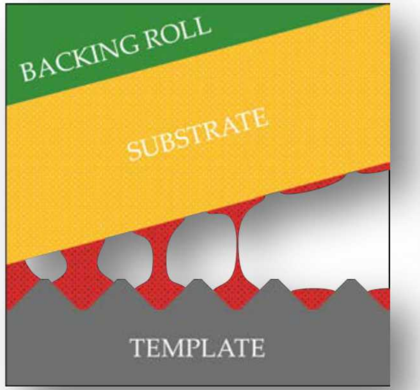
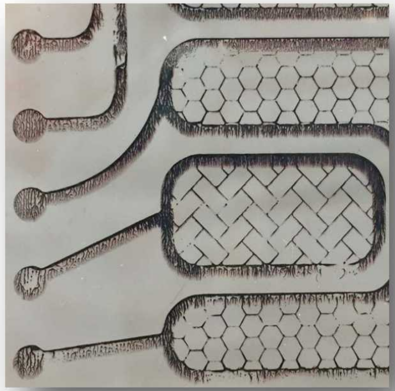
Briefing to DOE/EERE Advanced Manufacturing Office and Lab-Leads from NREL, ORNL, LBNL, and ANL by P. Randall Schunk, 4 August 2020

SAND2020-8324PE

GRAVURE PRINTING DEFECT PREDICTION VIA MACHINE LEARNING





Robert Malakhov
Kristianto Tjiptowidjojo
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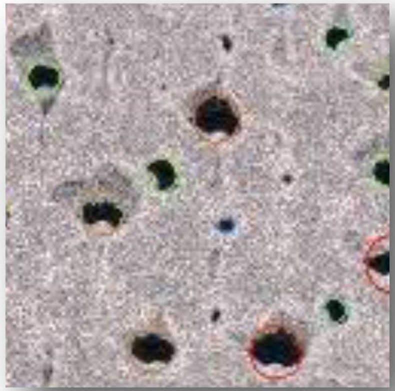
2020 August 4th



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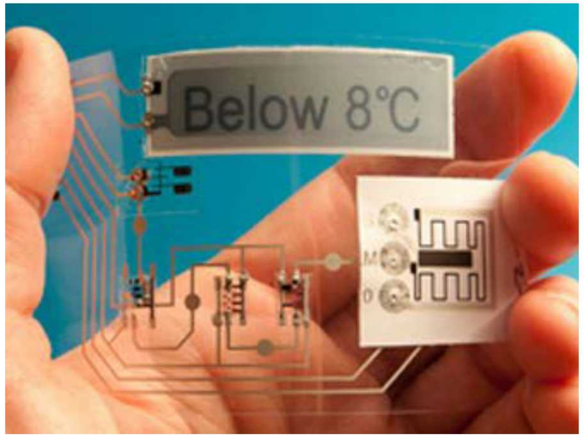
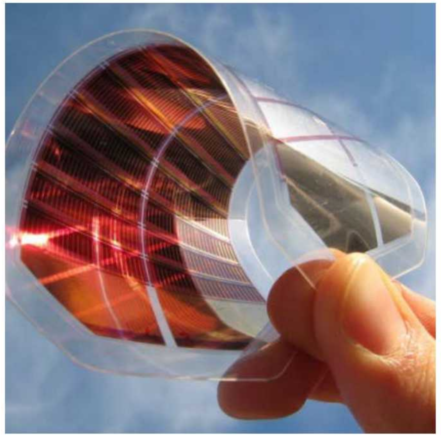
Enabling the Future

- Printed Electronics and Flexible Systems enable future innovations and applications
  - Low cost sensors in smart and connected devices (Internet of Things (IoT))
  - Smart-packaging, RFID tags
  - Healthcare wearable devices
  - Flexible displays
  - Organic Photovoltaics
  - $9.8 billion (2019)
    $19.8 billion (2024)
    (2019 Markets and Markets)

