Simulation of thin water layers on wafer surfaces during bond chamber evacuation

COMSOL Conference 2023 – Computational Fluid Dynamics I

Max Huber, Andreas Zienert, and Jörg Schuster
Fraunhofer Institute for Electronic Nano Systems ENAS
October 25, 2023

Simulation of ultra-thin liquid layers on solid surfaces

Models and methods

Goal of the simulations

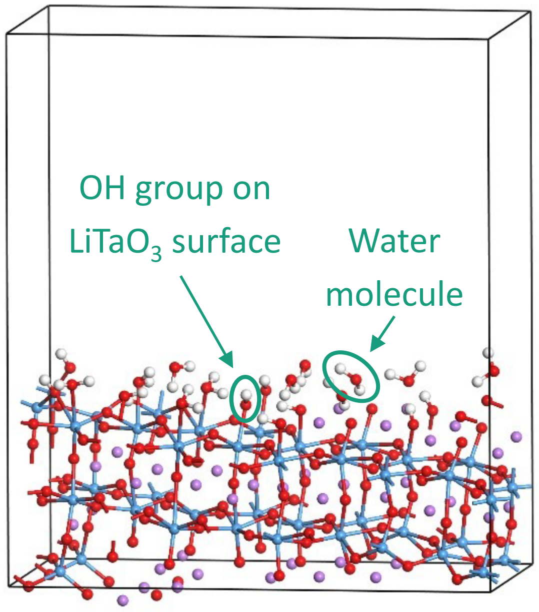
- Simulation of temporal evolution and stability of thin water layers on different wafer materials during complete technological process from wafer rinsing to bonding

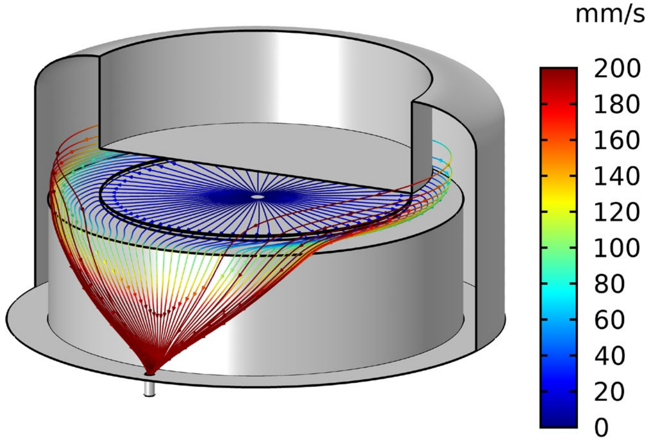
Models and methods depending on length scale and physical situation

- Interaction of water molecules with surfaces: density functional theory
- Evaporation during wafer handling: Diffusion-based continuum models
- Evacuation of bond chamber:
  - Different models depending on current pressure in the chamber (continuum flow, transitional flow, free molecular flow)
  - Analytical modeling of wafer temperature

Viable with COMSOL

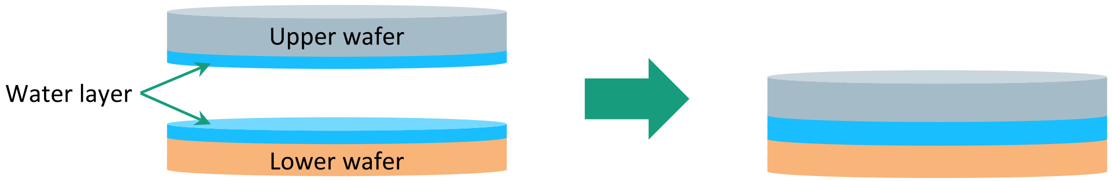
- Pre-treatments of the surface can be incorporated, e.g., spin drying after wafer rinsing





Example process: Direct wafer bonding

- Wafer rinsing → Handling → Pump down



Modeling the temporal evolution of the layer from rinsing to evacuation

Which steps are needed and what is the idea behind the models?

1

Spin drying of wafers
Simple model based on balance of forces to estimate initial water layer thickness [1].

