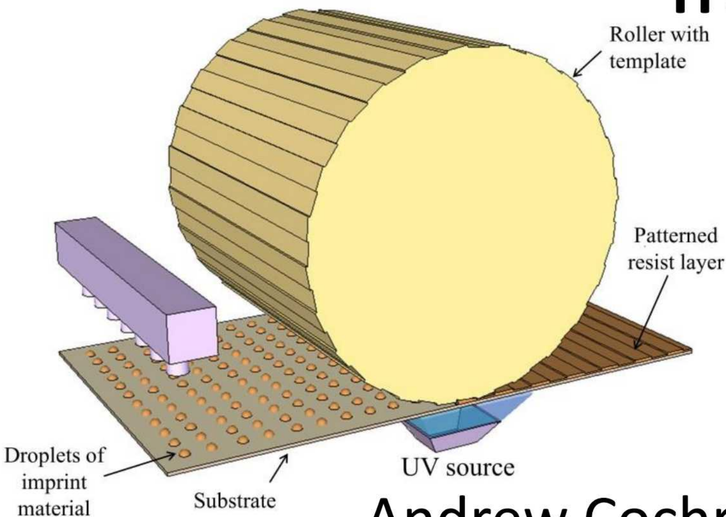
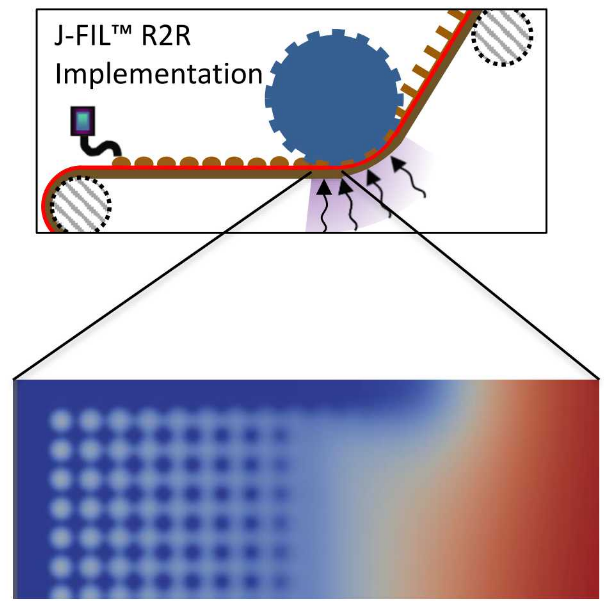
SAND2018-11560C

Two-phase flow and structural deformation models for nanoimprint lithography

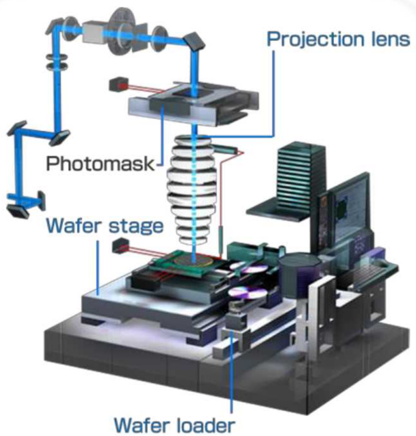


Andrew Cochrane, Kristianto Tjiptowidjojo, Roger T. Bonnecaze, P. Randall Schunk*

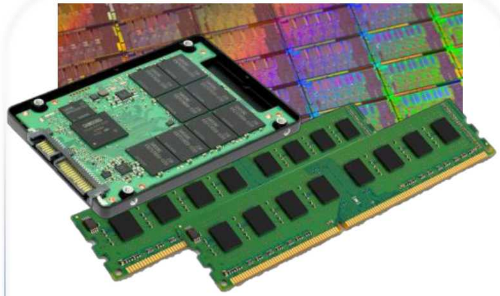


* Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Manufacturing Nano-Featured Materials



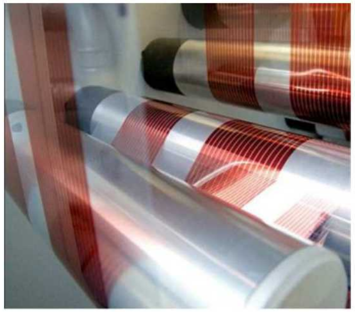
Optical Lithography



CPU, SSD, RAM

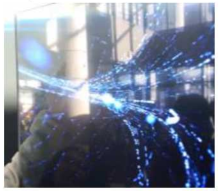
High Price Point
High Volume

- Simpler processing steps
- More product



Roll-to-Roll Nanoimprint

Transparent Electronics



Flexible Batteries

Flexible Displays

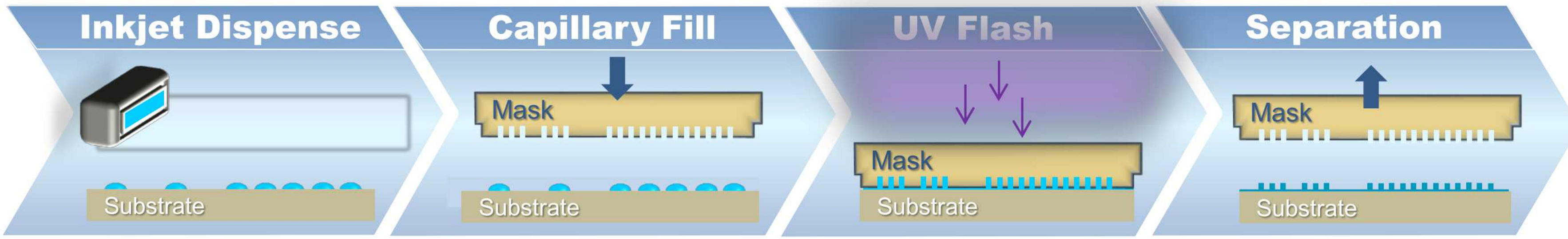
Flexible Polarizers

Flexible Solar Cells

Lower Price Point
Higher Volume

Developing economic nano-patterning for higher volume market

Process Configuration of Jet and Flash Imprint Lithography (J-FIL™)



Dispense Photo-Polymer (Resist) via Ink-Jet

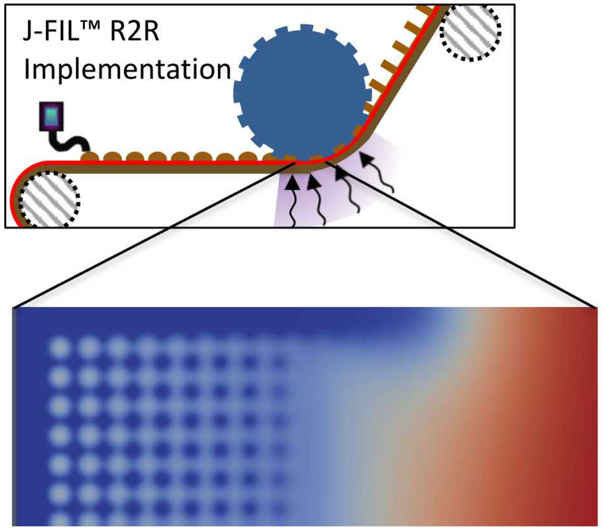
- Inkjet - reduces resist volume, viscous resistance and layer thickness
  - allows resist delivery to features