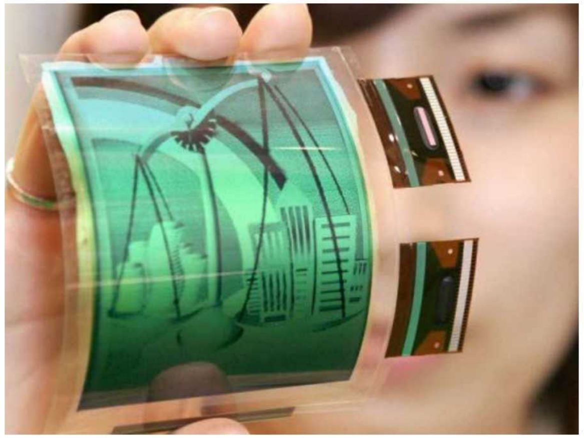
Sensors



Printable Electronics



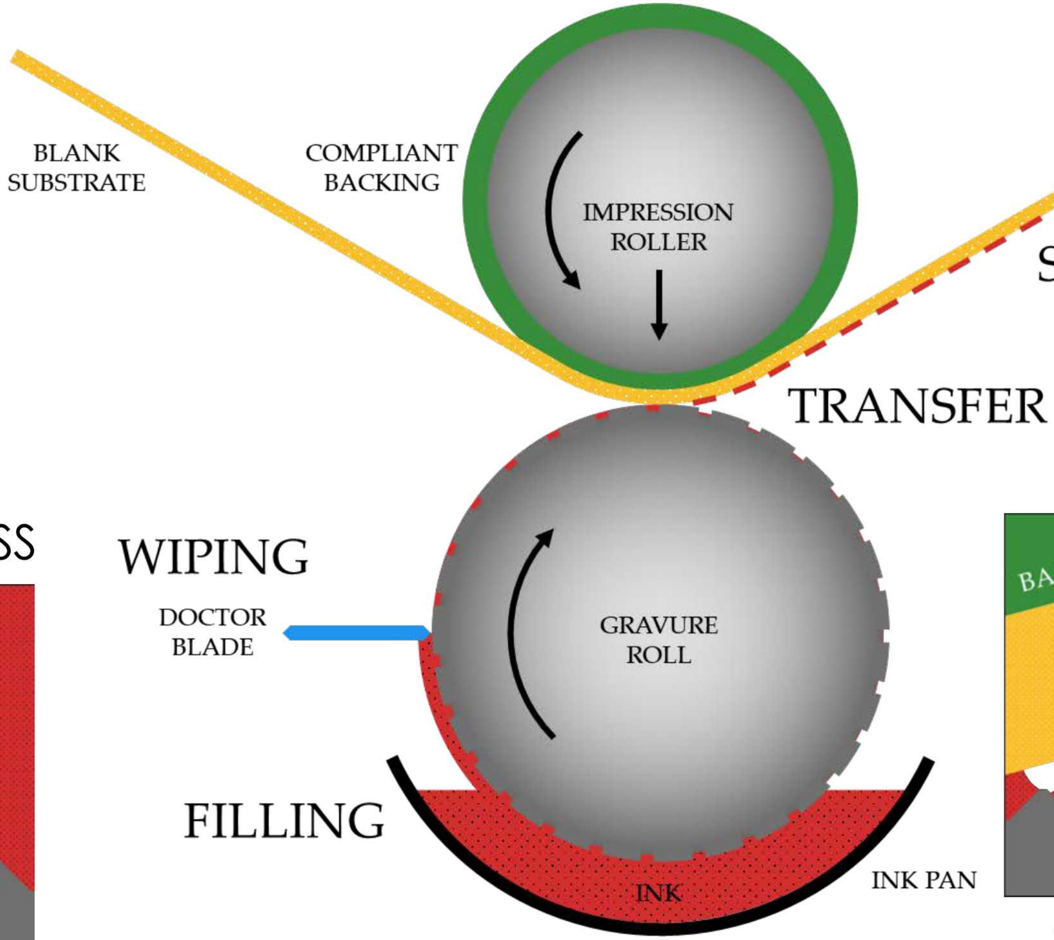
Organic Photovoltaics

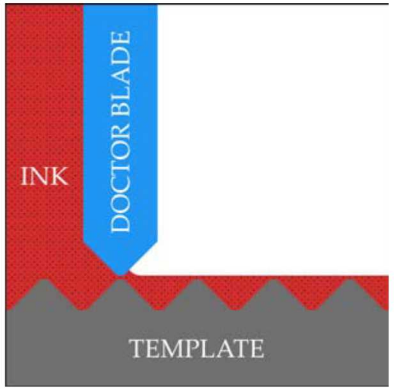


Flexible Screens

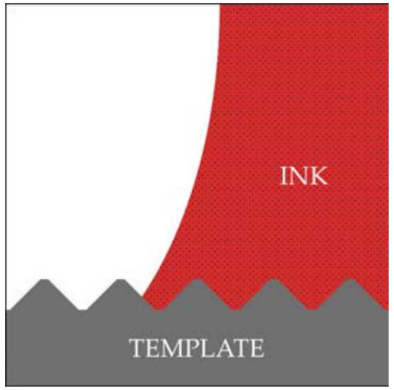
Challenge lies in understanding complex physical mechanisms to generate smaller features

Gravure Printing Process

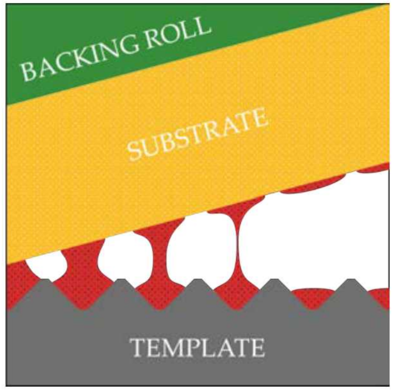




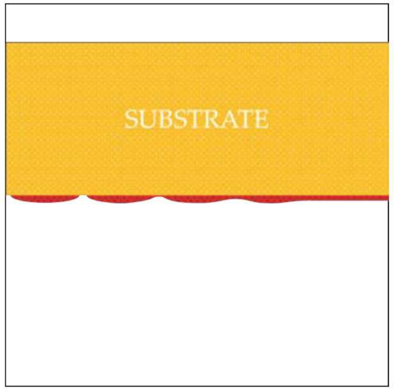
2. Wiping
Blade removes excess



1. Filling
Cells filled with ink



3. Transfer
Substrate pressed and separated



4. Solidification

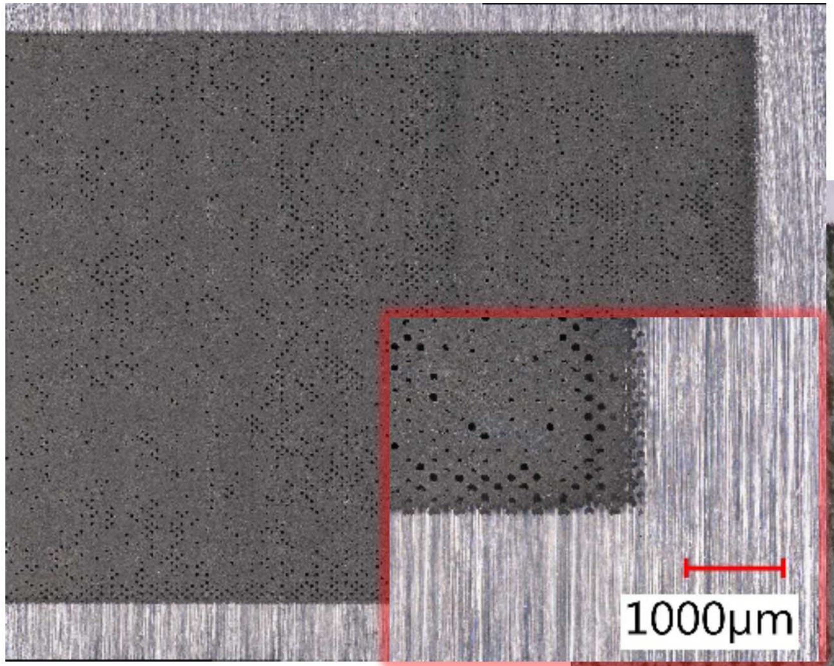
Ideal for PE:

+ Over wide areas
+ High throughput
+ Durable
+ Wide solvent compatibility
+ Combine with other mechanisms
+ **Pattern resolution**
+ **Print speed**
- Overlay and registration is challenging

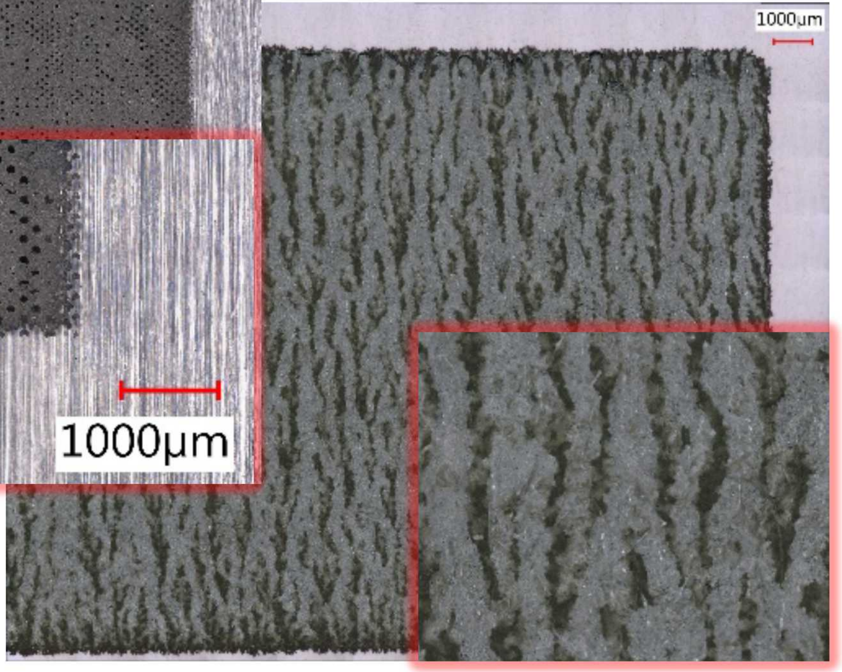
Gravure printing is a complex process with multiple steps and physical mechanisms

