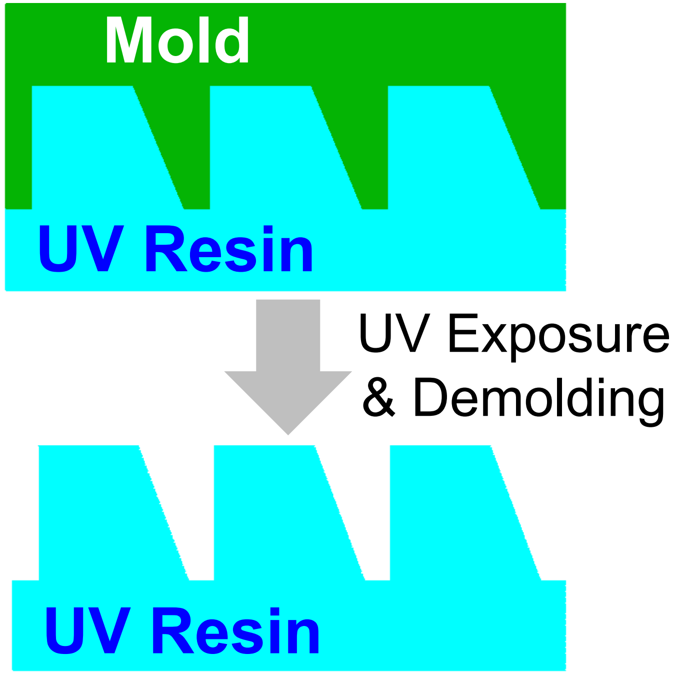
Numerical modeling method to reproduce UV imprint process using thermo-viscoelastic constitutive law

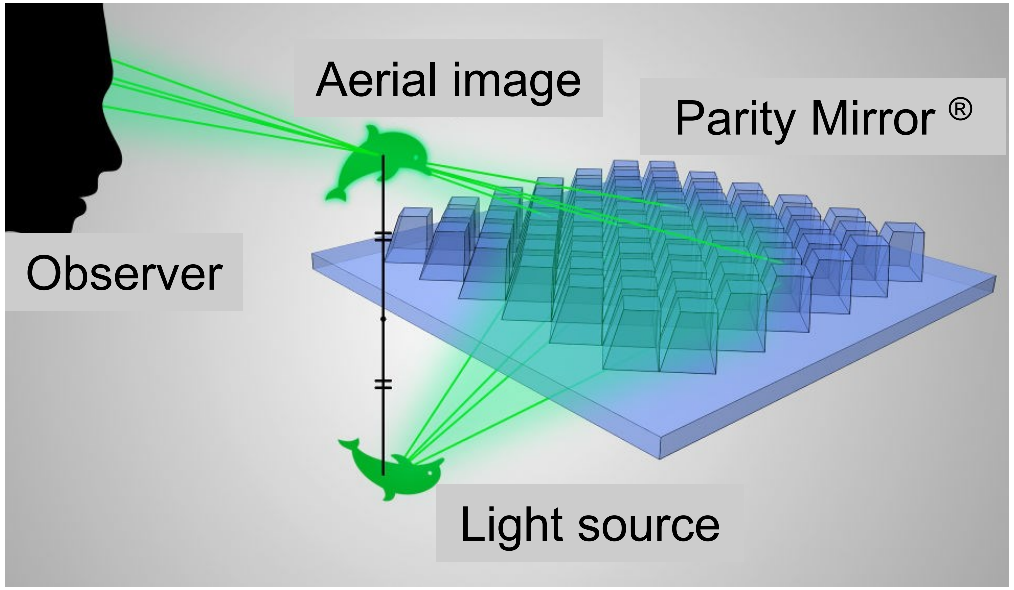
Ryunosuke YAMASHITA, Yuki ONISHI, Kenji AMAYA

Tokyo Institute of Technology, Japan

Background

- **UV imprinting** is a low cost and high throughput production method.
- It has been adopted to the production of various **optical devices requiring high surface accuracy** such as micro mirror array.

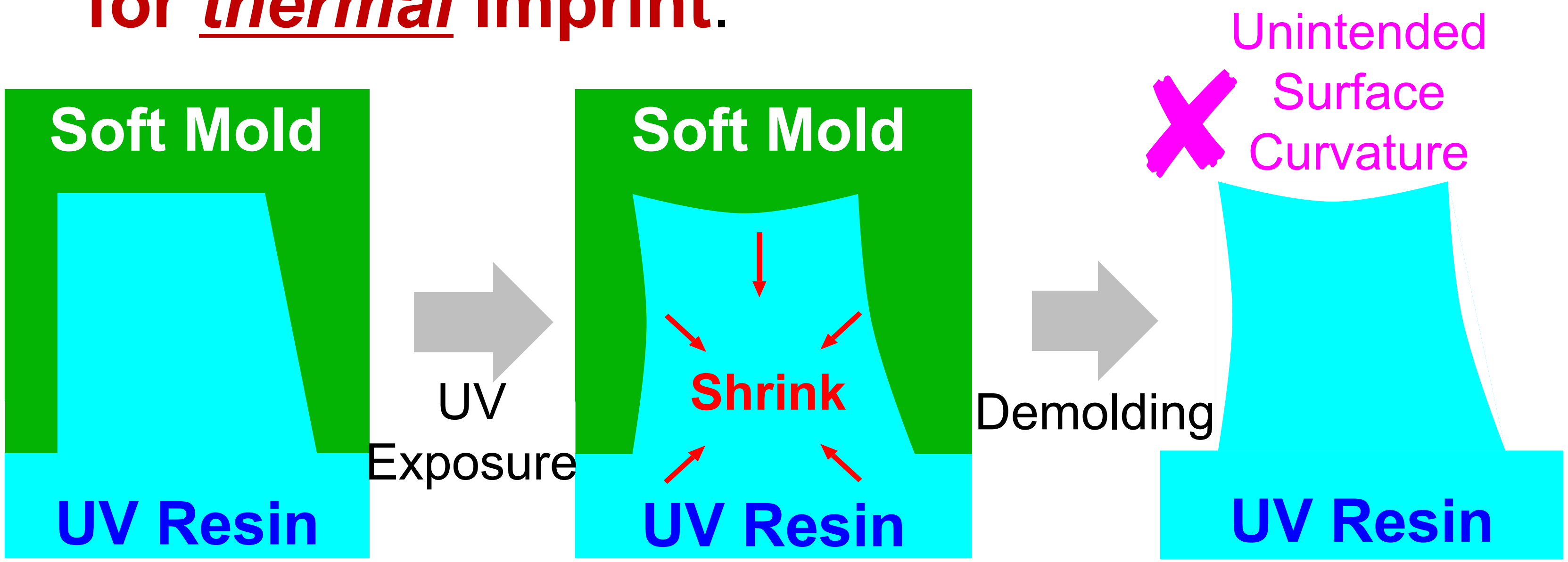


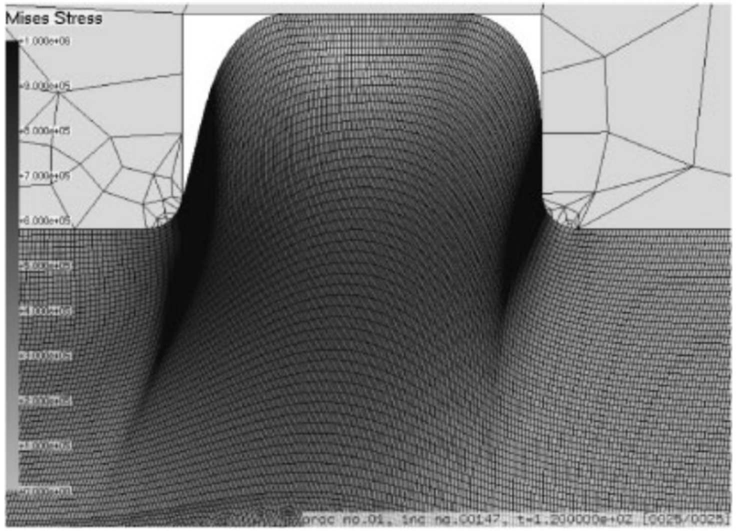


Example of optical product produced by micro imprint. (Parity Innovations Co., Ltd.)

Issues

- In the curing process, **volume shrinkage of UV resin** arises and may cause **unintended surface curvature** when a soft mold such as PDMS is used.
- There is **no numerical modeling method** to reproduce this type of error in UV imprint, although there are a few **conventional methods for *thermal* imprint**.

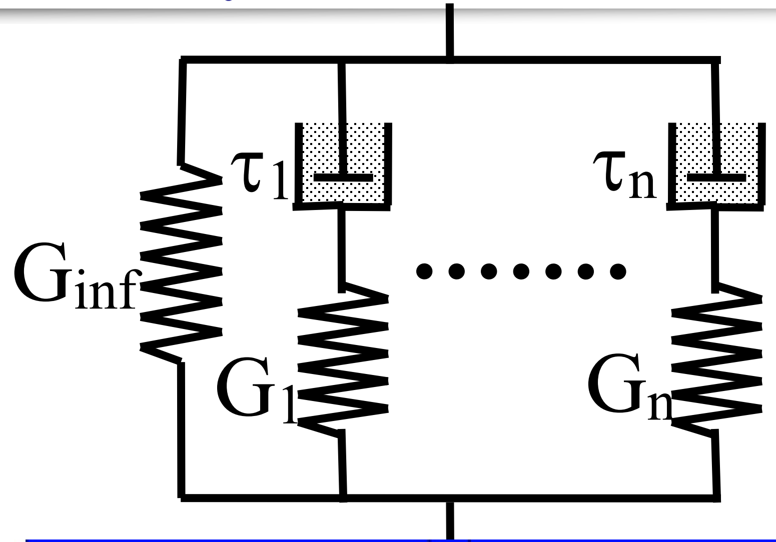


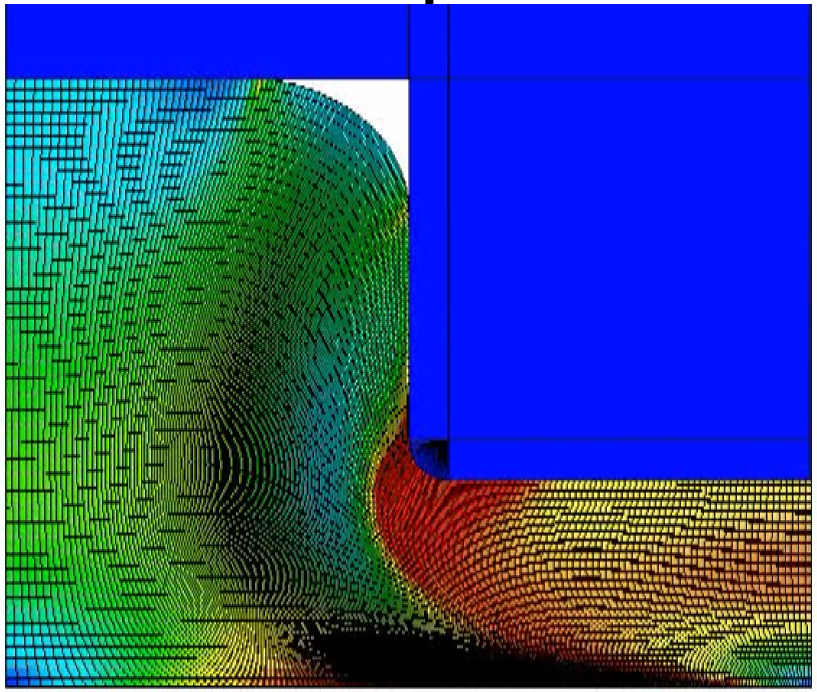


Y. Onishi *et al. Jpn. J. Appl. Phys.* **47** 5145 (2008)

Brief of Conventional Method for *Thermal* Imprint Simulation

- **Thermo-viscoelastic** constitutive model
  - Thermal contraction is described with **thermal expansion coefficient**.
  - Shear behavior is described with the **time-temperature superposition principle** and **Prony series** for the **generalized Maxwell model**.
  - Volumetric behavior is assumed to be independent of strain rate and temperature.
- Numerical simulation with the **finite element method (FEM)**





Our idea :
Similar numerical approach could be used for ***UV*** imprint simulation.

Objective

1. Propose a numerical method for **UV curing process simulation**.
2. Utilize the process simulation for **mold shape optimization**.

