Simulation of roll-to-roll and roll-to-plate NIL: modeling the effects of process speed, imprinting load, roller elasticity, and pattern design

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We contribute a fast numerical approach to simulating the roller-imprinting of complex patterns. The technique predicts the extent to which imprinted patterns are fully formed, as well as variation of the imprinted material's residual layer thickness (RLT).

Process development for roller imprint is often done experimentally, which is laborious and wasteful of materials. Some use has been made of analytical squeeze-flow models [1], which predict average RLTs but take no account of material flow at the scale of nanofeatures. Our new technique integrates material deformations from the feature to the roller scale, enabling simulation of a wide range of ultraviolet-curing and thermal roller-based processes.

Our method encapsulates the behavior of the imprinted material using the response of its surface topography to a normal mechanical impulse applied to a small region. The elastic deformations of the roller(s) and substrate are modeled via point-load responses. We previously validated this concept for chip-scale NIL with several thermoplastic resists [2–3]. The new, roller-based technique finds the evolving pressure distribution experienced by the web it moves in contact with the roller and then separates from it. By differentiating between the displacement of resist forwards and backwards along the web, we can capture the 'pile-up' of resist behind the roller that occurs when the average resist thickness is reduced by imprinting (Fig 1a).

The approach can be used for roll-to-roll and roll-to-plate configurations, and for rollers with or without elastomeric coatings (Fig 1b). If patterns vary in pitch, shape or areal density across the roller, RLT and the completeness of pattern transfer can vary with position as well as with processing parameters, and our technique is able to model these effects.

We have validated our new technique against published data from two roller-based processes. When the resist is a UV-curing resin, we use a purely viscous resist model, and our technique reproduces the inverse-square-root relationship between roller pressure and RLT, and the square-root relationship between web speed and RLT observed by Ahn and Guo for epoxysilicone (Fig 2a–b) [1]. When the imprinted material is thermoplastic, a viscoelastic model is needed, particularly if the material is a high-molecular-weight, highly entangled network that constitutes the web itself. We show that a Voigt model—with a viscous component and a limiting elasticity—can explain the relationship that Mäkelä *et al.* found between the depths of imprinted nanostructures and the speed of a cellulose acetate web softened only at its surface (Fig 2c) [4].

In many roller imprint processes (*e.g.* as proposed by Ulsh [5]), resist is not completely solidified before the imprinting pressure is removed. In such cases, we predict that there exists an *optimal* web speed that maximizes pattern fidelity (Fig 2d). While slower web speeds allow nanostructures to be more fully formed by the patterned roller, longer delays before resist solidification permit shape recovery driven by material stresses or by surface tension. We argue that pattern formation and dissipation compete to give an optimal processing rate that maximizes final pattern height. This insight could inform machine design as well as process development.

[1] Ahn and Guo, *ACS Nano*, **3**, 2304 (2009)
[2] Taylor and Boning, *Proc NNT* (2009)
[3] *Ibid.*, *Proc SPIE* 764129 (2010)
[4] Mäkelä *et al.*, *Microelectron Eng*, **88**, 2045 (2011)
[5] Ulsh *et al.*, U.S. Patent 6,096,247 (2000)

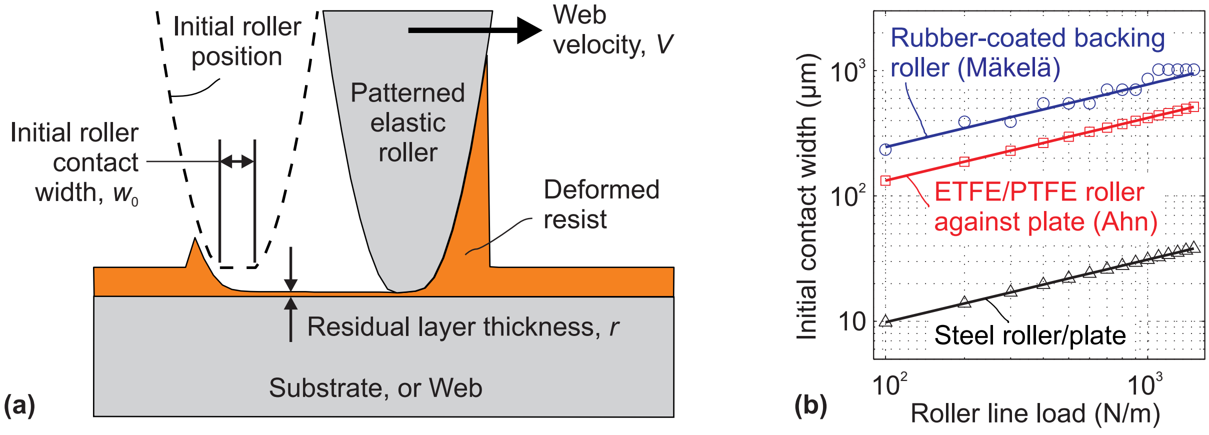

Fig. 1: Cross-section of roller, deformed resist and web (a). Completeness of pattern formation and final RLT depend on roller load, web speed, resist properties and roller/web elasticity. Resist 'pile-up' behind the roller, as described by Ahn [1], is captured. (The vertical axis is exaggerated for clarity; individual features are much smaller than RLT and are not shown.) Simulated roller contact widths (b) are consistent with those reported by both Mäkelä [4] and Ahn [1].