Defects Lead to Performance Disruption

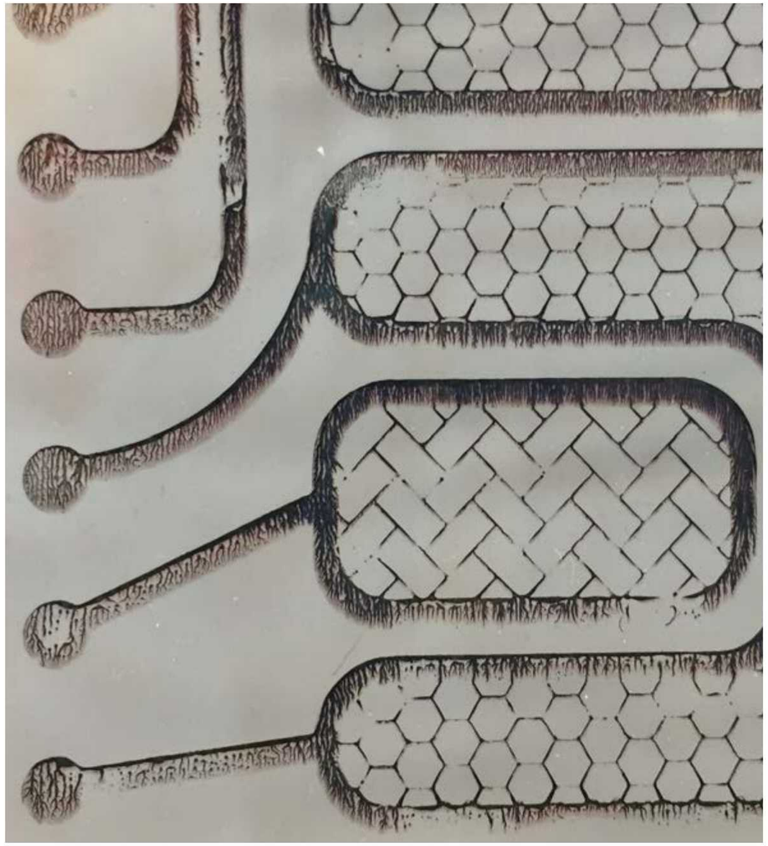
What is the cause of these defects?



Pinholes



Striations

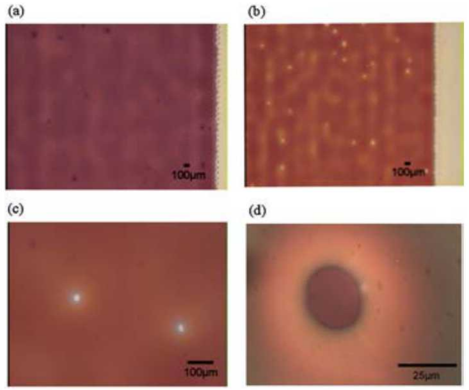


Loss of conductivity

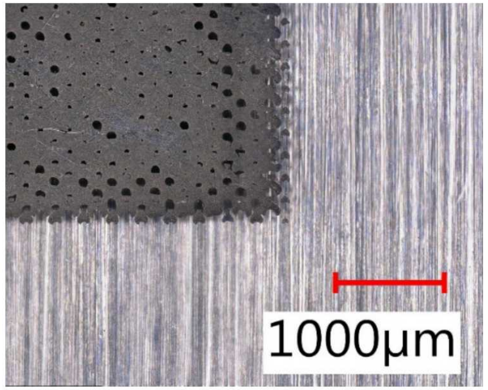
Pinholes: Not All Pinholes are the Same

- May be controlled for
  - Template defects
  - Ink impurities
  - Missing particulate
  - Irregular template contact
  - Environmental contaminants
- Less understood
  - Ink spreading / leveling
  - Gravure cell gas trapping

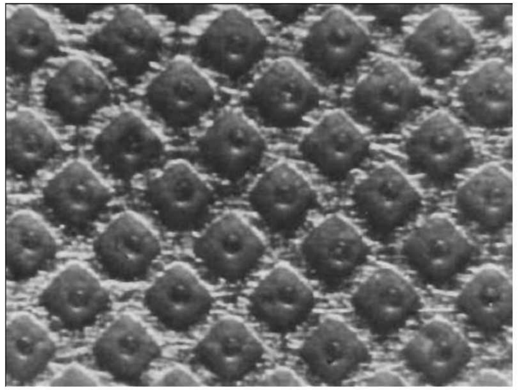
What is the cause of these process-based pinholes?



Missing dots 2015 Apilo et al.



Not enough ink spreading



Gas trapping 1985 Bery et al.

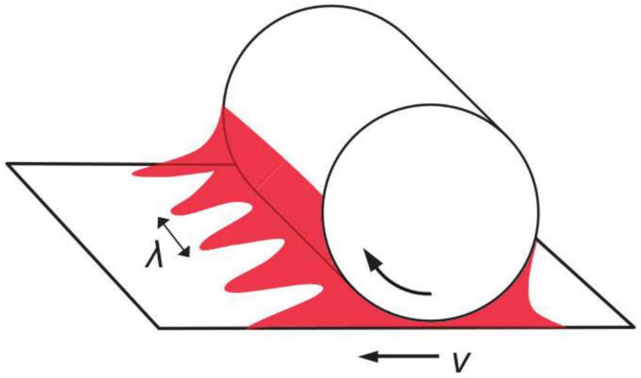
Environmental contaminants

STRIATIONS: VISCOUS FINGERING VS RIBBING

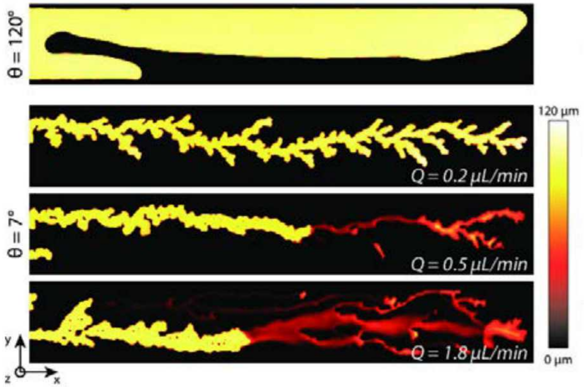
What is the cause of these striations?

Viscous Fingering

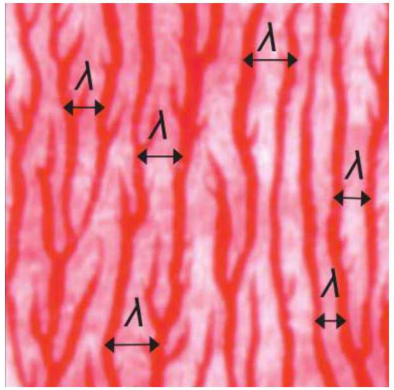
- Brumm et al. speculated due to viscous fingering
- Upstream transfer nip instabilities generate air fingers that index striations
- Can only occur in transfer nip where gas can be entrained



2019 BRUMM ET AL.



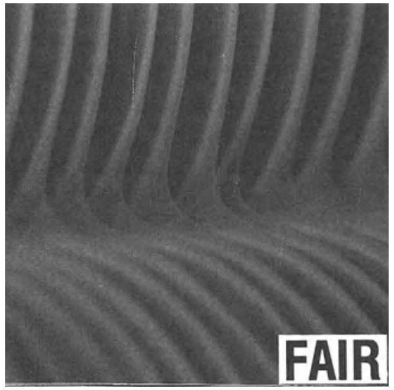
2014 LEVANCHE ET AL.



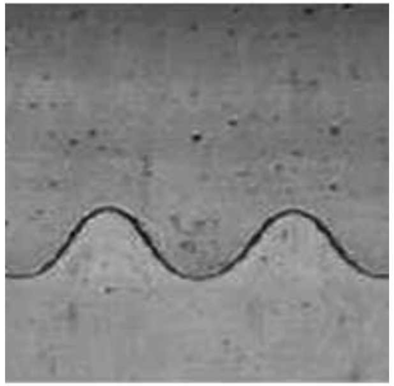
2019 BRUMM ET AL.

