Convective Flow Simulation of Supercritical Carbon Dioxide Fluid in Cold Wall Type Reactor

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ABSTRAT

Deposition method using a supercritical carbon dioxide fluid has been proposed and developed along with the miniaturization of fabrication process for semiconductor and MEMS devices. It has been reported that the convection has considerable effect on deposition. To understand the convective flow in a deposition reactor, we performed a computational fluid simulation of supercritical carbon dioxide fluid. The availability of the supercritical fluid simulation is evaluated in this study, and the fluid simulation will be useful for the design of a deposition reactor.

INTRODUCTION

Novel thin film fabrication method called supercritical fluid deposition (SCFD), which is a reduction/oxidation of metal organics with hydrogen in supercritical carbon dioxide ($scCO_2$), has been proposed [1-3]. This method realizes conformal deposition and complete gap-filling of metals and metal oxides onto high aspect ratio features, which is required by the electronic device fabrication such as ULSI and MEMS. Cold wall type SCFD reactor was proposed to prevent the unwilling reaction in the fluid, where a substrate was heated up in order to facilitate the deposition reaction, and a wall of the reactor was kept at relatively low temperature. However, in this configuration of the reactor, a temperature gradient of the substrate and surrounding fluid is apt to create a convective flow and/or turbulence due to high molecular density and low viscosity of supercritical fluid. We have found the turbulence generated in the cold wall reactor caused non-uniform film on the substrate during SiO_2 deposition. Accordingly, understanding of the mechanism and optimization of deposition conditions are pressing issue. In this paper, behavior of the convective flow depending on the deposition conditions are simulated using computational fluid dynamics (CFD). Firstly, fluid turbulence caused by the natural convection near the substrate was examined. Secondly, the effect of the forced convective flow on the natural convective flow was calculated, that is, global convective flow in the reactor with/without an inlet flow was evaluated.

SIMULATION SET UP

The deposition reactor (cold wall type reactor) is shown in Fig.1. In the deposition reactor in which a substrate is directly heated up with the installed heater, a convective flow is created by the temperature gradient of supercritical carbon dioxide fluid.

To evaluate the behavior of the convective flow in the deposition reactor, we use the ANSYS/FLUENT software. Solver type is selected as "Density Based Model" and Material property is set to be Carbon Dioxide which is defined in NIST (National Institute of Standards and Technology) Database. When the natural convection near the substrate is examined, we perform a transient fluid simulation to recognize a turbulent flow. On the other hand, the steady flow simulation is selected to evaluate the global convection in the deposition reactor. In this case, "Reynolds Stress Model (7 equations model) is used for the turbulence model.

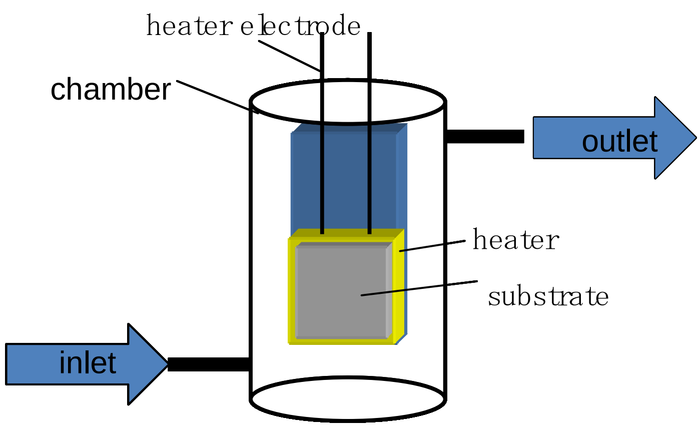
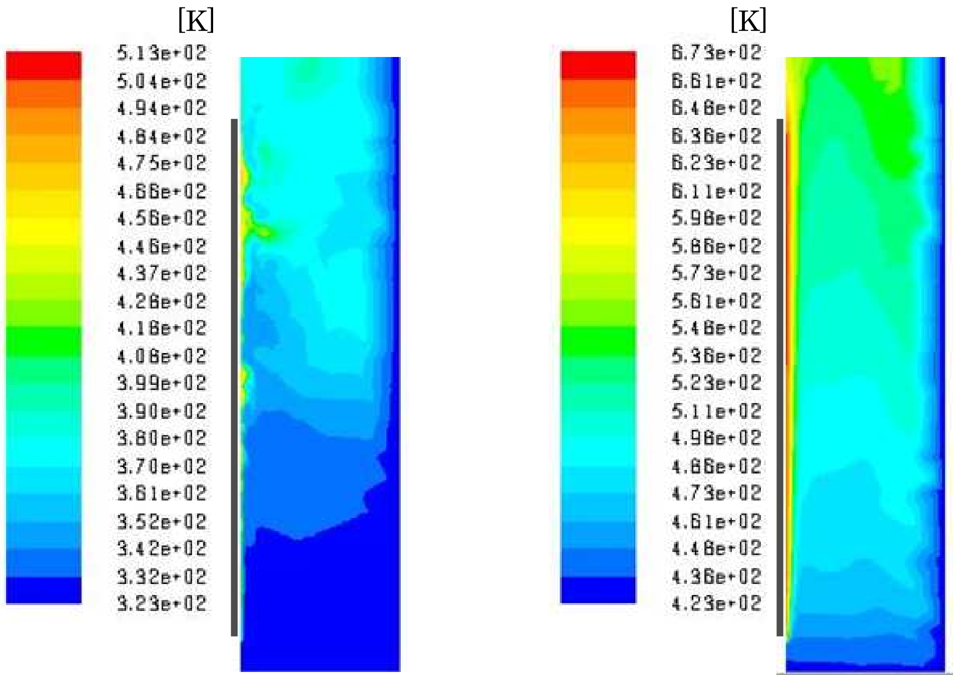


