Karlsruher Institut für Technologie

Institute for Applied Materials

VIRTUAL MATERIALS DESIGN

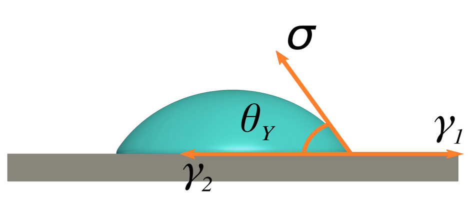
Digital Twin for Electronic Devices on Patterned Substrate

F. Wang, B. Nestler

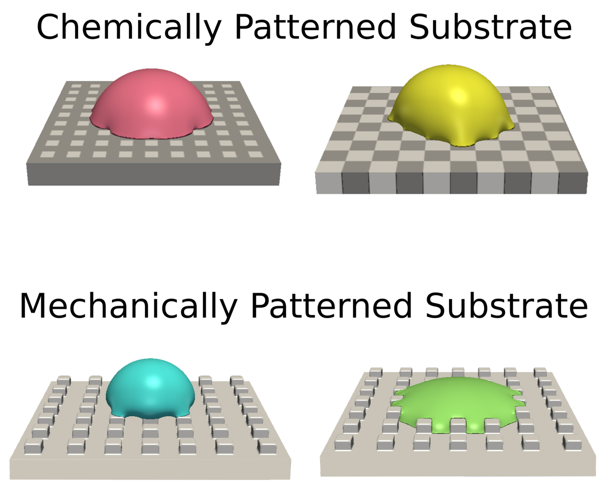
Theory

Young's theory

$$\cos\theta_Y = \frac{\gamma_1-\gamma_2}{\sigma}$$

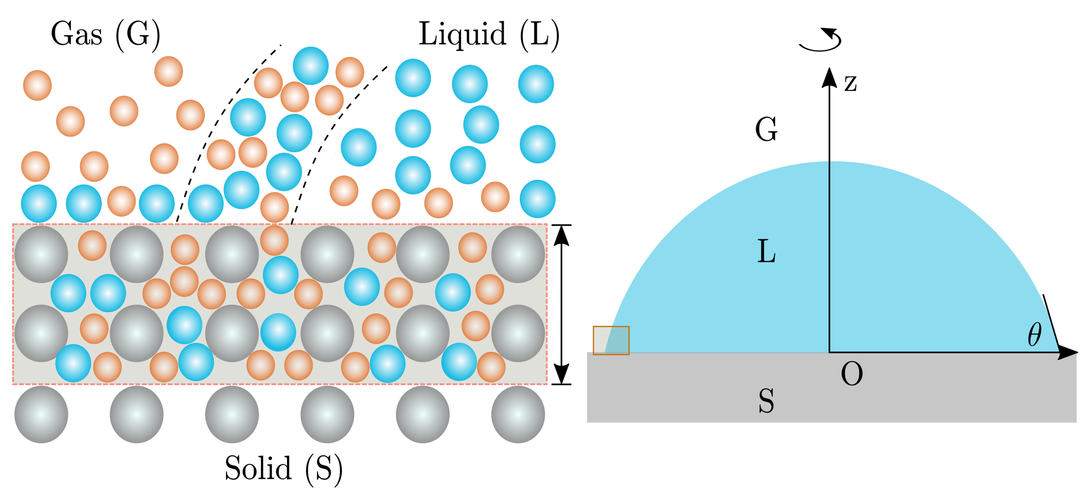


Cassie-Baxter-Wenzel theory

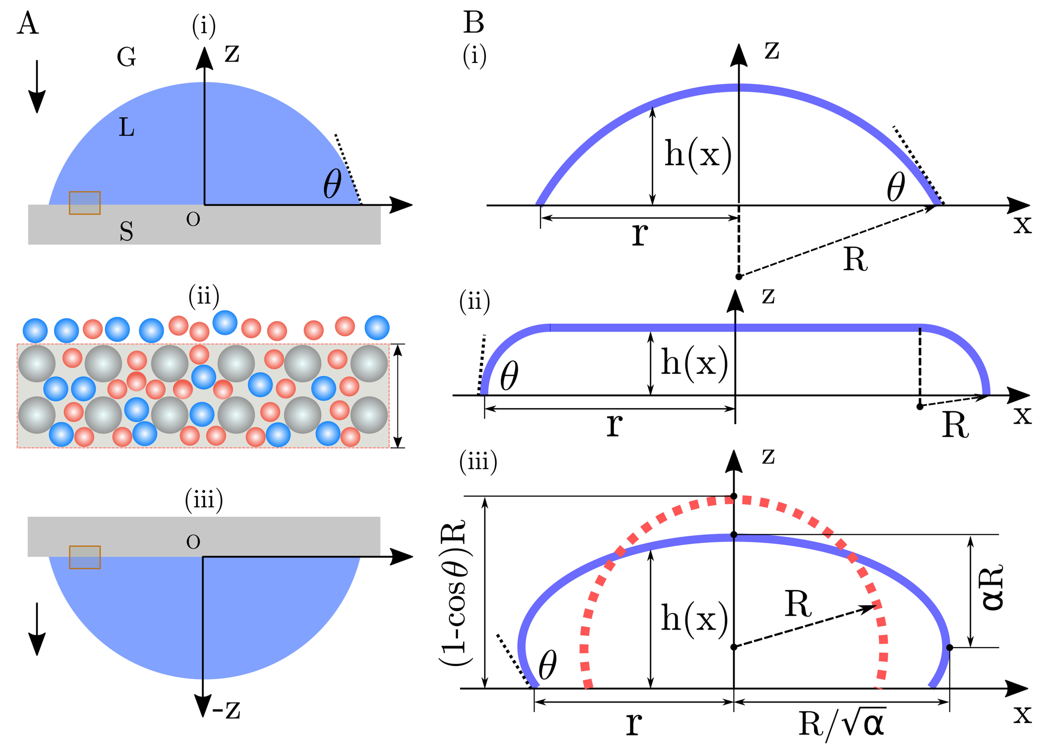


Current theory

$$\cos\theta_\pm = \varrho[1 \pm (\Delta p - \Delta\chi)/\chi]^2$$



Gravity and line tension