Ribbing

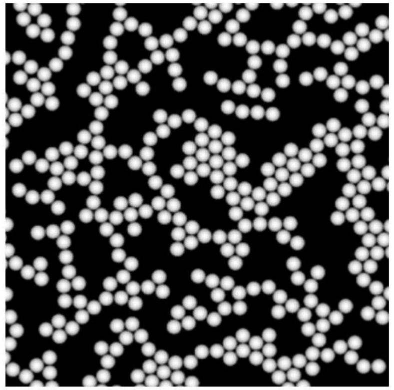
- May be due to instability common in separating flows
- Ribbing instability leads to peaks and troughs that drive differential drying and colloidal aggregation that index striations



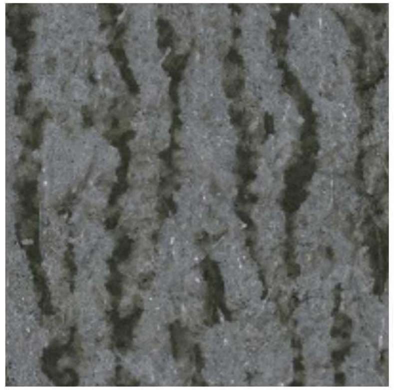
1988 SOULES ET AL.



2002 VARELA LOPEZ ET AL.



2007 FUJITA ET AL.

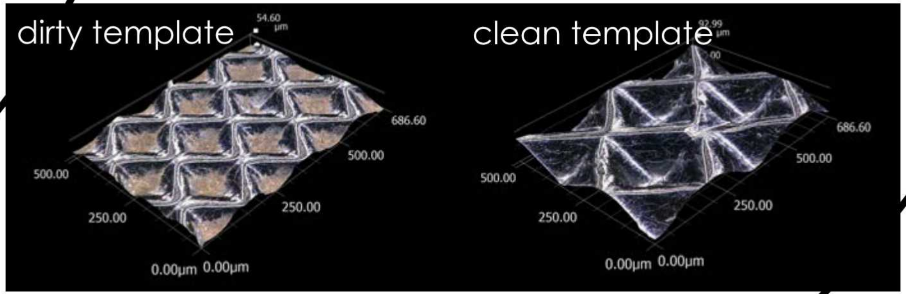


Informatics Approach & Results Collection

Gravure is a complex process so use machine learning to see big picture!

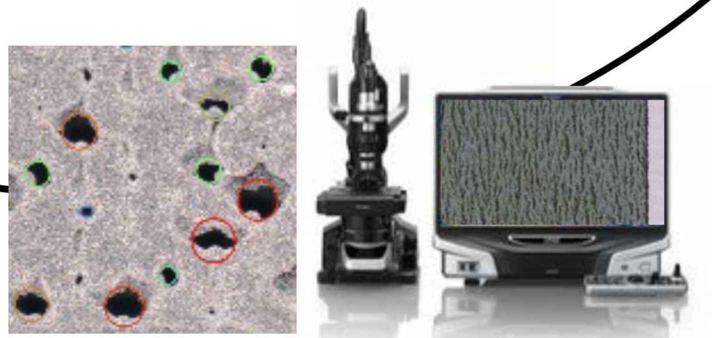
Extensive Database of many Features → Machine Learning → Predictions via algorithms

