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Virtual sensing and virtual metrology for spatial error monitoring of roll-to-roll manufacturing systems

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ABSTRACT

Roll-to-roll (R2R) manufacturing techniques are promising for the high-volume continuous production of substrate-based products for a variety of emerging technologies such as flexible printing electronics, biosensors, thin film batteries. However, meeting the tight tolerance requirements of the R2R printed products has become a major challenge in R2R. This paper focuses on integrating kinematics modelling and data-driven surrogate models to fundamentally understand the spatial error generation and variation propagation mechanism within a multi-step R2R system, and provides a novel method to devise accurate virtual sensing for effective process monitoring, fault detection and diagnosis with limited physical in-situ sensors, and how they can be used to achieve unprecedentedly accurate process control.

1. Introduction

Roll-to-roll (R2R) printing techniques are promising for high-volume continuous production of substrate-based products such as nano- and micro-scale flexible electronics, as opposed to sheet-to-sheet (S2S) approach suited for low-volume work. However, meeting the tight alignment tolerance requirements of multilayer printed electronics specified by device resolution (micrometer accuracy) has become a major challenge in R2R printing, preventing the fabrication technology from being transferred from conventional S2S to high-speed R2R production. Registration of multiple layers on a flying substrate is important. For electrolytes, surface integrity of printed layers with poor registration accuracy of the could generate severe problems such as missing or disconnected printing patterns causing device malfunction, which seriously impedes the successful deployment of fully scalable processes for R2R electronics printing. The main goal of this paper is to advance the fundamental understanding of the spatial variation generation and its propagation and accumulation mechanism within a high-speed R2R printing with a flexible substrate, and to apply the underlying science to devise accurate virtual sensing and virtual metrology techniques. The new method enables accurate process monitoring and fault detection in real time, and facilitates smarter process control in the creation and integration of features that will form the foundation of flexible electronic devices R2R printing.

1.1. Background

Recent research and development for printing electronics have shifted from flexible displays towards sensors for medical applications and integrated electronic circuits. Inkjet printing is the current state of nanoscale flexible electronics printing technology. High-throughput R2R manufacturing technique provides significantly greater manufacturing economies of scale, though the required upfront capital investment is higher than sheet-based manufacturing systems [1,2]. The global market for flexible devices manufactured by R2R technologies totalled $21.2 billion in 2018 and is expected to reach $41.3 billion by 2023 at a compound annual growth rate of 14.3% from 2018 to 2023 [3]. Due to its flexibility and high speed in integrating preparation of materials, deposition, patterning, and encapsulation [4–7] in a continuous manner, scalable R2R processing techniques will have a widespread impact on flexible electronics mass production, nanomanufacturing (graphene films [8], and carbon nanotubes [9]), and renewable energy.

1.2. Metrology for R2R process and quality control

Accurate spatial alignment and registration in printing electronics remain a major challenge for high-speed R2R processes. Any inter-layer misalignment greater than the desired resolution of the printed device will cause severe device functional problems. Fig. 1 illustrates the various misalignment scenarios web in an R2R printing process. The main cause of longitudinal misalignment is the change of substrate tension, roller or web speed. The root cause of lateral deviation is web tilt and the causation of altitudinal error

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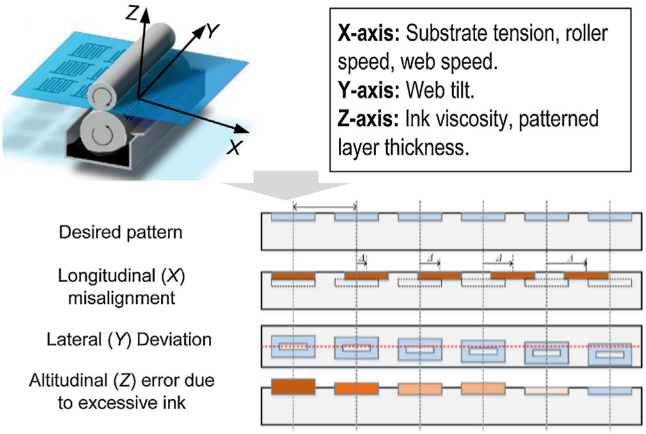

Fig. 1. Various misalignment scenarios in an R2R printing process.

is related to thickness change of ink and substrate. Dimensional errors occur in any direction would lead to quality issues in the printed devices.