Resist fills template pattern

- Imprint

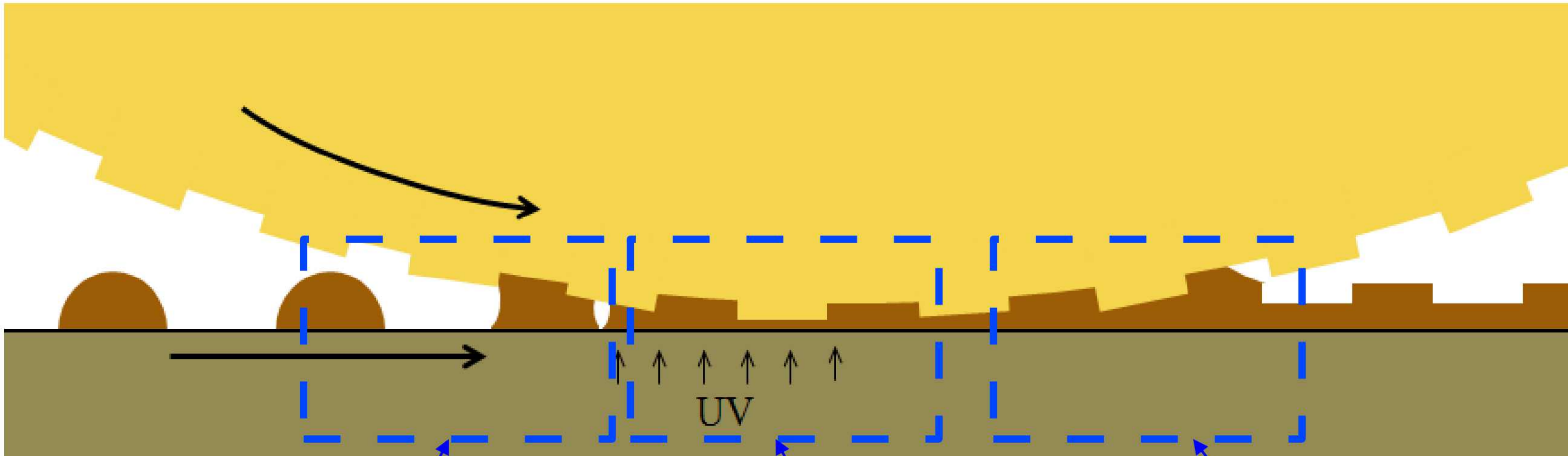
Resist is cured with light

- Flash



Many challenges arise when implementing this process

Physics Regimes of Nanoimprint Lithography



Droplet Merge
Gas Trapping
Capillary Forces
Substrate Deformation
Pattern Filling

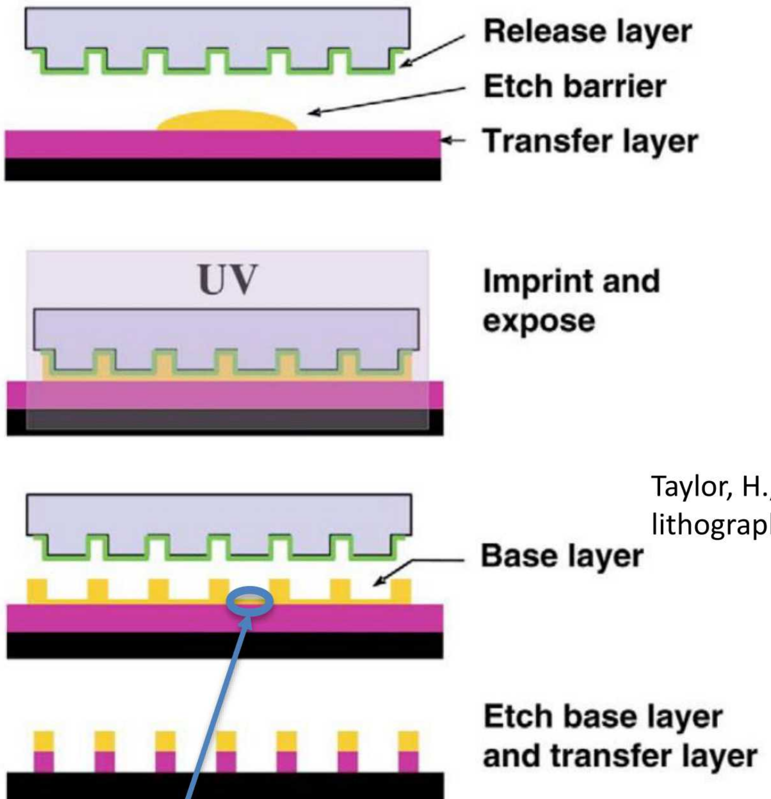
Flash
Phase/Volume Change
Residual Stresses

Peel-Off
Pattern De-adhesion
Feature Deformation

Focus on processing barriers in the droplet merge regime

Courtesy of Akhilesh Jain

Process Scaling Barriers

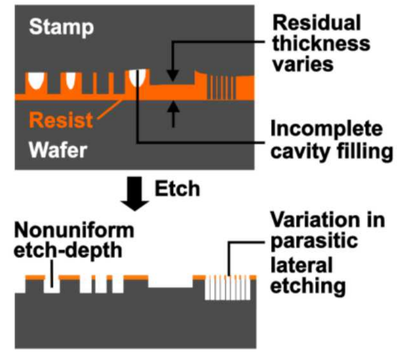


Residual layer is any resist that is not part of the pattern

Resnick, D. J., Sreenivasan, S. V. and Wilson, G. C., 2005, Step & flash imprint lithography: Materials Today, February.

Non-Uniform Residual Layer Thickness

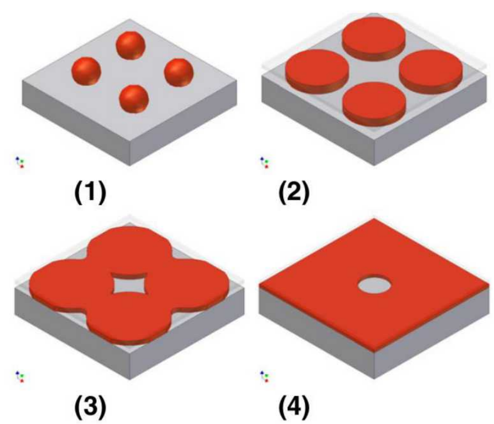
Results in non-uniform etch depth



Taylor, H., 2011, Simulation and mitigation of pattern process dependencies in nanoimprint lithography: Journal of Photopolymer Science and Technology, v. 24, n. 1, p. 47-55.

Gas Trapping

Results in non-fill defects



Model are used to optimize processes and minimize these barriers

Liang, X., Tan, H., Fu, Z., Chou, S. Y., 2007, Air bubble formation and dissolution in dispensing nanoimprint lithography. Journal of Photopolymer Science and Technology, v. 24, n. 1, p. 47-55.

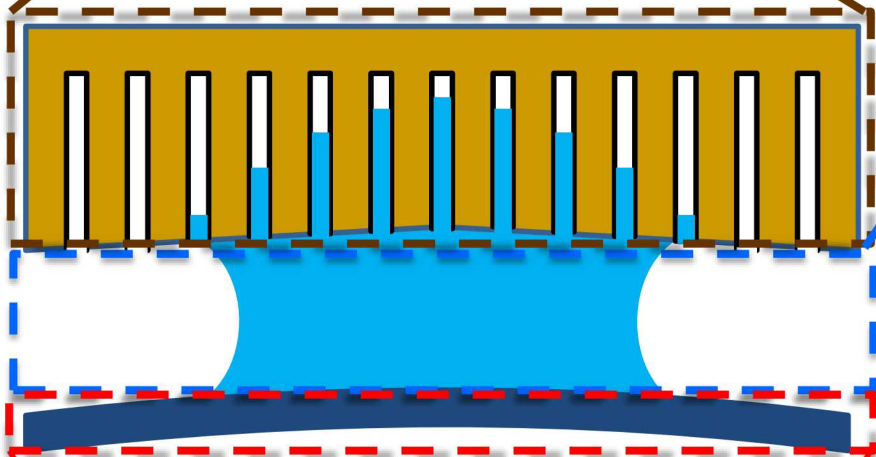
Breaking Down the Droplet Merge Regime

Not drawn to scale!