1. Print Sample



2. Clean Template

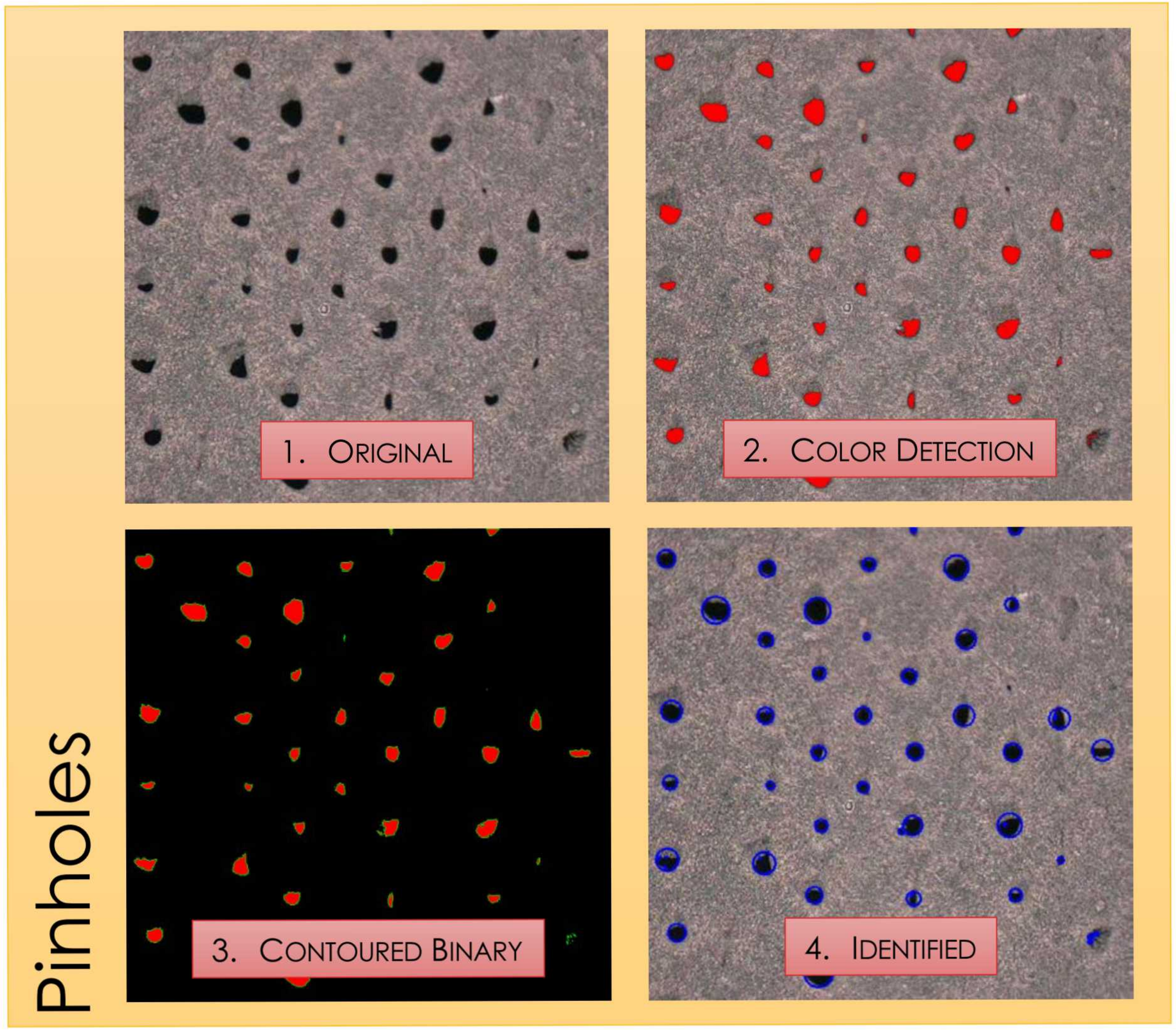
3. Dry with minimal dust and handling

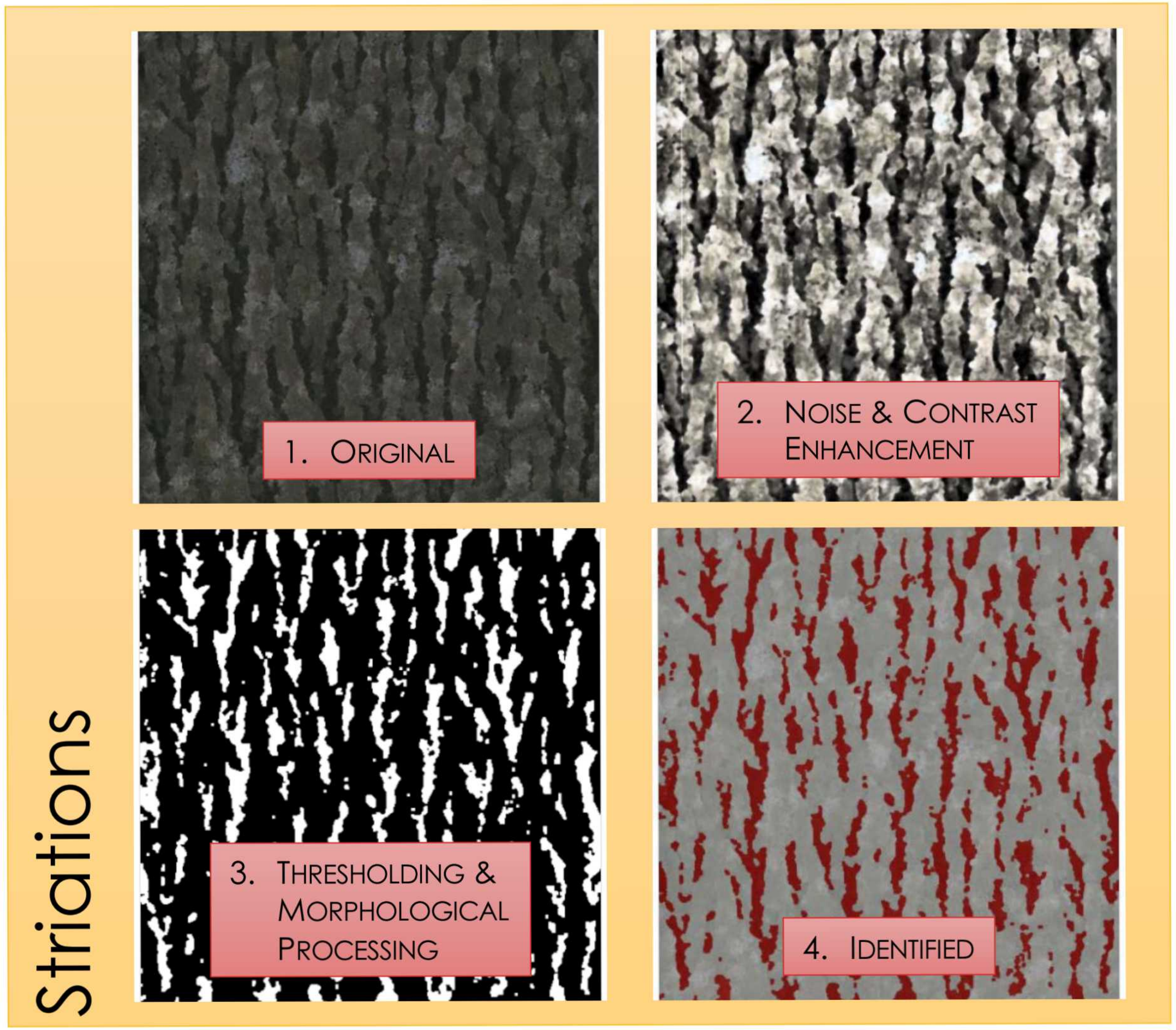


4. Characterize Prints

5. Input Data

Characterization via Computer Vision





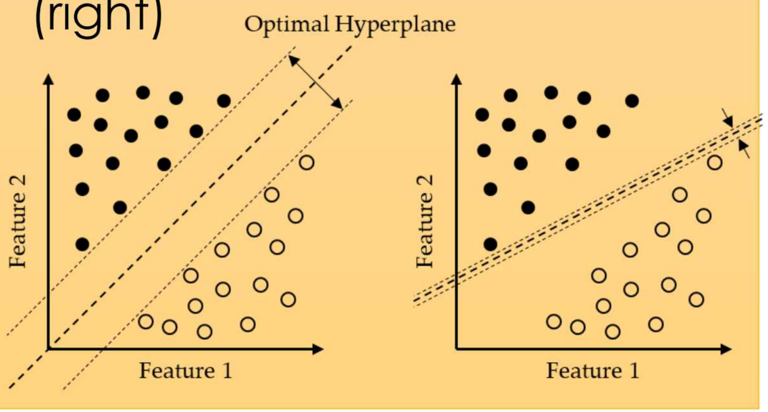
ML Algorithms

Learn which features are most sensitive and which set of features is enough to accurately predict defects

Support Vector Machine (SVM)

Separates data into groups (classifications) in n-dimensional feature space

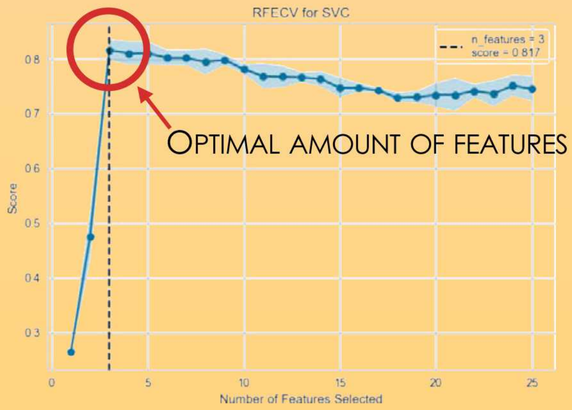
Uses the large margin principle to find a hyperplane with a large margin (left) versus that of a small margin (right)



Recursive Feature Elimination (RFE)

Simply a parameter sensitivity analysis

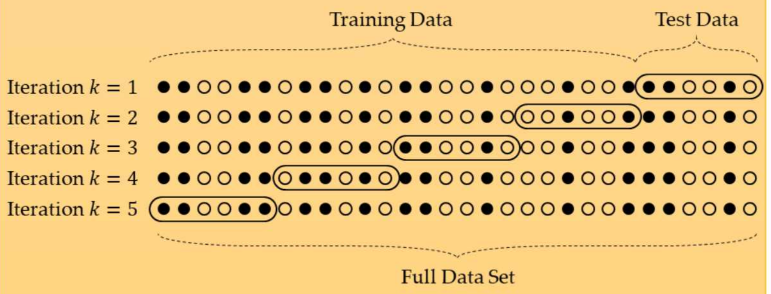
Tests removal of least sensitive features to minimize features necessary to accurately predict the classification



Stratified K Fold Cross-Validation

Makes sure all the data is used in training and testing

Semi-random partitioning of data so that all data (including each classification) is used once in the training and once in the testing of the model



PREDICTIONS & CONFIDENCE

Pinholes

Classification	0.94±0.01
Optimal Features	viscosity, substrate

- Viscosity
  - Higher viscosity resists complete filling of gravure cells
  - Multiple components including particle size, shape, loading, temperature, etc.
- Substrate
  - Porosity difference between paper and plastic
  - Surface energy variation causing incomplete wetting or dewetting mechanics

