Analysis of microspectroscopy images based on a PDEs model for electrodeposition metal growth

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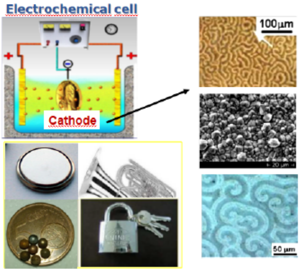
Motivation

Mathematical model for electrodeposition and metal growth

Goals:

- rationalise formation of patterns in electrochemical process
- control strategy of morphology/composition



Electrodeposition: process of depositing material onto a conducting surface from a solution containing ionic species, used to apply thin films of material to the surface of an object to change its external properties

Motivation

Mathematical model for electrodeposition and metal growth

Fields of applications of electrodeposition:

- Corrosion protection, increase abrasion resistance (aeronautics...);
- Surface decoration (silver Au plating, jewellery);
- Biomedical materials;
- Heritage (preserving/recovering ancient materials);
- Energetics (fuel cells, batteries)
  a technological challenge:
  optimization of novel metal-air batteries:
  - energetic efficiency of the recharge process
  - durability of the energy storage device.

PDEs model

Mathematical model for electrodeposition and metal growth

- Morpho-chemical model:
morphology (surface profile) $\eta(x, y, t) \in \mathbb{R}$
surface chemistry (composition) $0 \leq \theta(x, y, t) \leq 1$

$$\begin{cases} \frac{\partial \eta}{\partial t} = \Delta \eta + \rho f(\eta, \theta) \\ \frac{\partial \theta}{\partial t} = d\Delta \theta + \rho g(\eta, \theta) \end{cases}$$

$\rho > 0$ and $d = \frac{D_\theta}{D_\eta}$ dimensionless diffusion coefficient.
- The nonlinear reaction terms f and g account for generation (deposit) and loss (corrosion) of the relevant material:

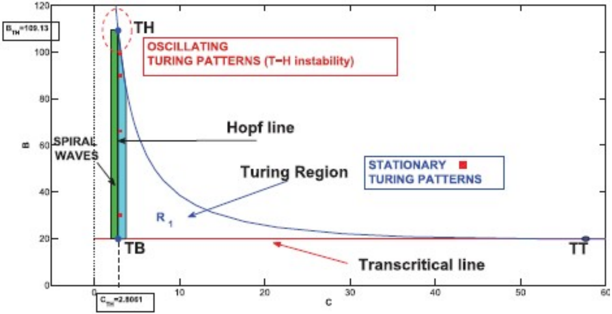
$$f(\eta, \theta) = A_1(1-\theta)\eta - A_2\eta^3 - B(\theta - \alpha)$$

$$g(\eta, \theta) = C(1 + k_2\eta)(1-\theta)(1-\gamma(1-\theta)) - D(\theta(1-\gamma\theta) + k_3\eta\theta(1+\gamma\theta))$$

- B and C bifurcation parameters, $P_e = (0, \bar{\alpha})$ homogeneous steady state.

PDEs model

Mathematical model for electrodeposition and metal growth

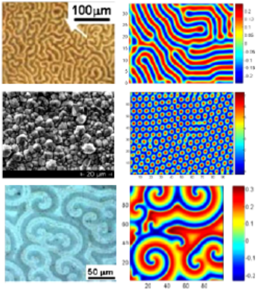


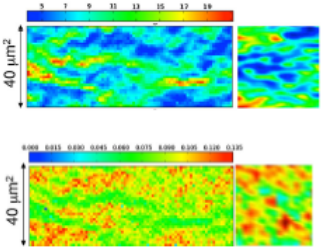
Bifurcation diagram in the parameter space (C, B)
Spatio-temporal pattern formation due to: TURING instability, HOPF instability $\Rightarrow$ TURING-HOPF interplay

Lacitignola D, Sgura I and Bozzini B, 2015 *Spatio-temporal organization in a morphological electrodeposition model: Hopf and Turing instabilities and their interplay* European Journal of Applied Mathematics **26** 143-173

Qualitative comparisons

In each panel qualitative comparisons between experimental data (left microscopy images) and numerical simulations (right images).
Left panel: structured patterns (labyrinths, spots, spirals); right panel: unstructured map.