Feature length ~ 50 – 100 nm
Substrate width ~ 1 cm
Gap thickness ~ 100 nm – 2 μm

Template

- Feature flow
- Solid deformation



Gap

- Two fluid phases
- High viscous stresses
- Gas dissolution
- Capillary forces

Substrate

- Solid deformation
- Web tension
- Rigid flexure

Fast simulations are needed to effectively integrate modeling into process design

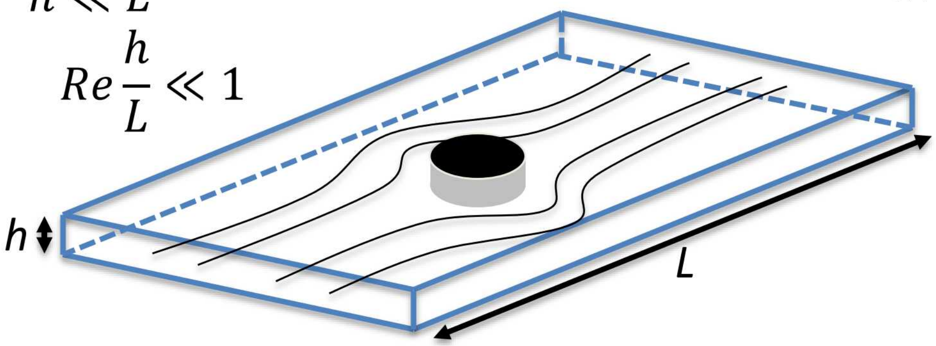
Reduced–order models are needed

Courtesy of Kristianto Tjiptowidjojo

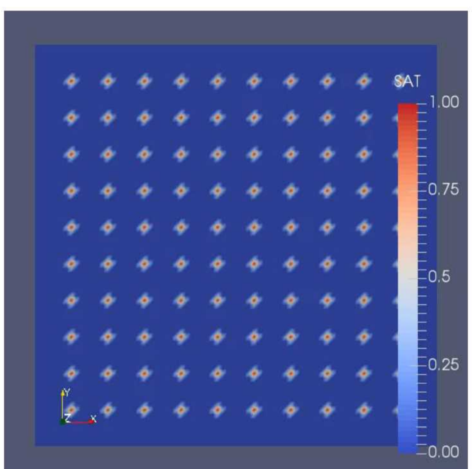
Reduced-Order Models for Thin Gap Multiphase Fluid Flow

$$h \ll L$$

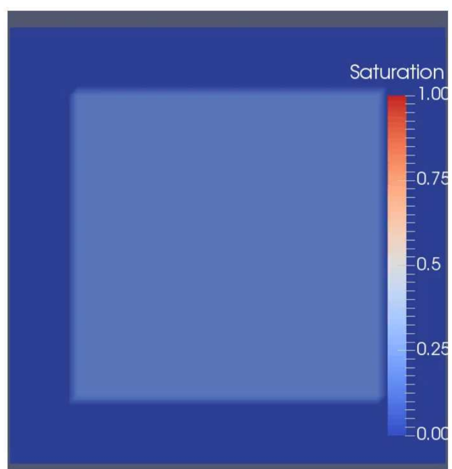
$$Re\frac{h}{L} \ll 1$$



Reynolds, O., 1886, On the Theory of Lubrication and Its Application to Mr. Beauchamp Tower's Experiments, Including an Experimental Determination of the Viscosity of Olive Oil: Philosophical Transactions of the Royal Society of London, v. 177, p. 157-234.



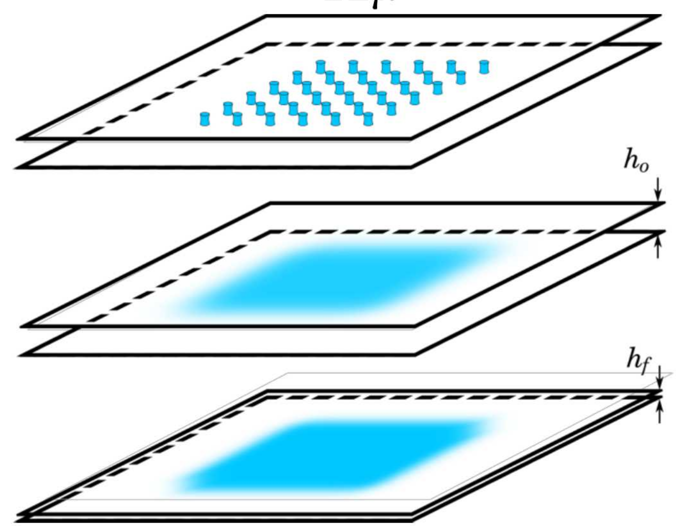
Separated



Disperse

In thin gaps momentum equations reduce to 2-D expression

$$\boldsymbol{v}_{\mathrm{II}} = -\frac{h^2}{12\mu}\boldsymbol{\nabla}_{\mathrm{II}}P$$



Relative Permeability

$$\boldsymbol{v}_{\alpha} = -\frac{h^2}{12\mu}k_{r\alpha}\boldsymbol{\nabla}_{\mathrm{II}}P$$

Disperse representation enables large area simulations with coarse discretization

Gas Dissolution

Gas Mass Balance

$$\frac{\partial((1-S)h\rho_g)}{\partial t} + \nabla_{\mathrm{II}} \cdot (h\rho_g \boldsymbol{v}_g) + J = 0$$