---

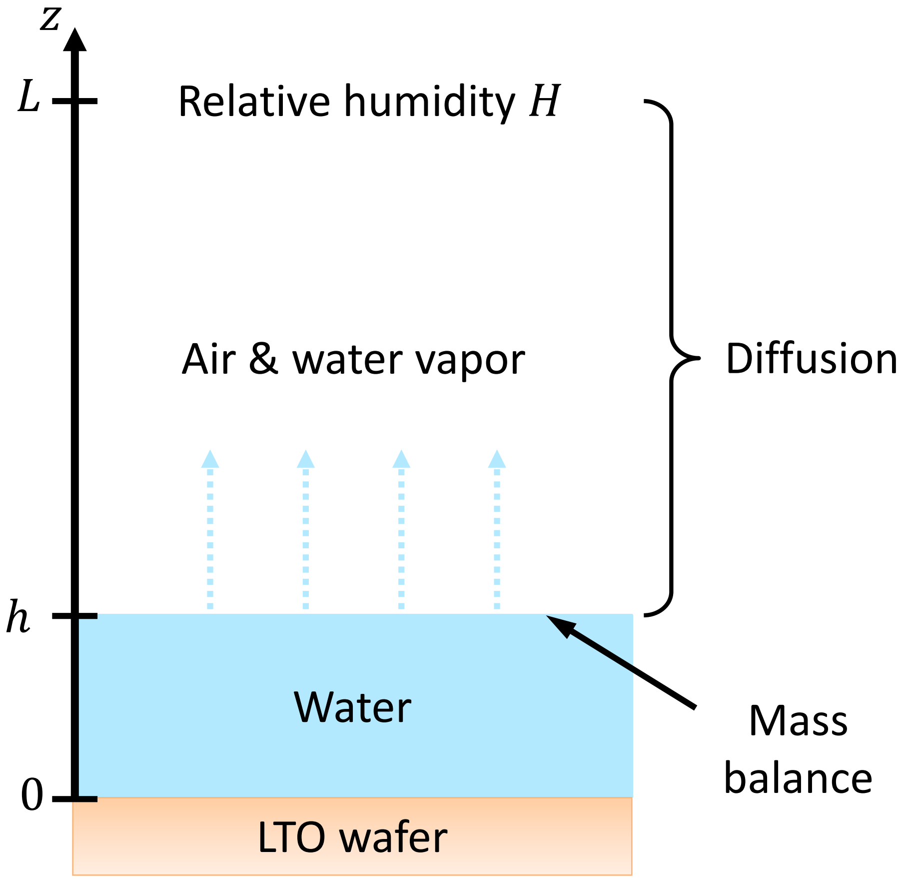
[1] A. G. Emslie et al.: J. Appl. Phys. 29, 858 (1958)

Modeling the temporal evolution of the layer from rinsing to evacuation

Which steps are needed and what is the idea behind the models?

1 Spin drying of wafers
Simple model based on balance of forces to estimate initial water layer thickness [1].

2 Handling time / transport of wafers
Evaporation of water under ambient conditions [2].



[1] A. G. Emslie et al.: J. Appl. Phys. 29, 858 (1958)

[2] V. S. Ajaev et al.: Microgravity Sci. Technol. 22, 441 (2010)

Modeling the temporal evolution of the layer from rinsing to evacuation

Which steps are needed and what is the idea behind the models?