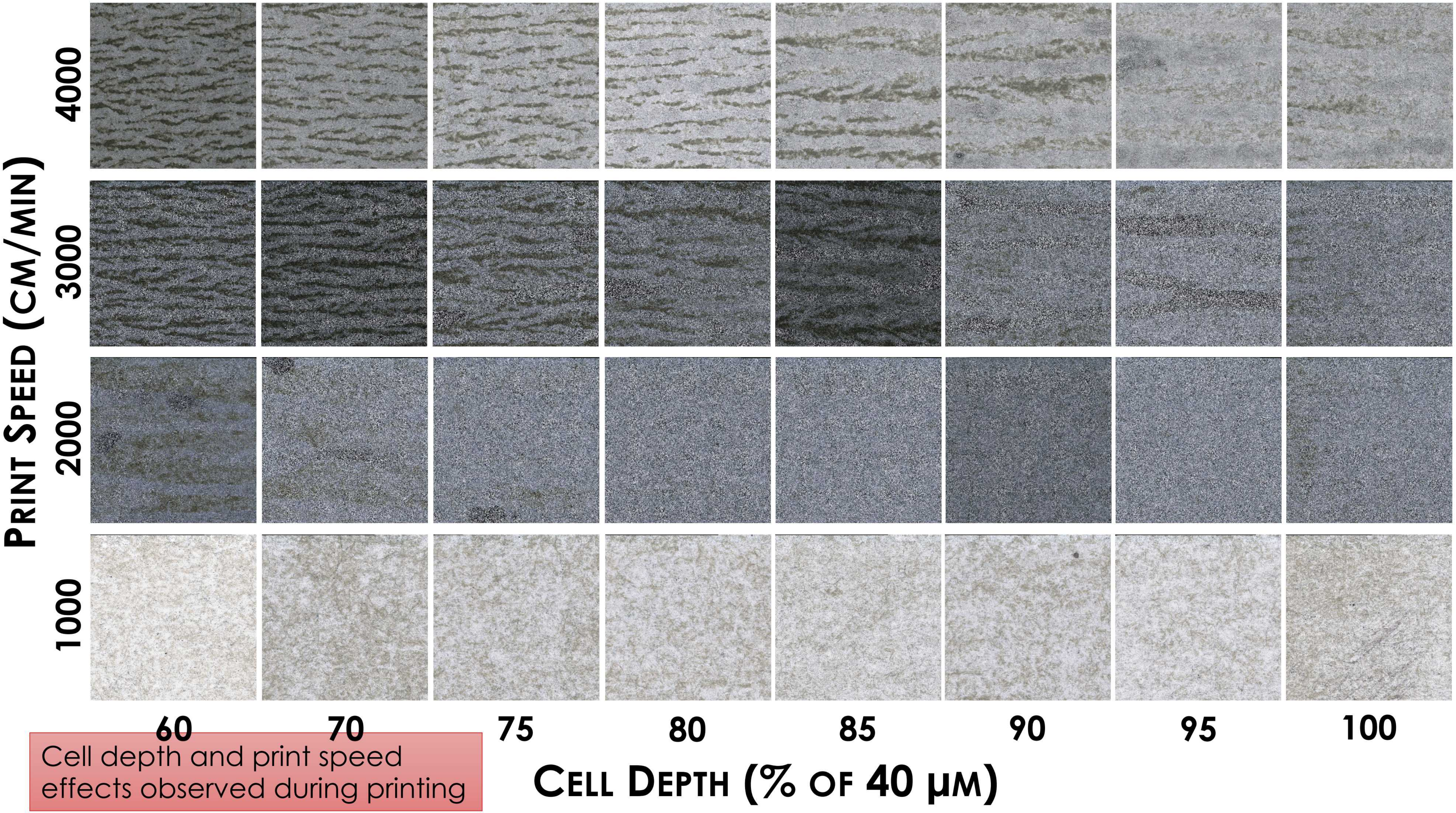
Managing cell to substrate transfer vital

Striations

Classification	0.87±0.05
Optimal Features	particle size, cell depth, print speed

- Particle Size
  - Unexpected result from the ML
  - Fewer large particles fit in a cell
  - Reduced mobility affecting leveling when drying
- Cell Depth
  - Smaller cells deposit thinner films that dry before particles can level
- Print Speed
  - Main ribbing instability criterion

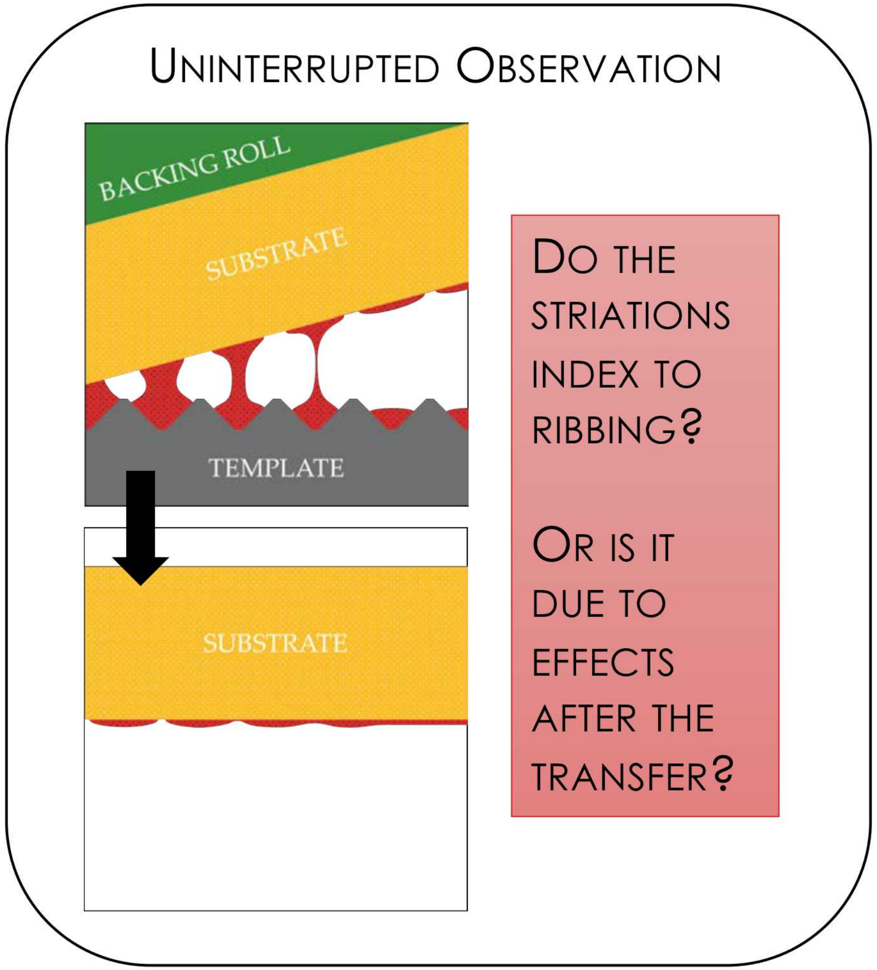
Ribbing consistent with critical features