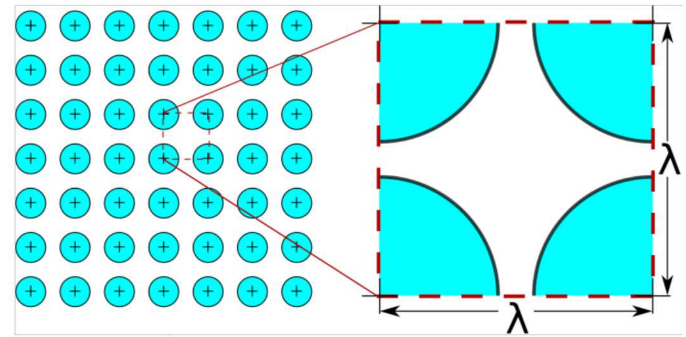
Ideal Gas Law

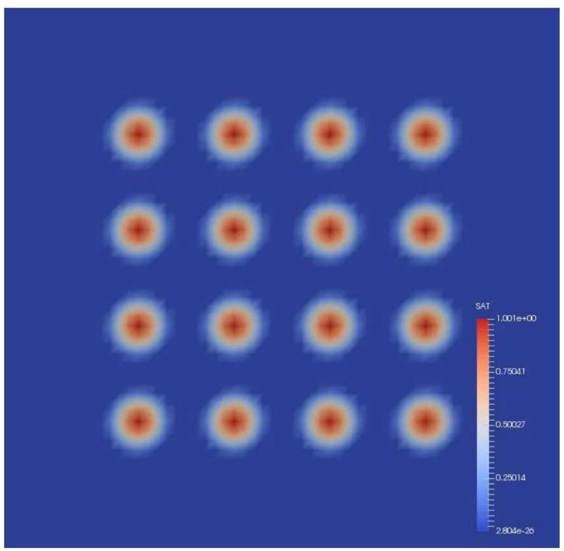
$$\rho_g = \frac{M_g P}{RT}$$

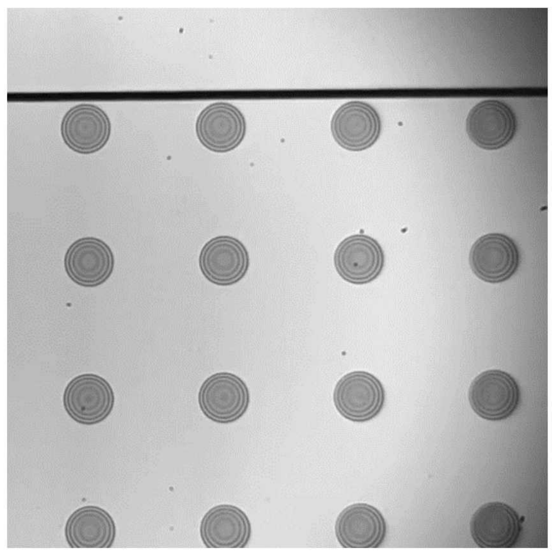
Lumped Parameter Dissolution Model

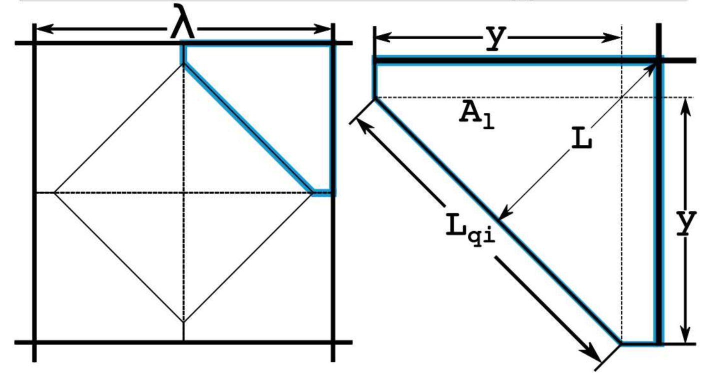
$$J = h\frac{A_i}{V_G}\frac{D}{L}H(P - P_{\mathrm{atm}})$$

Regular/known drop pattern









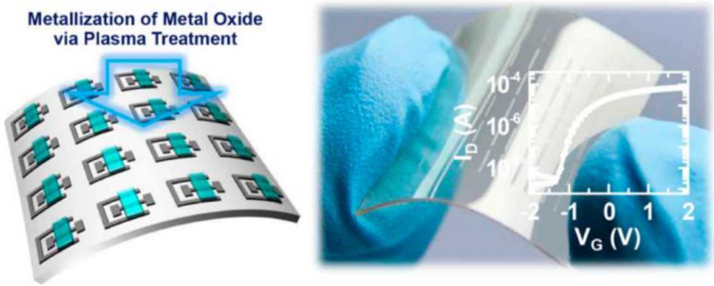
Analytic dissolution model

Reduced order models for two-phase, thin-gap, gas dissolving flow

Cochrane, A., Tjiptowidjojo, K., Bonnecaze, R. T., Schunk, P. R. 2018 *Multiphase model for nanoimprint lithography*. International Journal of Multiphase Flow.

Drop Density Varied for Fill of Non-Uniform Pattern

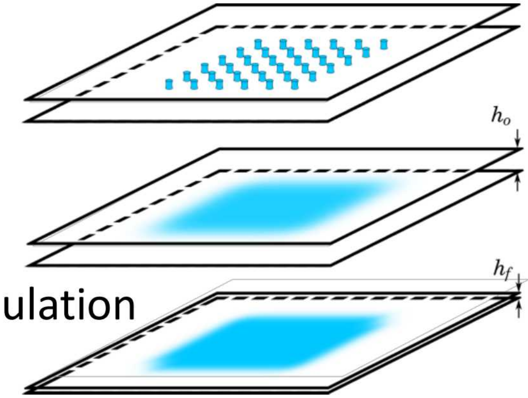
Thin film transistor



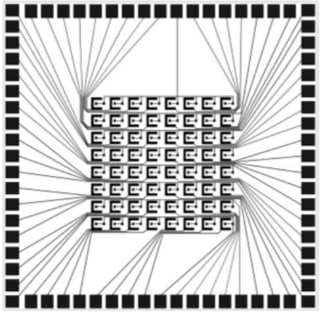
Choi, Y., W.-Y. Park, M. S. Kang, G.-R. Yi, J.-Y. Lee, Y.-H. Kim, and J. H. Cho, 2015, Monolithic metal oxide transistors, ACS Nano, p. 4288-4295.

NIL processing model

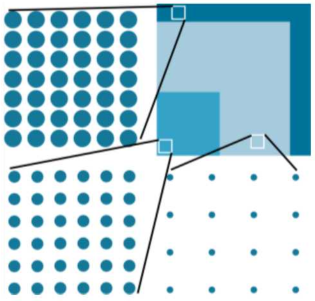
Disperse flow formulation



Pattern mask



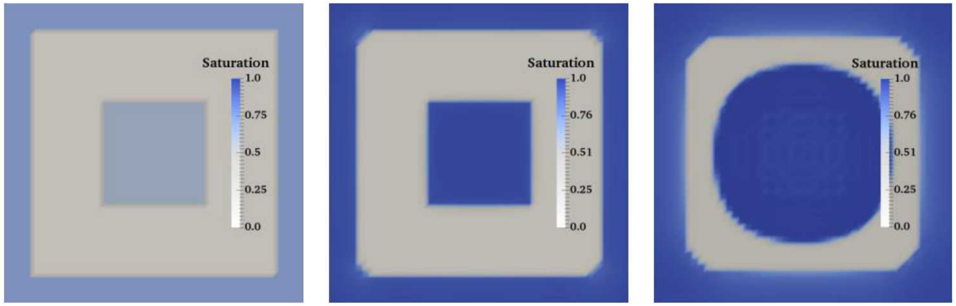
Regions require different amounts of resist



Liquid bridge formation

Full gap

Overfull gap



Model can represent varied density drop pattern by variation across initial saturation field

Sensitivity Analysis
Relative Work Comparison

Comparative Work Function

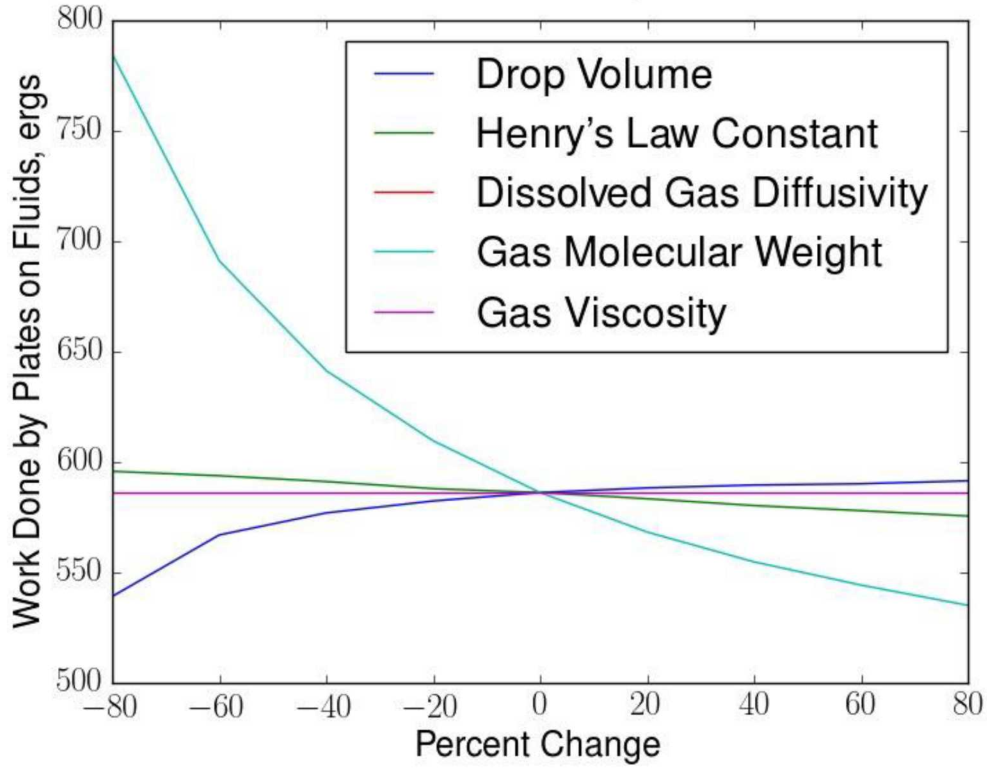
- No Surface Tension
- No Deformation

$$E = \int_0^{t_f} \int_A P \mathrm{d}A \frac{\mathrm{d}h}{\mathrm{d}t} \mathrm{d}t$$

Base Case:
6 pL water drops in N_2
Squeezed from 1 micron to 100 nm

Is processing rate increased because viscous dissipation is high or because it takes a long time to dissolve the gas?

