Technology

Simulation of Material Gas Supply System for Semiconductors Using Surrogate Model

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1. Introduction

We have been working on the development of a material gas supply system for semiconductors using solid materials [1]. This system fills a cylinder with solid material at room temperature and pressure, heats it with a heater installed around the cylinder to vaporize the solid material, and supplies it as material gas for semiconductors.

It is necessary for this system to maintain the gas-phase pressure in the cylinder at a predetermined pressure to ensure a stable supply of material gas for semiconductors. To do so, controlling the heating of the cylinder by the heaters appropriately is important. For example, heating can be controlled by changing the heater arrangement (number of heaters). However, experimenting with all combinations of heater arrangements is not realistic due to the too large number of combinations and the limited cost and time involved.

Therefore, in our study to be presented in this paper, we assumed multiple heater arrangements and used 1D simulation (a simulation in which the behavior of fluid pressure and temperature is represented by a simple mathematical model such as a simultaneous differential equation) [2] in designing heaters to understand the behaviors of the gas-phase pressure in the cylinder depending on various arrangements, and used this simulation to examine the heater arrangement. We used Modelica language (OpenModelica Ver. 1.18.1) [3] for the 1D simulation.

2. Issue and solution of 1D simulation

2.1 Issue of 1D simulation

Figure 1 shows the change in gas-phase pressure over time. In the figure, the "Experimental result" is the actual gas-phase pressure when the cylinder is heated under certain conditions in a supply experiment using this system, the "Saturated vapor pressure" is the gas-phase pressure obtained from the approximate formula of the saturated vapor pressure for the solid material, and the "Surrogate model" is the gas-phase pressure obtained from a surrogate model described below.

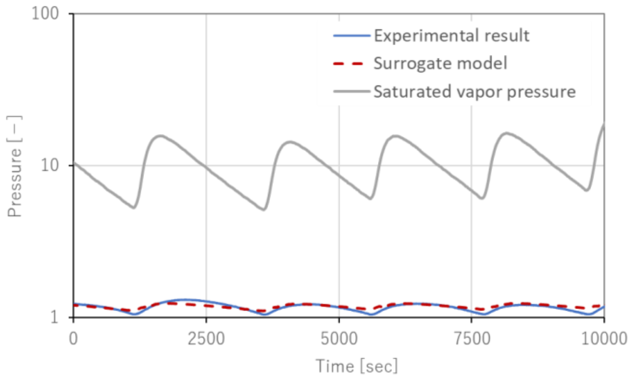

Figure 1　Examination result of gas-phase pressure estimation

The wavy behavior shown by the "Experimental result" is due to the effect of the heater temperature fluctuations caused by heater ON-OFF control for maintaining the gas-phase pressure in the cylinder. In Figure 1, the gas-phase pressure is normalized and displayed in logarithmic scale for visibility. Initially, it was assumed that the gas-phase pressure in the cylinder would equal the saturated vapor pressure, but as shown in Figure 1, the "Experimental result" and the "Saturated vapor pressure" differed significantly.

2.2 Solution

To address the above-mentioned issue, in this study, we estimated the gas-phase pressure using a surrogate model instead of the saturated vapor pressure and performed 1D simulation commensurate with the "Experimental result".

In general, a surrogate model is a model that finds a law between known explanatory and objective variables based on existing data to predict an unknown objective variable using the found law [4]. This law can be found by

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response surface methods using approximate functions or by machine learning.

In this study, we obtained approximately 100,000 samples of combinations of two explanatory variables (two gas-phase temperatures in the cylinder) and objective function (one gas-phase pressure in the cylinder) from the experimental results of two cases to generate response surfaces using a second-order polynomial approximation. For the generation of response surfaces, a general-purpose design exploration tool, Simcenter HEEDS Ver. 2021.2 [5]), was used.

An important point in generating a surrogate model is to perform pre-processing to eliminate noise and outliers in the experimental result. Due to the pre-processing, the accuracy of the surrogate model was improved, and the output gas-phase pressure accuracy with a coefficient of determination (R2) of 0.8 or higher was achieved. As shown in Figure 1, the "Surrogate model" and the "Experimental result" are generally in agreement with each other.

