Advantages of a Slim Vertical Gas Channel at High $SiHCl_3$ Concentrations for Atmospheric Pressure Silicon Epitaxial Growth

Kenta Irikura[1], Mitsuko Muroi[1], Ayami Yamada[1], Miya Matsuo[1], Hitoshi Habuka[1], Yuuki Ishida[2, 3], Shin-Ichi Ikeda[2 3] and Shiro Hara[2 3]

[1] *Yokohama National University, Yokohama, Japan*

[2] *National Institutes of Advanced Science and Technology, Tsukuba, Japan*

[3] *Minimal Fab Development Association, Tsukuba, Japan*

Effective process conditions to utilize a slim vertical silicon chemical vapour deposition reactor were studied. Based on a numerical analysis taking into account the gas flow, heat and species transport, particularly over a wide range of the trichlorosilane gas concentrations from 1% to 40 % in ambient hydrogen, a heavy and cold gas was shown to quickly go downward to the hot wafer surface through the slim vertical gas channel. The gas phase near the wafer was sufficiently cooled to produce a cold wall thermal condition which enabled the trichlorosilane gas consumption only at the wafer surface, even in a non-axisymmetric and non-steady condition. The slow wafer rotation, less than 30 rpm, had a considerable effect, such as that increasing the gas phase temperature gradient for suppressing the gas phase reaction.

Keywords: Minimal Fab, chemical vapor deposition reactor, silicon, trichlorosilane gas concentration, wafer rotation

1. Introduction

Significant advances in the information and communication technology has expanded the semiconductor silicon device demand. The silicon electronic device manufacturing technology has acknowledged the trend in the large diameter wafer with the shrinking design rule [1, 2]. While the large diameter wafer can produce a huge number of low cost electronic devices, the significant initial cost for the equipment is a serious issue. Currently, various electronic devices are customized to various kinds of applications. The customized devices are produced by a small lot using rather small diameter wafers, such as 150- and 200-mm diameter wafers. Thus, in the future, an electronic device manufacturing system will be further flexible for allowing the frequently changing designs and amounts of the devices.

For this purpose, the Minimal Fab [3, 4] is the new practical choice, which adds a half-inch (12.5 mm) diameter wafer to typical large diameter wafers. The process using a half-inch diameter wafer and small instruments having a small footprint can quickly and flexibly produce a reasonable and sufficient number of devices from one to a million.

The Minimal Fab should have the chemical vapour deposition (CVD) process, similar to the present semiconductor device process. The Minimal CVD reactor [5 - 7] has been developed by employing the slim vertical gas channel, the trichlorosilane-hydrogen system and the concentrated infrared light heater. The transport phenomena in the Minimal CVD reactor was numerically evaluated [7] in order to show the characteristic gas flow caused by the slim vertical gas channel. The calculation performed at the low trichlorosilane gas concentration of 1% showed that the precursors were effectively transported to the wafer surface by the recirculating flow initiated by the upward flow due to natural convection around the wafer.

For further pursuing the way to improve the precursor transport accounting for the least gas flow rate through the significantly slim vertical gas channel, a method to achieve the direct and quick downward stream to the wafer surface from the inlet should be designed. However, such a downward stream may be very difficult because of the upward natural convection formed due to the geometry having a cold inlet at the top and a high temperature wafer at the bottom. In the existed notable studies [7-19], the fast gas stream, the reduced pressure and the high-speed wafer rotation were preferred. However, a large volume of gas, a large vacuum pump and a customized rotation module unfortunately make the reactor big. These are not suitable for achieving the small instrument of the Minimal Fab.

By considering a downward natural convection, a significant effect is expected by the heavy gas consisting of a trichlorosilane ($SiHCl_3$) gas at high concentrations in ambient hydrogen. Because the molecular weight of trichlorosilane, 135, is significantly greater than that of hydrogen, 2, even a small amount of trichlorosilane gas in hydrogen ambient easily produces a heavy gas mixture. Additionally, such a heavy gas may help producing a stable downward flow and a cold wall thermal condition, even non-axisymmetric, through the very slim vertical gas channel.

In this study, the transport phenomena in the slim vertical CVD reactor for the Minimal Fab were studied using numerical calculations accounting for the heat, flow and chemical species with chemical reaction. Particularly, the influences of the trichlorosilane gas concentration, from low to significantly high, on the entire phenomena in the slim vertical gas channel were evaluated in order to develop a highly-productive process. The calculations in this study evaluate a possibility that a heavy gas can directly approach the hot wafer surface through the slim vertical gas channel to quickly initiate and continue the epitaxial growth with maintaining a cold wall thermal condition.

2. Numerical calculation

Figure 1 shows the configuration of the Minimal CVD reactor. This reactor consists of a half-inch silicon wafer (12.5-mm diameter and 0.25-mm thick), a tubular chamber made of transparent quartz, a wafer holder made of quartz glass, gas inlet, and three lamp heating modules. The inner diameter of the quartz tube is 24 mm. The wafer holder diameter is 19 mm. The infrared light emitted from the halogen lamp in the lamp heating module is concentrated on the wafer surface. The quartz tube wall is cooled by flowing air [6]. The quartz wall between the reflector body and the wafer is assumed to have a temperature near 500 ^{o}C, because the quartz wall near the wafer is heated by the hot wafer and the body of the three reflectors, which are directly heated by the halogen lamps placed inside the reflector [6].

Trichlorosilane gas and hydrogen gas are introduced from the gas inlet at the top of the reactor at atmospheric pressure. Trichlorosilane gas is the popular and important precursor for the silicon epitaxial growth, as well as dichlorosilane and monosilane [20-22]. The silicon epitaxial growth from the trichlorosilane gas follows the surface chemical reaction and the rate equation of the Eley-Rideal model [23].

Chemisorption: $SiHCl_3 \rightarrow {}^{*}SiCl_2 + HCl$. (*: Surface species) (1)

Silicon production: ${}^{*}SiCl_2 + H_2 \rightarrow Si + 2\ HCl$. (2)

Growth rate: $$R_{\mathrm{Si}} = \frac{k_{\mathrm{ad}} k_{\mathrm{r}} [\mathrm{SiHCl_3}][\mathrm{H_2}]}{k_{\mathrm{ad}} [\mathrm{SiHCl_3}] + k_{\mathrm{r}} [\mathrm{H_2}]}. \quad (3)$$

R_{Si} (mol m^{-2} s^{-1}) is the silicon epitaxial growth rate, and $[i]$ (mol m^{-3}) is the concentration of species i at the wafer surface. k_{ad} (m s^{-1}) and k_{r} (m s^{-1}) are the rate constants of equations (1) and (2), respectively. At a sufficiently high $k_{\mathrm{ad}}[\mathrm{SiHCl_3}]$ value, equation (3) is simplified as follows:

$$R_{\mathrm{Si}} = k_{\mathrm{r}} [\mathrm{H_2}]. \quad (4)$$

For evaluating the gas flow, heat and gas species transport in the reactor, the governing equations of mass, momentum, enthalpy and chemical species following the ideal gas law are numerically evaluated using the Fluent 15 software (Ansys Inc., USA). The wafer temperature and the gas velocity at the inlet are fixed at 1000 ^oC and 0.004 m s^{-1} (110 sccm), respectively, which are set as the boundary conditions for the calculation. The trichlorosilane gas concentration at the inlet and the wafer rotation rate are 1 – 40 % and 0 - 30 rpm, respectively.