Sensitivity of Work to Percent Change in Base Case Processing Parameter



Experimentally Realizable parameter adjustment
Reduce liquid viscosity 20% → Reduce Work by 9%
Change N_2 to CO_2 → Reduce Work by 8%

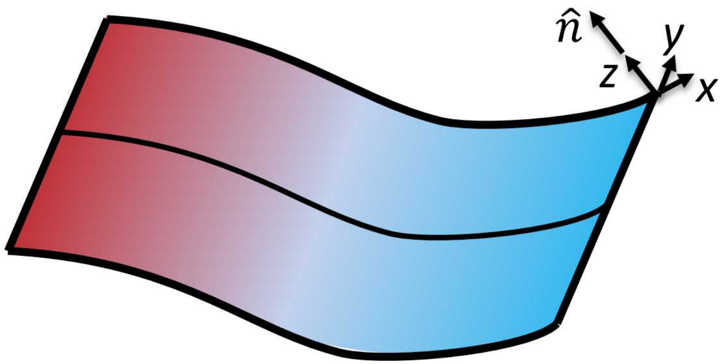
Both viscous dissipation and gas dissolution can have an effect on processing rate

Structural Model

Membrane Mechanics

$$\boldsymbol{\nabla}_{\text{II}} \cdot \overline{\overline{\boldsymbol{T}_{\text{II}}}} + \boldsymbol{\tau}_{\text{II}} = 0$$

$$T_{xx}\kappa_x + T_{yy}\kappa_y + P_s = 0$$



- Constitutive Relationship

$$\boldsymbol{v}_{\text{II}} = -\frac{h^2}{12\mu}\boldsymbol{\nabla}_{\text{II}}P$$

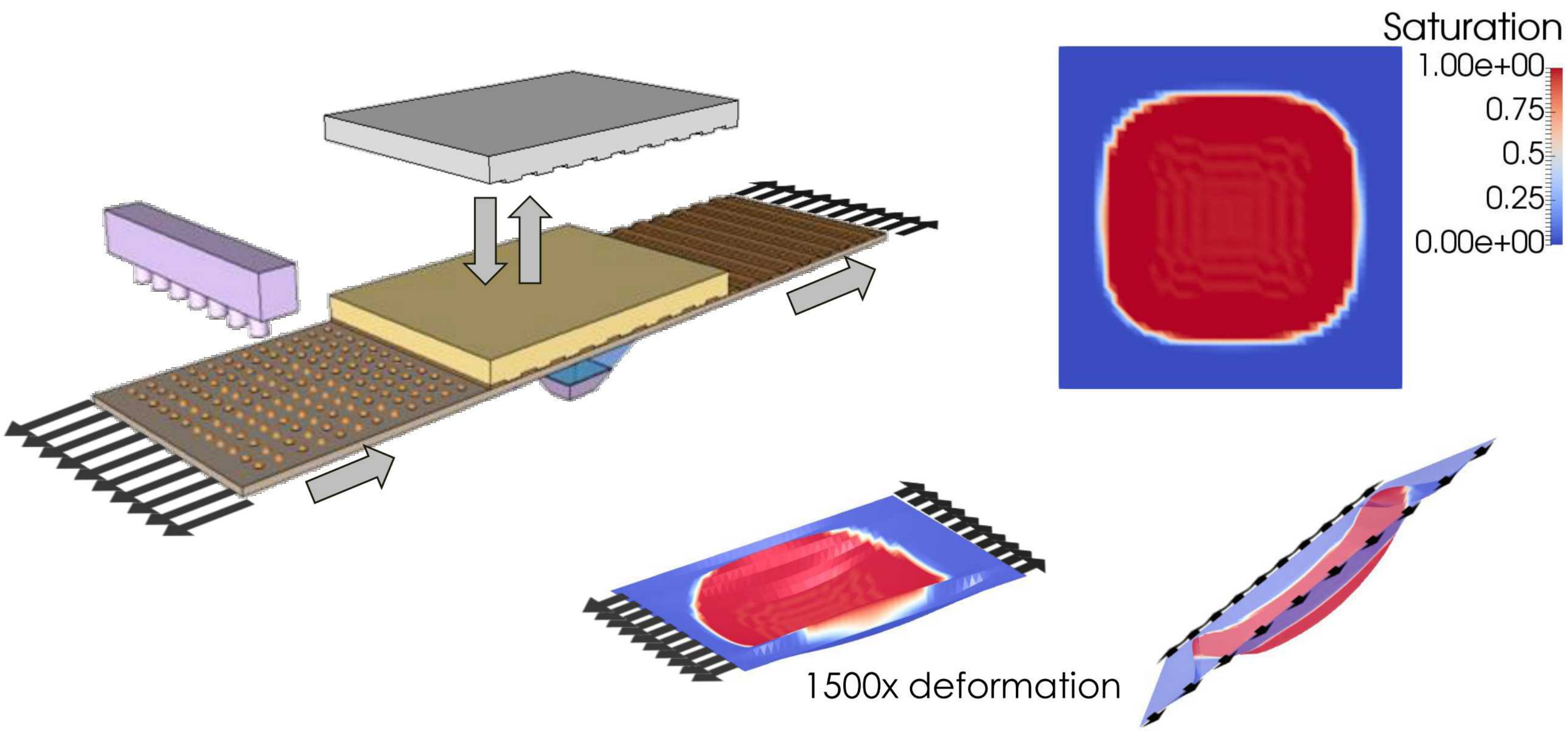
$$P_s = P + S\sigma\kappa$$

Wrinkled membrane

Reduced order model for web-structure mechanics

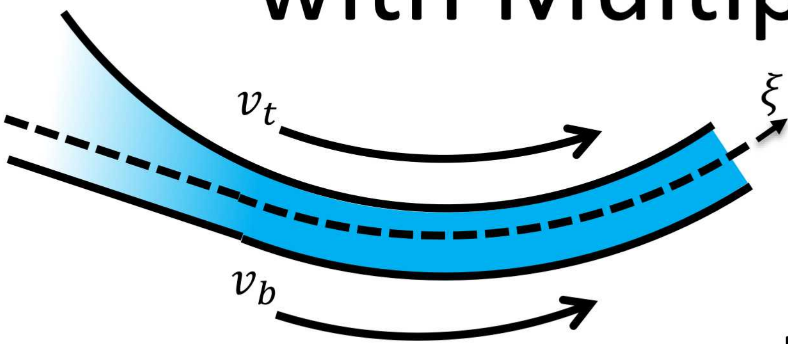
Tjiptowidjojo, K., 2014, Structural Mechanics of Roll-to-Roll Nanoimprint Lithography: 17th International Coating Science and Technology Symposium.