3. Mathematical model for 1D simulation

In the 1D simulation of this study, it is assumed that a cylinder filled with solid material is covered with a heater, thereby increasing the temperature inside the cylinder, and the vaporized gas is supplied from a single point of the cylinder. It is also assumed that the cylinder is a hollow cylinder, and that the inside of the cylinder consists of a region where the solid material exists uniformly (solid phase) and a region where the gas vaporized from the solid material exists uniformly (gas phase).

3.1 Mathematical model for mass balance

Figure 2(a) shows a schematic of the mass relationship in the cylinder. The mass in the cylinder is the sum of the mass of the gas phase m_g and the mass of the solid phase m_s. Equation (1) and Equation (2) represent the change of each mass over time.

$$\frac{dm_g}{dt} = -(F_{\mathrm{sup}} - F_{\mathrm{vp}}) \tag{1}$$

$$\frac{dm_s}{dt} = -F_{\mathrm{vp}} \tag{2}$$

Where, F_{sup} is the supply amount and F_{vp} is the vapor amount. The mass of the gas phase m_g and the mass of the solid phase m_s are expressed in terms of the volume of the solid phase Vs as in Equation (3) and Equation (4).

$$m_g = \rho_g(V_T - V_s) \tag{3}$$

$$m_s = \rho_s V_s \tag{4}$$

Where, V_T is the volume in the cylinder and is constant. ρ_g is the density of the gas phase and ρ_s is the density of the solid phase.

3.2 Mathematical model for energy balance

Figure 2(b) shows a schematic of the energy relationship in the cylinder. Equation (5) represents the change of the total energy in the cylinder over a small time period.

$$\frac{dH_T}{dt} = Q_{zg} + Q_{rg} + Q_{zs} + Q_{rs} - (Q_{g,\mathrm{out}} + Q_{s,\mathrm{out}}) \tag{5}$$

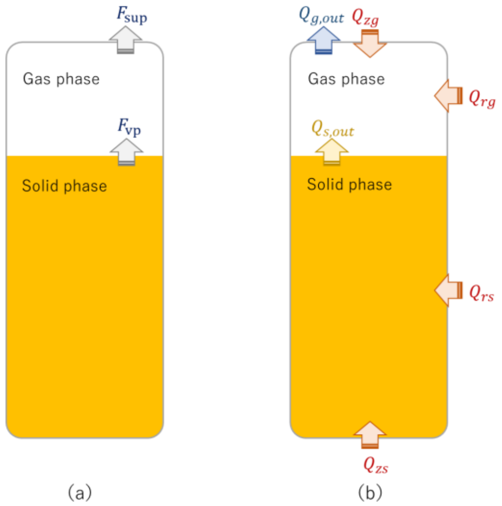

Figure 2 (a) Schematic of mass relationship (b) Schematic of energy relationship

Where, H_T is the total energy (sum of gas-phase and solid-phase enthalpies). Q_{zg} is the energy gained by the gas phase from the top of the cylinder, Q_{rg} is the energy gained by the gas phase from the side of the cylinder, Q_{zs} is the energy gained by the solid phase from the bottom of the cylinder, Q_{rs} is the energy gained by the solid phase from the side of the cylinder, $Q_{g,out}$ is the energy lost by the gas phase due to supply, and $Q_{s,out}$ is the energy lost by the solid phase due to vaporization. Energies (heat transfer quantity) Q_{zg}, Q_{rg}, Q_{zs}, and Q_{rs} in Equation (5) are defined by the summary heat transfer coefficient, heat transfer area, and temperature difference (between the gas-phase temperature and cylinder temperature, and the solid-phase temperature and cylinder temperature).

The gas-phase temperature is calculated by solving the mathematical model shown in Equations (1) to (5), and the gas-phase pressure is calculated by inputting the gas-phase temperature into the surrogate model.

4. 1D simulation calculation example

As mentioned above, there are many combinations of heater arrangements. By assuming a heater arrangement that can be designed or manufactured and conducting 1D simulation, limited experimental costs and time for heater arrangement examinations can be effectively utilized.

Figure 3 shows examples of heater arrangement types. The arrows in the figure represent the heating by each heater, and the higher the number, the higher the heater temperature. L1, L2, and L3 in the figure represent the width of the heater installed on the side of the cylinder for each arrangement type.

Figure 4 shows the simulation result of the gas-phase pressure for each heater arrangement type. From the simulation results, it was found that there was no significant difference in the gas-phase pressure between the assumed heater arrangements. Therefore, we selected the type 1 heater arrangement, which can be manufactured at fewer man-hours and a lower cost, for the actual supply experiment.

