A thermomechanical approach to mold filling in roll-to-roll nanoimprinting lithography

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In a typical Roll-to-Roll NanoImprinting Lithography (R2RNIL) process, a substrate coated with a fluid film is continuously transported through the nip region between the mold roller and the backup roller. The process involves the following sequential steps: filling of the mold pattern with the fluid film on the substrate (mold filling), the phase change from liquid to solid of the fluid in the mold pattern, and the debonding of the patterned surface from the mold roller; see the illustration provided in Figure 1. One critical aspect of large area patterning using R2RNIL is to obtain quality imprinted features at reasonable web transport speeds (> 10 m/min). This has been a challenge due to the lack of appropriate models of the process which could be employed to evaluate the effect of key process and transport parameters, such as web speed, pattern geometry, film thickness, viscosity, stress relaxation time, etc. From a mechanics viewpoint, most existing models have one or more of the following deficiencies: lack of physical compliance with conservation laws and material properties, consideration of the free surface that is formed inside the mold pattern, and the evolutionary nature of the problem.

A preliminary model that addresses the aforementioned deficiencies with regard to mold filling was described in [1]. In this paper, we will improve this model by applying the thermomechanical framework developed in [2]. Employing this framework and considering specific forms of the stored energy and rate dissipations functions, we derive the constitutive equations which along with the conservation laws of continuum mechanics describe the mold filling process of viscoelastic fluid films at the nanoscale. Kinematic equations associated with the geometry of the mold pattern, rollers, and the substrate with the fluid film are derived and integrated into the governing equations; see the illustration provided in Figure 2. The available time for mold filling is defined based on these kinematic equations. To show the qualitative behavior of the evolution of mold filling within the pattern via numerical simulations, we assume that the displacement gradient is small to derive linearized governing equations with dynamic boundary conditions. A numerical scheme based on the Marker and Cell method first proposed in [3] is derived for the R2RNIL process to solve the governing equations and obtain the evolution of the dynamic free surface of the fluid film in the mold cavity. A number of numerical simulations were conducted with this numerical scheme, and Figure 3 provides the non-dimensional pressure and strain for one pattern feature at the end of the mold filling phase. The proposed model is capable of predicting the evolution of the free surface profile within the pattern feature. The model may be employed to study the effects of various key process, material and transport parameters, which could be utilized for the process and control design. Although the focus in this paper is on the mold filling process only, the problem formulation will set the theoretical background and general assumptions that can be applied to phase change and demolding aspects of the process.

References:

[1] Gomez-Constante, J. P., Pagilla, P. R., and Rajagopal, K. R., 2019, "Effect of the Processing

and Transport Parameters on Mold Filling in Roll-to-Roll Nanoimprint Lithography," Proc. of the 15th Intl. Web Handling Conference, Stillwater, OK.
[2] Rajagopal, K.R. and Srinivasa, A.R., 2000. "A thermodynamic frame work for rate type fluid models". Journal of Non-Newtonian Fluid Mechanics, 88(3), pp.207-227.
[3] Harlow, F.H. and Welch, J.E., 1965. Numerical calculation of time- dependent viscous incompressible flow of fluid with free surface. The physics of fluids, 8(12), pp.2182-2189.

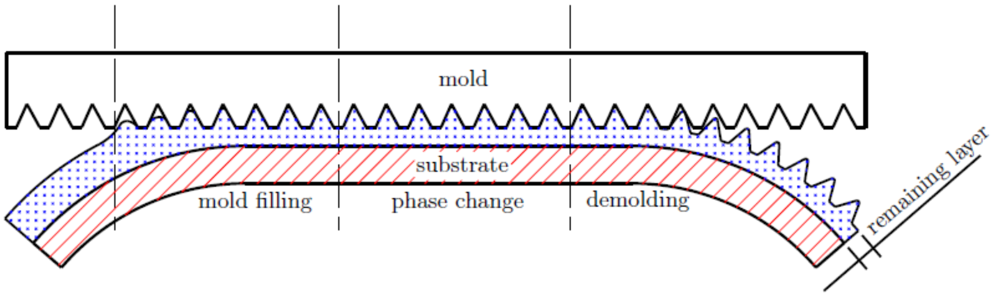

Figure 1. Mechanical sub-processes of R2RNIL process.