3. Results and discussion

3.1 Trichlorosilane gas concentration

Figure 2 shows the gas velocity vectors in the reactor at various trichlorosilane gas concentrations. The dotted lines indicate the main stream in the gas phase. The wafer surface temperature, the inlet gas velocity and the wafer rotation rate were 1000 ^oC, 0.004 m s^{-1} and 4 rpm, respectively. As shown in Fig. 2 (a), the upward flow from the wafer center is produced at the trichlorosilane gas concentration of 1 %. The main stream in this figure was recognized to be symmetric. With increasing trichlorosilane gas concentration, the entire stream tended to be asymmetric. At the trichlorosilane gas concentration of 5 %, there is downward flow from the right top of the chamber, as shown in Fig. 2 (b). Simultaneously, the main stream rises from the wafer center to the chamber top. At the trichlorosilane gas concentration of 10 %, Fig. 2 (c) shows that there seems to be two large streams in the regions near the wafer and in the top half of the chamber. At even higher trichlorosilane gas concentrations, the gas mixture introduced from the chamber top seems to directly go downward to the wafer surface, as shown in Figs. 2 (d) and (e). In Fig. 2 (d), the gas mixture, consisting of 20 % trichlorosilane gas and 80 % hydrogen gas, directly approaches the wafer surface and rises to the chamber top. The main stream at the trichlorosilane gas concentration of 40 % is similar to that at 20%, as shown in Fig. 2 (e). The gas mixture introduced from the inlet goes downward to the wafer and recirculates from the wafer surface to the chamber top. In Fig. 2, the gas velocity near the wafer becomes faster with increasing trichlorosilane gas concentration. At 1 and 5 %, the gas velocity near the wafer surface is quite low, as indicated by the dark blue coloured region in Figs. 2 (a) and (b). At 10 %, there is the light blue coloured region indicating a gas velocity around 0.05 m s^{-1}. Figs. 2 (d) and (e) show a green coloured stream which has a gas velocity near 0.2 m s^{-1} from the chamber top to the wafer surface at 20 % and 40 %.

The large recirculating flow directly approaching the hot wafer surface from the cold gas inlet is expected to decrease the gas phase temperature. Figure 3 shows the contour lines of the gas phase temperature in the chamber. At the trichlorosilane gas concentration of 1 %, the yellow coloured region, corresponding to about 700 ^{o}C, has a flat or convex shape as shown in Fig. 3 (a). This situation is produced by the upward flow from the center of the hot wafer, as shown in Fig. 2 (a). In contrast, at the trichlorosilane gas concentration of 5 %, the yellow coloured region shows a concave shape, because the cold gas can directly approaches the wafer, following the stream shown in Fig. 2 (b). This trend becomes significant with the increasing trichlorosilane gas concentration. The bottom position of the yellow coloured region exists very close to the wafer surface at the trichlorosilane gas concentration of 10 %, as shown in Fig. 3 (c). At the trichlorosilane gas concentrations higher than 20 %, the light green coloured region, indicating temperatures near 400 ^{o}C, comes very close to the wafer surface, as shown in Figs. 3 (d) and (e).

The change in thermal condition influences the temperature gradient in the gas phase immediately above the wafer surface. As shown in Fig. 4, the temperature gradient increases from 50 K mm^{-1} to more than 200 K mm^{-1} when the trichlorosilane gas concentration at the inlet increases from 5 % to 15 %.

The distribution of the trichlorosilane gas concentration changes with its concentration at the inlet. As shown in Fig. 5, the trichlorosilane gas concentration near the wafer increases with that at the inlet. Particularly, because the light blue coloured region and the green coloured region in Figs. 5 (d) and (e), respectively, are vertically long, the trichlorosilane gas is considered to directly approach the wafer surface from the inlet.

With the increasing trichlorosilane gas concentration, the wafer surface tends to be sufficiently covered with the intermediate species of $*SiCl_2$. The surface coverage, θ (-), is evaluated using the following equation [23].

$$\theta = \frac{k_{ad}[\mathrm{SiHCl_3}]}{k_{ad}[\mathrm{SiHCl_3}] + k_r[\mathrm{H_2}]}. \quad (5)$$

Figure 6 shows the surface coverage by $*SiCl_2$ at the various trichlorosilane gas concentrations at the inlet. The surface coverage is less than 0.8 at the trichlorosilane gas concentration of 1 %. It becomes higher than 0.95 at 5 %; it saturates near 1.0 at the trichlorosilane gas concentrations greater than 10%. This behaviour influences the growth rate and its profile, following equation (4).

Next, the silicon epitaxial growth rate is evaluated. At the trichlorosilane gas concentration of 1 %, the growth rate is about 1.2 μm min^{-1} at the wafer center, and is slightly lower than that at the outside position. The non-uniform growth rate profile indicates that the growth rate follows equation (3) and is still influenced by the trichlorosilane gas transport. In contrast, the growth rate profiles for the trichlorosilane gas concentrations above 5 % are uniform over the wafer. This indicates that the growth rate is governed by the hydrogen concentration at the wafer surface as described by equation (4). Consistently, as shown in Fig. 7, the values of the epitaxial growth rate show a maximum and slightly decrease for trichlorosilane gas concentrations at the inlet above 10 %, because the increase in the trichlorosilane gas concentrations results in a decrease of the hydrogen gas concentration.

3.2 Wafer rotation

Figure 8 shows the temperature and the trichlorosilane gas concentration near the wafer at rotation rates of 0, 20 and 30 rpm. This calculation was executed for a trichlorosilane gas concentration of 15 %, at which the surface coverage by the surface intermediate species is nearly 1.0, as shown in Fig. 6. The trichlorosilane gas concentration of 15 % is comparable to the industrial condition [18] for the high speed rotation vertical reactor which uses a trichlorosilane gas concentration of 20 % at the inlet. The value of 15 % is expected to to be the lowest for achieving the downward flow and the cold gas phase, with the moderately asymmetric gas flow and the acceptable growth rate decrease, as shown in Figs. 2 and 7, respectively.

With increasing rotation rate, the low temperature region approaches the wafer surface because the main gas stream from the cold inlet shifts close to the wafer surface. In Fig. 8 (c)-(T), the light blue coloured region indicating the temperature near 300 ^{o}C exists near the wafer at 30 rpm, in contrast to that shown in Fig. 8 (a)-(T) at 0 rpm. Such a gas phase thermal condition influences that in the vicinity of the wafer surface, as shown in Fig. 9. The temperature gradient in the gas phase close to the wafer surface is higher than 230 K mm^{-1} at the rotation rate of 30 rpm, while that at 0-10 rpm is about 220 K mm^{-1}. Although the temperature gradient seems to have some fluctuation in the magnified figure, Fig. 9, the temperature gradient is recognized to entirely and moderately increase with increasing wafer rotation rate. Such a cold wall condition can effectively suppress the gas phase chemical reaction by the trichlorosilane gas. This effect can give a wider process window which enable to increase the wafer temperature without generating particles.

The cold gas phase maintains the high trichlorosilane gas concentration near the wafer surface due to the lower gas expansion in addition to the direct transport from the inlet. Fig. 8(c)-(C) contains the green coloured region indicating nearly 0.003 kmol m^{-3}, which does not exist in Fig. 8 (a)-(C).

Figure 10 shows the silicon epitaxial growth rate profile over the wafer at the rotation rates of 0, 10, 20 and 30 rpm. The epitaxial growth rate is normalized using that at 0 rpm and at the distance of half radius from the water center. The epitaxial growth rate profile is entirely very flat, because its difference over the wafer is less than 0.5 %. At the rotation rate of 0 and 10 rpm, the silicon epitaxial growth rate is nearly 1.4 $\mu m\ min^{-1}$. The increase in the wafer rotation rate induced an increase in the trichlorosilane gas concentration along with a simultaneous decrease in the hydrogen gas concentration. Thus, following equation (4), the silicon epitaxial growth rate at 30 rpm slightly decreases to 99 % of that at 0 rpm. This behaviour is consistent with that shown in Fig. 7.

Overall, at sufficiently high trichlorosilane gas concentrations resulting in a surface coverage of nearly 1, the slow wafer rotation at the rotation rate below 30 rpm has a considerable influence on the gas stream, the gas phase temperature and the trichlorosilane gas concentration near the wafer surface. The wafer rotation rate between several to 30 rpm is practical, by the calculation in this study and by the experiment that the specular epitaxial film surface was empirically produced.

3.3 Advantages of heavy gas through slim vertical gas channel

Based on the conclusions obtained in this study, the combination of a heavy gas and a slim vertical gas channel has practical advantages for the silicon epitaxial growth, as shown in Fig. 11.

(i) Quick transport: The trichlorosilane gas transport to the wafer surface is direct and quick following the downward flow produced by the heavy gas mixture containing the trichlorosilane gas at high concentrations. The heavy gas can produce downward natural convection to reach the entire surface of the small-sized wafer placed in the significantly slim gas channel. Even if entirely in a non-steady state at an early stage, an unstable condition does not have a significant influence on the epitaxial growth, because the surface is quickly and fully covered with the intermediate species, $SiCl_2$. Thus, the very quick manufacturing utilizing the non-steady state is possible.