Methods

Overview of Our Method

Considering the analogy of thermal and UV imprint,

- Our approach uses **<u>thermo-viscoelastic</u>** material constitutive model and replaces phenomena on UV resin as follows.
  - UV reaction progress ⟹ Cooling (temperature drop)
  - UV shrink ⟹ Cooling contraction
  - UV curing ⟹ Cooling solidification

Becomes similar to thermal imprint simulation

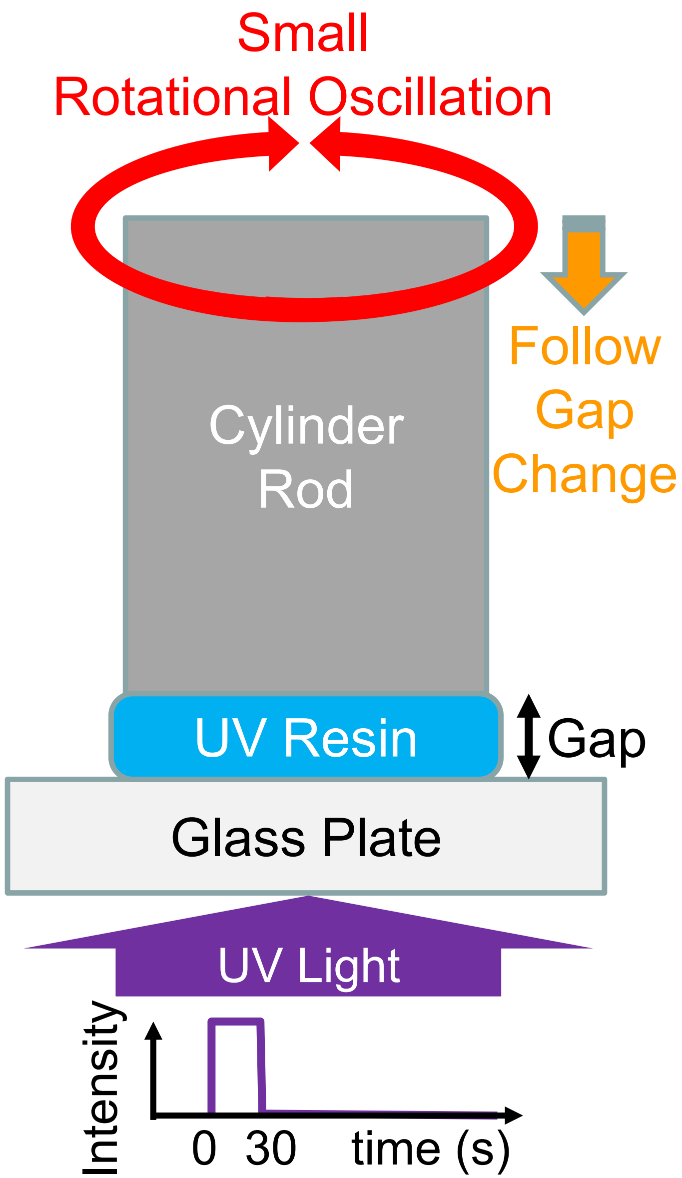
- The model parameters are identified through **rheology measurement experiments**.

⇩

Numerical UV process simulation is realized as the result.

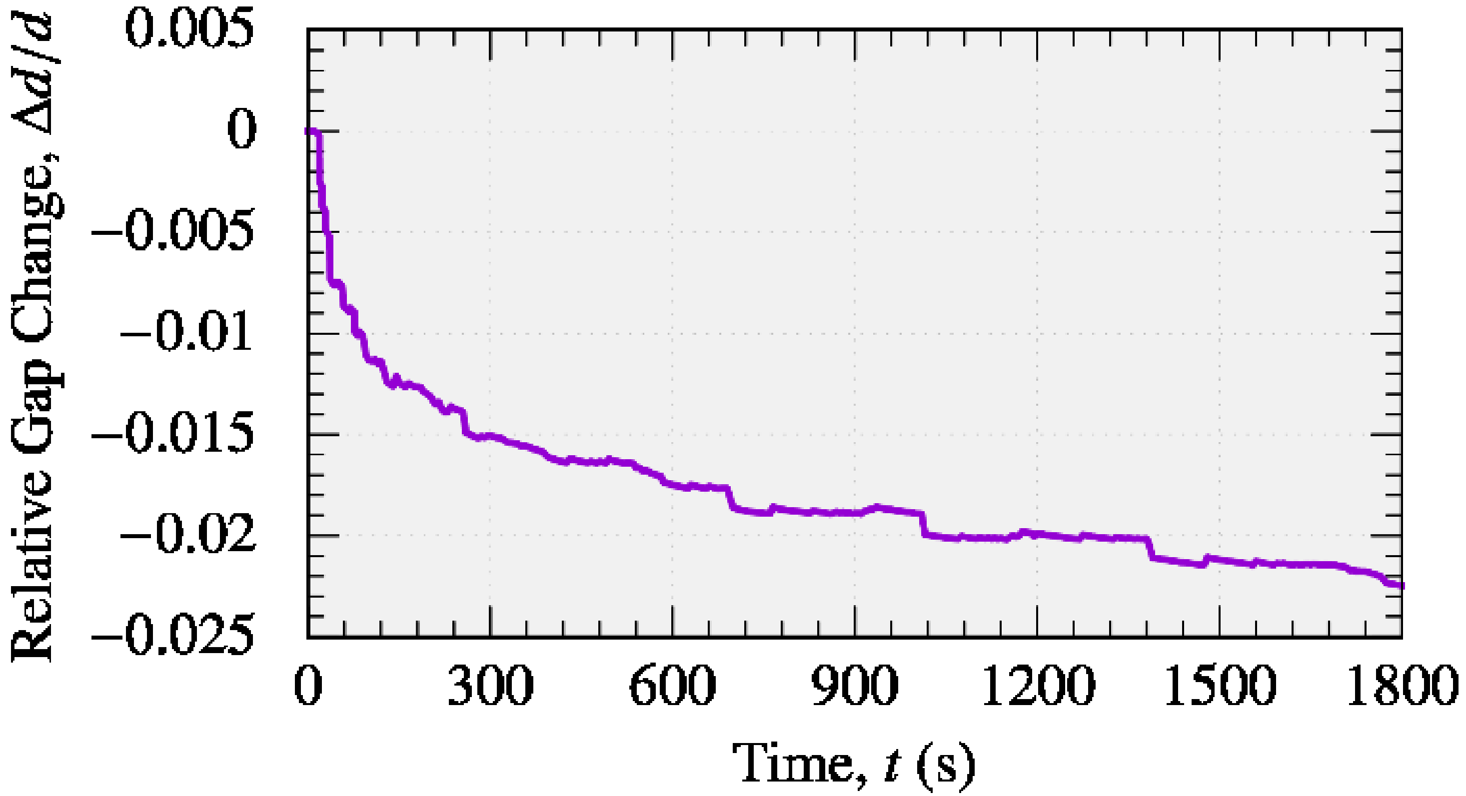
Experimental Conditions

- Rotational oscillatory rheometer (Anton Paar MCR301) is used.
- The measurement object is an UV resin from Daicel Co..
- Room temperature is 25℃ (const.).
- UV exposure condition is constant (30 s exposure in a constant intensity).
- The oscillation frequency is varied from 0.1 to 10 Hz.
- The gap between the cylinder rod and the glass plate changes over time due to UV shrink.
- Long time measurement is conducted to consider the dark curing.



Relative Gap Change (Experimental Result)

Time History of Relative Gap Change

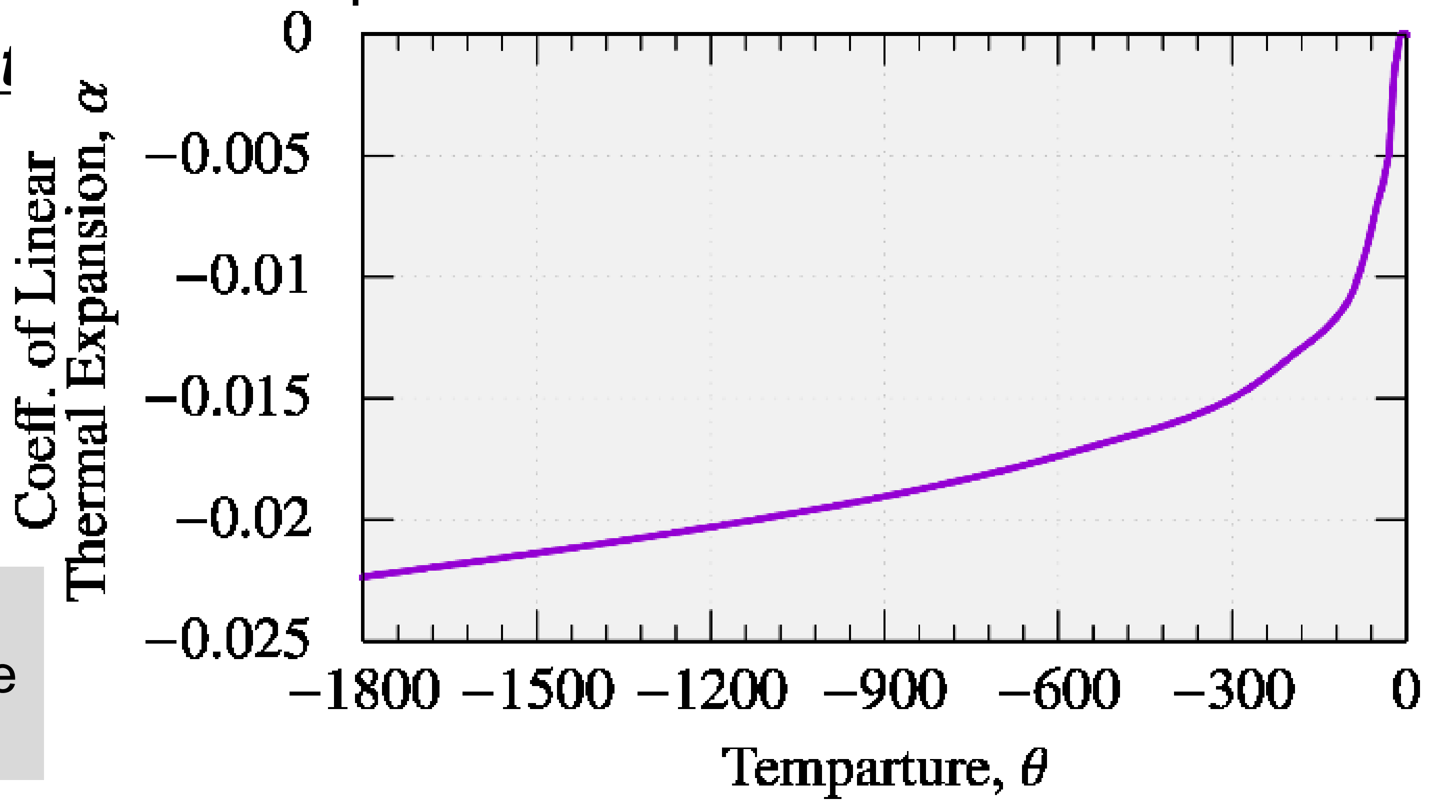


- Note: the time history of the relative gap change is always the same in all cases (∵ UV exposure condition is constant).
- UV shrink progresses with time, but the shrink speed gradually decreases.

Relative Gap Change (Model Parameter Identification)

- UV shrink is modeled as **thermal (cooling) contraction**.
- For the UV reaction progress measure, the time history of temperature is given as $\boldsymbol{\theta(t) = -t}$. (Note that θ is not a real physical quantity but just a virtual value.)
- The time history of relative gap change is converted into the temperature-dependent coefficient of thermal expansion.

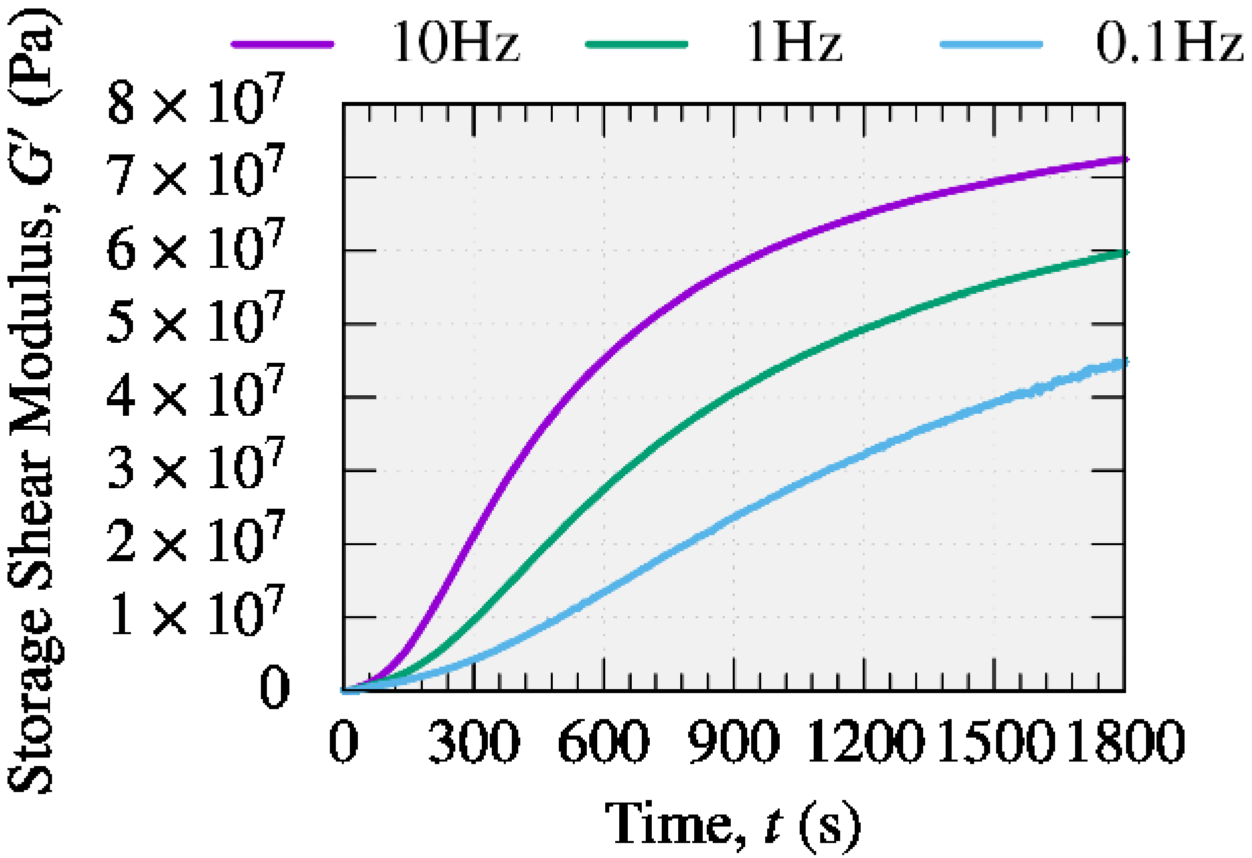
Temperature-Dependent Coefficient of Thermal Expansion