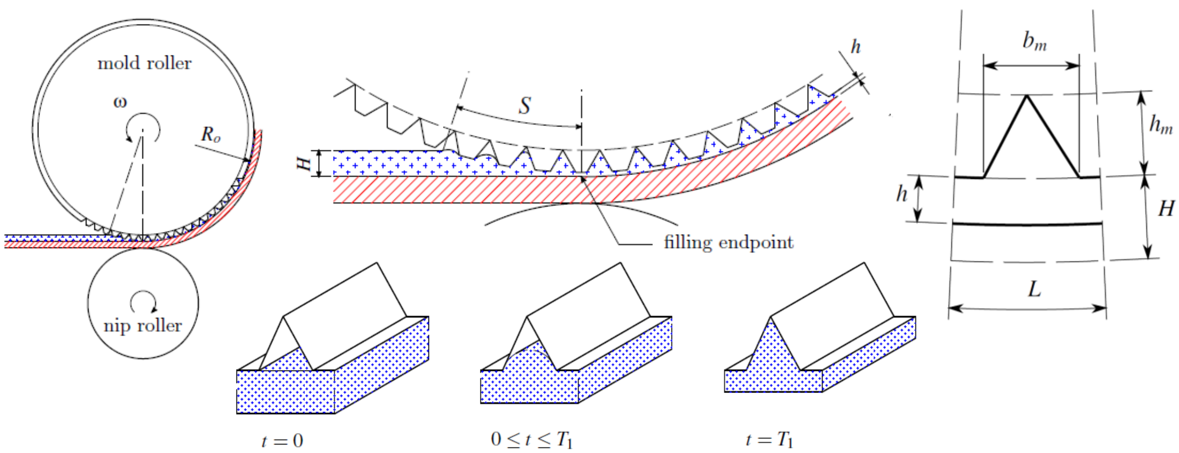

Figure 2. Kinematics and spatial domain for one feature.

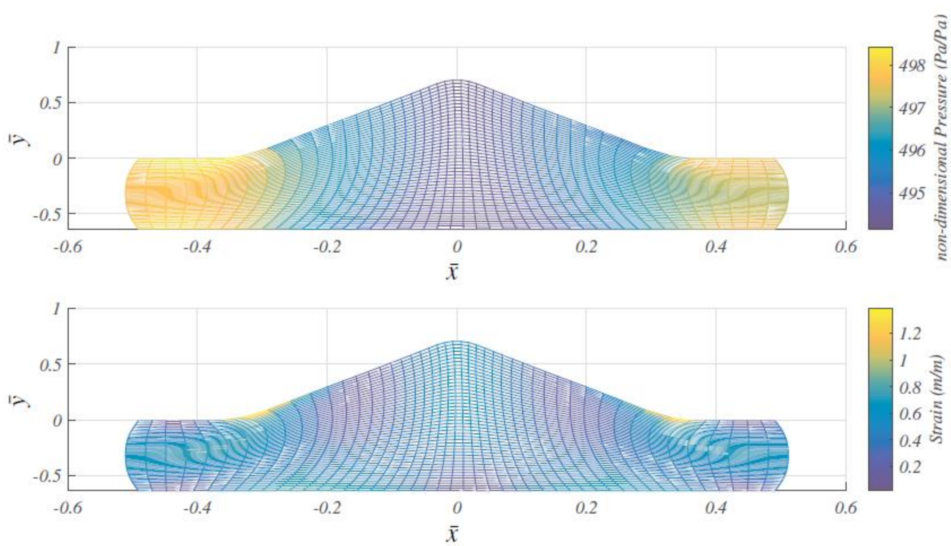

Figure 3. Non-dimensional pressure and strain for one feature at the end of mold filling process.