(ii) Cold wall thermal condition: The cold wall thermal condition is produced by the downward flow of the heavy gas mixture. Particularly, a sufficiently cold gas phase can exist in the vicinity of the wafer surface. The surface chemical reaction only at the wafer surface produces the specular epitaxial film, because no silicon particle formation in the gas phase occurs. Simultaneously, because the parasitic silicon deposition is suppressed over the entire quartz tube wall, the reactor cleaning process can be skipped till the parasitic deposition on the wafer holder becomes thick.

These advantages were experimentally recognized and verified by the specular silicon epitaxial film surface, no parasitic deposition and the real-time process information, as reported elsewhere [24].

4. Conclusions

The combination of a heavy gas and a slim vertical gas channel was studied for the silicon chemical vapour deposition reactor in the Minimal Fab, by means of a numerical analysis taking into account the gas flow, heat and species transport, particularly over a wide range of trichlorosilane gas concentrations from 1% to 40 % in ambient hydrogen. A heavy and cold gas introduced from the top of the chamber was shown to quickly go downward to the hot wafer surface through the slim vertical gas channel, for achieving a quick process. While the main gas stream was asymmetric, the gas phase in the vicinity of the wafer surface was sufficiently cooled to produce a cold wall thermal condition allowing the stable trichlorosilane gas consumption only at the wafer surface. A slow wafer rotation, below 30 rpm, was shown to be sufficient for the small wafer.

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Figure captions

Figure 1 Chemical vapour deposition reactor for Minimal Fab.

Figure 2 Gas flow vectors calculated at the wafer surface temperature of 1000 ^{o}C, the inlet gas velocity of 0.004 m/s and the wafer rotation rate of 4 rpm. The trichlorosilane gas concentration at the inlet was (a) 1%, (b) 5 %, (c) 10 %, (d) 20 % and (e) 40 %.

Figure 3 Gas phase temperature, calculated at the wafer surface temperature of 1000 ^{o}C, the inlet gas velocity of 0.004 m/s and the wafer rotation rate of 4 rpm. The trichlorosilane gas concentration at the inlet was (a) 1%, (b) 5 %, (c) 10 %, (d) 20 % and (e) 40 %.

Figure 4 The gas phase temperature gradient in the vicinity of wafer surface at various trichlorosilane gas concentrations at the inlet calculated at the wafer surface temperature of 1000 ^{o}C, the inlet gas velocity of 0.004 m/s and the wafer rotation rate of 4 rpm.

Figure 5 Trichlorosilane gas concentration in the gas phase calculated at the wafer surface temperature of 1000 ^{o}C, the inlet gas velocity of 0.004 m/s and the wafer rotation rate of 4 rpm. The trichlorosilane gas concentration at the inlet was (a) 1%, (b) 5 %, (c) 10 %, (d) 20 % and (e) 40 %.

Figure 6 Surface coverage by the intermediate species at the silicon wafer surface at various trichlorosilane gas concentration at the inlet calculated at the wafer surface temperature of 1000 ^{o}C, the inlet gas velocity of 0.004 m/s and the wafer rotation rate of 4 rpm.

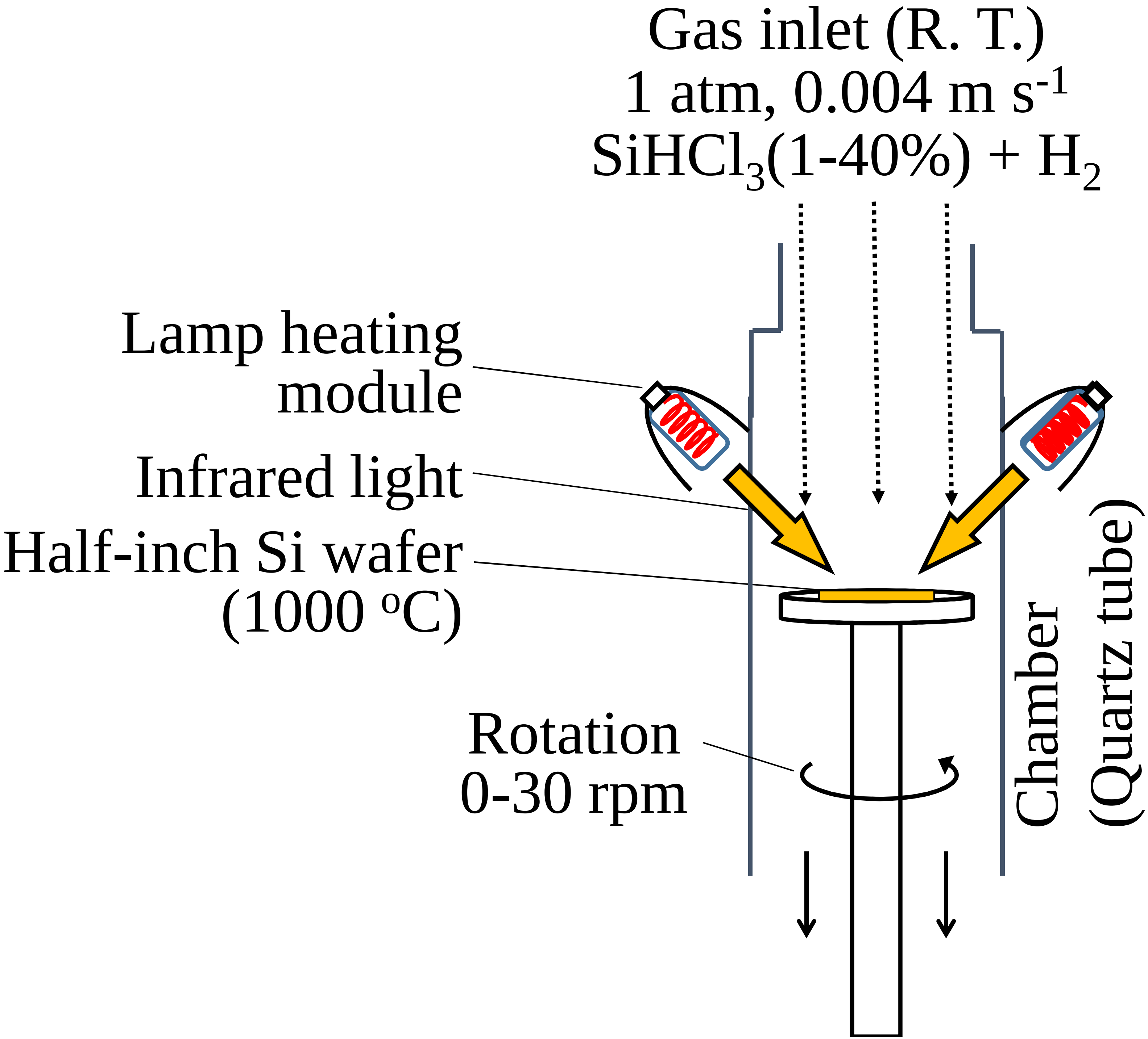
Figure 7 Epitaxial growth rate calculated at the wafer surface temperature of 1000 ^{o}C, the inlet gas velocity of 0.004 m/s and the wafer rotation rate of 4 rpm. The trichlorosilane gas concentration at the inlet was 1 - 40 %.

Figure 8 Gas phase temperature and trichlorosilane gas concentration near the wafer calculated at the wafer surface temperature of 1000 ^{o}C, the inlet gas velocity of 0.004 m/s and the wafer rotation rates of 0, 20 and 30 rpm. The trichlorosilane gas concentration at the inlet was 15 %.

Figure 9 The gas phase temperature gradient in the vicinity of wafer surface at various wafer rotation rates. The trichlorosilane gas concentrations at the inlet was 15%. The wafer surface temperature was 1000 ^{o}C. The inlet gas velocity was 0.004 m/s.

Figure 10 Epitaxial growth rate profile calculated at the various wafer rotation rates. The growth rates were normalized using the value at the wafer center and at 30 rpm. The wafer surface temperature, trichlorosilane gas concentration at the inlet and the gas velocity at the inlet were 1000 ^{o}C, 15 % and 0.004 m/s, respectively.

Figure 11 Advantages of slim vertical gas channel caused by heavy gas mixture.