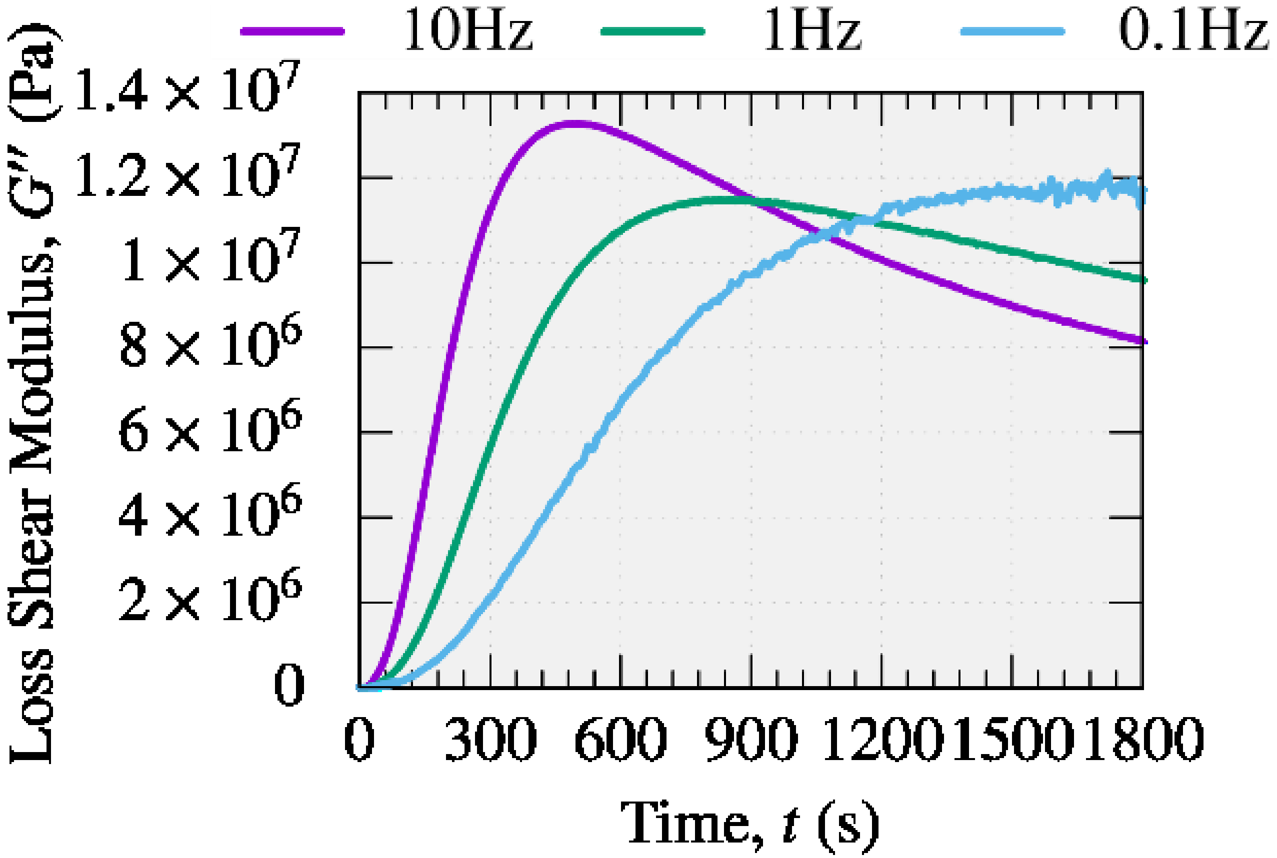


Note: α is negative because it represents the volume change compared to the initial volume.

Viscoelasticity (Experimental Result)

Time History of Storage / Loss Shear Modulus (G' / G'')





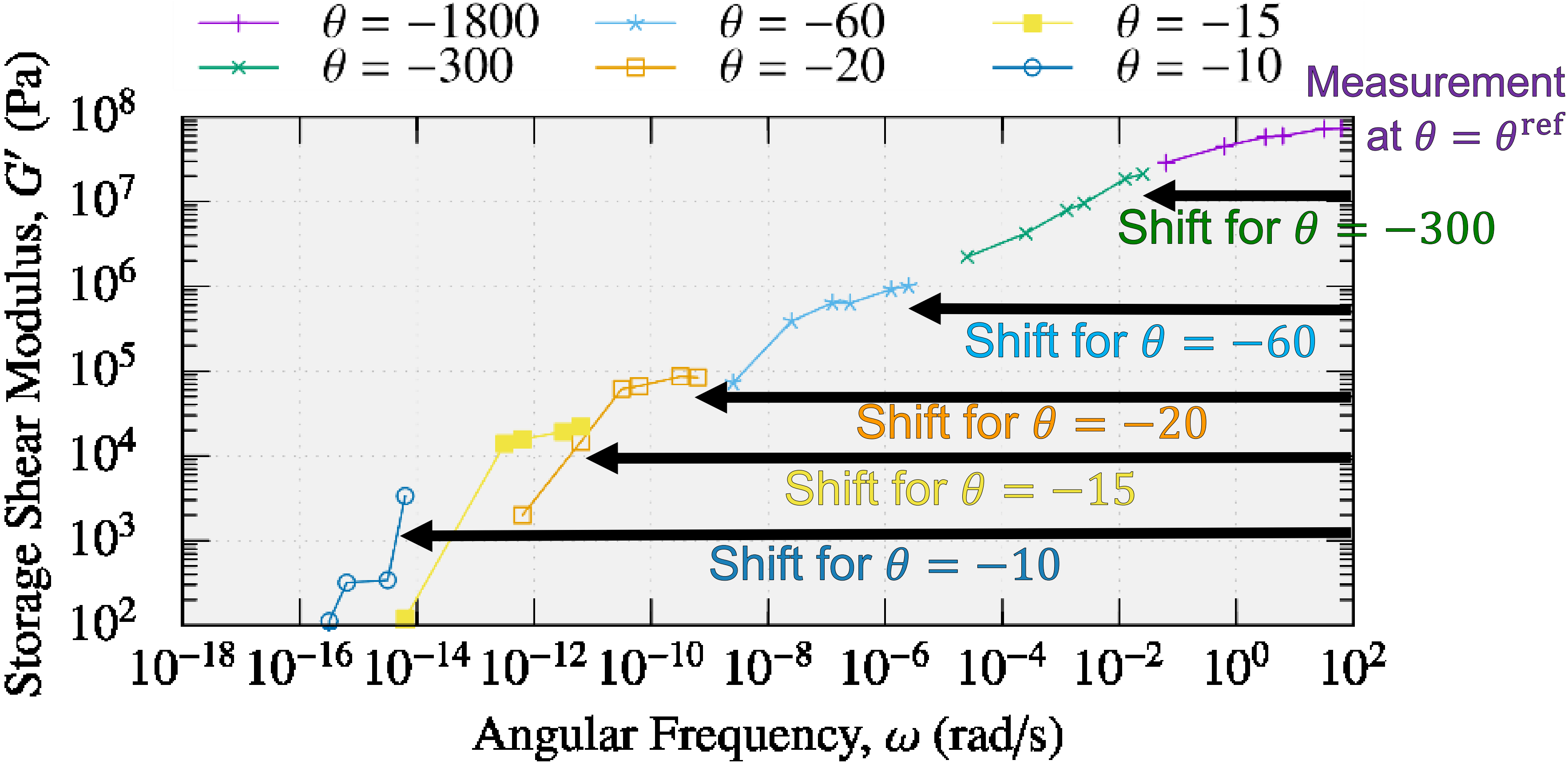
- Depending on the frequency, the time histories of G' and G'' are different (harder at higher frequencies).
- At any frequency, UV resin monotonically hardens with time.

Viscoelasticity (Model Parameter Identification 1/3)

- UV resin is modeled as viscoelastic material based on the **time-temperature superposition principle** and **Prony series** for the **generalized Maxwell model**.
- A certain temperature is set as a reference temperature (e.g., $\theta^{\mathrm{ref}} = -1800$).
- Pick G's and G''s at different temperatures and identify each time shift.

Time-Shifted Storage Shear Modulus $G'(\omega)$ at θ^{ref} (Master Curve)

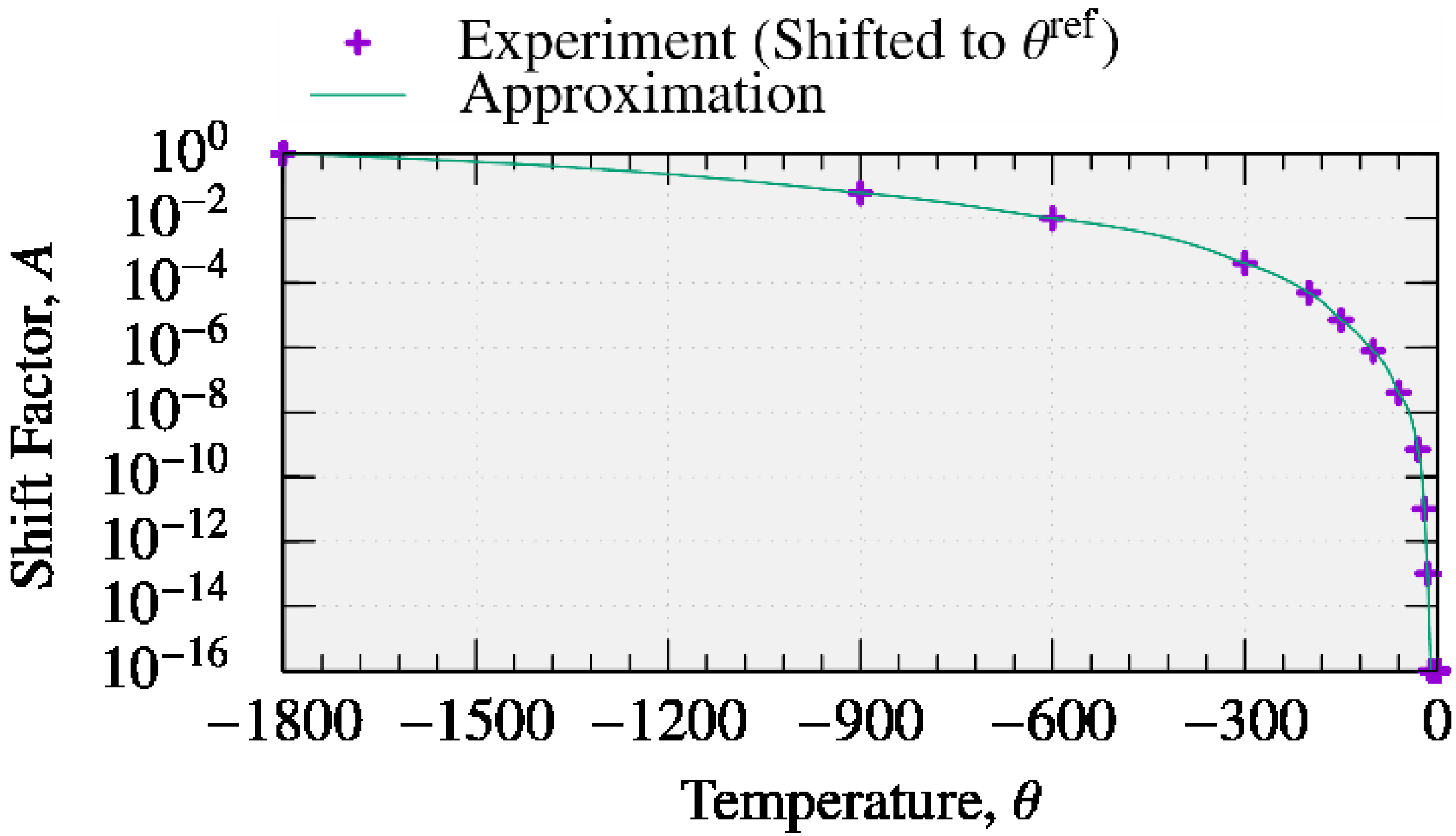
In practice, $G''(\omega)$ is also taken into consideration to determine the time shifts.



Viscoelasticity (Model Parameter Identification 2/3)

- A temperature-dependent shift factor (i.e., time-temperature superposition) is obtained by fitting the time-shifts at various temperatures.

