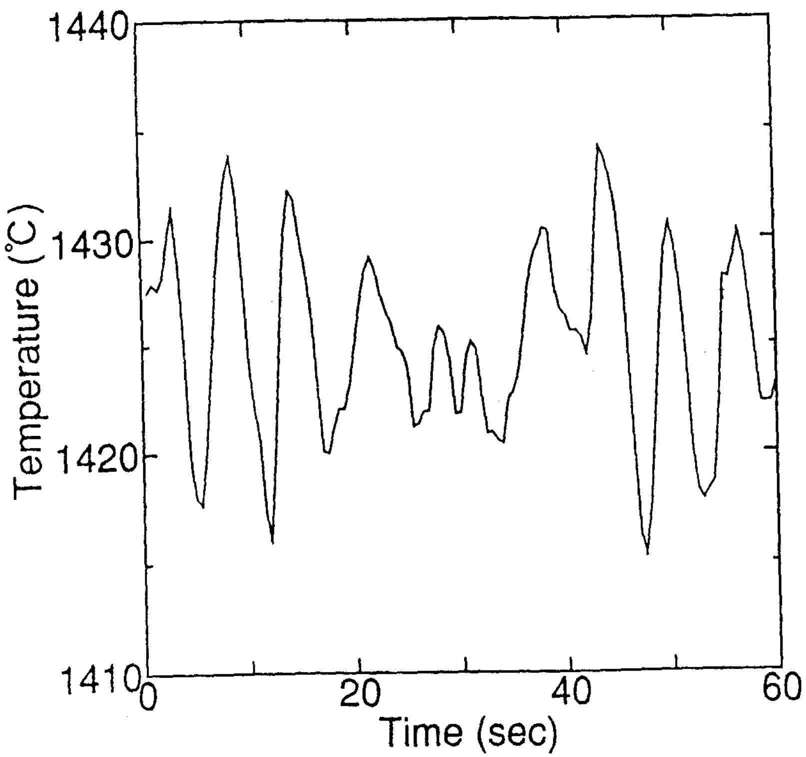
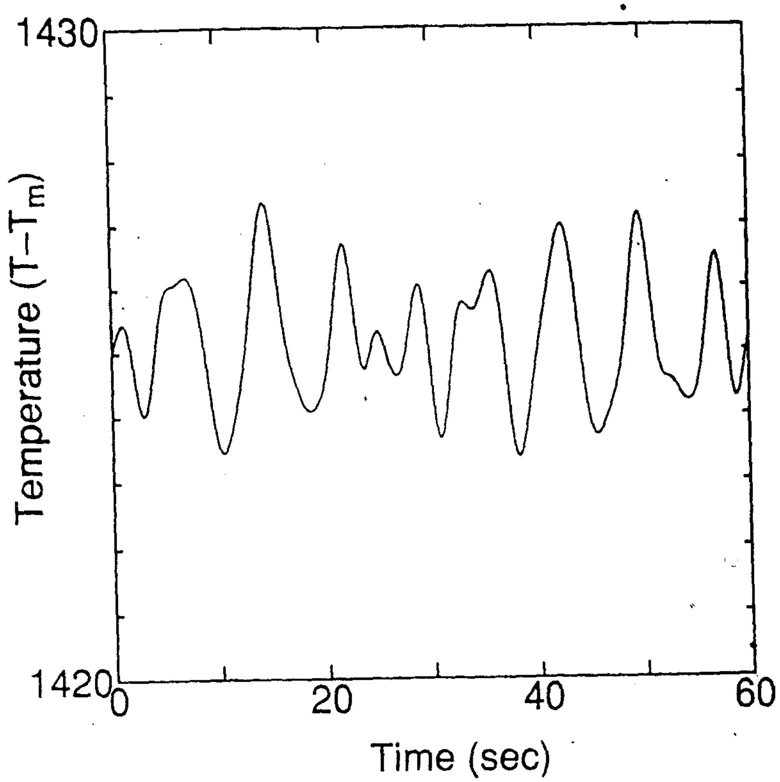


Fig. Isothermal lines and velocity profiles.