Gas inlet (R. T.)
1 atm, 0.004 m s-1
SiHCl3(1-40%) + H2
Lamp heating module
Infrared light
Half-inch Si wafer (1000 oC)
Rotation 0-30 rpm
Chamber (Quartz tube)

Fig. 1

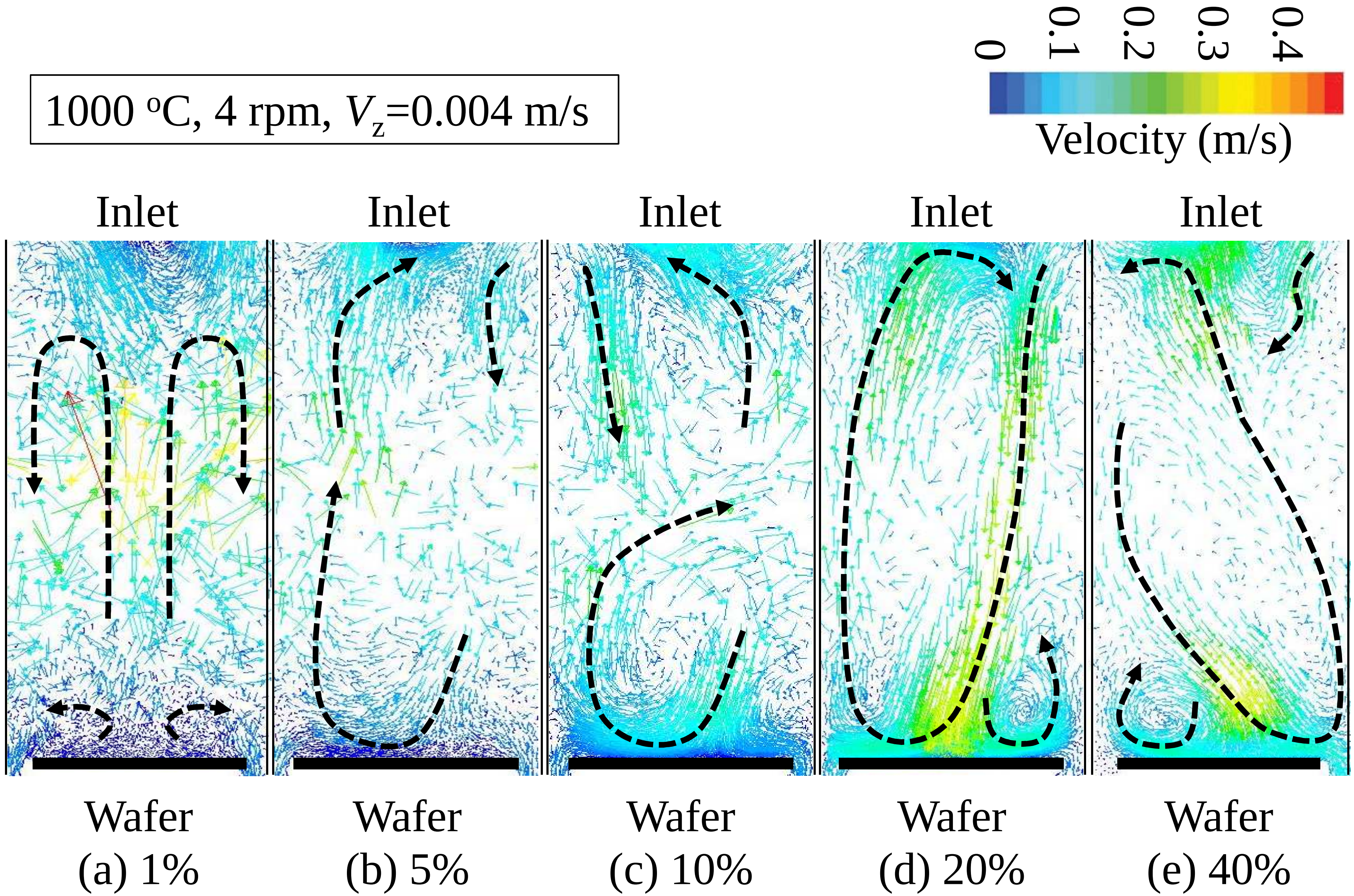
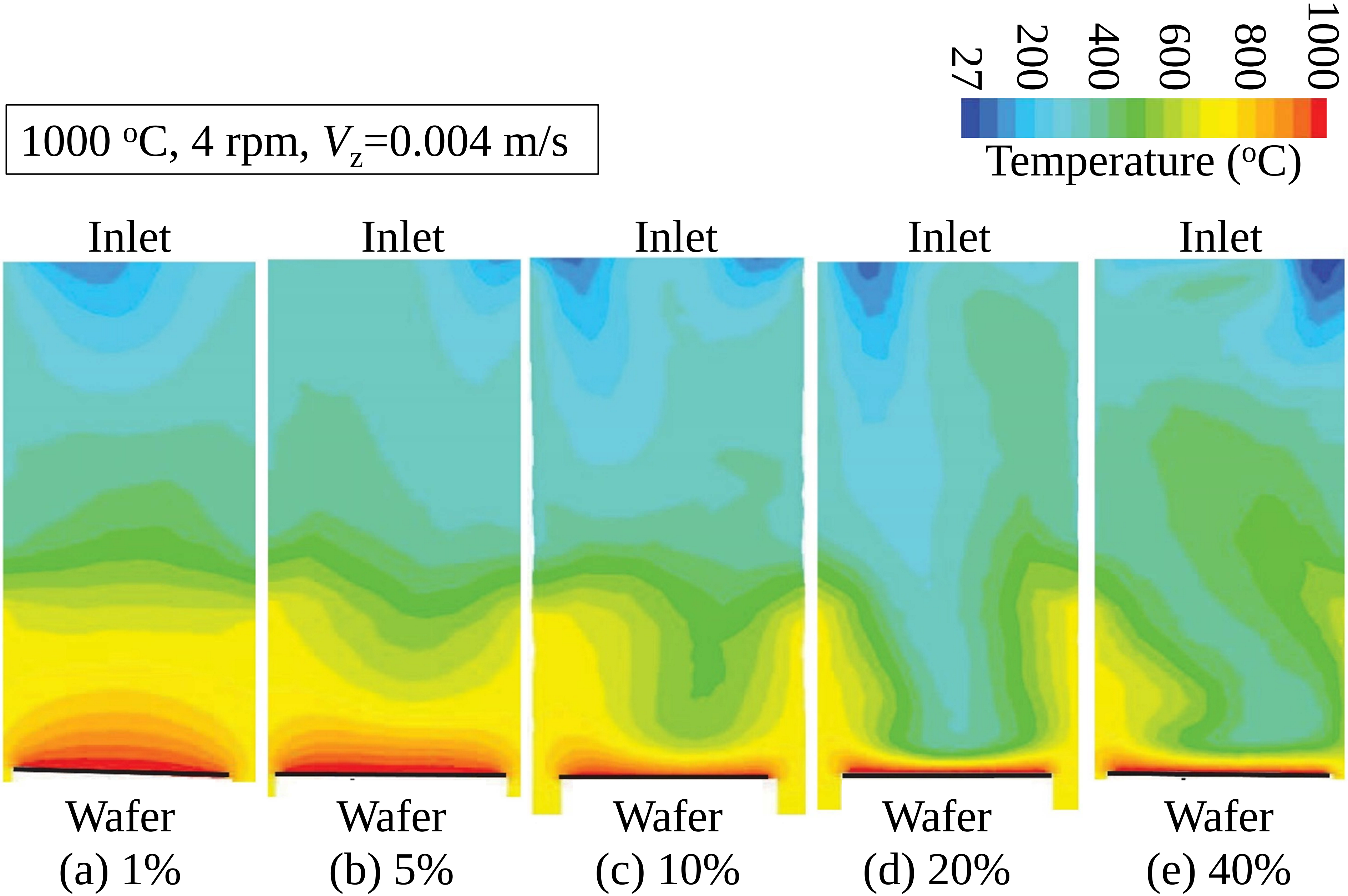

1000 °C, 4 rpm, Vz=0.004 m/s
0
0.1
0.2
0.3
0.4
Velocity (m/s)
Inlet
Inlet
Inlet
Inlet
Inlet
Wafer
(a) 1%
Wafer
(b) 5%
Wafer
(c) 10%
Wafer
(d) 20%
Wafer
(e) 40%