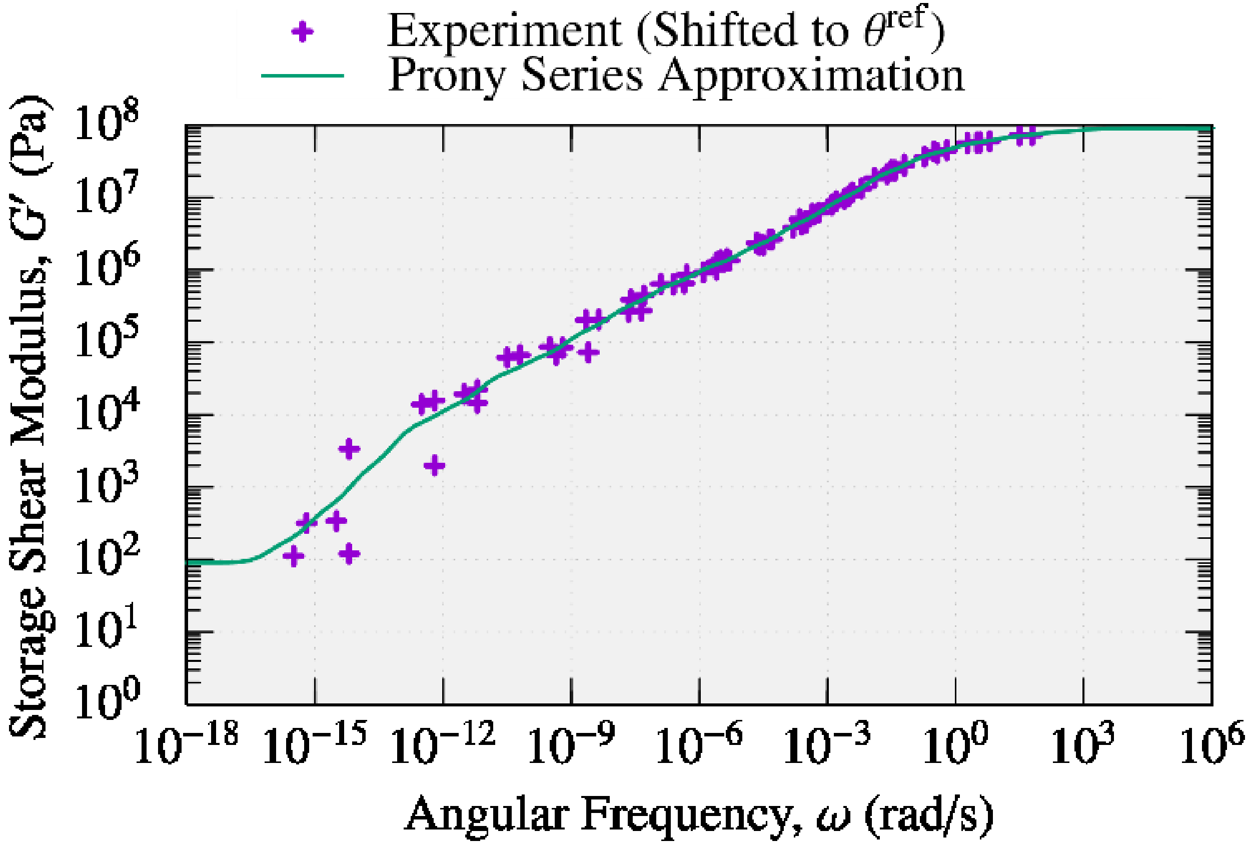
Temperature-Dependent Shift Factor $A(\theta)$

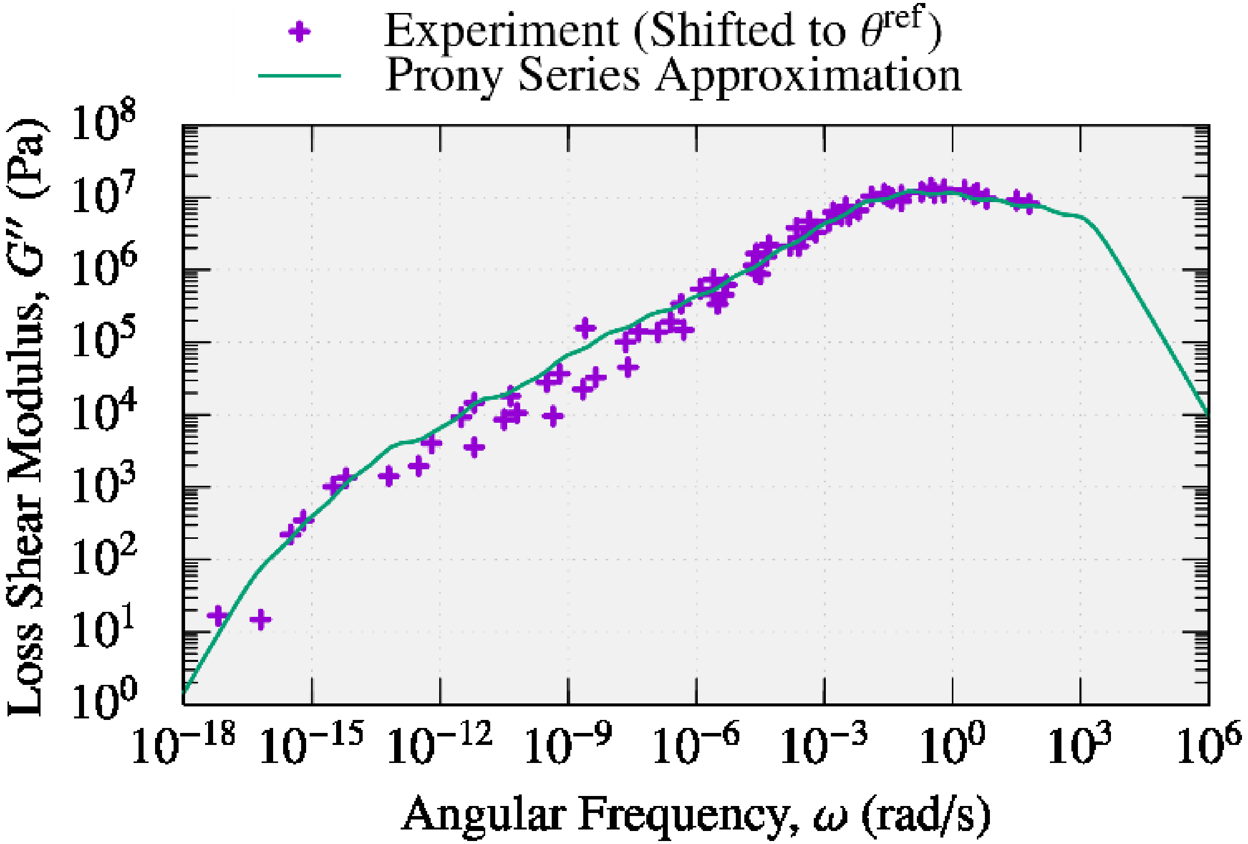


Viscoelasticity (Model Parameter Identification 3/3)

- Find the Prony series coeffs by fitting the master curve at the reference temp.

<u>Storage / Loss Shear Modulus at Reference Temp. Expressed by Prony Series</u>



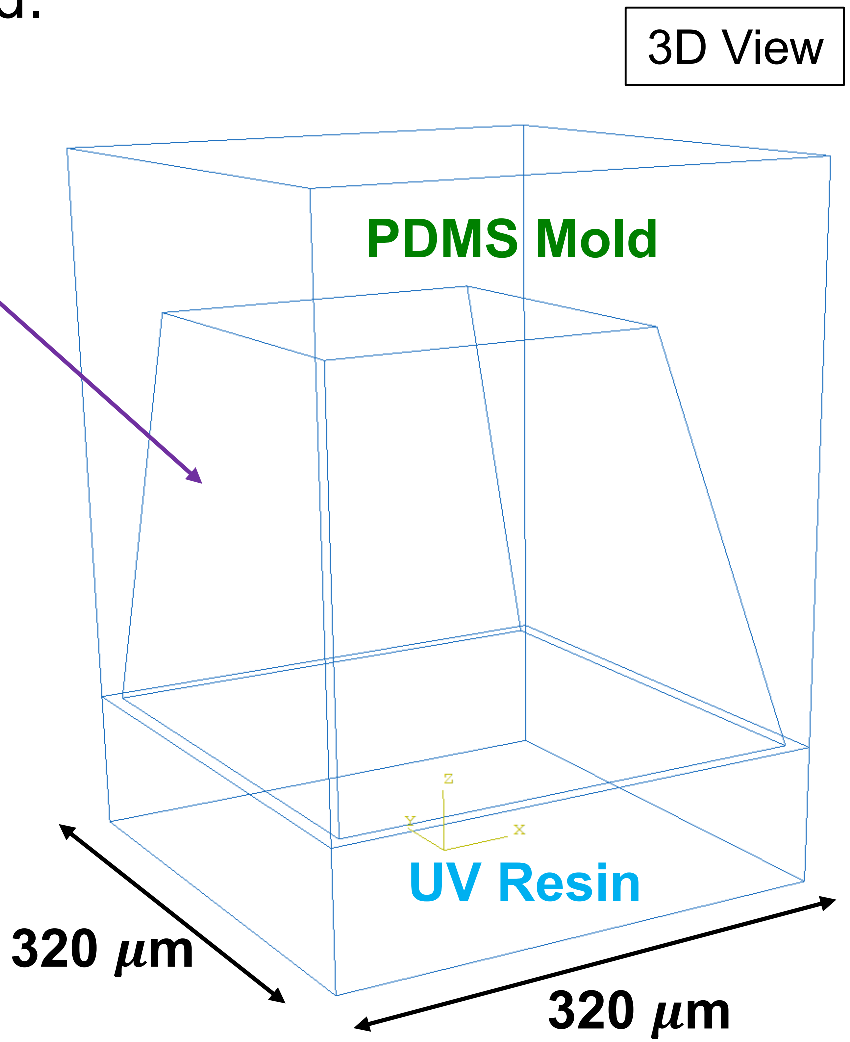


From the above, the constitutive model of thermo-viscoelasticity to simulate UV shrink and curing were identified.

Result & Discussion

UV Curing Process Simulation (Outline)

- Commercial finite element code, ABAQUS, is adopted.
- Target pattern is a **micro mirror array**.
- The mold pattern is periodic and thus only **one mirror is taken into account** with **periodic boundary conditions**.
- Mold cavity is filled with UV resin at the initial state.
- Temperature is given as $\boldsymbol{\theta(t) = -t}$.
- UV exposure condition is exactly the same as that of the rheology measurement experiments. (30 s exposure in a constant intensity).
- Demolding is conducted 70 s after the end of UV exposure.
- Mirror curvature is evaluated enough after the demolding (6000 s).