There has been growing research interest in developing and improving sensors and inspection techniques to provide rich information for quality control in R2R manufacturing systems [10,11]. Crosscutting quality control (QC) research and development needs have been identified by the National Renewable Energy Laboratory (NREL) [11], including the ability to measure thickness, mechanical defects such as pinholes and cracks, electrical properties, surface structure, morphology, inter-layer delamination and voids. Among those, dimensional metrology is of top interest and need. A wide variety of other optical systems (e.g., interferometric-based, X-ray) also exist for film or multi-layer thickness and dimension measurements [12,13]. However, very few noncontact measurement techniques are available for in-line control [14]. Even for the systems with in-line machine vision or imaging systems (e.g., infrared sensor, optical coherence tomography (OCT) [15,16]), it is incredibly difficult for an automated vision system to tell the difference between a defect and naturally occurring variation. In cases of multiple layers, especially when patterned or patch coating is employed, over-layer registration and 3D dimensional accuracy are essential.

Therefore, the performance and condition of R2R processes currently applied in the manufacturing industry are not yet fully observable due to the lack of cost-effective sensors and in-process metrology systems. As such, there exists a need for a standardized modeling approach for process monitoring and precision control by utilizing data from controllers, sensors and limited in-situ metrology and ex-situ metrology systems. The latent process state estimation (e.g., web tension) and output prediction (e.g., longitudinal distortion, lateral displacement) based on the spatial variation model could be used as virtual sensors and virtual metrology, respectively, enabling to enhance the visibility and diagnosability of the system. The main goal of this study is to develop a systematic and generalizable methodology for codifying the process model and data analytics into a process monitoring and diagnosis method and a simplified control algorithm for misalignment correction and reduction.

2. The model for error generation and propagation

2.1. Overall methodology framework

In this paper, a fundamental understanding of both dimensional error propagation mechanism is established and the impact of these errors on the alignment precision of printed pattern is quantified, by extending the model in [17] from one dimensional (longitudinal) to all three dimensions, i.e., longitudinal, lateral and altitudinal; a systematic methodology for modeling the process dynamics and variation propagation and accumulation is developed. The source of error or variation in final print quality could be in any direction caused by deviation or changes in components. Table 1 summarizes the critical components and the associated error sources of misalignment in an R2R system.

Table 1
Summary of critical components and the associated error sources of misalignment.

Component	Attribute	Source of spatial variation
Rollers: components for transporting web in a continuous manner	Various types of rollers: pressure roller, engraved roller, unwinder, rewinder, driven rollers, idlers.	Roller surface roughness, orientation, position (height offset), rotational speed.
Ink: deposited/ printed material	Mechanical & material properties: ink viscosity, conductivity, thermal properties when applied to the substrate surface.	Variations in ink viscosity, thermal expansion, conductivity.
Substrate: surface for printed pattern	Mechanical & material properties: printability, adorability, initial tension, modulus, orientation.	Variations in ink absorbability, initial tension, modulus, web orientation and location; web breakage.
In-situ sensors: sensor for process monitoring and control	Various types of rollers: Ultrasonic diameter gauge, tension sensor, machine vision system for end-of-line dimension measurement.	Measurement errors, measurement disruptions, calibration.

In order to monitor the process condition and identify the root causes of spatial errors, a generalized *two-pronged* error propagation model is developed to understand the source of dimensional and positional deviation. The model will enable a more accurate process state estimation as a virtual sensor (VS) technique and predict dimensional quality as virtual metrology (VM) with sparse *in-situ* sensing and high-resolution metrology including ultrasonic-base radius, web tension, web speed, concentric circular imaging. This proposed error propagation model offers significant potential to enhance nano/micro-scale R2R printing capabilities by providing critical information for misalignment detection, diagnosis, and process control in real time. The proposed overall framework is shown in Fig. 2.