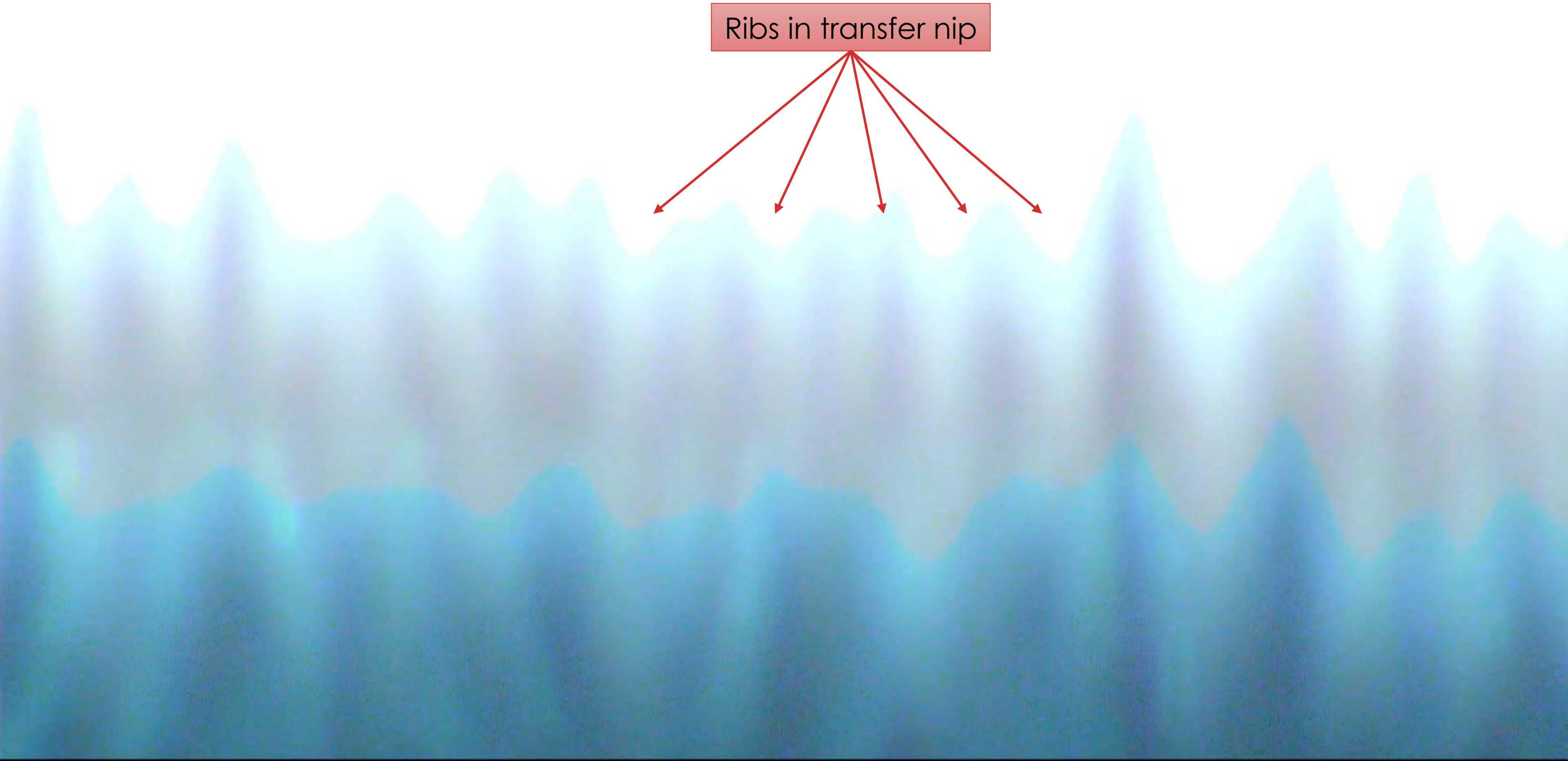
Cell depth and print speed effects observed during printing