Fig. 2



1000 °C, 4 rpm, V_z=0.004 m/s
27
200
400
600
800
1000
Temperature (°C)
Inlet
Inlet
Inlet
Inlet
Inlet
Wafer
Wafer
Wafer
Wafer
Wafer
(a) 1%
(b) 5%
(c) 10%
(d) 20%
(e) 40%

Fig. 3

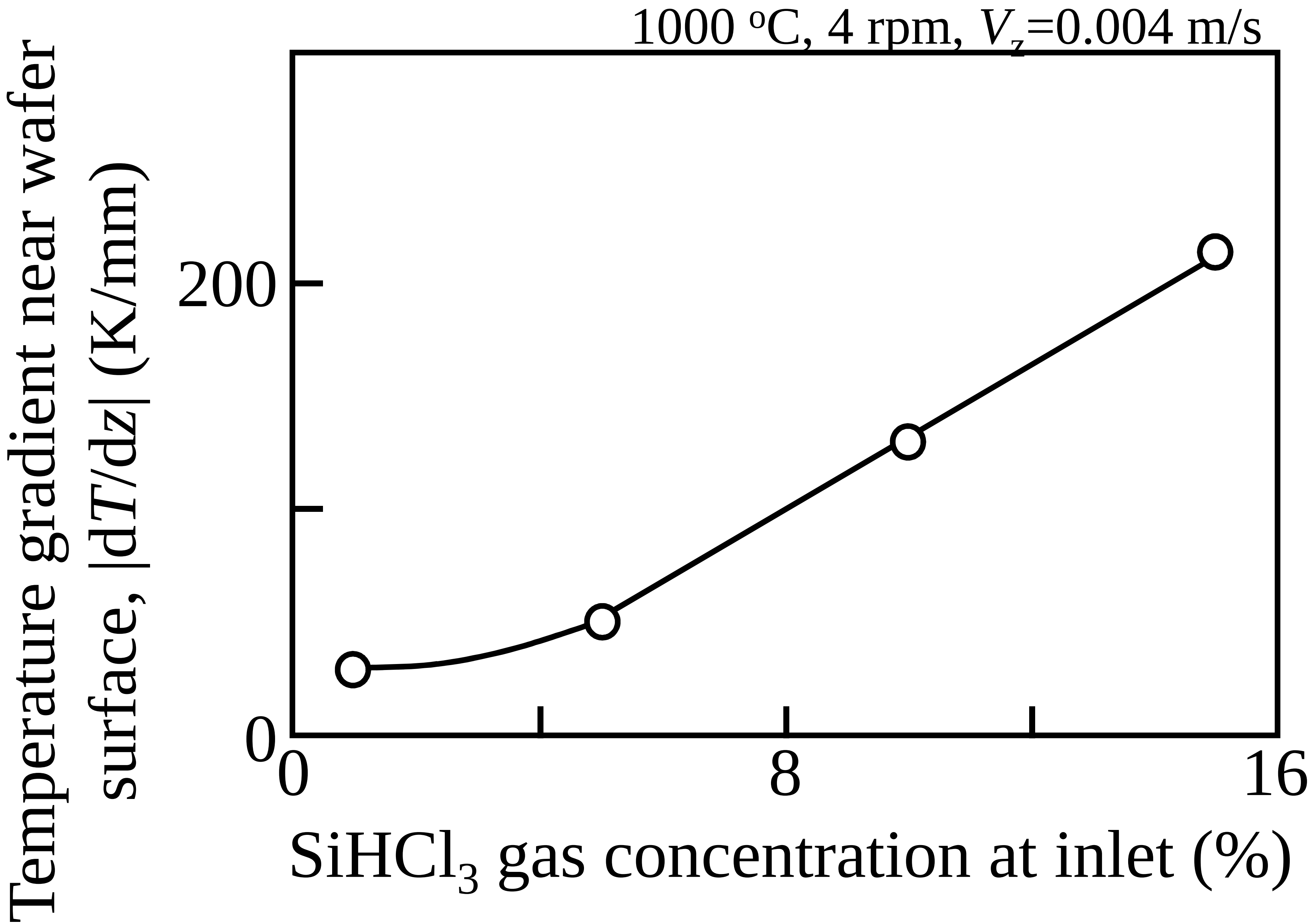
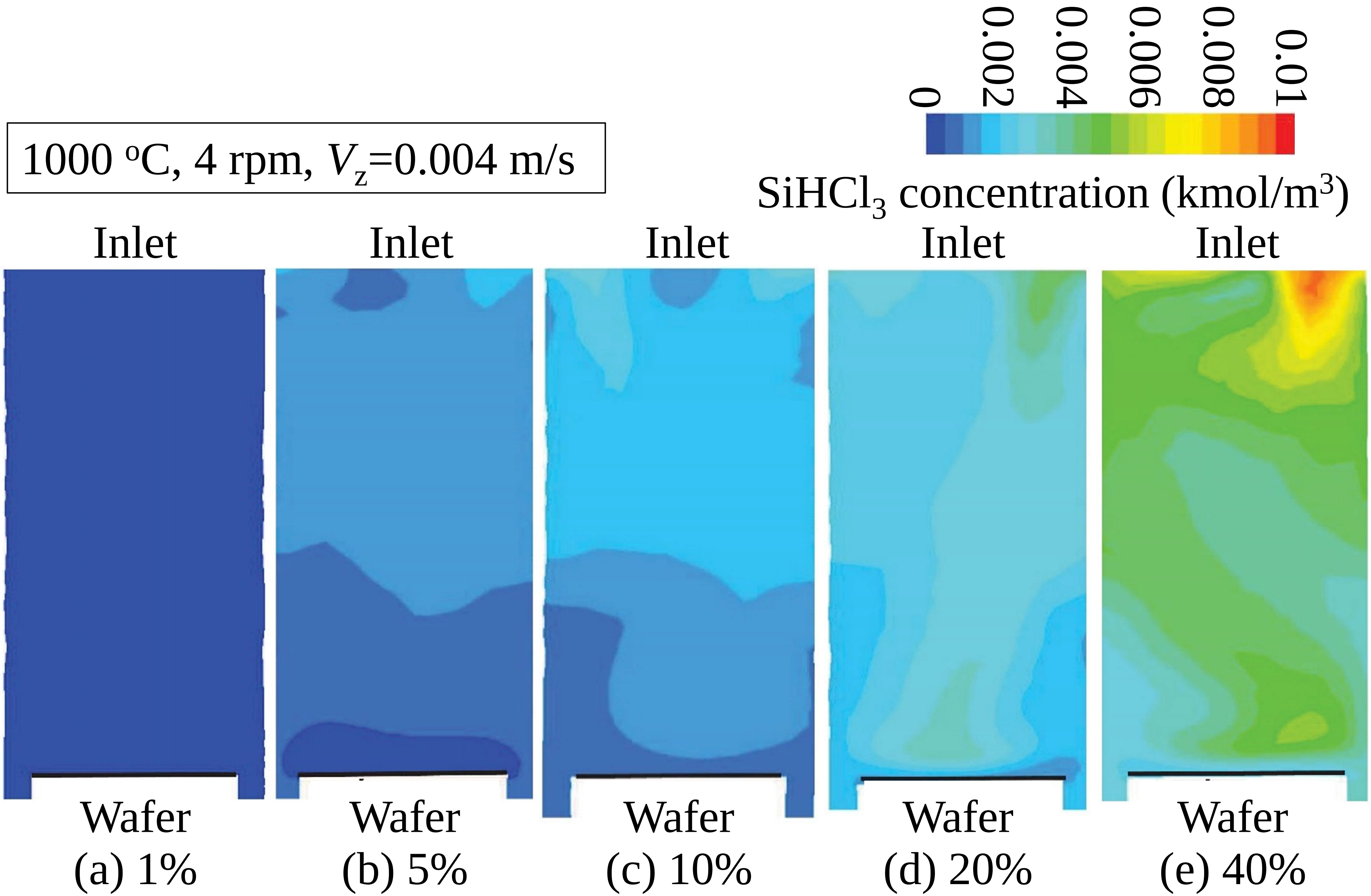