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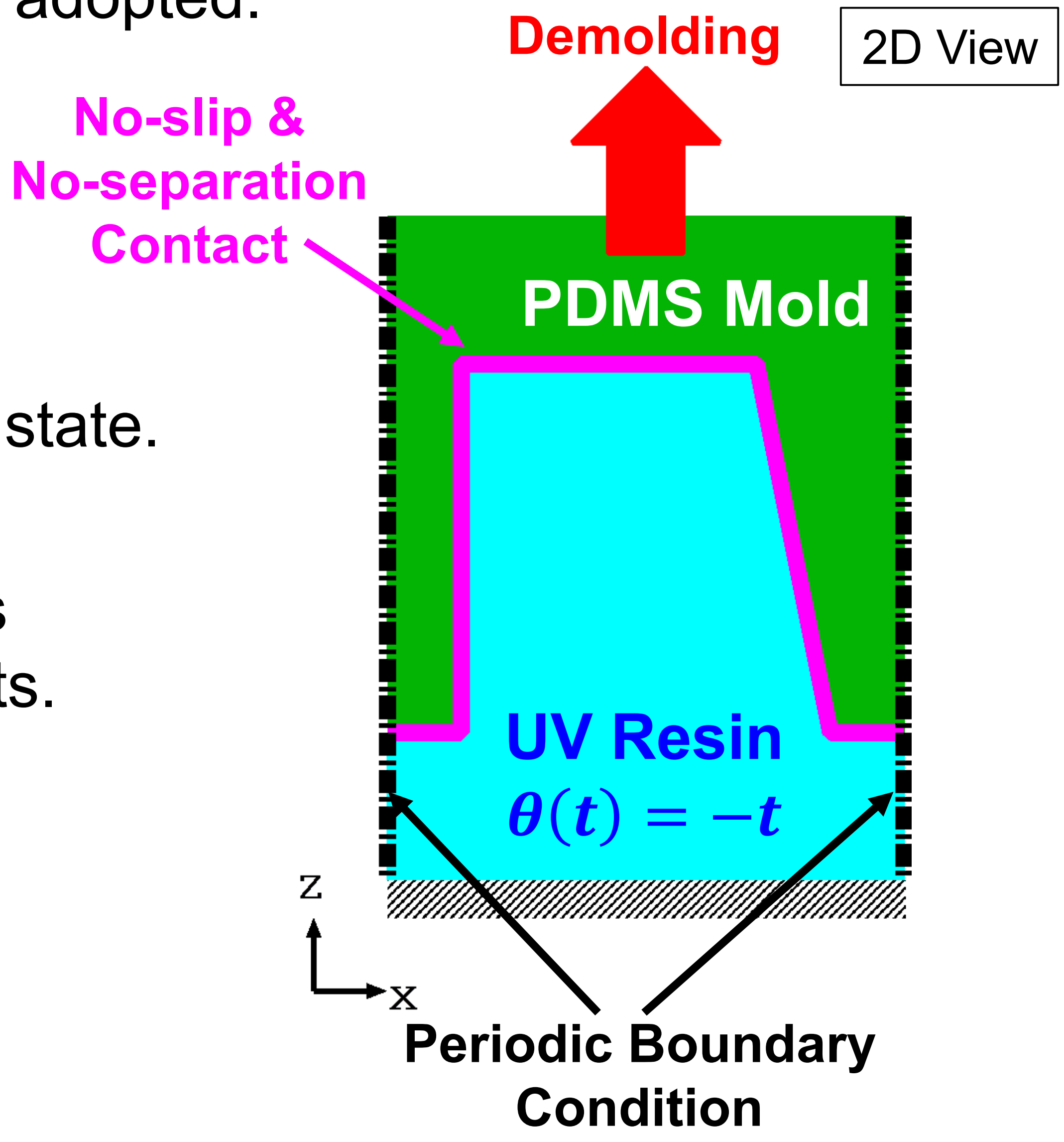
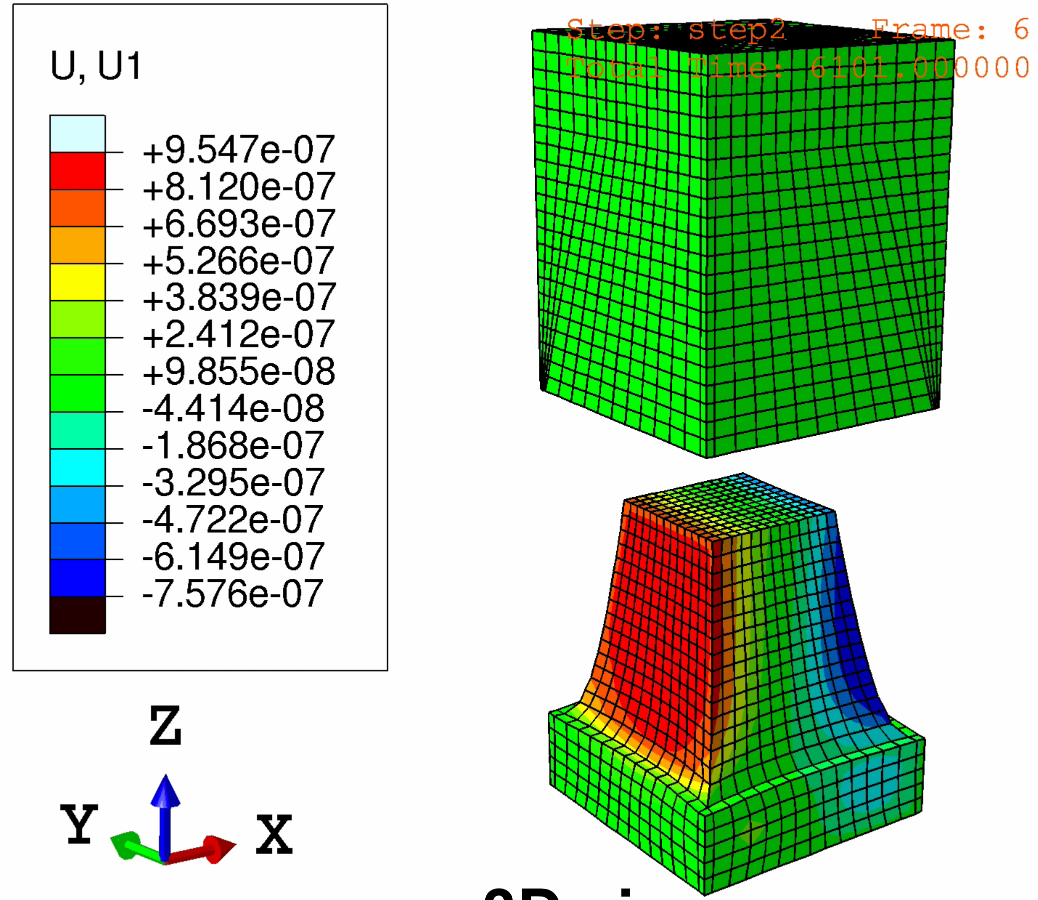


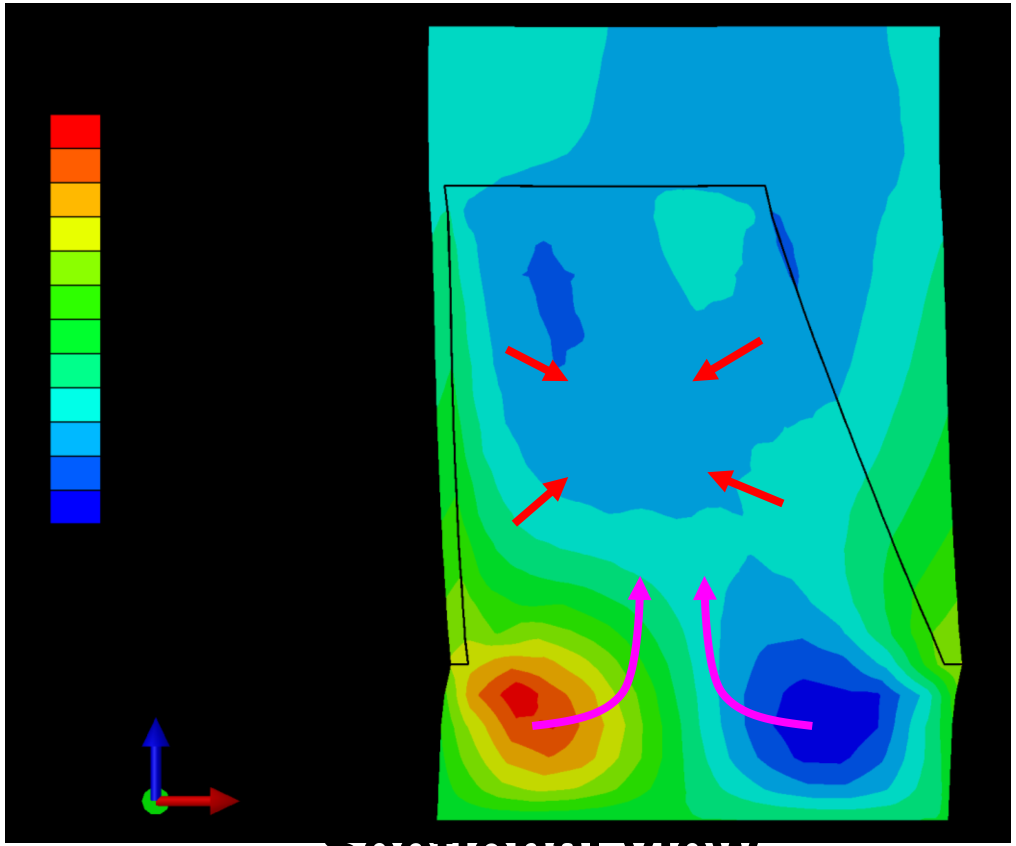
UV Curing Process Simulation (Simulation Result)

Displacement Dist. in X Direction

Deformation Scale Factor: 30 x 30 x 1 in *XYZ*



3D view



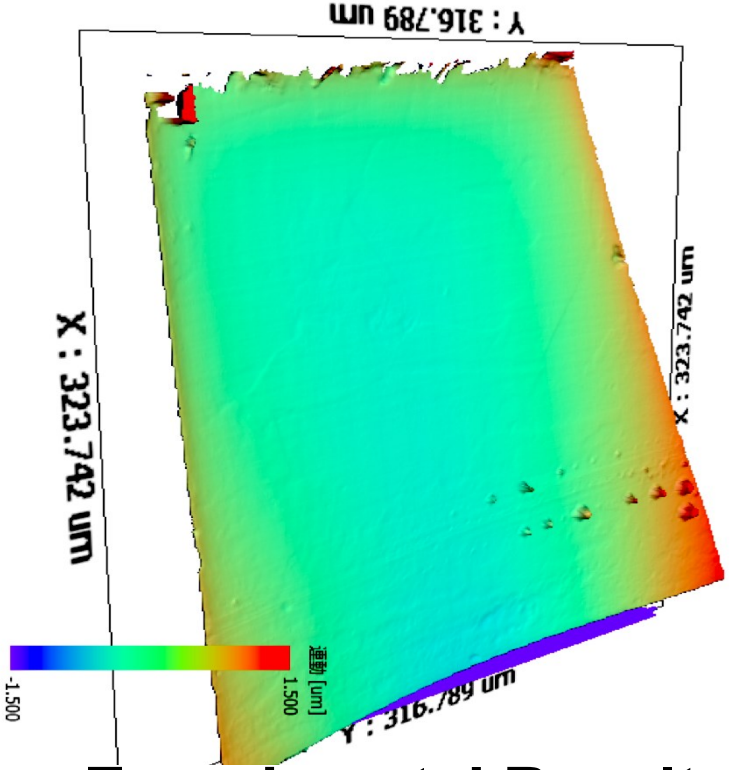
Sectional View (cut on *Y* plane)

Surface curvature due to the mold deformation is observed.

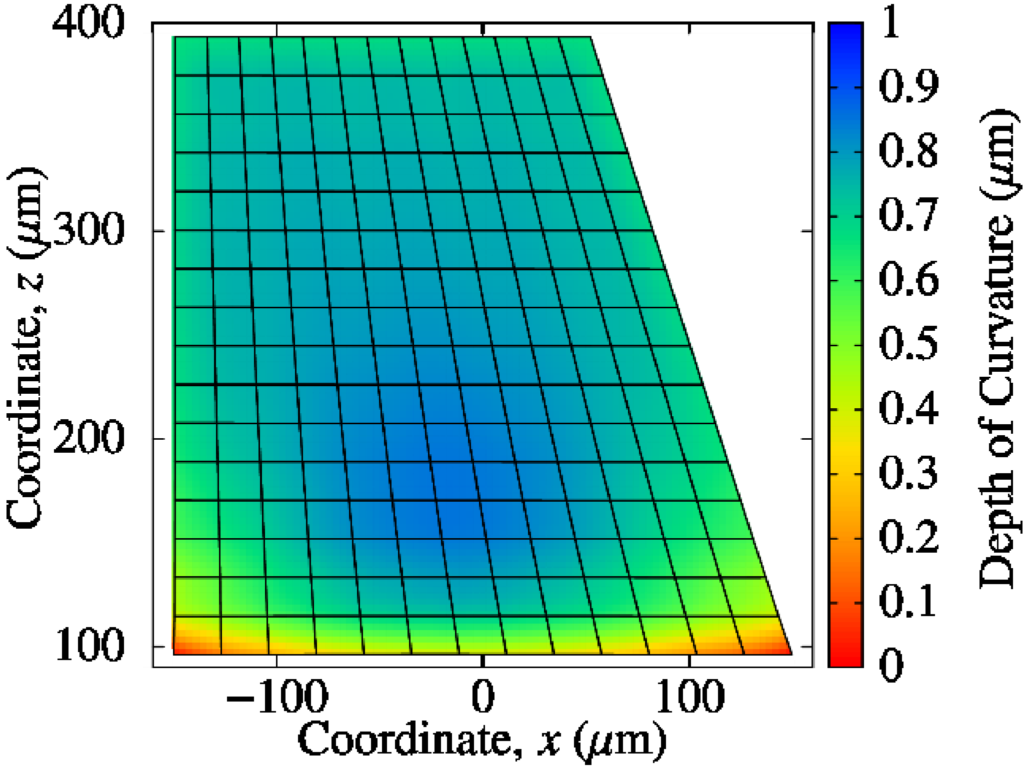
Flow of UV resin due to the UV shrink is observed.

UV Curing Process Simulation (Validation)

Curvature Depth Dist. on Mirror Surface



The maximum curvature depth is about 1 μm located at lower center of the surface.



Experimental Result

(Measured with scanning probe microscope)

Simulation Result

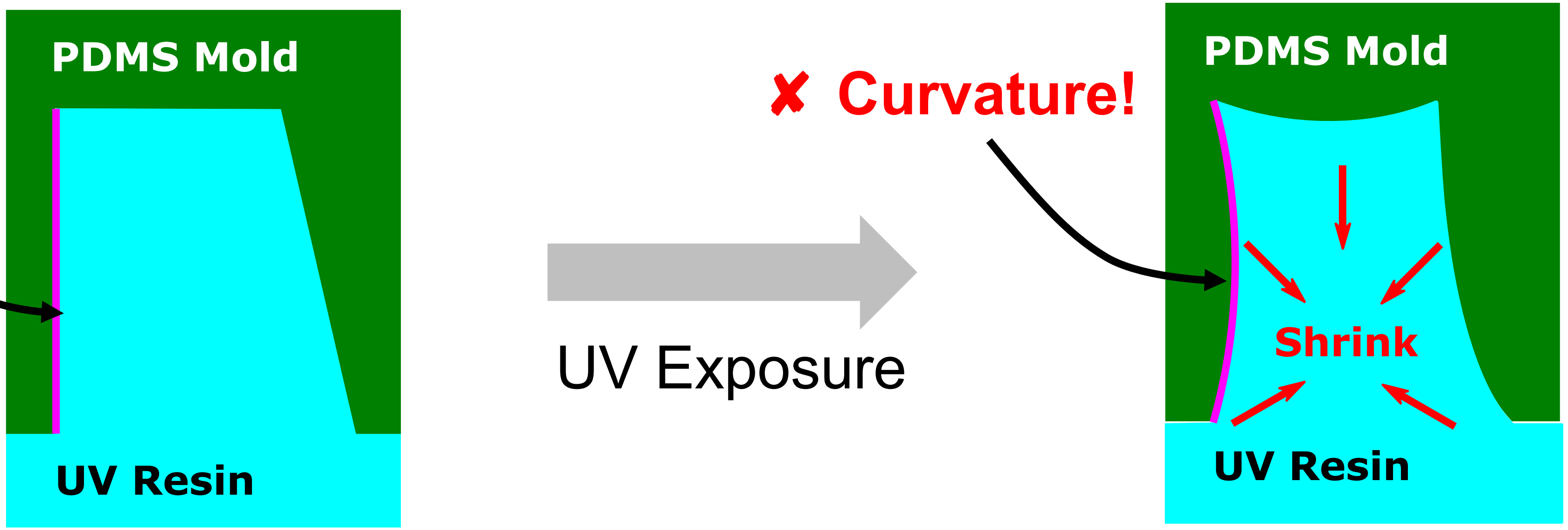
(For ease of comparison, the contour color scheme uses “reversed rainbow”.)