1

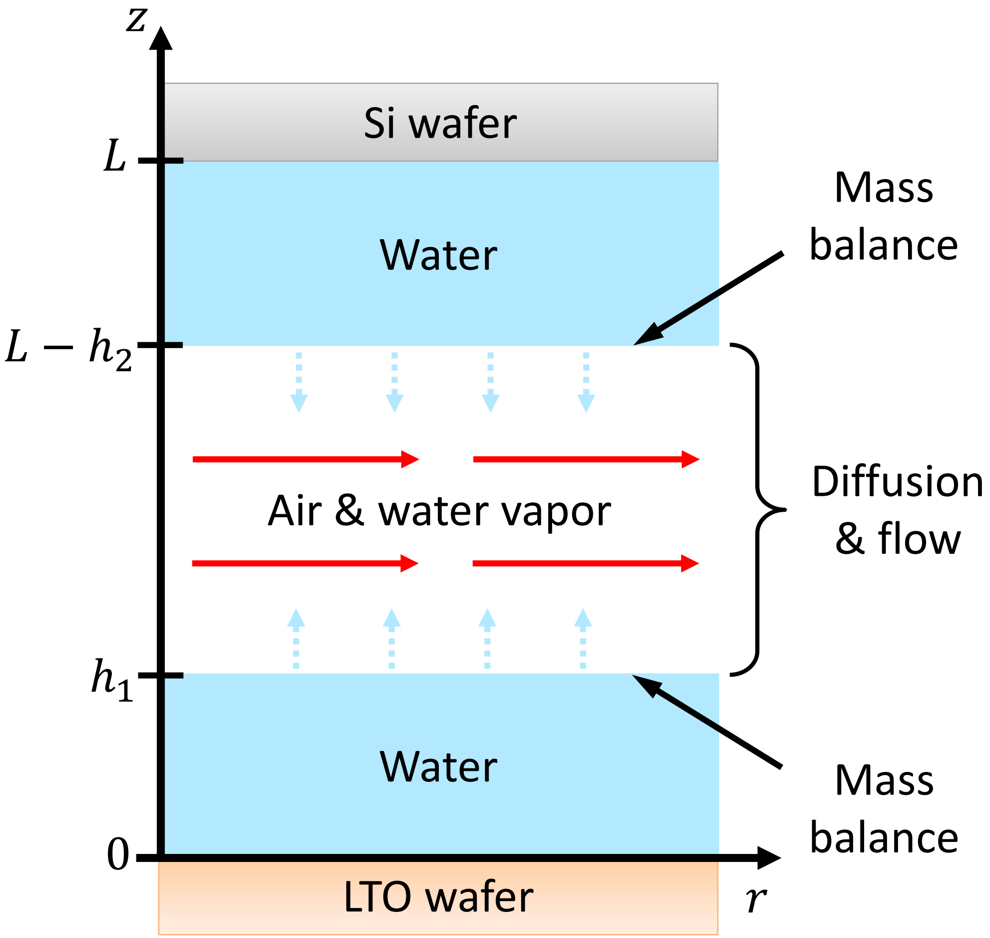
Spin drying of wafers
Simple model based on balance of forces to estimate initial water layer thickness [1].

2

Handling time / transport of wafers
Evaporation of water under ambient conditions [2].

3

Evacuation of bond chamber
Evaporation of (residual) water while total pressure decreases.



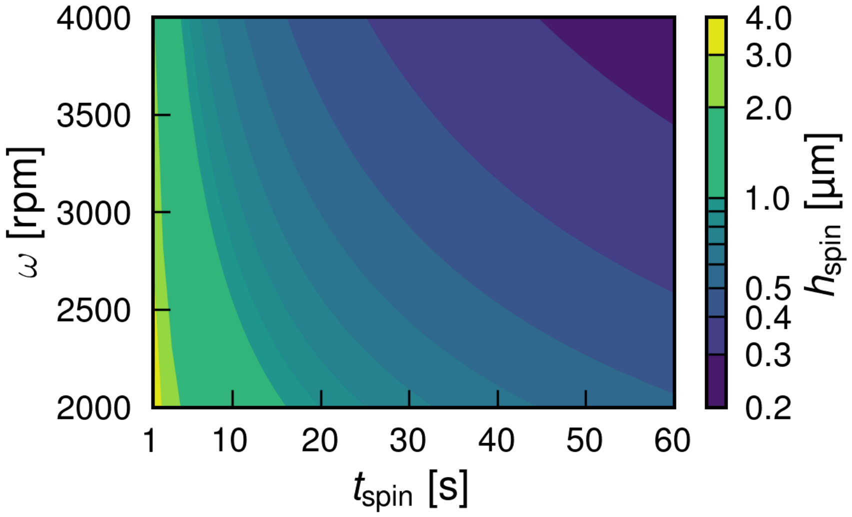
[1] A. G. Emslie et al.: J. Appl. Phys. 29, 858 (1958)

[2] V. S. Ajaev et al.: Microgravity Sci. Technol. 22, 441 (2010)