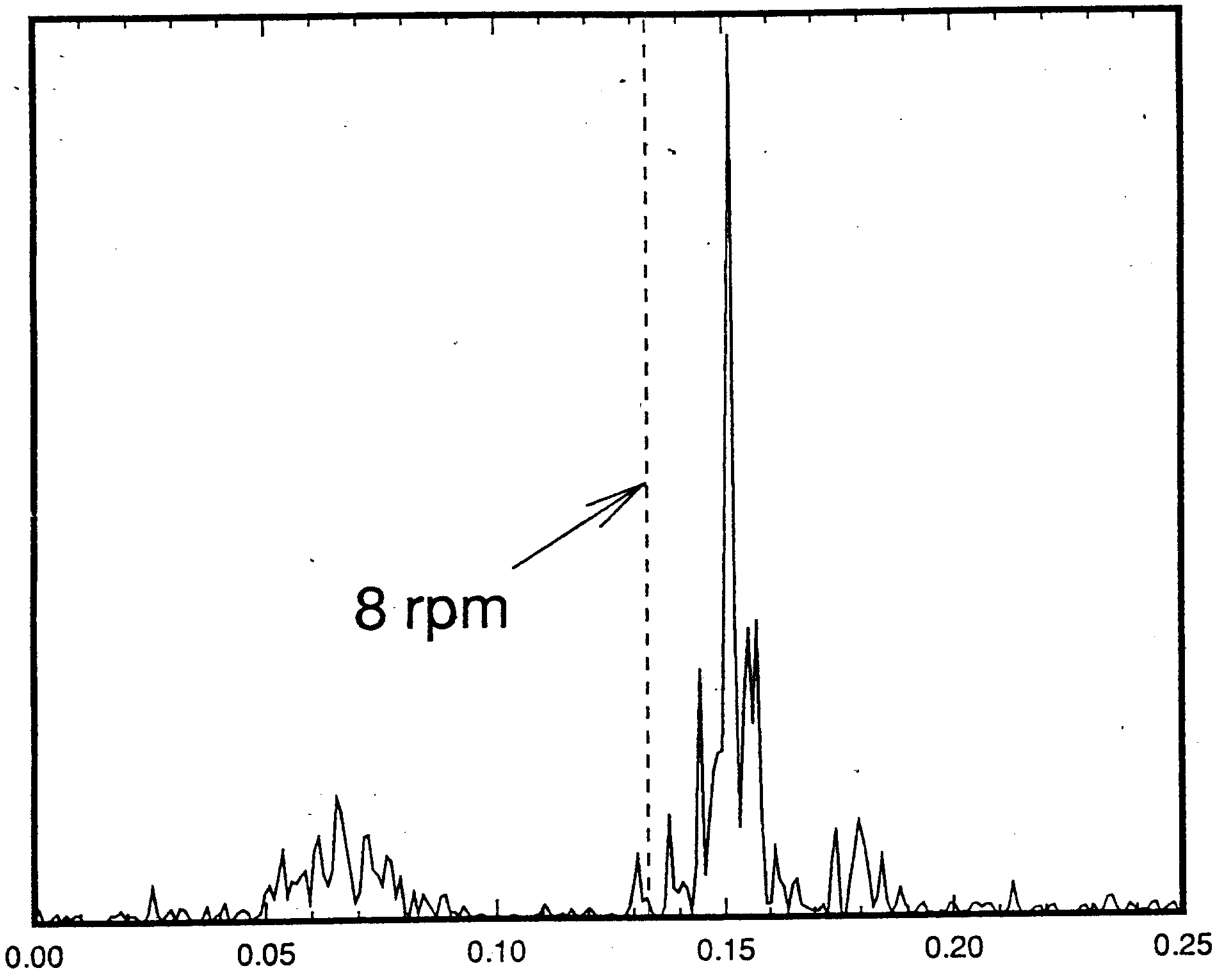
Experimental results

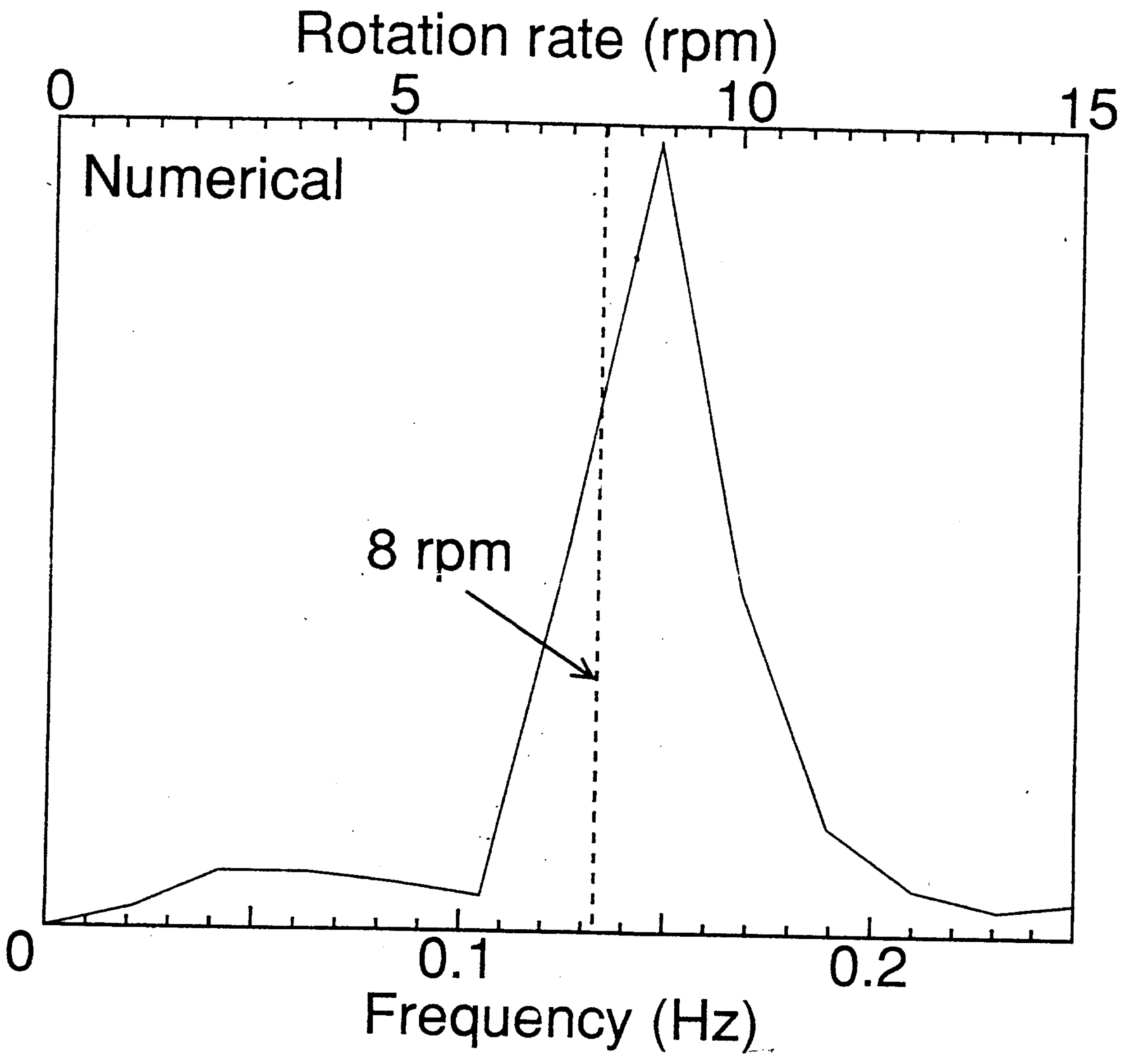


Results calculated

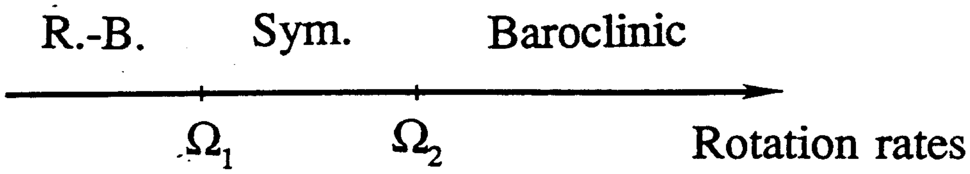


8rpm Case




Rotation rate (rpm)
0
5
10
15
Numerical
8 rpm
0
0.1
0.2
Frequency (Hz)

Instabilities at a rotational case



Rayleigh-Benard instability : $\Omega < \Omega_1$

Baroclinic instability : $\Omega > \Omega_2$

Small crucible ($\phi = 7$ cm) : $\Omega_1 < \Omega_2$

Large crucible ($\phi = 20$ or 40 cm) : $\Omega_1 > \Omega_2$

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