Membrane Mechanics Model Coupled with Disperse Flow Model



Pinch-off in crossweb direction suggests membranes are too pliant

Cylindrical Shell Model Coupled with Multiphase Lubrication



Cylindrical Shells

Tangential Force Balance

$$\frac{dT}{d\xi} + \kappa \frac{\partial}{\partial \xi}(\kappa D) + P_t = 0$$

Normal Force Balance

$$-\kappa \frac{\partial^2}{\partial \xi^2}(\kappa D) + \kappa T + P_n = 0$$

Geometry

$$\frac{d^2 x}{d\xi^2} + \kappa \frac{dy}{d\xi} = 0$$

Liquid Mass Balance

$$\boldsymbol{v}_l = -\frac{h^2}{12\mu_l} k_{rl} \frac{\partial}{\partial \xi} P$$

$$\underbrace{\frac{\partial (Sh)}{\partial t} + \frac{\partial}{\partial \xi}(h v_l)}_{\text{Pressure driven flow}} + \underbrace{\frac{\partial}{\partial \xi}(S h v_a) - \frac{1}{2} S v_d \frac{\partial}{\partial \xi} h}_{\text{Top/Bottom boundary motion terms}} = 0$$

Pressure driven flow — Top/Bottom boundary motion terms

Displacement-Gap Thickness Coupling

$$h = h_o - \boldsymbol{n} \cdot \boldsymbol{\delta}$$

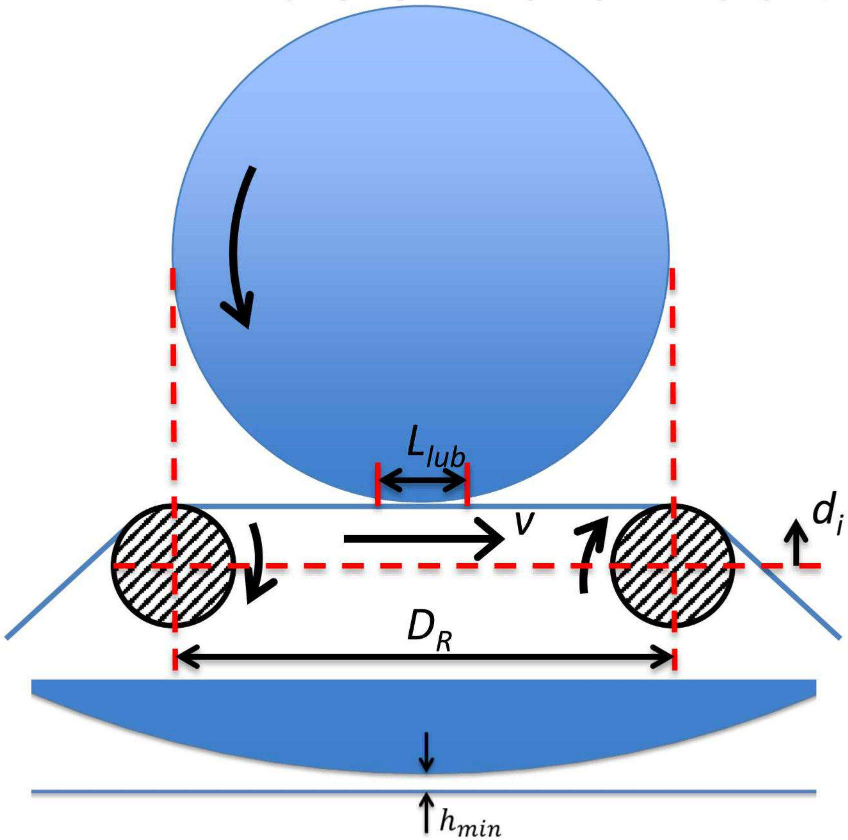
Lubrication-Normal Pressure Coupling

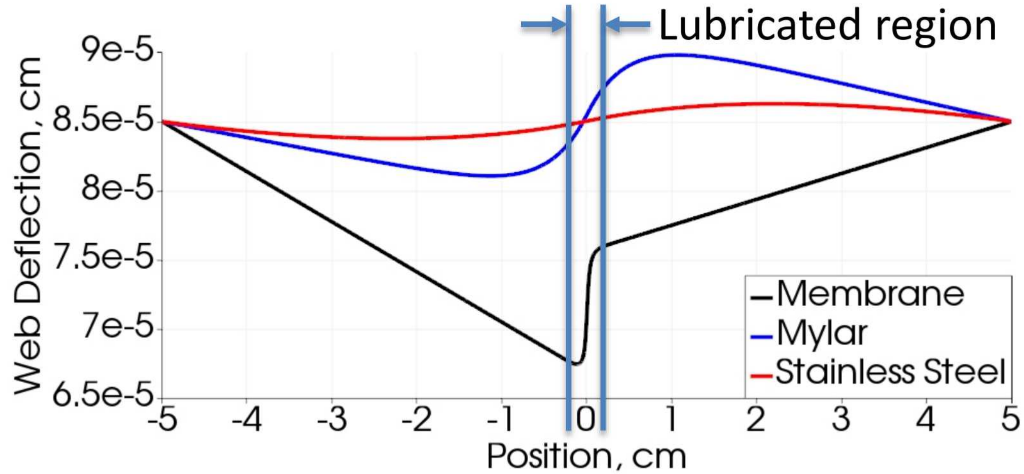
$$P_n = P - P_{\text{atm}}$$

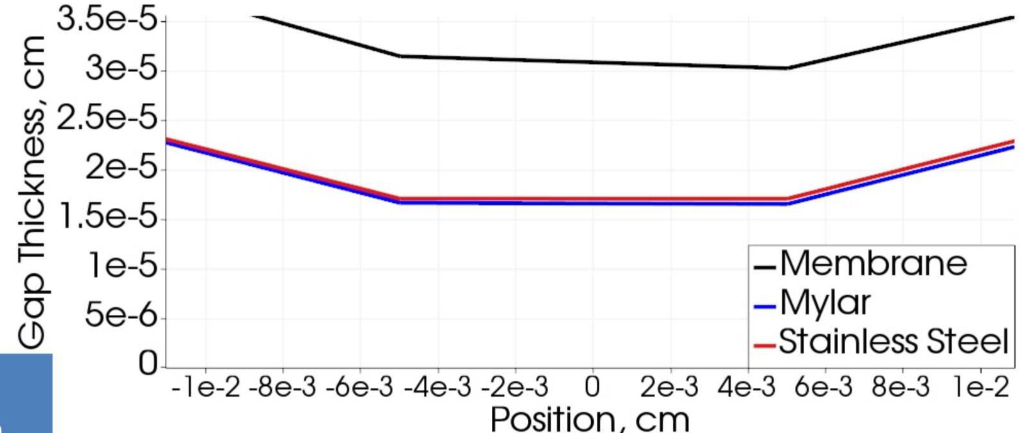
With this coupled model we explore how bending stiffness affects web deformation in a closing nip

Carvalho, M. S. (2003) Elastohydrodynamics of tensioned web roll coating process. *International Journal of Numerical Methods in Fluids,* 41**,** 561-576.

Effects of Web Stiffness on Single Phase Lubrication Thickness Profile







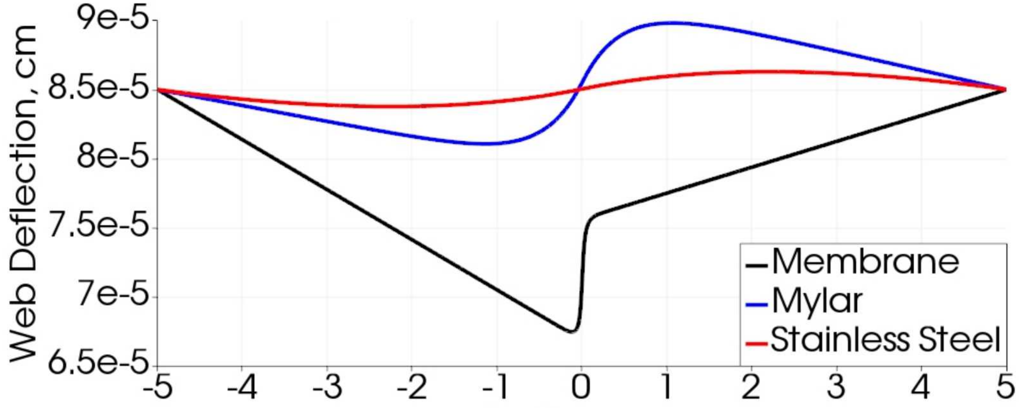
L_{lub} = 6.6 mm
D_R = 10 cm
v = 1 micron/s
d_i = 850 nm
h_{min} = 1 micron