F. Wang et al., Adv. Mater. 35, 2210745 (2023). F. Wang et al., Phys. Rev. Lett. 132, 126202 (2024). F. Wang et al., Phys. Rev. Lett. accepted.

Phase-field Model and Experiment

Phase-field model

Free energy functional:

$$\mathcal{F} = \int_\Omega \left[f(\phi) + \epsilon a(\phi,\nabla\phi) + \frac{1}{\epsilon} w(\phi)\right] d\Omega + \int_S f_w(\phi)\, dS$$

Time evolution in the domain:

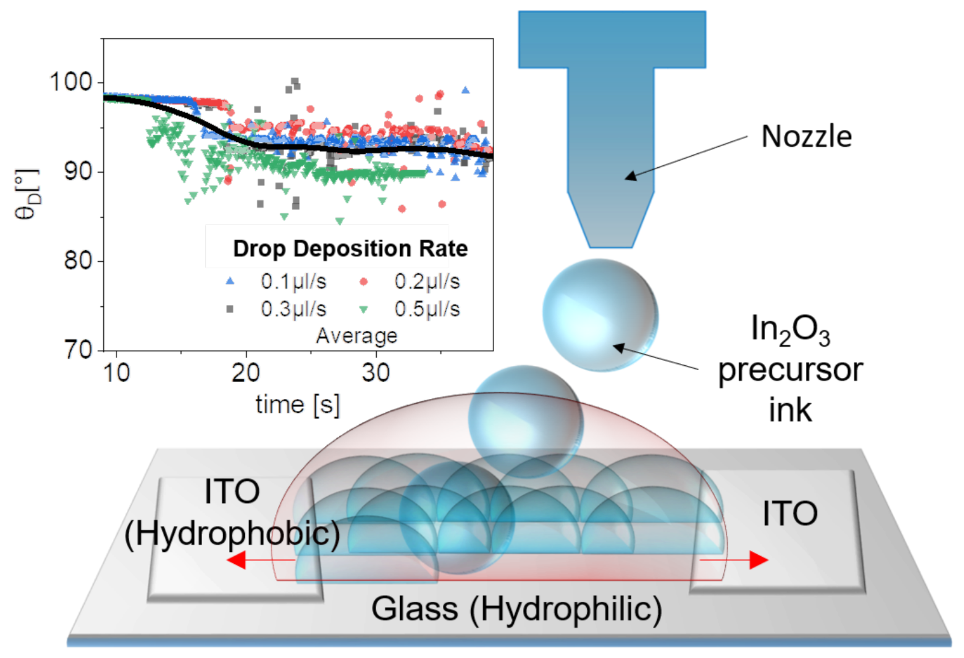
$$\tau\epsilon \frac{\partial\phi}{\partial t} = 2\gamma\epsilon\nabla^2\phi - \frac{16}{\pi^2}\frac{\gamma}{\epsilon}(1-2\phi) - \frac{\partial f}{\partial\phi}$$