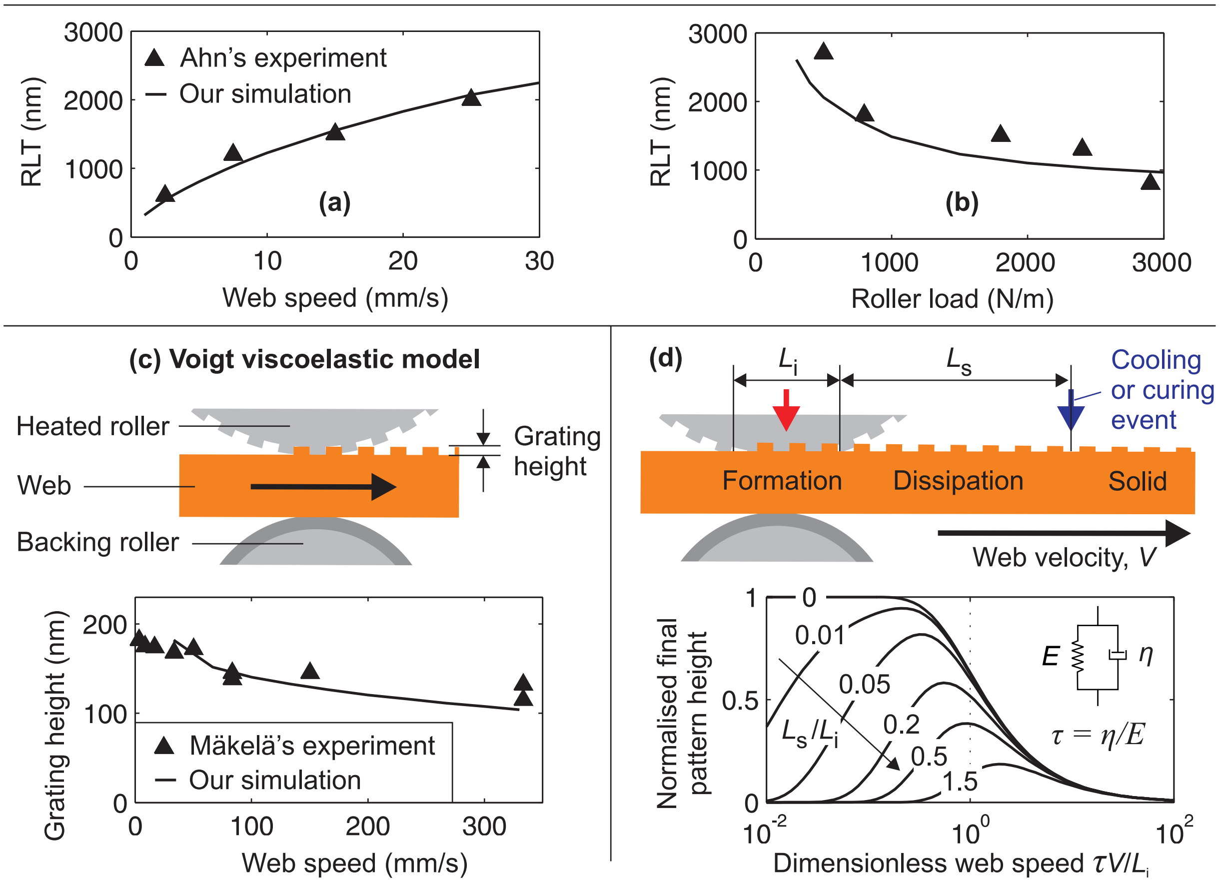

Fig 2: Our technique captures the dependencies of RLT on (a) web speed and (b) roller load seen experimentally by Ahn [1] using a polymeric roller, a solid backing plate and epoxysilicone resist. A Newtonian resist with viscosity 0.8 Pa.s is assumed. Meanwhile, by adopting a Voigt viscoelastic model (c), the technique captures the dependence of an imprinted grating's height on web speed as measured by Mäkelä for a cellulose acetate web heated on one side by a metallic roller. Here, grating height falls more slowly with increasing web speed than would be consistent with a purely Newtonian model. If solidification of the imprinted material finishes after the load is removed (d), pattern dissipation can occur, implying an optimal web speed.