Material	Bending Stiffness, Nm
Membrane	0
Mylar	$0.21(10)^{-3}$
Stainless Steel	$7.7(10)^{-3}$

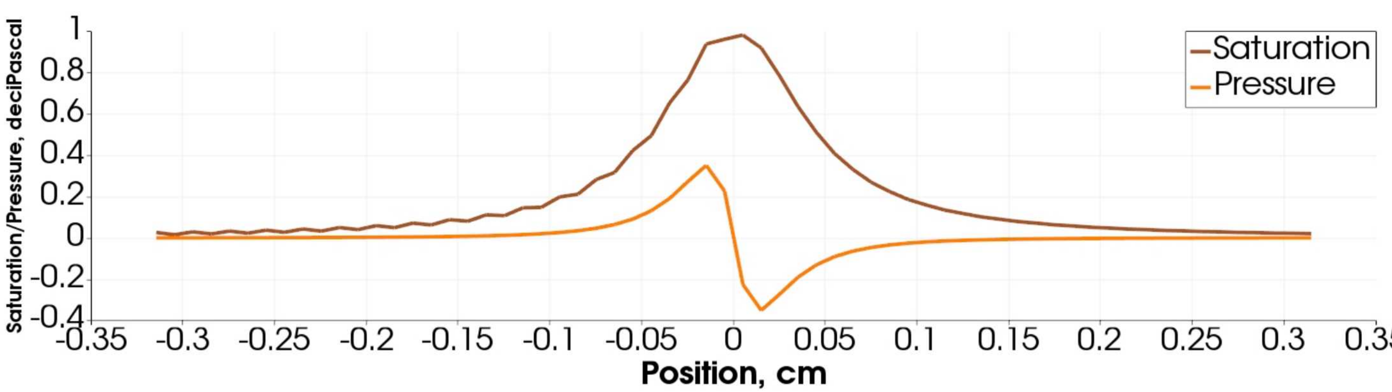
Even for pliant web material, bending stiffness has an effect on web deformation

Conclusions & Future Work

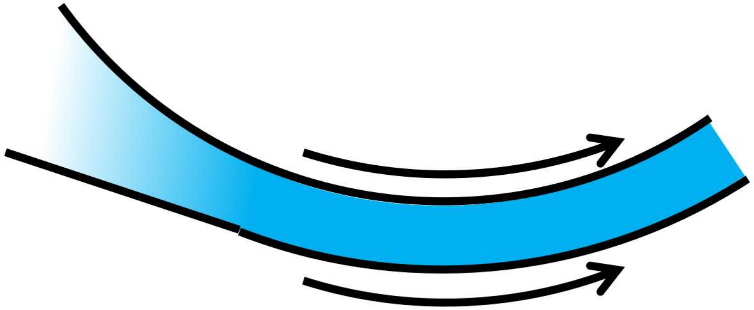
- In drop merger, both viscous dissipation and gas dissolution can effect processing rate
- Bending stiffness is an important physical aspect that needs to be included in simulations of web deformation
- Using coupled reduced order models many simulations can be iterated through quickly to determine effects of various properties in a given process



- Push forward with cylindrical shell model and two-phase flow



Questions and Acknowledgements



Is the instability due to physical model, mathematical formulation or numerical implementation?

Schunk Group:
P. Randall Schunk
Rekha Rao
Kris Tjiptowidjojo
Daniel Hariprasad
Rich Martin
Weston Ortiz

Bonnecaze Group:
Roger T. Bonnecaze
Akhilesh Jain
Andrew Spann

Experimental Support:
Shrawan Singhal

THE UNIVERSITY OF NEW MEXICO

TEXAS
The University of Texas at Austin

GOMA

https://github.com/goma/goma

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Schunk, P. R., R. R. Rao, K. S. Chen, D. A. Labreche, A. C.-T. Sun, M. M. Hopkins, H. K. Moffat, R. A. Roach, P. L. Hopkins, P. K. Notz, S. A. Roberts, P. A. Sackinger, S. R. Subia, E. D. Wilkes, T. A. Baer, D. R. Noble, and R. B. Secor, 2013, GOMA 6.0 : a full-Newton finite element program for free and moving boundary problems with coupled fluid/solid momentum, energy, mass, and chemical species transport : users guide.

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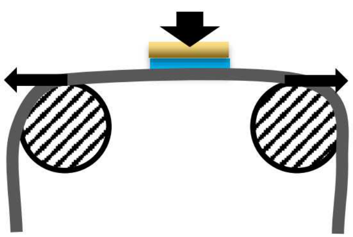
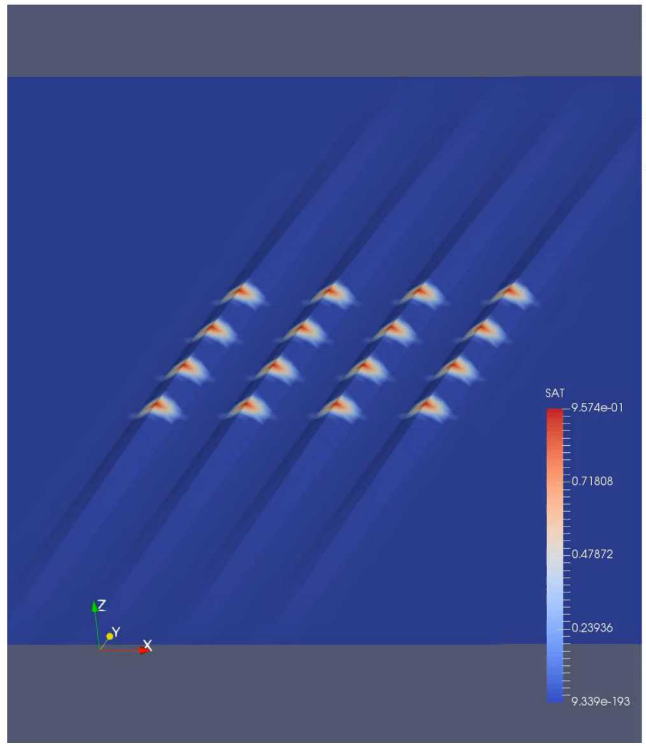
Membrane + Reduced-Order, Separated Reynolds Lubrication

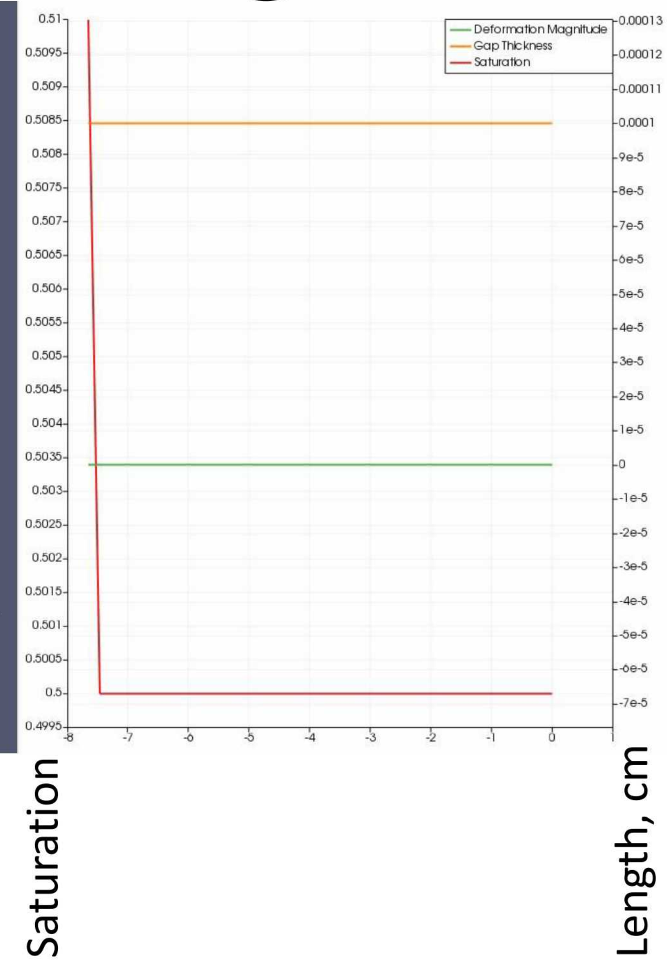
Squeezing of liquid film
Membrane Deformation
+ Reynolds Lubrication
+ two-phase model