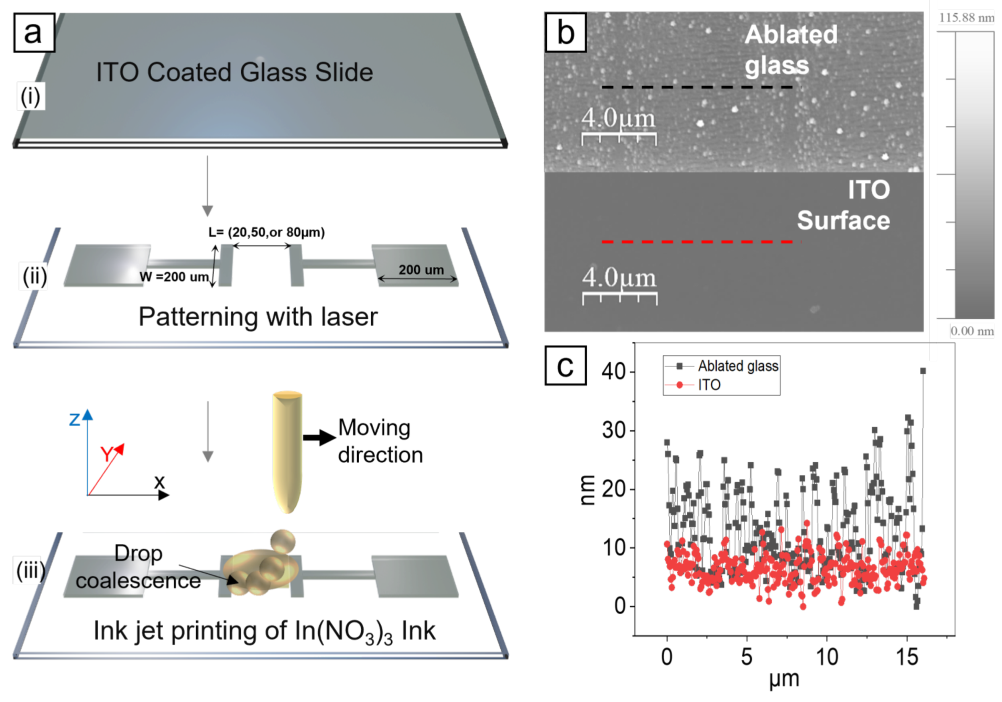
Time evolution on the substrate:

$$\tau_w \frac{\partial\phi}{\partial t} = 2\gamma\epsilon\nabla\phi\cdot\mathbf{n} - \frac{\partial f_w}{\partial\phi}$$

