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Physics-Informed Neural Networksを用いた回転基板上の液膜流動予測

Prediction of liquid film flow on rotating wafers using Physics-Informed Neural Networks

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1. Introduction

In semiconductor manufacturing processes, the behavior of liquid films during wet processing is a critical factor that can ultimately lead to the degradation of device quality. The standard wet processing procedure involves dispensing a chemical solution onto a rotating wafer from a scanning nozzle to coat the entire surface. To determine the optimal application conditions for achieving the desired processing effect, simulating the liquid film flow on the rotating wafer is indispensable. However, predicting the flow of this thin film, especially with complex nozzle trajectories, is often impractical with general-purpose two-phase flow simulation methods like the Volume of Fluid (VOF) method, due to the prohibitive computational cost. On the surface of a rapidly rotating wafer, the centrifugal force is overwhelmingly dominant compared to gravitational force. This creates a unique situation where the fluid dynamics are governed primarily by surface tension, inertial forces, and viscous forces, effectively creating an environment analogous to microgravity. Understanding the behavior of thin films in such conditions is paramount. The challenges in simulating these flows necessitate more efficient computational approaches. To address this issue, this study explores two advanced computational approaches. The first is the introduction of the lubrication approximation to the governing equations to reduce calculation time 1). The lubrication approximation is a method that simplifies equations by leveraging the fact that the length-scale ratio between the direction parallel to the substrate and the film thickness direction is extremely small, allowing negligible terms to be ignored. Although this approximation is widely used for thin-film flows, its application to the wet processing problem has not yet been reported. The second approach involves using Physics-Informed Neural Networks (PINNs) 2), a machine learning method that embeds physical laws directly into the neural network. Similarly, the application of PINNs to the wet processing problem is a novel endeavor. In this paper, we apply both the lubrication approximation and PINNs to the wet processing problem. We report on the verification of their effectiveness and validity as efficient and accurate methods for simulating thin-film dynamics in this specialized, microgravity-like environment.

2. Model Formulation

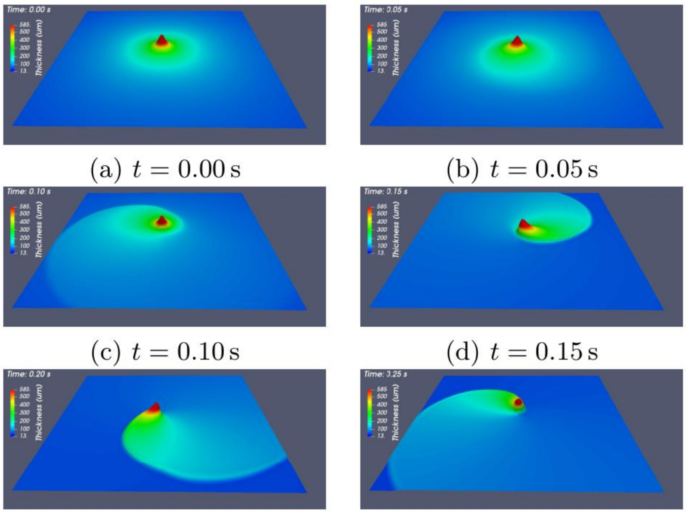
In this study, a physical model is constructed to describe the process in which a liquid dispensed onto a rotating wafer forms a thin film. The model is derived by simplifying the Navier–Stokes equations based on the lubrication approximation.

2.1. Governing Equation

Under the assumptions of the lubrication approximation, the spatio-temporal variation of the liquid film thickness h is described by a single partial differential equation. This equation is valid under the condition that the film thickness is much smaller than the wafer radius ($h \ll R$). For computational efficiency, the model considers gravity, centrifugal force, and liquid supply from the dispensing nozzle (source term) as the primary

Table 1. List of variables and constants

Symbol	Description	Units
h	Liquid film thickness	m
t	Time	s
$\boldsymbol{x}$	Position vector on the wafer	m
∇	Nabla operator	$1/\mathrm{m}$
ρ	Density of the liquid	kg/m^3
g	Gravitational acceleration	m/s^2
μ	Viscosity of the liquid	Pas
r	Distance from the center of rotation	m
$\boldsymbol{e}_r = x/r\boldsymbol{e}_x + y/r\boldsymbol{e}_y$	Radial direction vector	N.D.
ω	Angular velocity of the wafer	rad/s
$S(\boldsymbol{x}, t)$	Source term for the dispensing nozzle	m/s



(a) $t = 0.00\,\mathrm{s}$ (b) $t = 0.05\,\mathrm{s}$ (c) $t = 0.10\,\mathrm{s}$ (d) $t = 0.15\,\mathrm{s}$ (e) $t = 0.20\,\mathrm{s}$ (f) $t = 0.25\,\mathrm{s}$

Figure 1. Predicted film thickness during nozzle scanning using the lubrication approximation model

effects contributing to the film flow. The term corresponding to the Laplace pressure due to surface tension is neglected. Finally, the governing equation to be solved in this study is given by:

$$\frac{\partial h}{\partial t} = -\nabla \cdot \left[-\frac{\rho g h^3}{3\mu} \nabla h + \frac{\rho r \boldsymbol{e}_r \omega^2}{3\mu} h^3 \right] + S(\boldsymbol{x}, t), \tag{1}$$

where the variables and constants appearing in Eq. (1) are listed in **Table 1**.

2.2. Modeling of Dispensing Nozzle

The liquid supply from the nozzle is modeled as the source term $S(\boldsymbol{x}, t)$ in the governing equation Eq. (1). This term is a space- and time-dependent function that represents the supply of liquid at a specific position $\boldsymbol{x}$ and time t. In the spin coating process considered in this study, the nozzle performs linear scanning motion with respect to the stationary reference frame. However, because the wafer is rotating, the nozzle trajectory appears as a complex spiral when observed from the rotating reference frame fixed to the wafer. Accurately incorporating this complex trajectory into $S(\boldsymbol{x}, t)$ is critically important for predicting the final film thickness distribution.

3. Physics-Informed Neural Networks (PINNs)

Physics-Informed Neural Networks (PINNs) are a machine learning method that uses physical laws in the learning process. Unlike traditional methods, PINNs do not need a large amount of training data. Instead, they train the neural network to reduce the error between the prediction and the governing equation. This makes it possible to quickly predict the solution. In this study, we use PINNs to solve the governing equation shown in Section 2. By doing this, the neural network can predict the film thickness on the wafer.

4. Results

Figure 1 shows the predicted film thickness during nozzle scanning. The prediction was made using the lubrication-approximation-based model. The result shows that this model can describe the film thickness shape even when the nozzle is moving. This means the lubrication approximation is useful for practical spin-coating cases. We also used this model inside the PINNs method. The predictions from PINNs showed a similar trend. This suggests that combining physics-based models and machine learning can be useful for process simulation.

References

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