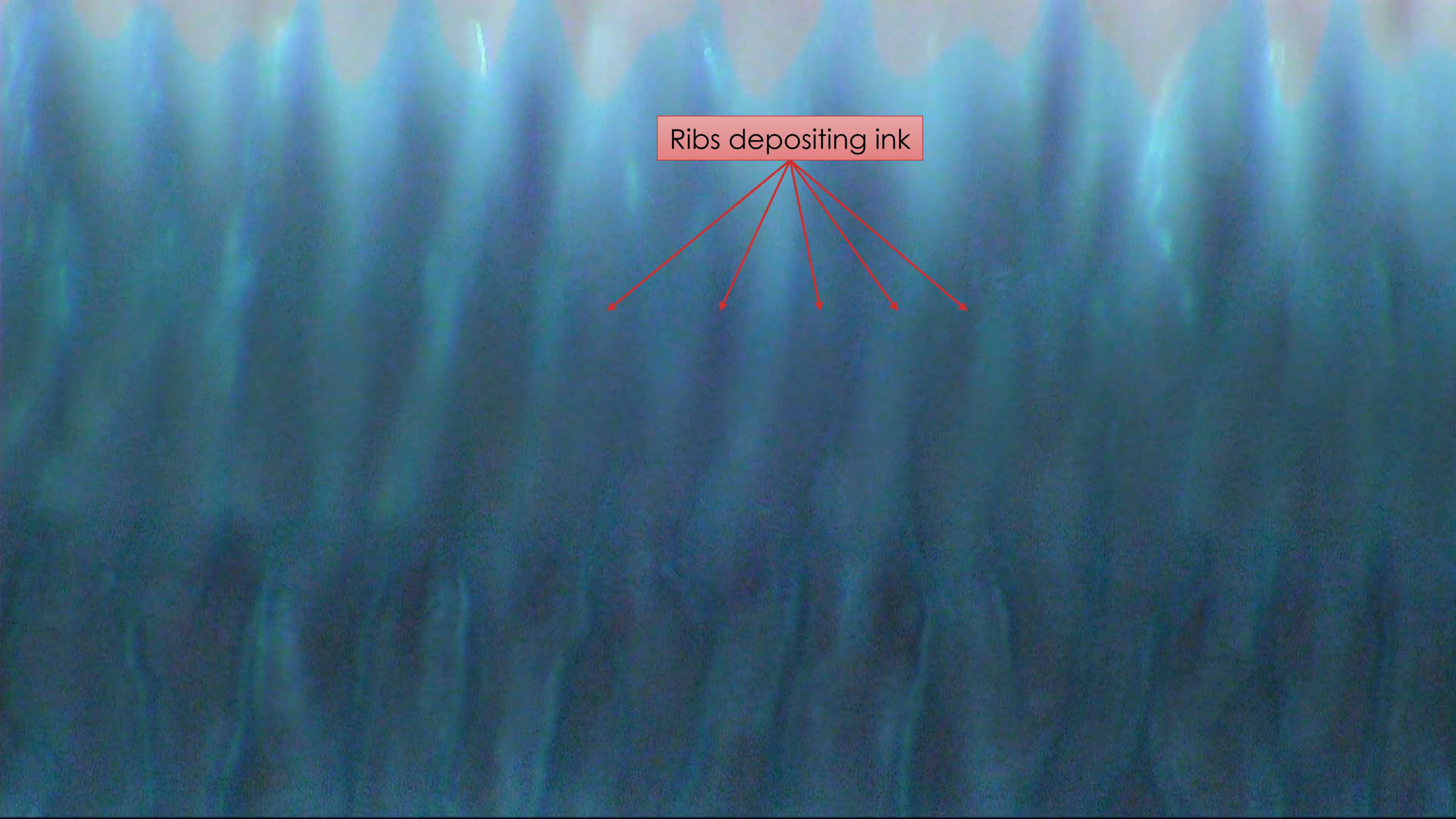
High Speed Visualization of Transfer

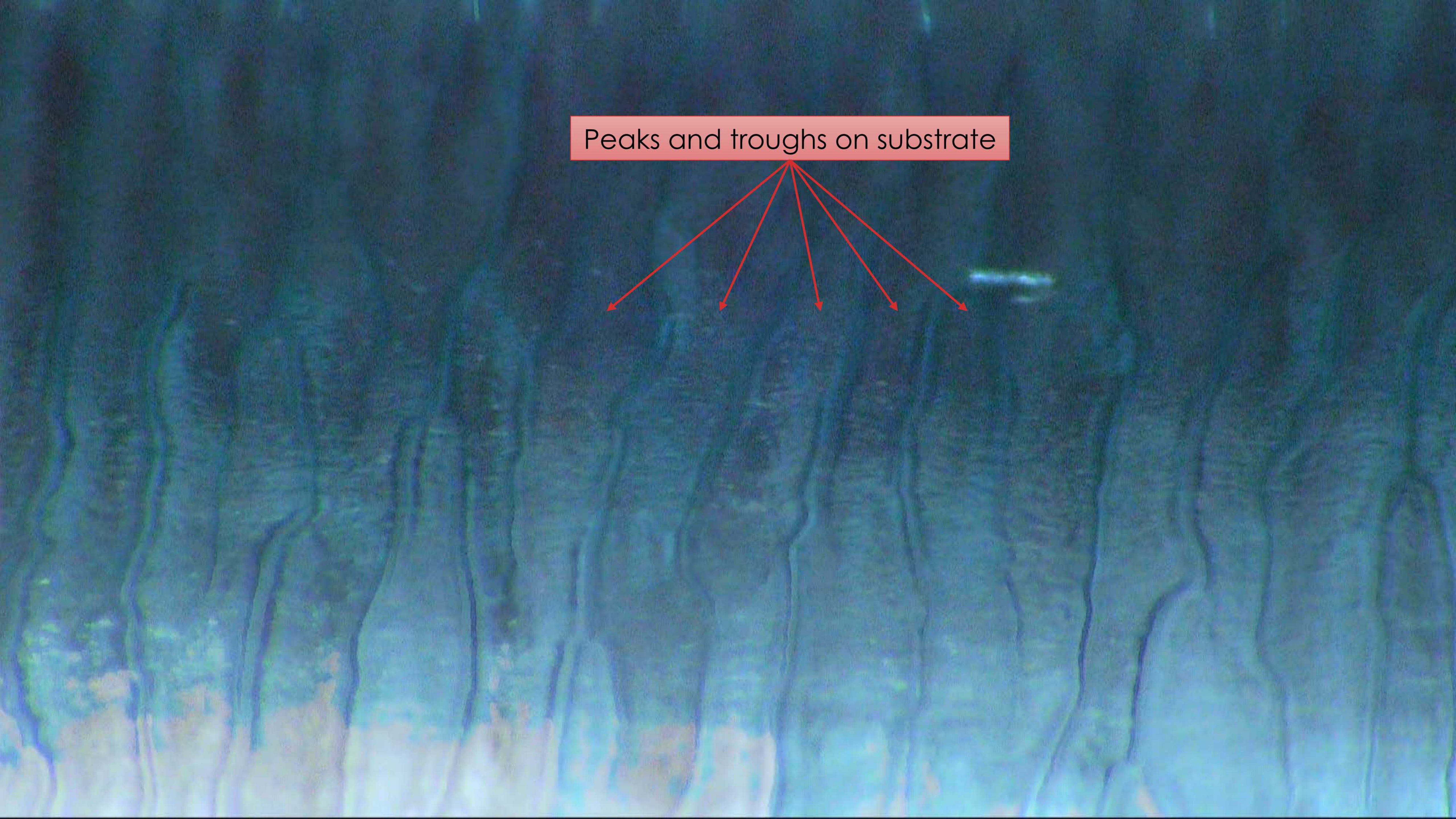
- Observe transfer process in situ
- Maintain view of transferred material
- Observe spreading

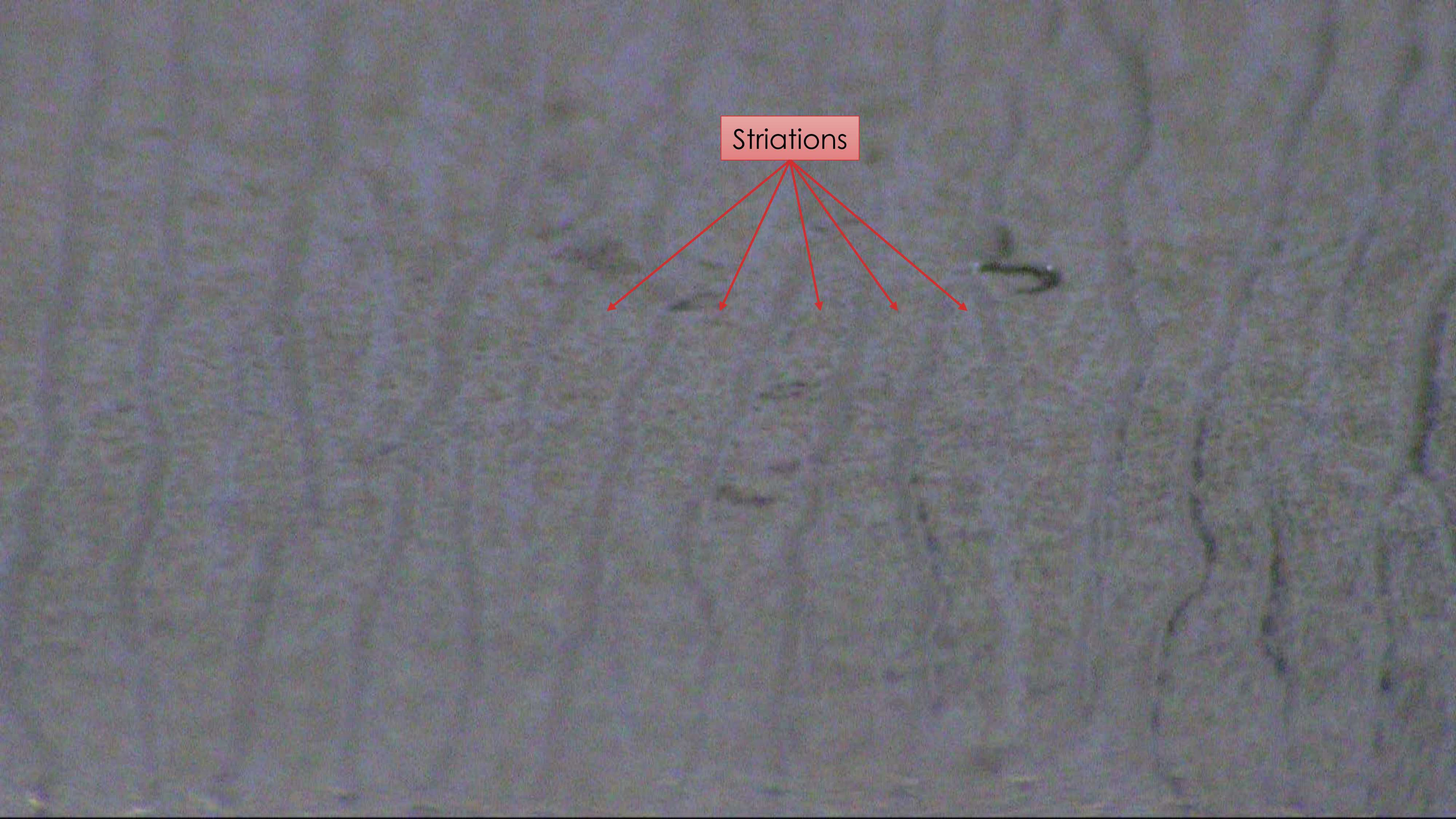


Ribbing into striation visualization




Ribs depositing ink


Peaks and troughs on substrate


Striations

Acknowledgements

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