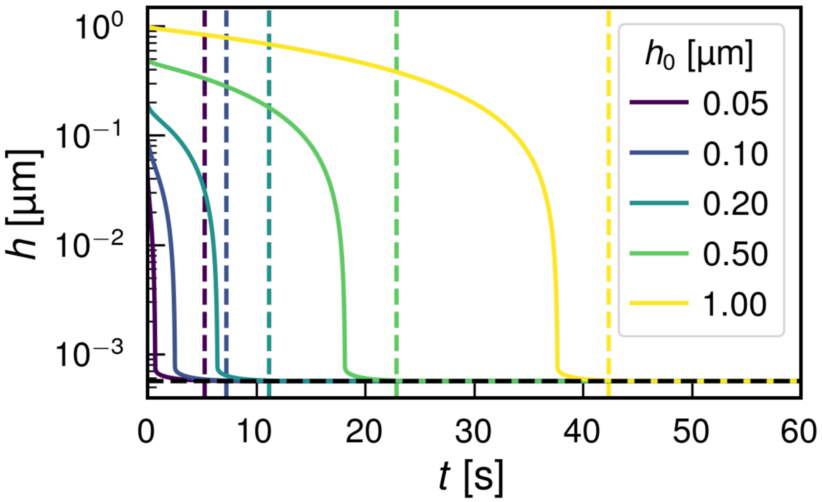
Investigation of an example process

From spin drying to the evacuation of the bond chamber

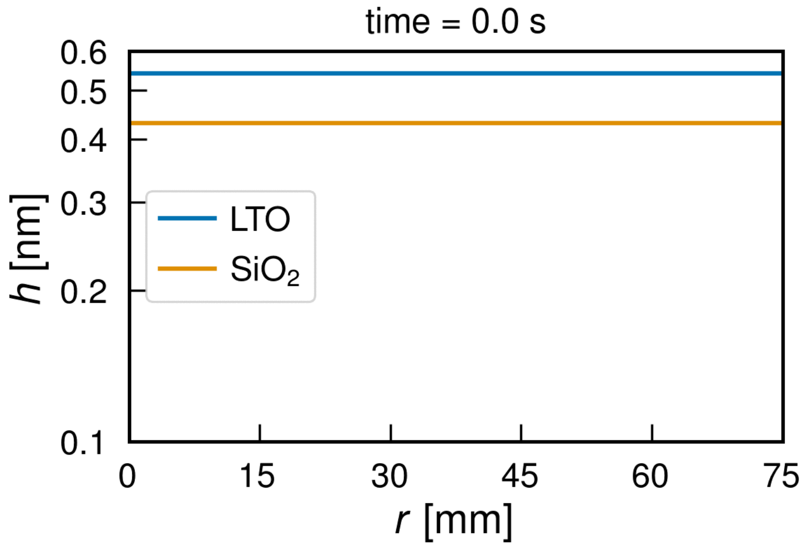
(1) Spin drying



(2) Transport



(3) Evacuation



(1) Water layer thickness after spinning h_{spin} decreases for higher angular velocities ω and longer spinning times t_{spin}
(2) Equilibrium layer thickness (here $2 \text{ monolayers} = 6.2$ Å for water on LTO) is reached after several seconds of evaporation
(3) Different wafer materials result in different equilibrium layer thicknesses which depend also on total pressure