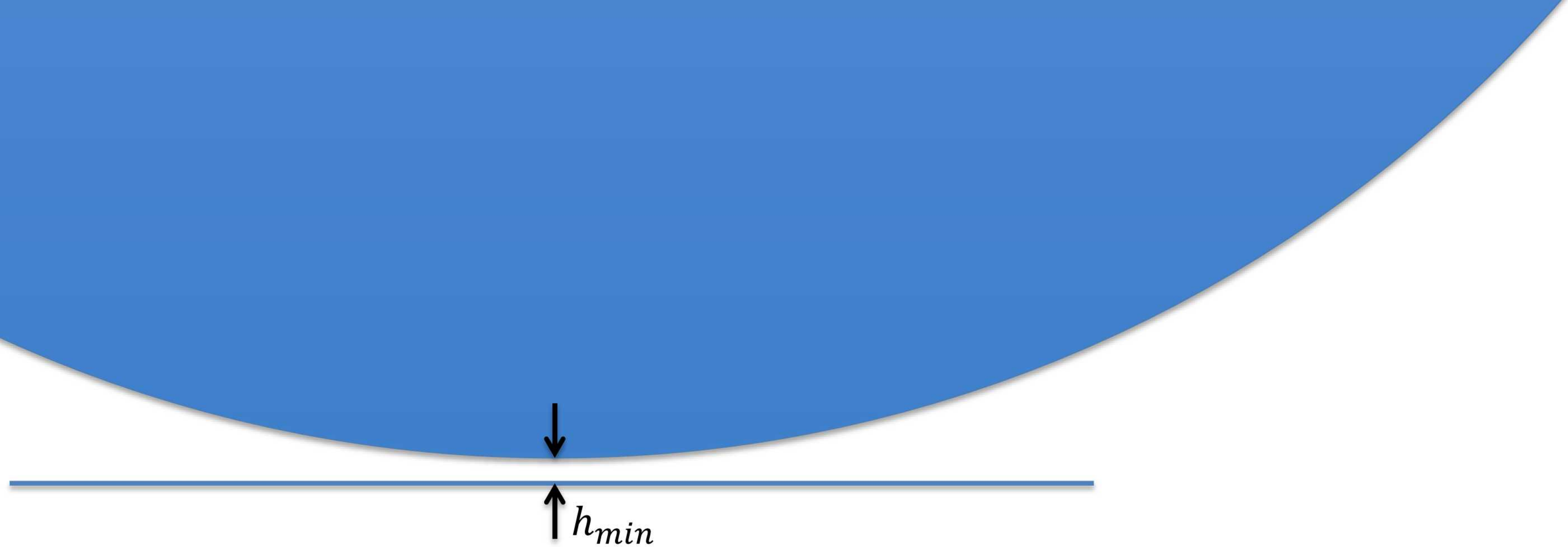


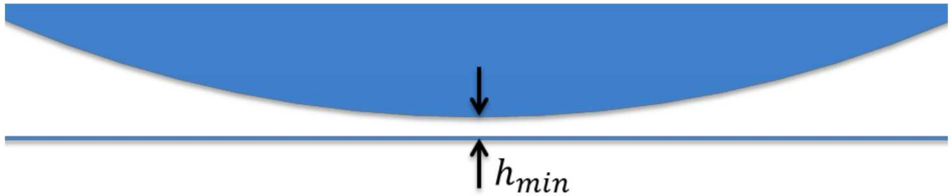
Demonstrated coupling of multiphase flow and structural mechanics

Disperse Drop Merger Between Tensioned Web and Rotating Roller

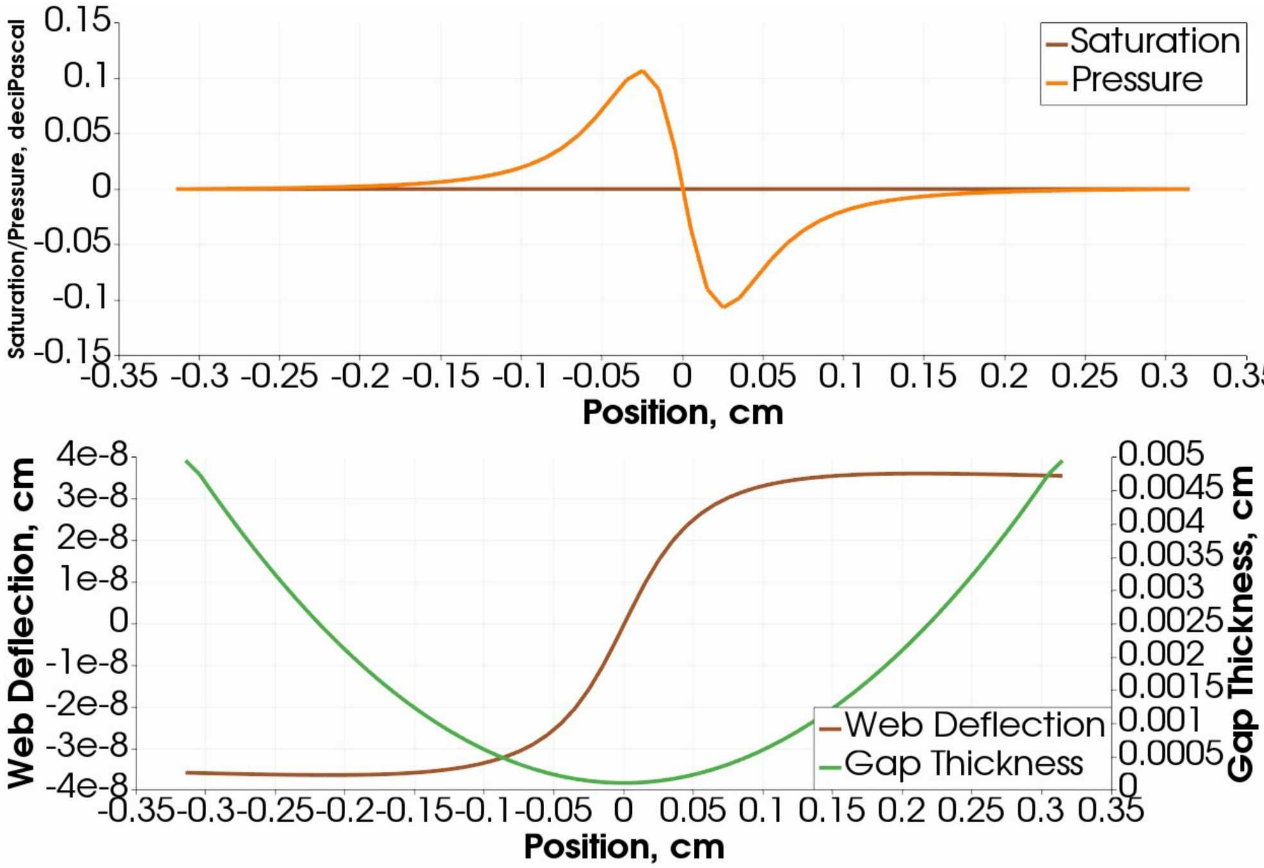


Model implementation continues with boundary condition formulation


h_{min}


h_{min}

Two Phase Lubrication Flow in Rolling Imprint Mode



The next challenge is to smooth out the intersection of partially saturated and fully saturated zones