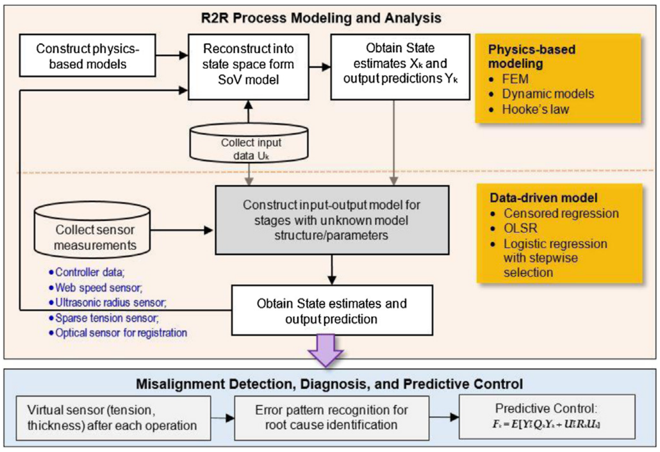

Fig. 2. Overall framework for R2R process modelling and analysis.

2.2. Multistage R2R process modeling

The main challenge to achieving high precision in R2R printing processes is to model the spatial variation dynamics and understand the error propagation mechanism for better process monitoring and control. An R2R printing process can be regarded as a variant of the discrete multistage manufacturing process, as it contains a continuous web with discrete processing stages on the web. In the existing literature on multistage manufacturing systems, a variety of modeling methodologies including model-based and data-driven models have been developed to describe the interactions among stages and errors on individual workpieces that propagate along stages [18,19]. The model-based approaches are established based on first principles and physical laws, thus requiring a comprehensive understanding of the process dynamics. Model- based models can provide physical insights and eliminate the requirement for sensors and inspections.

Among the model-based approaches, the Stream of Variation (SoV) theory has been widely used as a model-based approach for discrete multistage system modelling [18,20–22], compliant-part assembly processes [23,24], and machining processes [25,26]. The traditional SoV models utilize a stage-index state space model to illustrate error propagation across multiple stages. In this paper, the existing SoV model for a discrete system setting is transformed to a semi-continuous R2R system with high temporal and spatial independence, through a unique process segmentation method. A discretized *multistage* R2R system and its generic form of state space model are shown in Eq. (1).

System equation: $X_k = A_k X_{k-1} + B_k U_k + W_k$ (1a)

Observation equation: $Y_k = C_k X_k + V_k$ (1b)

In Eq. (1), X_k is the state vector representing the key quality characteristics of the product at stage k ($k = 1, \ldots, N$). X_k describes the dimensional variation in process stage k. Especially, X_k can be represented by a vector composed of a *spatial error* (SE) state vector X_k^s and a *temporal error (TE)* state vector X_k^t or a nonlinear combination of them i.e., $X_k = f(X_k^s, X_k^t)$. The dynamic equation for the *SE* describes how errors are generated in each printing stage, so the superscript s indicates the stage index. The dynamics of the *TE* describes how each error propagates as the substrate moving through the rollers from upstream to downstream. U_k is the system input related to the stage-specific operation. Y_k is the measurement vector. W_k and V_k are random errors. $A_k X_{k-1}$ represents the state transformation from stage k–1 to stage k while $B_k U_k$ is the transformed impact from operational inputs. C_k links the state to the output. If prior knowledge of the process and its physical model are difficult to obtain, data-driven surrogate models using factor analysis, graphical models and Bayesian approach can be used to identify the interactions among stages and estimate the state transition matrix in a multi-sensor environment.