We conducted a supply experiment using the heater arrangement type 1 and compared the result with the 1D simulation result. In the supply experiment, we confirmed that stable supply was achieved from start to finish. Figure 5 shows the change in the gas-phase pressure over time. The "Experimental result" is the result of the experiment with the heater arrangement type 1, the "Simulation result" is the result of the simulation with the heater arrangement type 1 described earlier, and the "Average value" is the average of the gas-phase pressure during one ON-OFF control of the heater in the experimental result. As in Figure1, the experimental result shows the wavy behavior due to the effect of the heater temperature fluctuations caused by the heater ON-OFF control for maintaining the gas-phase pressure in the cylinder.

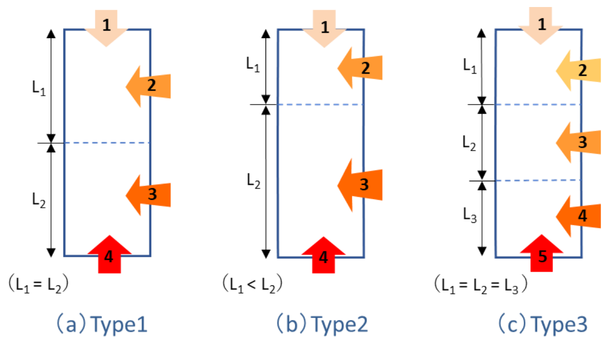

Figure 3　Examples of heater arrangement types

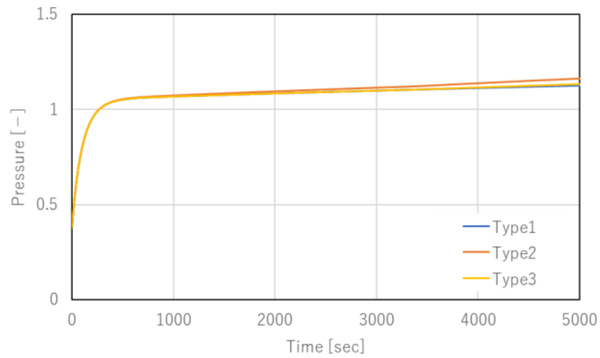

Figure 4　Simulation result of each heater arrangement type

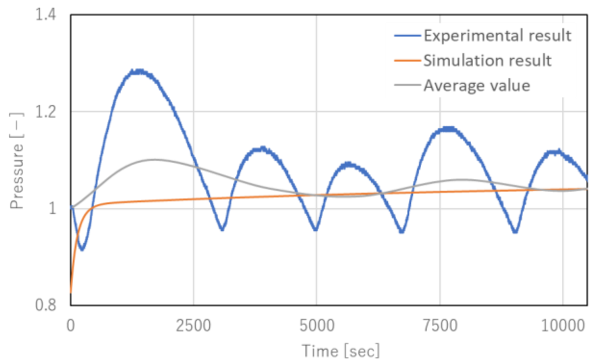

Figure 5　Experimental result and simulation result of type 1

On the other hand, the simulation result, which is calculated by a surrogate model with the assumption that the cylinder temperature is constant when heated by the heaters, shows estimated values with gentle behavior. Comparing the experimental result and the simulation result, the error shown by the experimental result with respect to the average gas-phase pressure during a single heater ON-OFF control was within about 3%, except for the behavior up to about 3000 seconds after the start of the supply. Thus, we were able to generally capture the behavior of the gas-phase pressure by the 1D simulation.

5. Conclusion

In this study, with regard to the material gas supply system for semiconductors using solid materials, we conducted a 1D simulation in order to roughly capture the behavior of the gas phase pressure when the vessel is heated by a heater and the gas is supplied, and aimed to study the heater arrangement.

In the calculation of gas-phase pressure in 1D simulation, there was a problem that the saturated vapor pressure differed significantly from the experimental results.

To solve this issue, we used a surrogate model generated from experimental results to estimate the gas-phase pressure, and incorporated the surrogate model into the mathematical model of the 1D simulation. Therefore, we were able to run the simulation that was consistent with the experimental results. In addition, we determined the heater arrangement by utilizing the 1D simulation without conducting experiments on all of the many heater arrangement types.

In this way, we have been developing efficient systems by utilizing 1D simulation.

References

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