1000 °C, 4 rpm, V_z=0.004 m/s
Temperature gradient near wafer surface, |d*T*/dz| (K/mm)
200
0
0
8
16
SiHCl$_3$ gas concentration at inlet (%)

Fig. 4



1000 °C, 4 rpm, V_z=0.004 m/s
0
0.002
0.004
0.006
0.008
0.01
$SiHCl_3$ concentration (kmol/m^3)
Inlet
Inlet
Inlet
Inlet
Inlet
Wafer
Wafer
Wafer
Wafer
Wafer
(a) 1%
(b) 5%
(c) 10%
(d) 20%
(e) 40%

Fig. 5

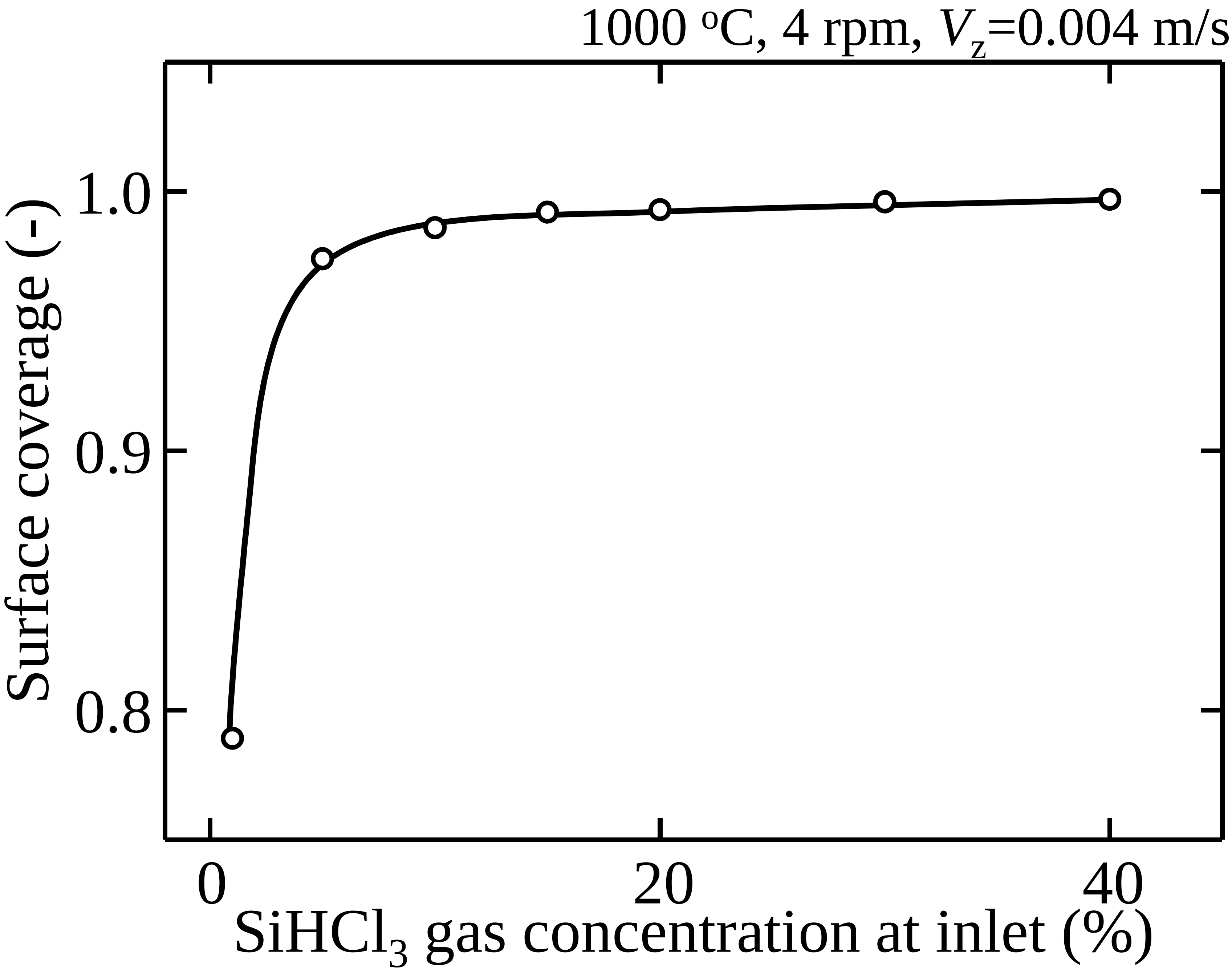

1000 °C, 4 rpm, V_z=0.004 m/s
Surface coverage (-)
1.0
0.9
0.8
0
20
40
$SiHCl_3$ gas concentration at inlet (%)