✔ Simulation result agreed with the experimental measurement data qualitatively.

Mold Shape Optimization (Outline)

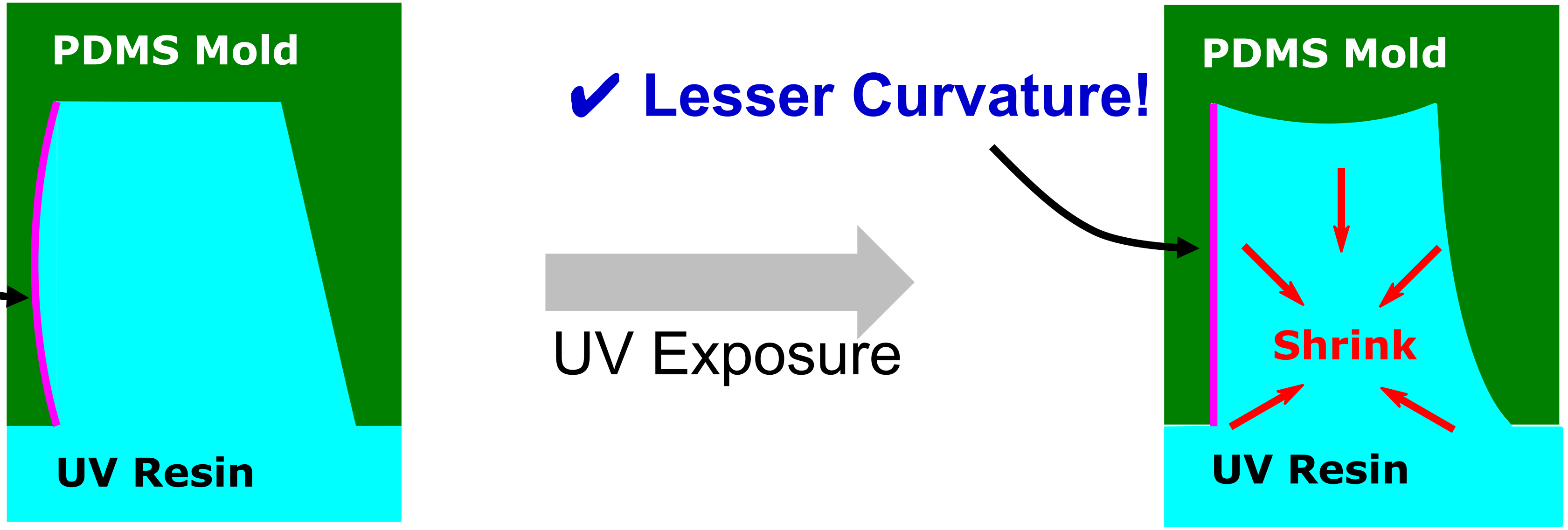
Unoptimized Mold Shape

Before Mold Optimization



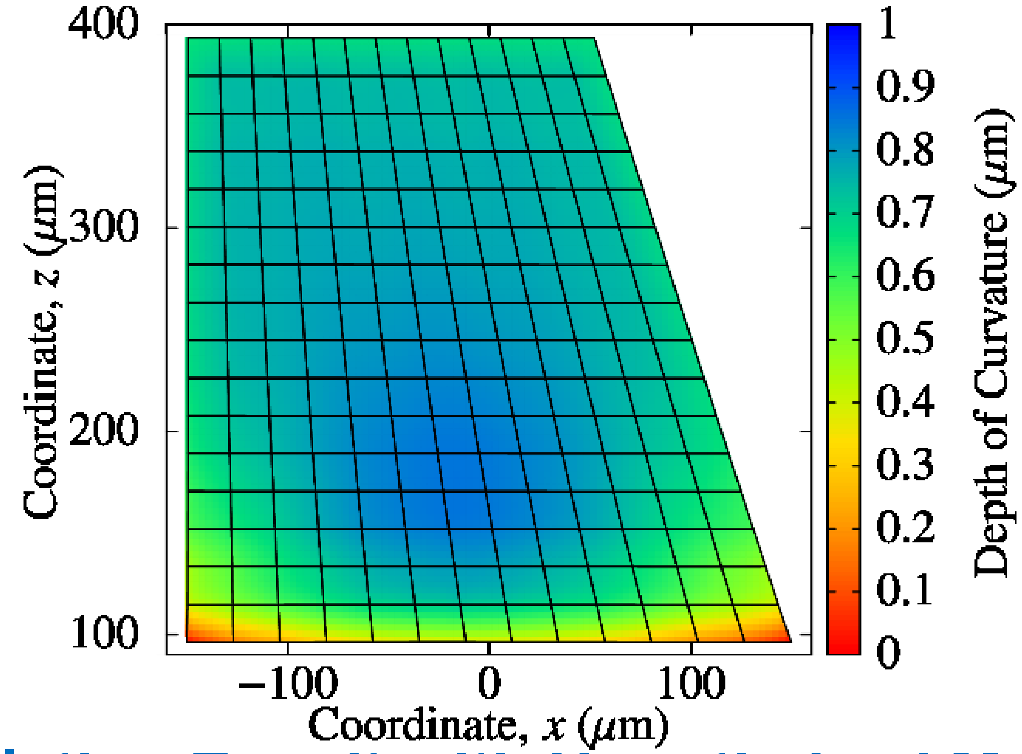
Optimized Mold Shape

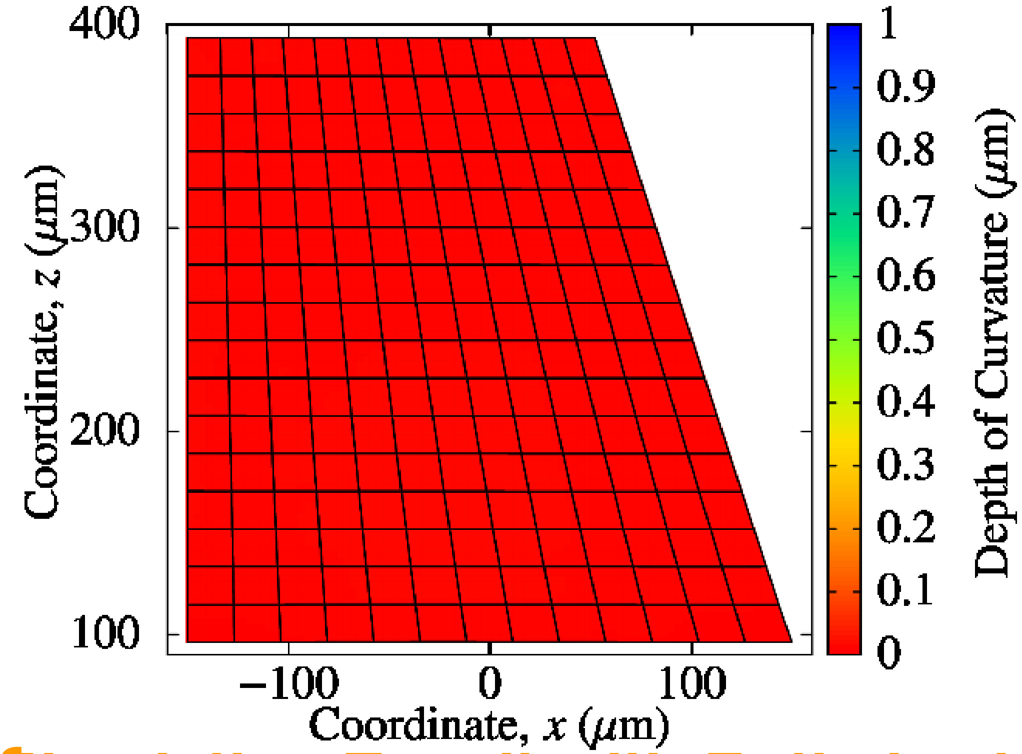
After Mold Optimization



Mold Shape Optimization (Simulation Result)

Curvature Depth Dist. on Mirror Surface





Simulation Result with Unoptimized Mold

✘ Maximum curvature depth: 1 μm

Simulation Result with Optimized Mold

✔ Maximum curvature depth: 0.01 μm

The optimized mold greatly suppressed the curvature and achieved a super-flat mirror surface!

Summary

Summary

- A numerical modeling method for **UV shrink & curing simulation** using **thermo-viscoelastic model** was proposed.
- The model parameters were identified through the **rheology measurement experiments**.
- A process simulation for micro mirror array using PDMS mold validated the **qualitative accuracy on mirror surface curvature.**
- A demonstration of **mold shape optimization** successfully suggested an optimal mold shape to achieve a flat mirror surface.
- Quantitative validation and application to other patterns (such as lens arrays) are our future work.

Acknowledgement

- This is a joint work with Daicel Co. and Osaka Prefecture Univ. (Prof. Hirai's group).
- Another joint work is scheduled for oral presentation tomorrow:
  - Yoshihiko Hirai et al., "3-Dimensional mold profile correction for resin shrinkage in micro-nano molding process"
  - Sep. 26 (Wed.), 16:25 -16:40, Auditorium 11 (06-11: Metrology)

Thank you for your kind attention.

Appendix

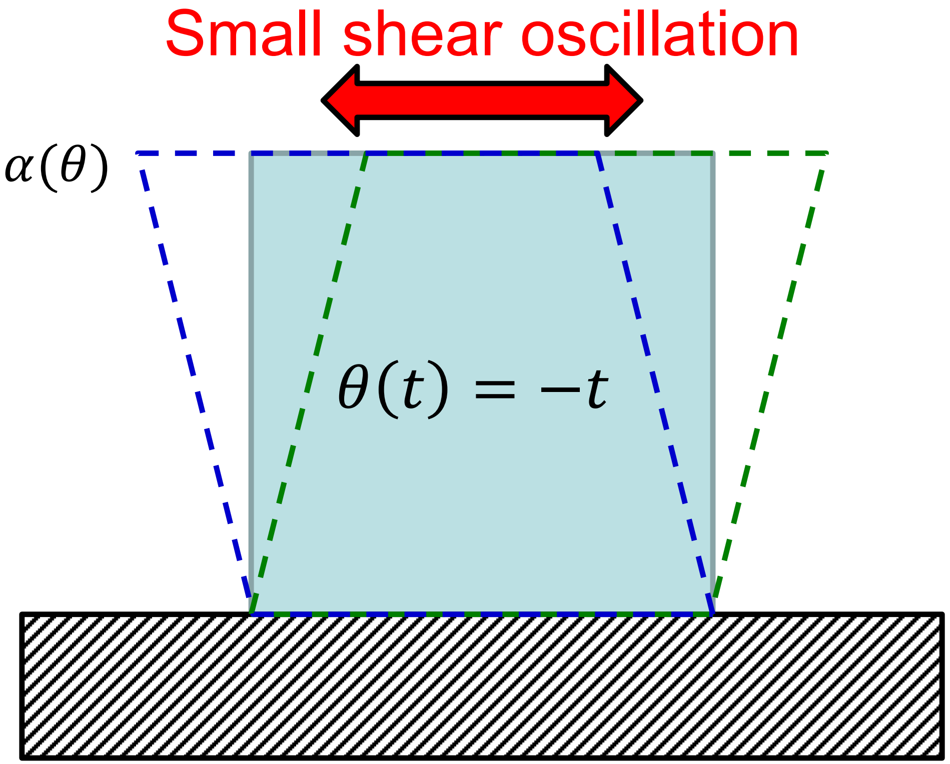
Limitation of Our Method

- UV exposure condition to simulate must be exactly the same as that on the rheology measurement experiments.
- The pattern size must be large enough to apply continuum approximation.