M. Huber et al.: J. Chem. Phys. 157, 0847066 (2022)

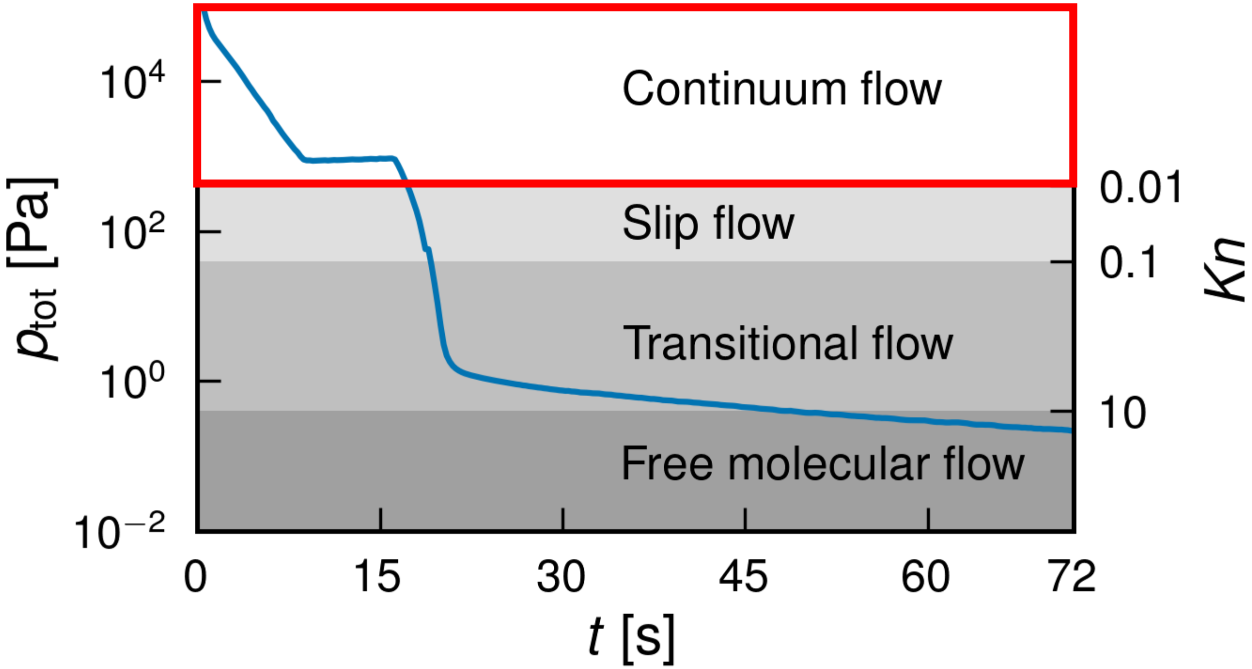
Evacuation of the bond chamber

Classification of flow regimes using the Knudsen number Kn

- Knudsen number *Kn* = mean free path / characteristic length scale

$$Kn = \sqrt{\frac{\pi R_s T}{2}} \frac{\eta}{pd} \approx \frac{4{,}05\ \mathrm{Pa}}{p}$$

Kn	p_tot [Pa]	Flow regime
$\leq 0{,}01$	≥ 405	Continuum flow
$0{,}01 \ldots 0{,}1$	$405 \ldots 40$	Slip flow
$0{,}1 \ldots 10$	$40 \ldots 0{,}4$	Transitional flow
> 10	$< 0{,}4$	Free molecular flow



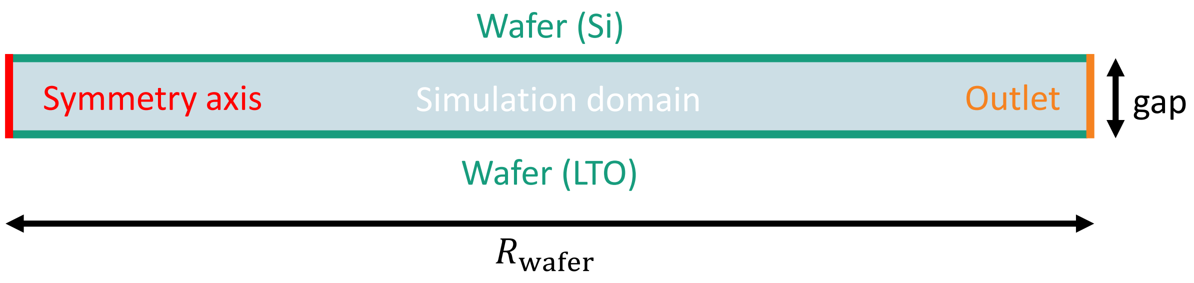
Already discussed on the slides before

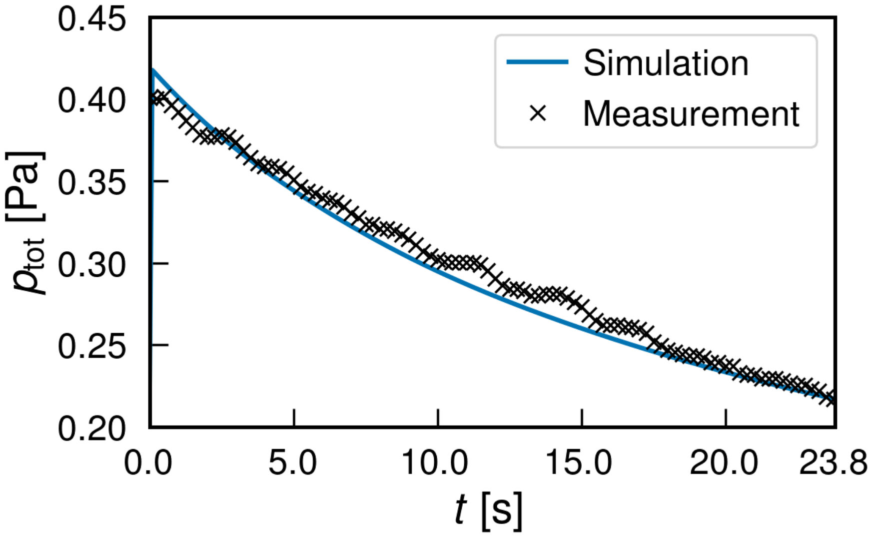
- For $p < 405$ Pa: Substitute *Laminar Flow Interface* for *Free Molecular Flow Interface* and *Transitional Flow Interface*, respectively
  - Focus on the gap between the wafers neglecting the rest of the bond chamber, use 2D axisymmetric model if possible
  - Transitional flow very time consuming and computational demanding → not shown here