Fig. 6

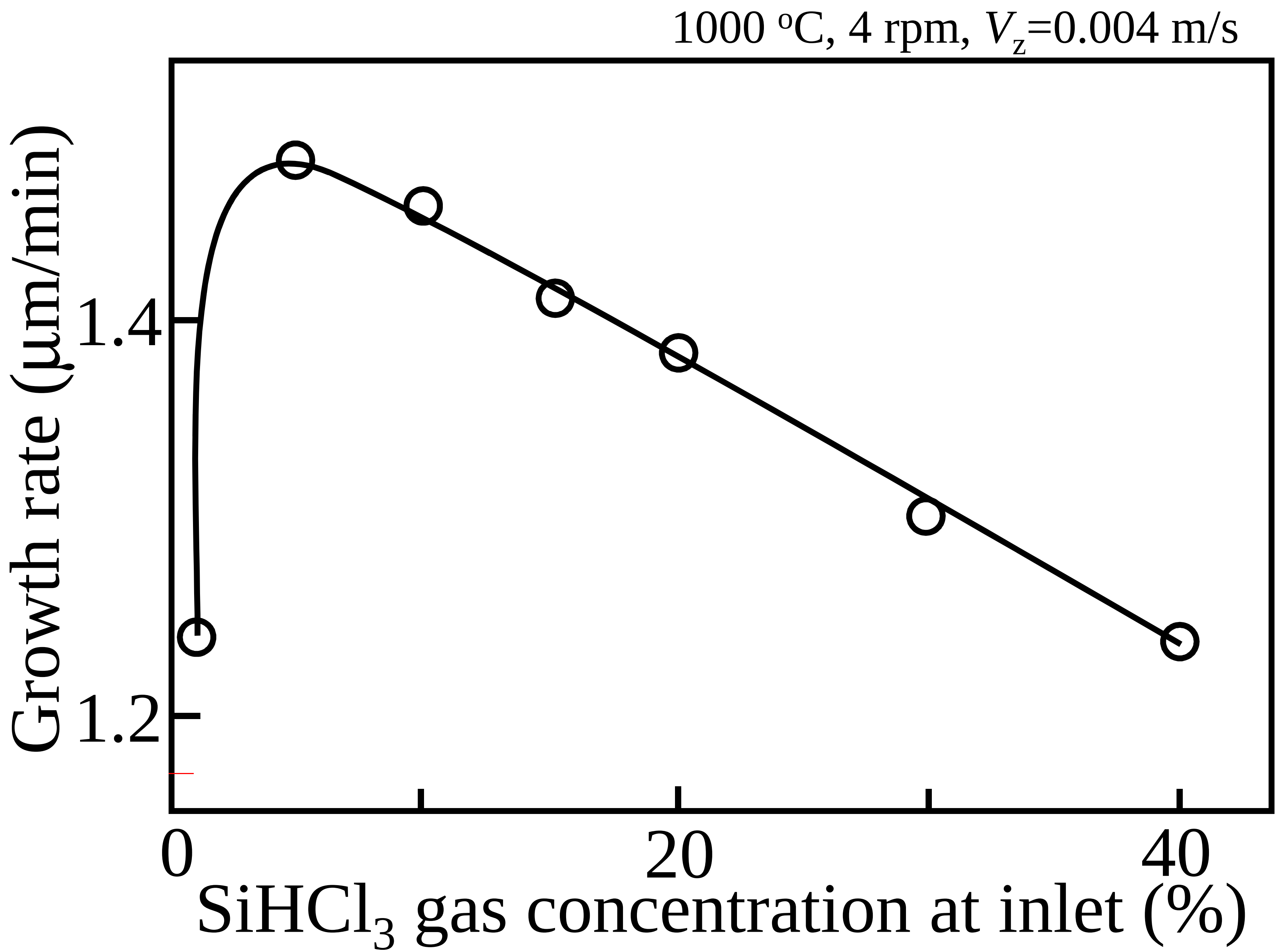
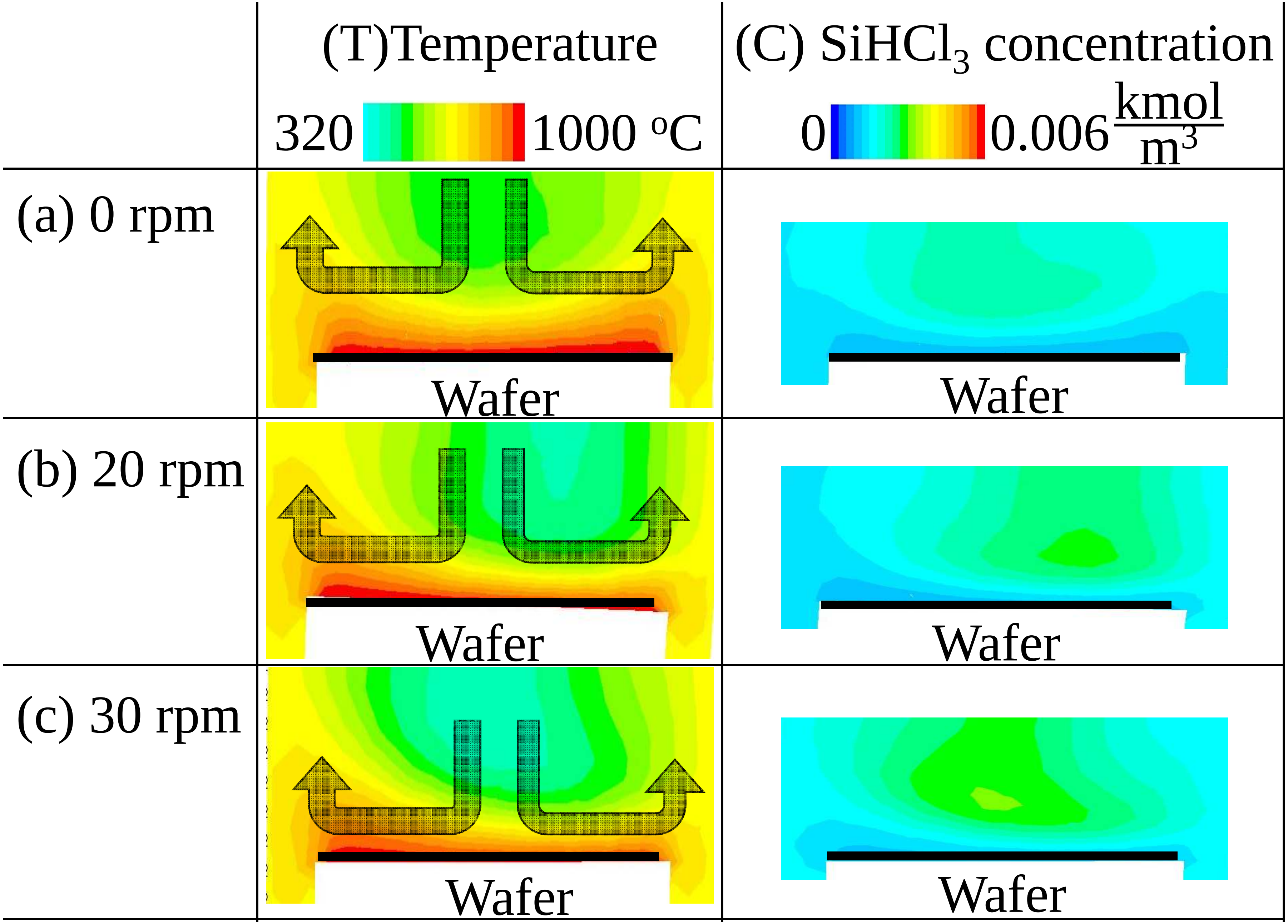
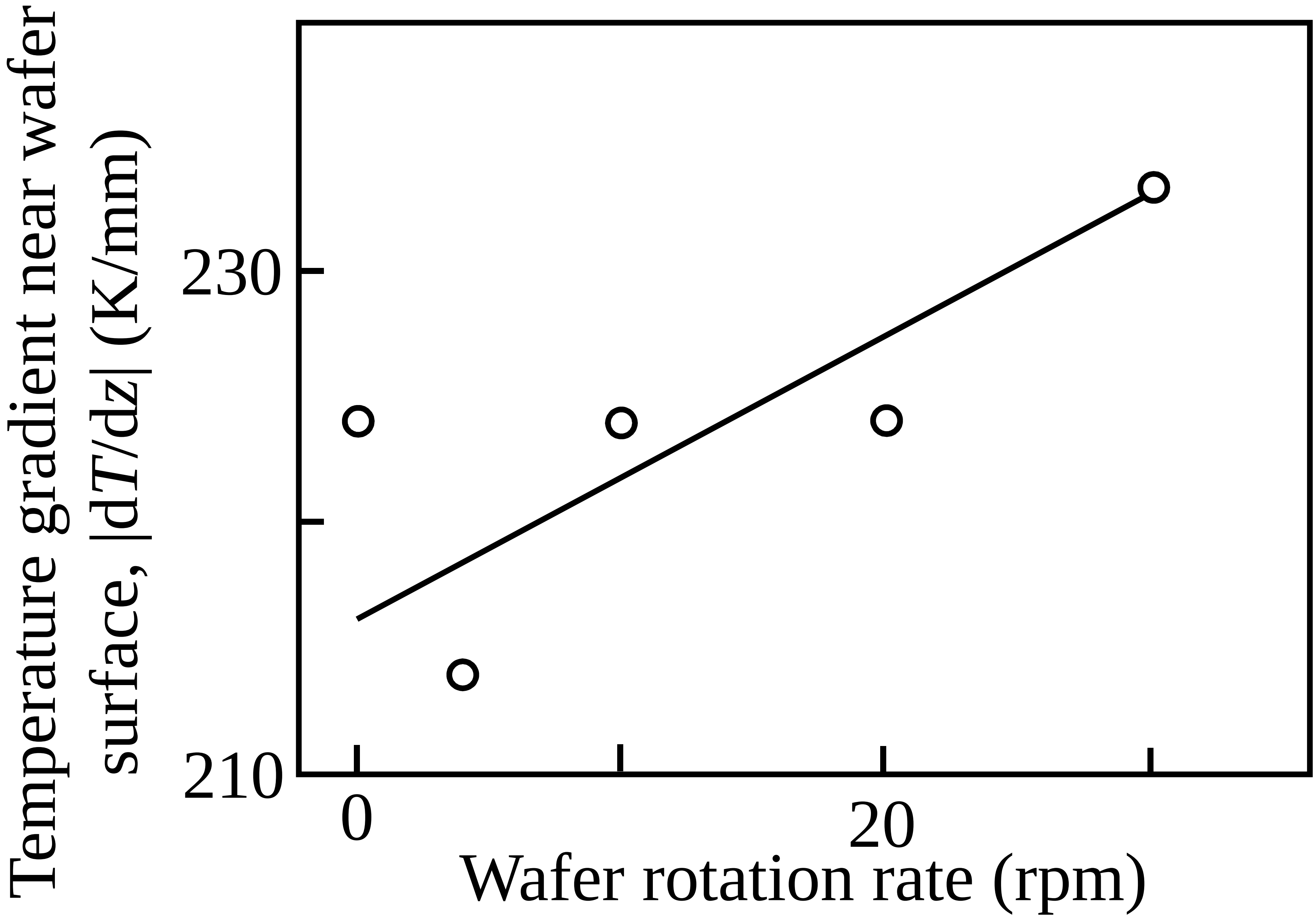

1000 °C, 4 rpm, V_z=0.004 m/s
Growth rate (μm/min)
1.4
1.2
0
20
40
$SiHCl_3$ gas concentration at inlet (%)

Fig. 7



1000 °C, $SiHCl_3$ at inlet = 15 %, V_z=0.004 m/s

Fig. 8



Temperature gradient near wafer surface, |dT/dz| (K/mm)
230
210
0
20
Wafer rotation rate (rpm)