Validation of Material Constitutive Model

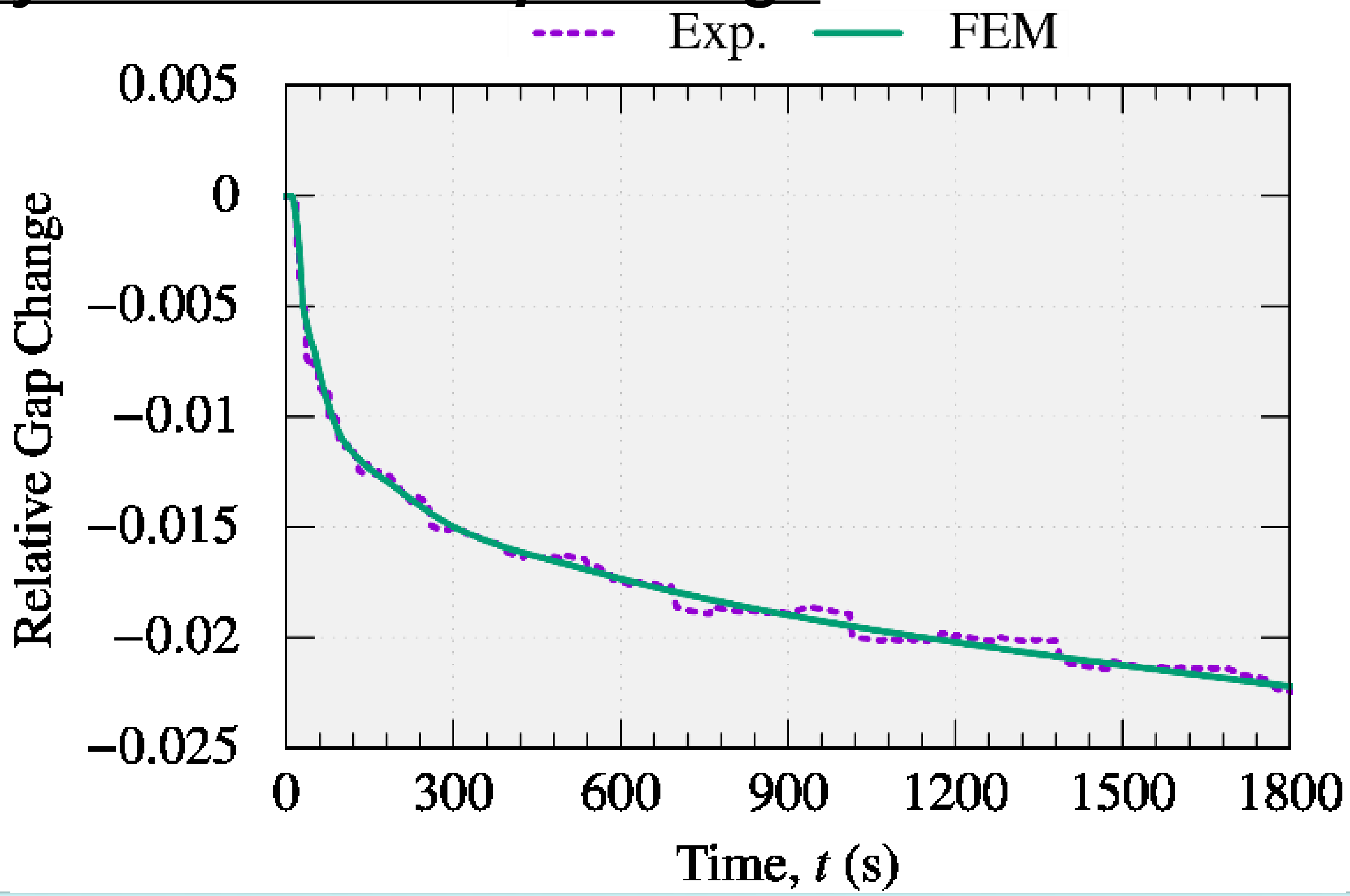
Outline

- Finite element analyses using the identified thermo-viscoelastic properties to reproduce the rheometer measurement data is conducted.
- For simplicity, time evolution analysis that gives shear vibration to one hexahedral element is performed.
- Defined thermo-viscoelastic properties are:
  - Temperature-dependent coefficient of thermal expansion, $\alpha(\theta)$
  - Temperature-dependent shift factor, $A(\theta)$
  - Prony series at reference temperature, g_i $(i = 1, \dots, 20)$
  - Instantaneous Young's modulus E^0 and Poisson's ratio ν^0
- Field condition of temperature $\theta(t) = -t$ is given.
- Boundary conditions are:
  - Perfect constraint on the lower surface
  - Small oscillatory disp. In shear on the upper surface.



Validation of Material Constitutive Model

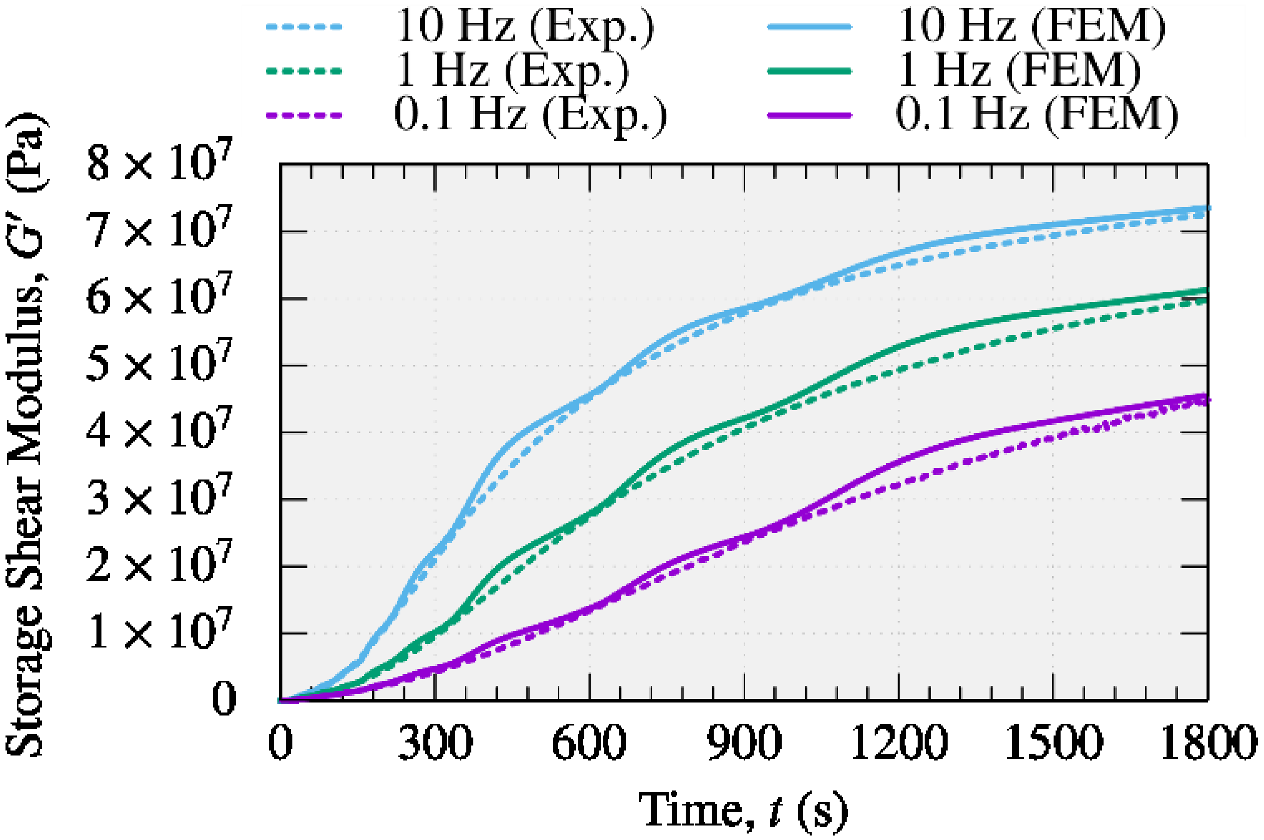
Time History of Relative Gap Change

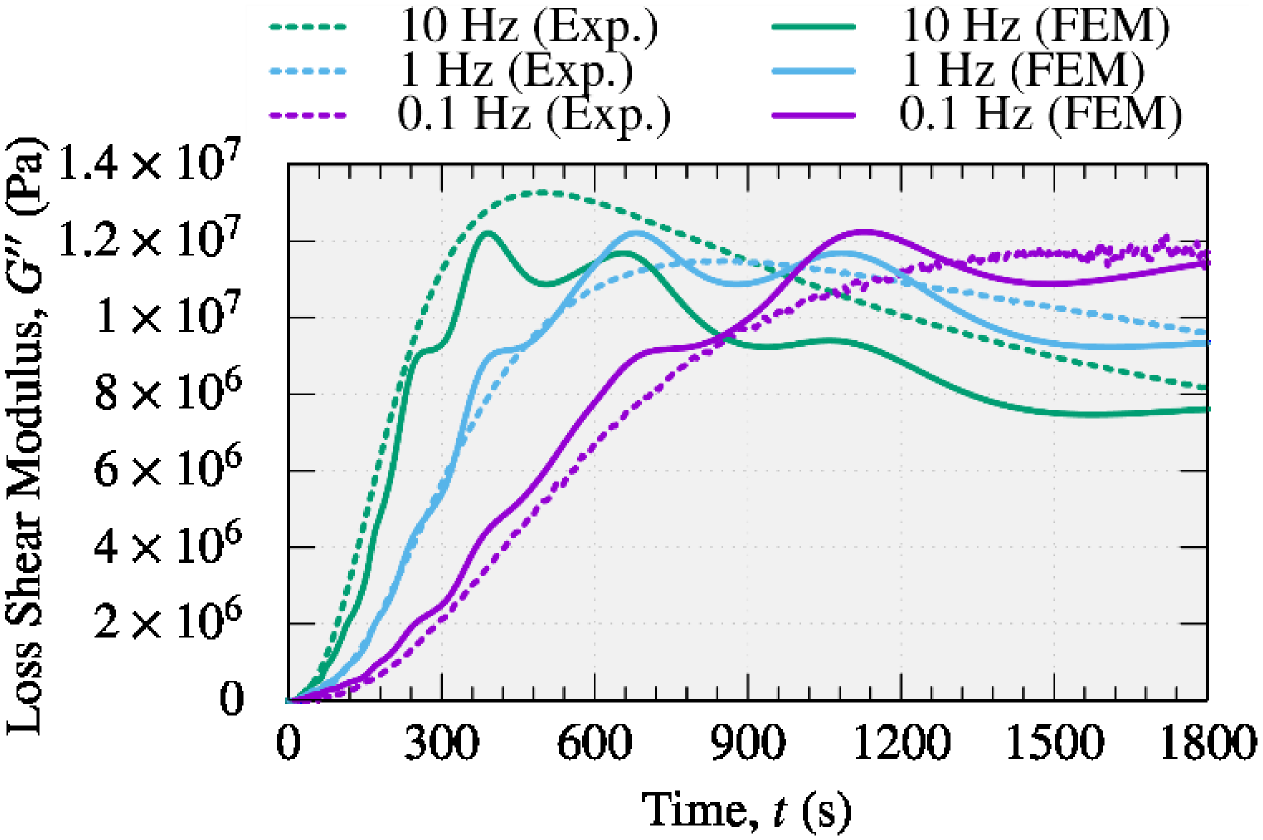


The relative gap change is accurately simulated.

Validation of Material Constitutive Model

Time History of Storage / Loss Shear Modulus





The storage shear modulus G' is accurately simulated.
On the other hand, minor problem remains in the accuracy of the loss shear modulus G'' because $G' \gg G''$.

Outline of UV Process Simulation

Step 1: Stationary (1 sec.)

- Static analysis
- Start no-slip & no-separation contact

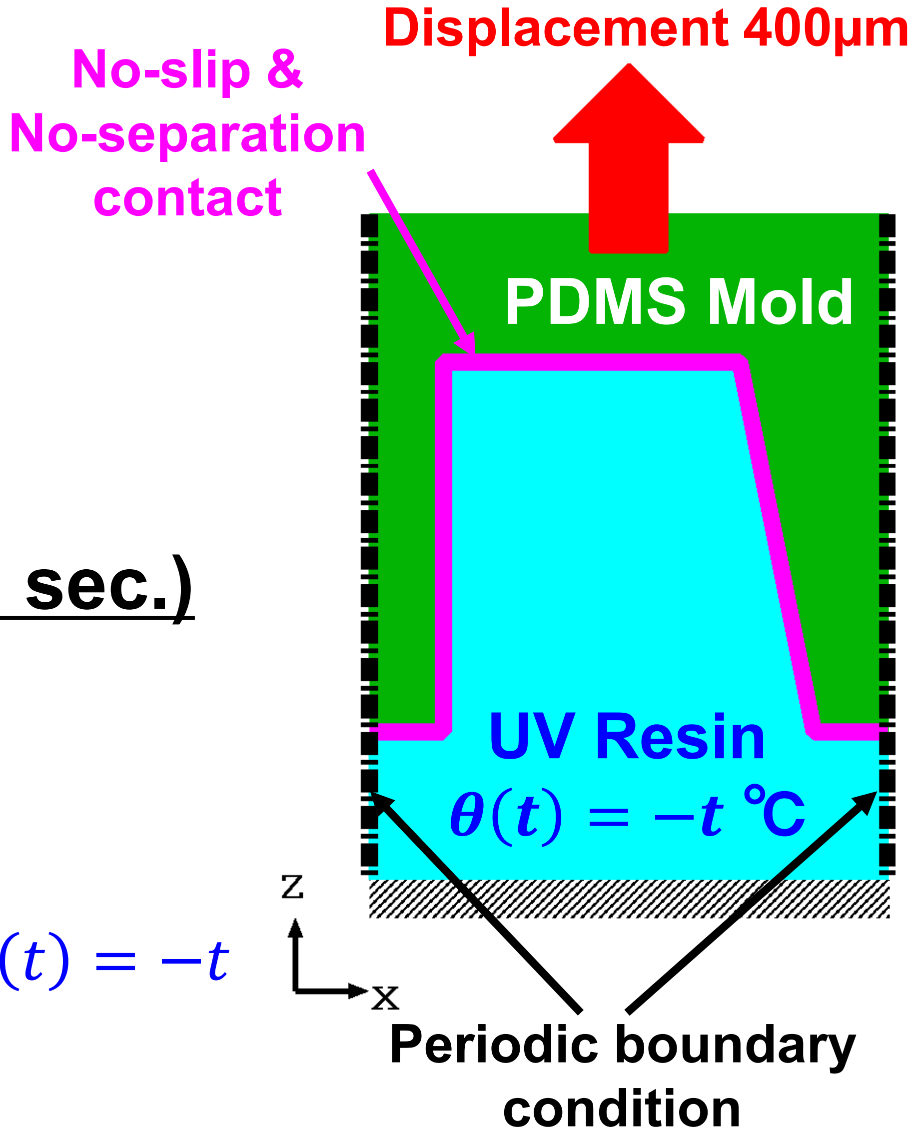
Step 2: UV curing (100 sec.)