Figure 1. Schematic drawing of cold wall type reactor.

SIMULATION RESULTS

The results of transient supercritical fluid simulation near the substrate are shown in Fig.2. In this figure, the snapshots of the temperature distribution are shown when a flow is fully developed. The heater temperature and fluid pressure are set to be 200℃ and 15MPa on left figure. A flow is disturbed by the natural convection at the upper substrate, and turbulent flow arises. On the other hand, all area on the substrate are laminar flow when the heater temperature and fluid pressure are set to be 400℃ and 8MPa. These results are consistent with the findings of the deposition experiment (data not shown), suggesting that the turbulence caused by buoyancy near the substrate is the reason of the non-uniform film formation during SiO_2 deposition.



(a) 200℃, 15MPa (b) 400℃, 8MPa

Figure 2. Temperature distribution.

Fig.3 shows the simulation results of global convective flow in the reactor with an inlet. The temperature distribution is shown in the left side, and the pathline with a color of transit time on the substrate is shown in the right side. The heated supercritical carbon dioxide fluid drifts upward along the substrate, and the heated fluid is cooled down on the chamber wall. As a result, a global circulation flow appears in the reaction chamber. The temperature of the fluid near the substrate gradually increases from the bottom to top of the chamber. Although a fluid and a precursor are injected from the inlet pipe at the bottom of the chamber, it is found that the injected flow could not overcome the natural convection on the substrate, suggesting a linear velocity of the fluid supplied from the inlet was inferior to that of the natural convection. One possible solution to make the forced-convection-dominant flow is to employ a reactor with a minute cross-sectional area enabling the higher linear velocity of the supplying fluid, which is our further challenge.

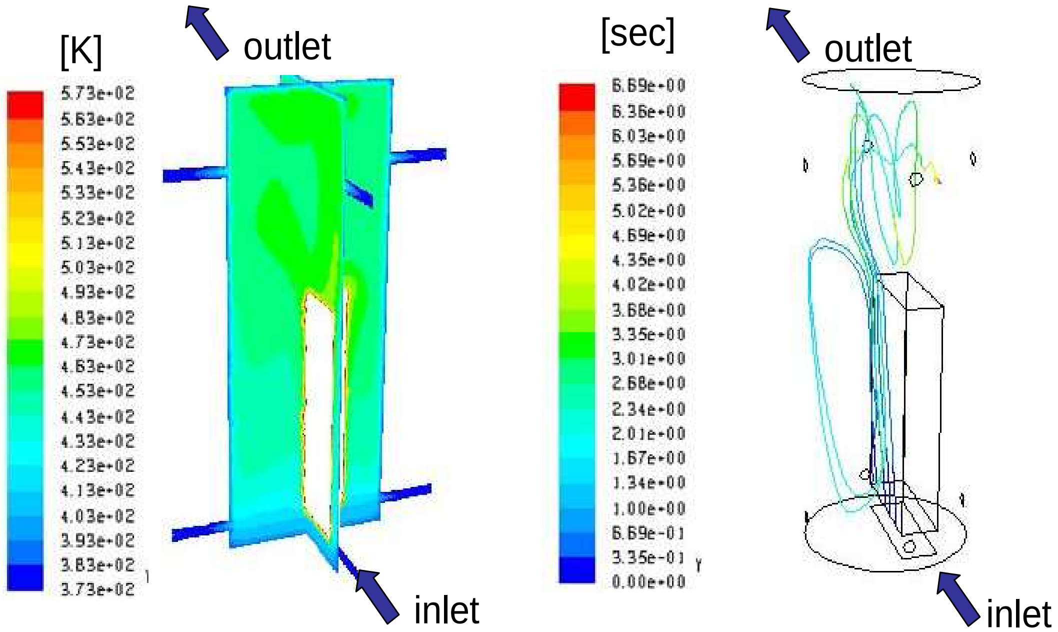


Figure 3. Temperature distribution and pathline.

CONCLUSION

The availability of the supercritical fluid simulation was evaluated in this study. The fluid simulation will be useful tool for the design of a deposition reactor.

ACKNOWLEDGEMENT

This work was supported by New Energy and Industrial Technology Development Organization (NEDO), Japan.

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