Fig. 9

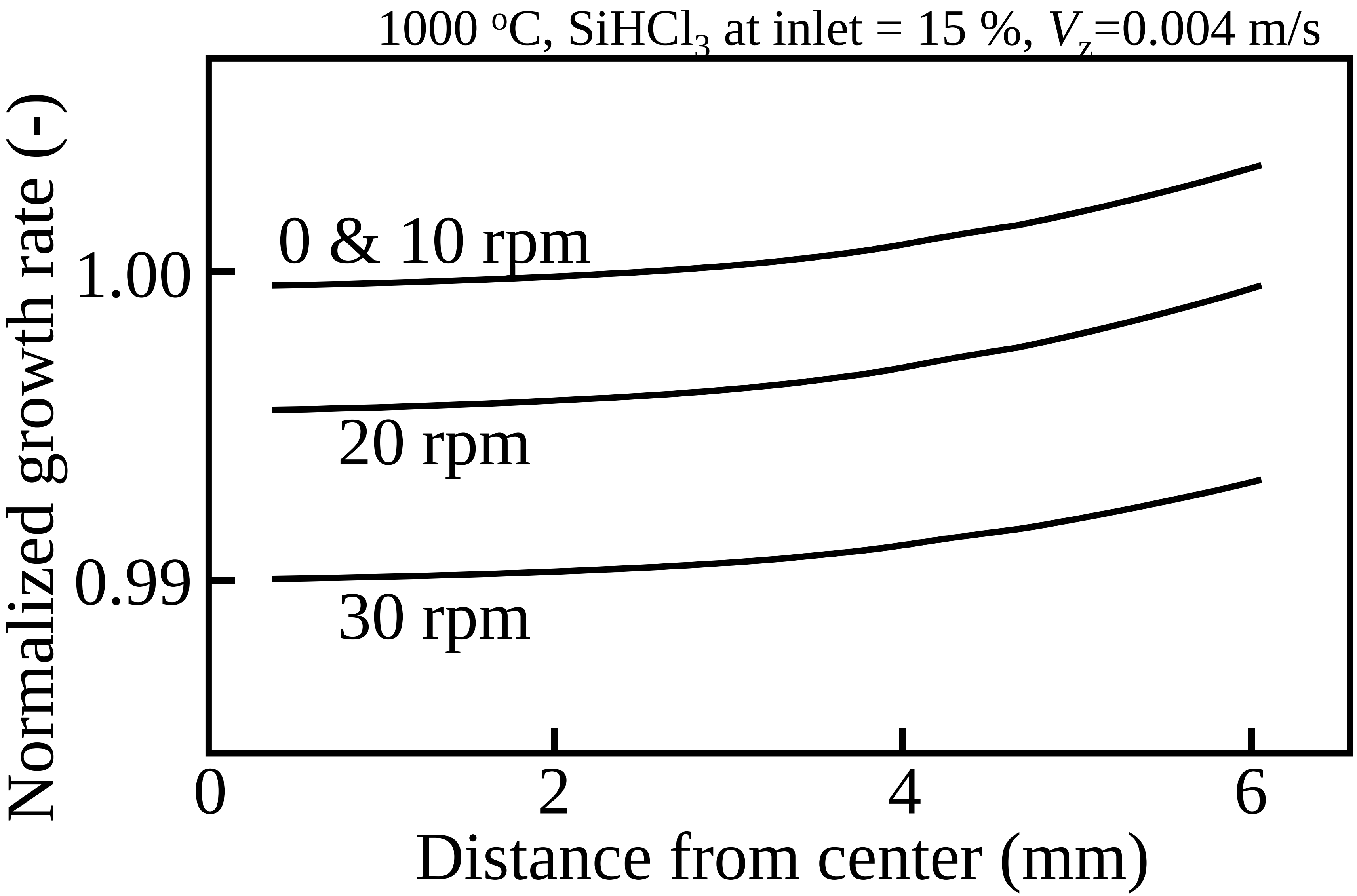
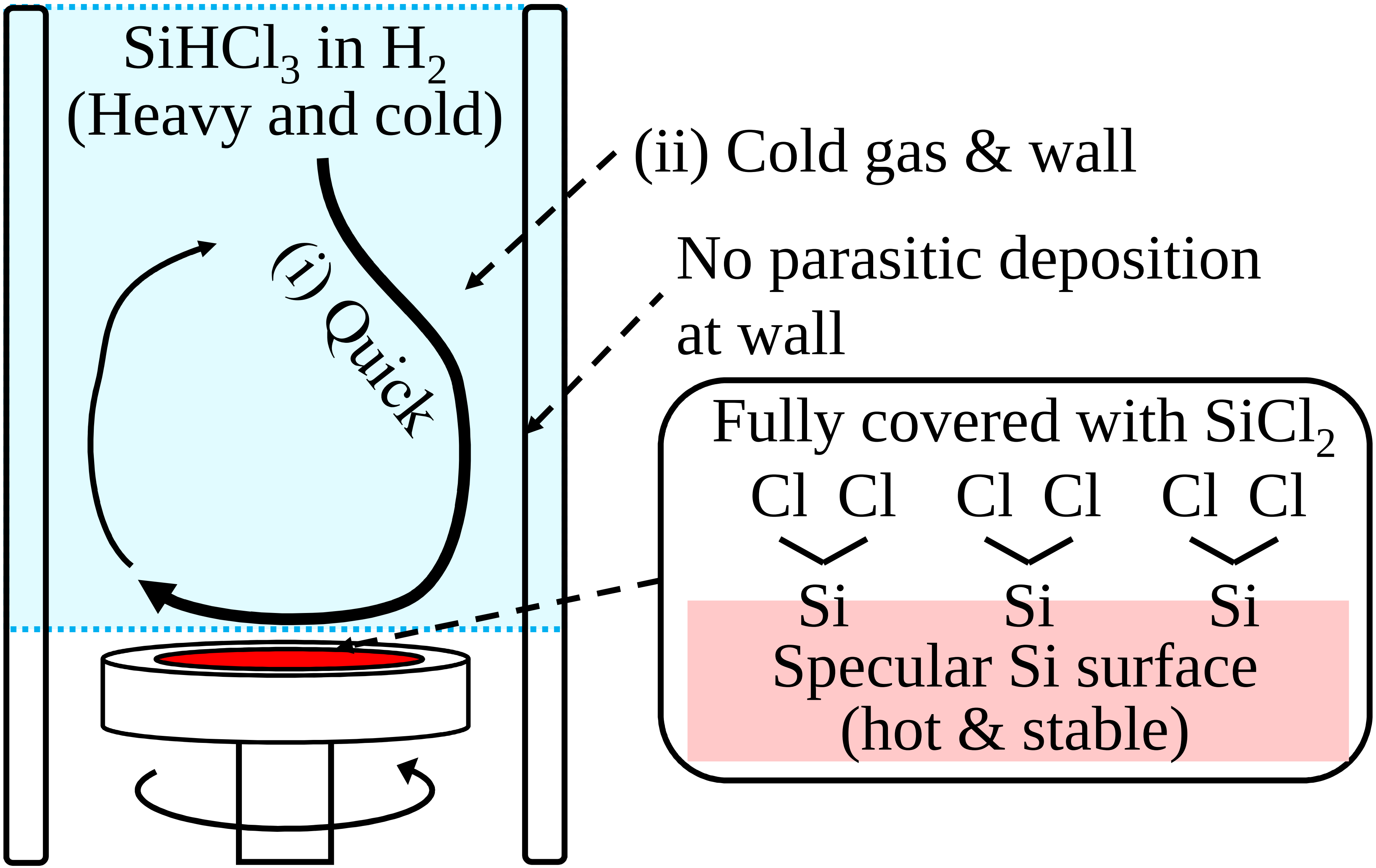

1000 °C, SiHCl3 at inlet = 15 %, Vz=0.004 m/s
Normalized growth rate (-)
1.00
0.99
0 & 10 rpm
20 rpm
30 rpm
0
2
4
6
Distance from center (mm)

Fig. 10



$SiHCl_3$ in H_2
(Heavy and cold)
(ii) Cold gas & wall
(i) Quick
No parasitic deposition
at wall
Fully covered with $SiCl_2$
Cl Cl Cl Cl Cl Cl
Si Si Si
Specular Si surface
(hot & stable)

Fig. 11