- Quasi-static analysis
- Lower UV resin temperature: $\theta(t) = -t$

Step 3: Demolding & Dark curing (6000 sec.)

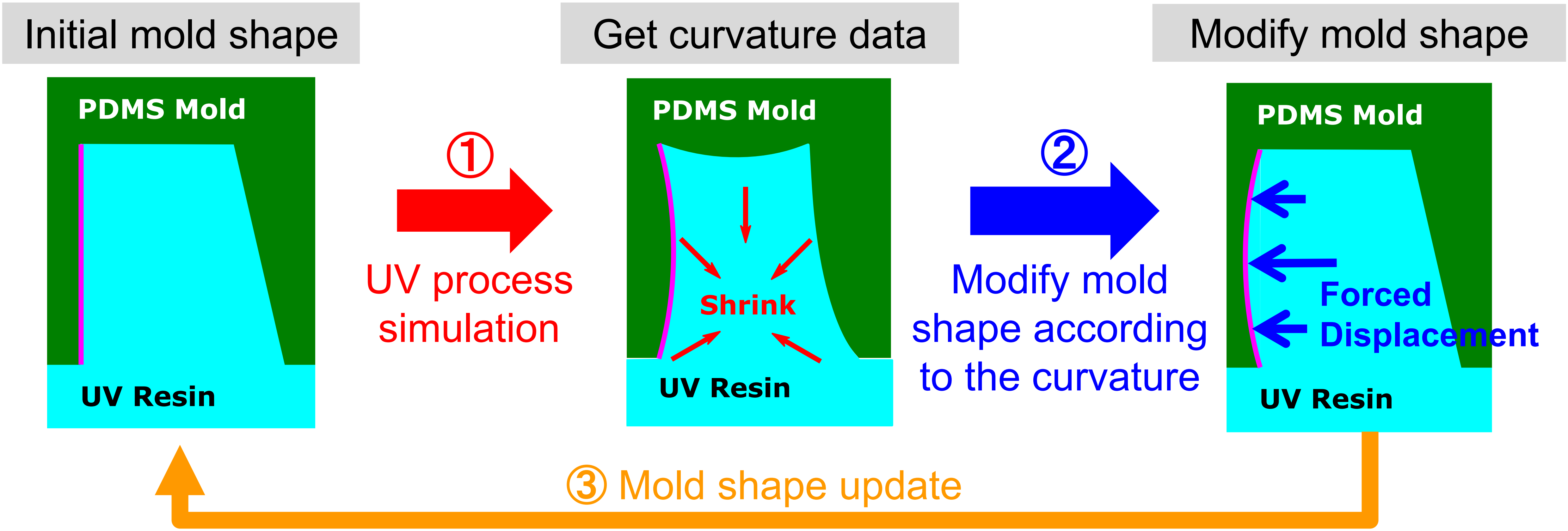
- Quasi-static analysis
- Remove no-slip & no-separation contact
- Lift mold upward
- Continue lowering UV resin temperature: $\theta(t) = -t$

ABAQUS/Standard C3D8 is used for FE analysis.



Search Flow of Optimized Mold Shape

Cost function: Squared sum of curvature depth
Optimization method: Quasi-Newton method



This optimization loop continues
until the curvature after UV shrink becomes flat within tolerance.

How to Find Optimal Mold Shape?

1. Perform proposed FE analysis using mold shape reprecented by $x_i^{(n)}$.

2. Get nodal coordinates $x_i'^{(n)}$ after the analysis.

3. Curvature depth $d_i^{(n)}$ satisfies $d_i^{(n)} < \epsilon \, \forall i$?

YES → Break loop

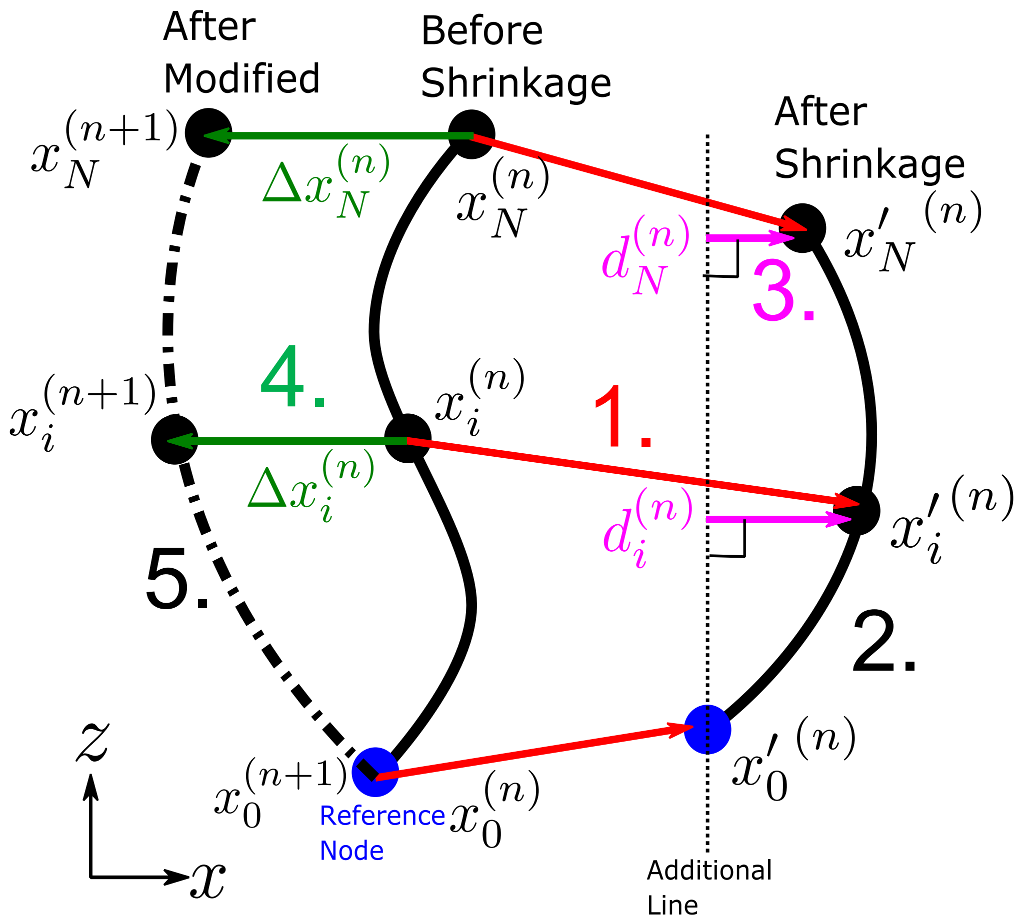
NO ↓

4. Apply forced displacement $\Delta x_i^{(n)} = -\alpha d_i^{(n)}$ to the nodes of the mold.

5. Mold shape coordinates are updated to $x_i^{(n+1)}$.

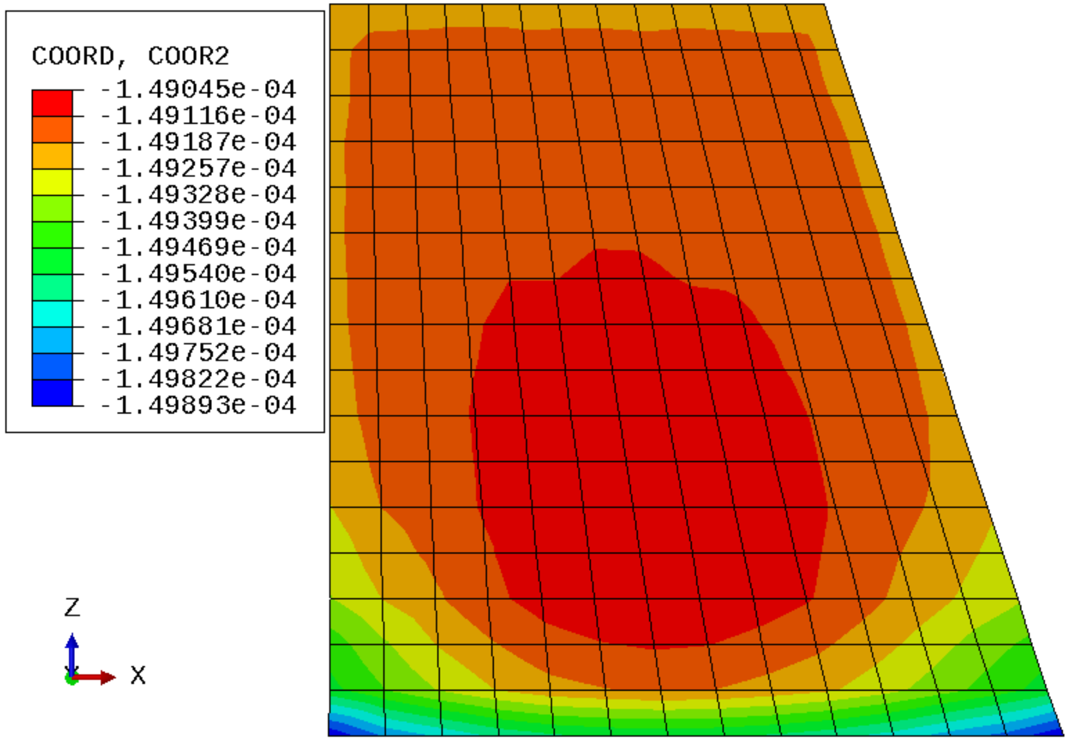
(return to 1.)

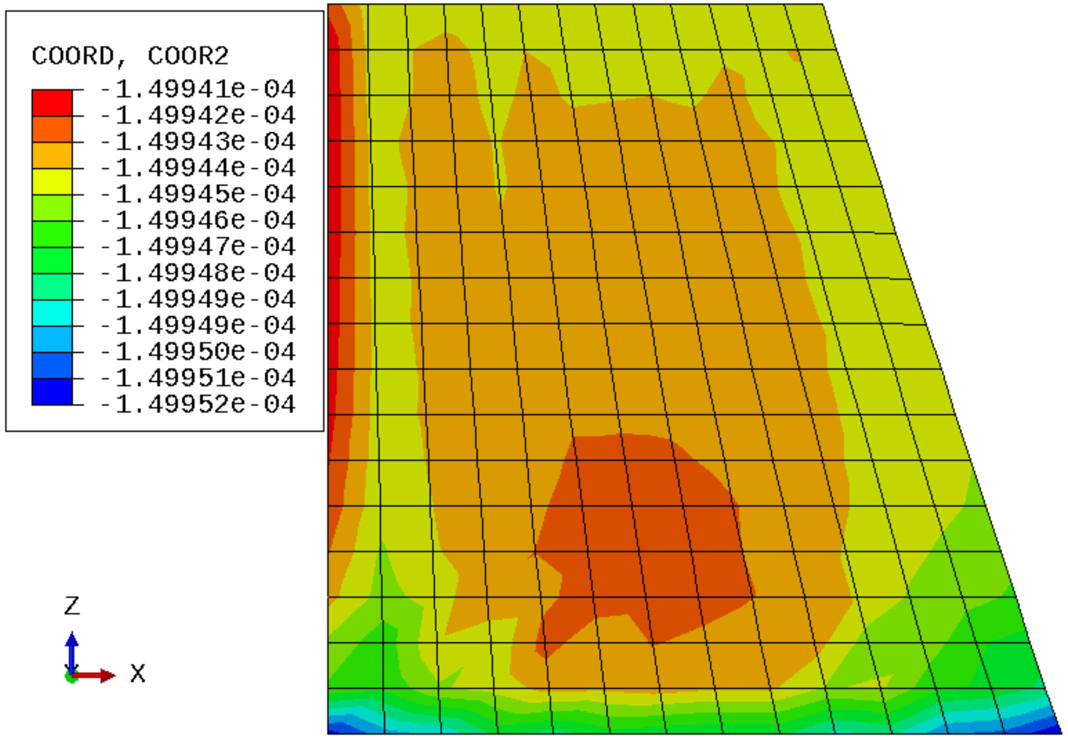
Find nodal coordinates set of the mold $\{\boldsymbol{x}_0, \dots, \boldsymbol{x}_N\}$ that minimize squared sum of curvature depth $\sum_{i=0}^{N} \|\boldsymbol{d}_i\|^2$.



Mold Shape Optimization (Simulation Result)

Curvature Depth Dist. on Mirror Surface





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