Free Molecular Flow

Model geometry and assumptions

- Based on *Adsorption and Desorption of Water in a Load Lock Vacuum System* from COMSOL Application Gallery
- Angular coefficient method to simulate the flow
- 2D axisymmetric model for the gap between the wafers:

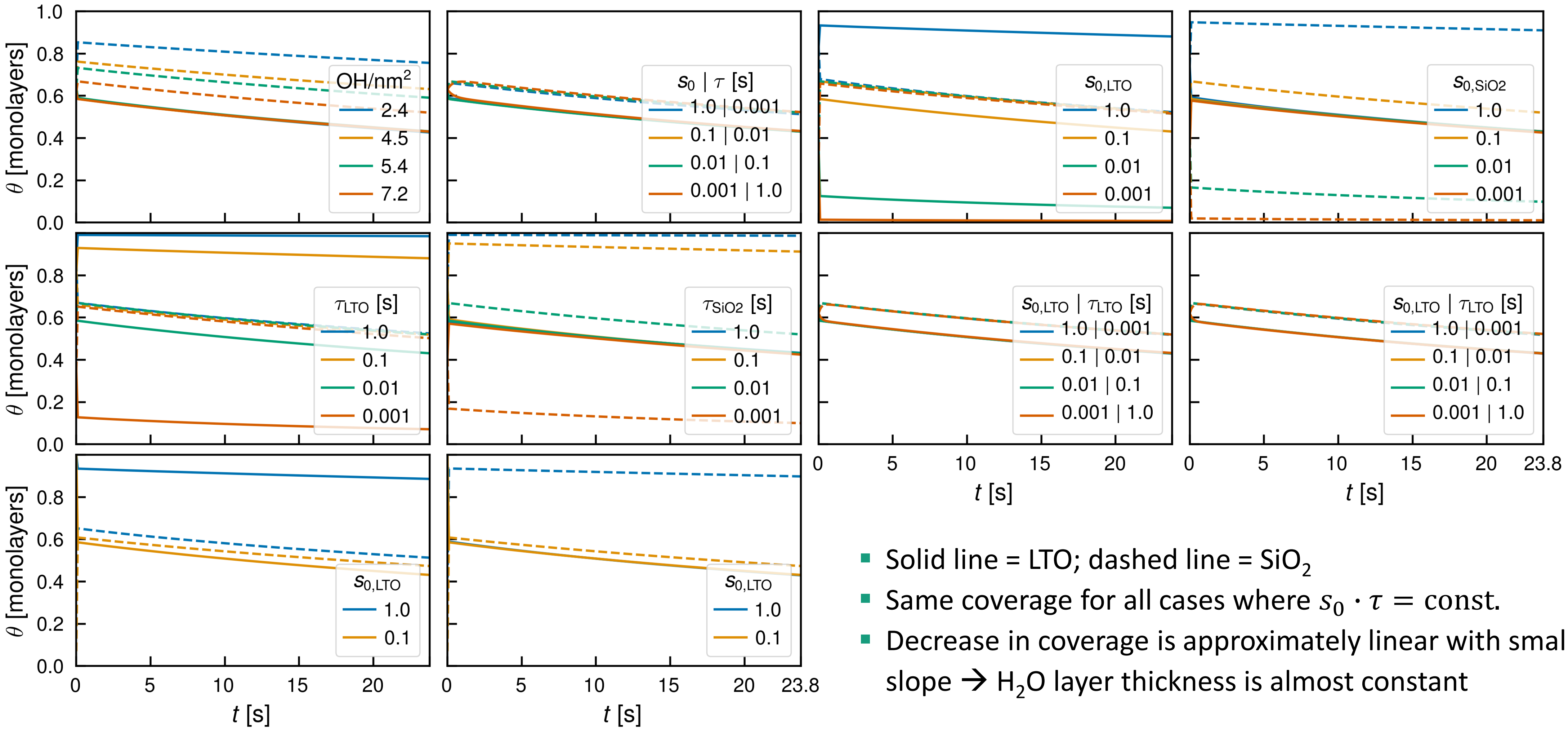




- Assumptions:
  - No multilayer coverage
  - Adsorption is described using sticking coefficient $s = s_0(1 - n_{\text{ads}}/n_{\text{sites}})$ and proportional to adsorbed molecules
  - Rate of desorption is proportional to number of adsorbed molecules: $D = n_{\text{ads}}/\tau$
  - Pumping speed of vacuum pump is fit parameter to match measured pressure
- Example on next slide: Parameter variation to find H_2O coverage of the wafers
  - Variation of s_0 and τ for both wafers

Free Molecular Flow

Results of the parameter variation



- Solid line = LTO; dashed line = SiO_2