Our prior study [17] has investigated a discretization method to transform a continuous R2R process into a discrete multistage system by lumping a set of consecutive rollers with the same function into a single stage. The SoV model is also adapted to a highly spatially and temporally interconnected R2R system that incorporates instantaneous dimensional error occurring at different stages. The method has been validated in longitudinal web tension monitoring in an elastic film R2R printing process. This paper aims to extend the work from one dimension to all three dimensions covering all possible critical variations and errors.

Kinematics and kinetics of the process will be studied to describe the torque balance and rotational motion of individual rollers or a set of rollers in each stage. For example, the longitudinal web tension at the "entrance" and the "exit" of a roller can be modeled as torque equilibrium equations. See Eq. (2) for materials roll and driven roll below:

$$T_k^{id} = A_k T_{k-1}^{id-1}(t) + B_k U_k + Z_k \quad (2)$$

where $\boldsymbol{T}_k^{id}(t)$ is the state vector describing the web tension of id^{th} span (or pitch) at k^{th} printing stage. The web tension of $(id\text{-}1)^{\text{th}}$ span at the preceding stage k-1 affects $\boldsymbol{T}_k^{id}(t)$ instantaneously. Matrices $\boldsymbol{A}_k$ and $\boldsymbol{B}_k$ represent how the upstream web tension affects that at the current stage, i.e., stage k. $\boldsymbol{U}_k(t)$ is the input vector characterizing the roller operations (e.g., driven roller, idle roller). Basically, the left-hand side of each equation represents the web tension going out of the current stage. The right-hand side consists of the tension generated by operations at the current stage and the upstream tension $T_{k-1}^{id-1}(t)$. This indicates that the web tension at one stage is not only determined by the downstream operations but is also instantaneously affected by its upstream operations, hence the SoV model is well adapted.

The kinematic equations for the lateral direction can be adopted from [27,28] to describe the roller-to-substrate interactions. The latitudinal displacement Δy of the web caused by a tilt angle (helix angle φ) of the wrapping substrate can be represented as below:

$$\Delta y_k = h(\theta_2) - h(\theta_1) + \int_{\theta_1}^{\theta_2} Jr\tan(\varphi)d\theta \quad (3)$$

where $h(\theta)$ represents the height function, the positions where the substrate first contacts it and the web loses contract are denoted by θ_1 and θ_2. r is the roller radius, φ denotes a helex angle with J equal to 1 for counter-clockwise wrapping and -1 for clock-wise wrapping. Then the lateral positional deviation (deflection) of the substrate going through multiple rollers and printing stages can be predicted and used as virtual metrology.

2.3. Virtual sensing and virtual metrology for diagnosis

The estimated state variables TE and SE from the error propagation dynamics are modeled by considering both temporal and spatial error propagation mechanisms, via an integrated (physics-based and data-driven) method. Fig. 3 shows a schematic of the multi-stage multilayer R2R gravure printing system with multiple physical sensors and metrology. Virtual Sensor (VS) provides real-time estimates of the latent process state (e.g., web tension, surface energy). The motor drivers follow a novel control scheme that makes use of the VS estimates to adaptively adjust the torque, hence changing stretch, web tension and web speed for variation mitigation and defect avoidance.

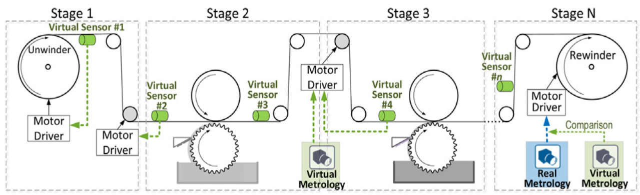

Fig. 3. A schematic of the multi-stage multilayer R2R gravure printing system with multiple physical sensors and metrology.