Wu et al., Soft Matter, 2020, **16**, 6115

Experiments



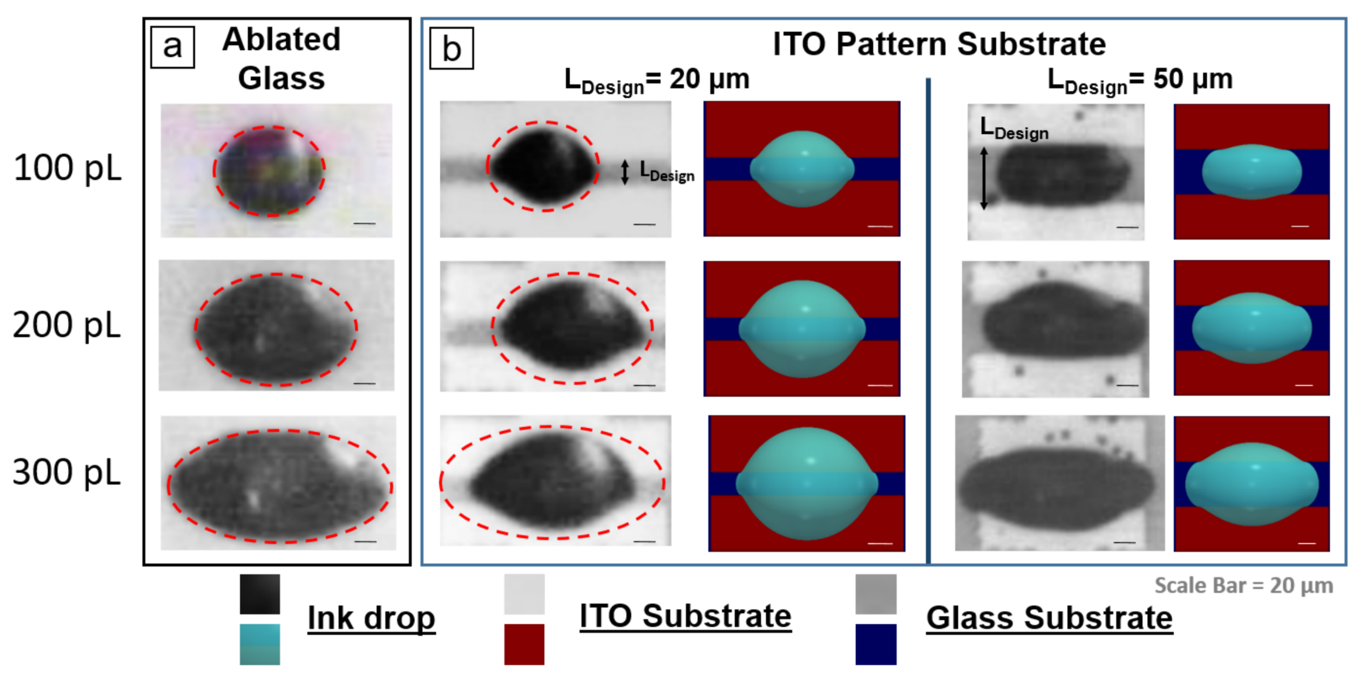


P. Arya, et al., Langmuir 40, 5162 (2024)

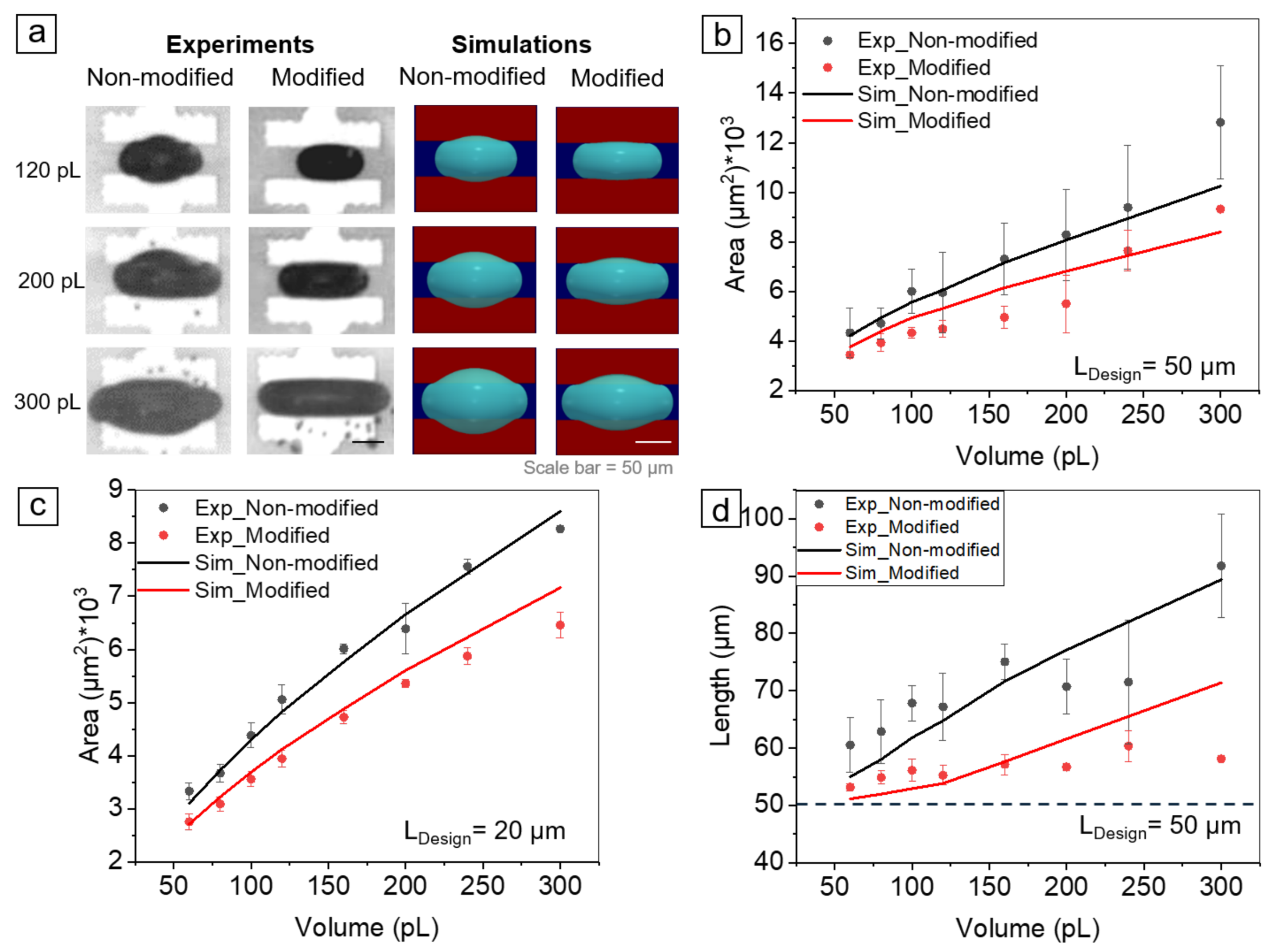
Simulation and Experimental Results

Aim: improve the printing quality by designing a patterned substrate

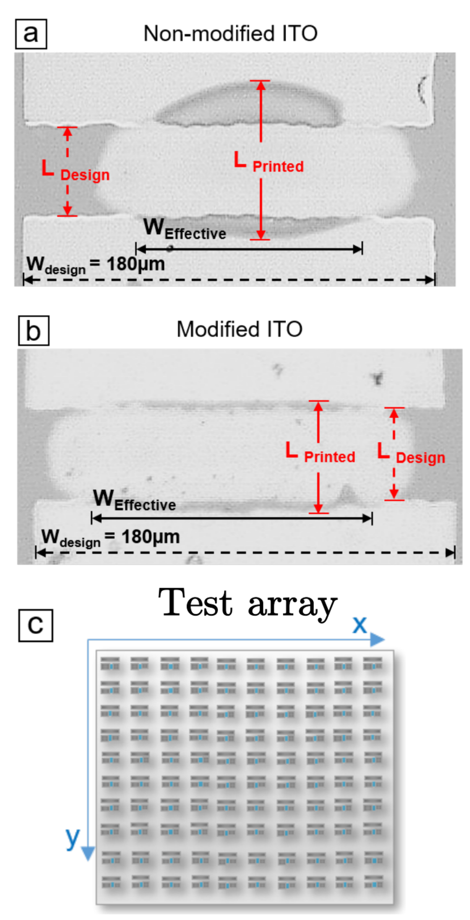
Inkjet-printed indium precursor ink drops of different volumes
(a) on laser ablated glass; (b) between two ITO electrodes



(Black/gray: experiments; Cyan/red: simulations)



Printing images based on
(a): Old device
(b): Optimized device



P. Arya, Y. Wu, F. Wang, Z. Wang, G.C. Marques, P.A. Levkin, B. Nestler, J. Aghassi-Hagmann, Langmuir 40, 5162 (2024)

Conclusion and Outlook

- Printing area versus volume and layout dimension
- Wetting morphologies when the substrate has multilayers (see right figure)
- Roughness, pinning, volume