- Same coverage for all cases where $s_0 \cdot \tau = \text{const.}$
- Decrease in coverage is approximately linear with small slope → H_2O layer thickness is almost constant

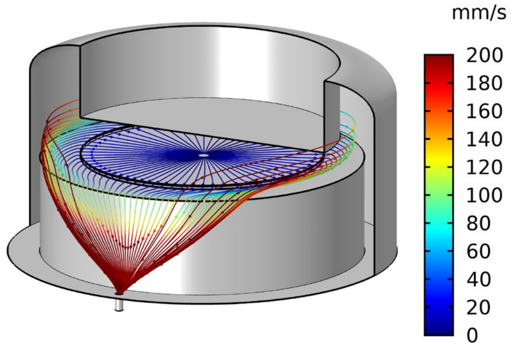
Summary and Outlook

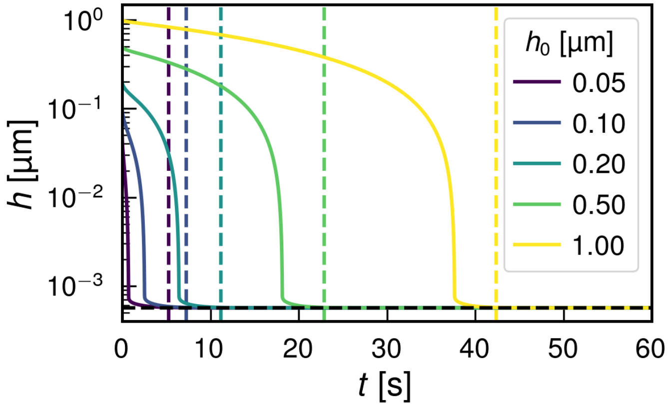
Summary

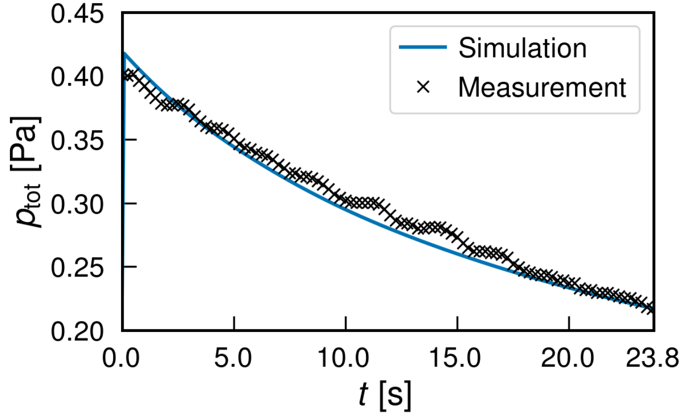
- Combination of simple models to describe the water layer on wafers at all steps in the process from rinsing to bonding in a vacuum chamber
  - Spin drying after rinsing
  - Evaporation during handling / transport to the bond chamber
  - Evaporation during evacuation of the bond chamber
- Different flow regimes require different models for flow and evaporation
  - Diffusion-based model in continuum regime
  - Angular coefficient method for free molecular flow

Outlook

- Implementation of 3D transitional flow model
  → Simulation of whole technological process possible







Thank you for your attention!