3. Results and discussion

3.1. Process monitoring and diagnosis

3.1.1. Detection of web damage

Precise tension control for web damage prevention is also critical to printing precision alignment. Too much tension can cause the web to be stretched beyond its elastic limit, resulting in a damaged web and that cannot be recovered in the later stages. Fig. 4 shows an example of a virtual tension sensor detecting the drifting or error of the R2R process web velocity and virtually

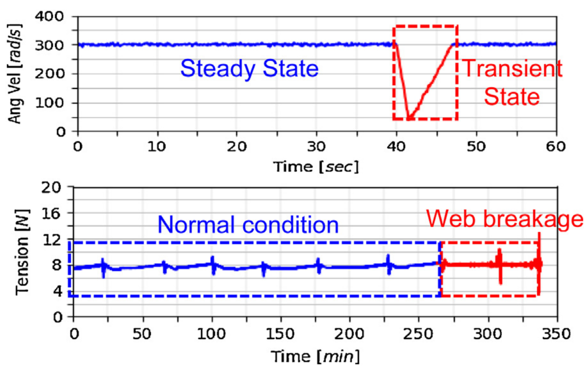

Fig. 4. Web velocity and tension monitoring for anomaly detection.

sensed web tension. The upper one shows the detection of the system entering a transient state from a steady state due to material roll changeover and splicing. The lower figure shows how the estimated web tension using the VS method is useful in detecting web breakage, i.e., the waveform in red shows different cycle-based patterns from the blue part (normal condition).

In addition, insufficient tension could cause wrinkles generated on the web or bubbles during lamination. Therefore, setting up reasonable control laws with the predictive misalignment information of intermediate products can effectively avoid web damage.

3.2. The solution: VS, VM and control synthesis

The developed modeling and analysis framework has provided and identified sources of variation in order to pinpoint the root causes of misalignment in earlier stages. The error information can be fed back to the motor controller to correct the system through appropriate controllers (e.g., robust PID control, predictive model control). A proper control law that is designed based on the predicted outputs would significantly mitigate defects caused by, registration misalignment (X axis), lateral drift (Y axis), thickness variation (Z axis), etc.

Currently, the most widely used control system in R2R systems is web tension control with a fixed PI gain, which requires extensive tuning and does not provide the desired performance for varying tension errors and material properties. It also relies on optical sensors to measure registration accuracy and tension sensor to provide inputs to the closed-loop control system. Given the VS and VM information resulting from the model, a novel model predictive control strategy based on the information will enable to adjust inputs adaptively and automate the parameter tuning in real time, avoiding the use of costly *in-situ* physical sensors and machine vision systems. The control action should also be punished based on its magnitude because large input adjustment might result in unstable system response. A generic mathematical representation of an optimization index at stage k is given by $\boldsymbol{F}_k = \boldsymbol{E}[\boldsymbol{Y}_k\ \boldsymbol{Q}_k\boldsymbol{Y}_k + \boldsymbol{U}_k\ \boldsymbol{R}_k\boldsymbol{U}_k]$, where $\boldsymbol{Y}_k$ denotes the intermediate product dimensional quality predicted at stage k, and penalty coefficient $\boldsymbol{Q}_k$ and $\boldsymbol{R}_k$ are weight matrices. A control scheme should work to proactively reduce the intermediate spatial errors with the real-time VS and VM information.

4. Conclusion

This paper introduced a novel framework to model the dimensional and positional error propagating of a thin, tensioned, and flexible substrate with multiple rollers and multi-stage operations in an R2R process. The framework integrates the physics-based (kinematics) process models with sensor data analysis to provide accurate estimates of latent state variables (e.g., web tension) and prediction of deflection and dimensional deviation in all three dimensions. The contribution of this study is threefold: (1) enhanced the fundamental understanding of the dynamics of spatial variation propagation (dimensional and positional) of print features across multiple printing steps by transforming stream-of-variation theory from discrete systems to a semi-continuous R2R system, (2) created a virtual sensing method for process monitoring and diagnosis and devise analytical virtual metrology for quality assessment and registration control “on the fly”, and (3) provided a guidance on a new R2R control scheme that makes use of virtual VS and VM to mitigate spatial variation and overlay misalignment issues for improved print patterning capability.

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