→ Next step: quantitative comparison between experimental images and PDEs simulations

Quantitative comparisons: Identification Problems (IP)

Given $\Theta^{exp} \in \mathbb{R}^{n_1 \times n_2}$ = experimental data given by digital images, given the integration domain $\Omega \times [0, T]$ and an appropriate numerical method to solve the PDEs:

Identification Problems

- Parameter Identification Problems (PIP): fixed $[0, T]$, find a set of parameters $p = (p_1, \ldots, p_m)$ such that:

$$\min_p J(P) = \min_p \|\Theta(p; T) - \Theta^{exp}\|$$

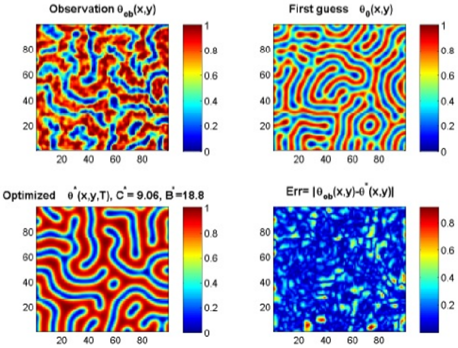
  comparison between experimental images and simulations at final time $T \Rightarrow$ stationary Turing patterns (spots, labyrinths...)
- Map Identification Problems (MIP): fixed a set of parameters $p = (p_1, \ldots, p_m)$ find $t^* \in [0, T]$ such that:

$$\min_t J(t) = \|\Theta(p; t) - \Theta^{exp}\|$$

  comparison between experimental images and simulations at each time step t_k, $k = 1, \ldots, N_t \Rightarrow$ unstructured oscillating patterns

PIP: stationary Turing pattern

Optimization problem solved by a "Discretize-then-optimize" procedure based on Conjugate gradients method



Top line: experimental image (left) and first guess pattern for optimization (right). Bottom line: optimal pattern Θ^* (left) and absolute error *Err* map (right)

Sgura I, Lawless A S, Bozzini B, 2018 *Parameter estimation for a morphochemical reaction-diffusion model of electrochemical pattern formation*, Inverse Problems in Science & Engineering

MIP: oscillating - unstructured pattern

- $M_\theta := \Theta^{exp} \in \mathbb{R}^{n_1 \times n_2}$: experimental XRF data image
- Given a set of parameters (B, C) in the Turing-Hopf zone (oscillating PDEs solutions)
- $e_\theta(t) = |M_\theta - \Theta(t)| \in \mathbb{R}^{n_1 \times n_2}$: absolute error matrix

$$\Downarrow$$

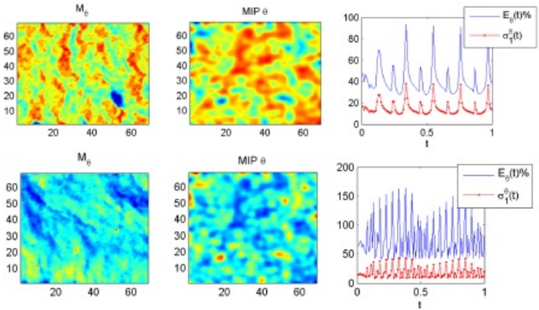
σ_i^θ, $i = 1, \ldots, p = \min\{n_1, n_2\}$: singular values of $e_\theta(t)$

Find: minimum of the first singular value:

$$\sigma_1^\theta(t_\theta^*) = \min_{t \in [0,T]} \sigma_1^\theta(t)$$

$$\Rightarrow \Theta^* = \Theta(t_\theta^*) \approx M_\theta$$

MIP: oscillating - unstructured pattern

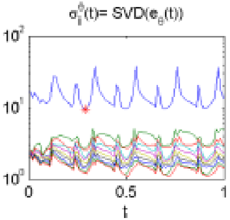


Data: top line: Mn-Co-based electrocatalyst; bottom line: Mn-Ag-based electrocatalyst. Original XRF data images (left column), MIP_{θ} solutions (middle column), time dynamics of the first singular value and Frobenius errors (right column).

Sgura I and Bozzini B 2017 *XRF map identification problems based on a PDE electrodeposition model* J. Phys. D: Appl. Phys. **50** 154002 doi:10.1088/1361-6463/aa5a1f

Remarks

- The information of the first singular value $\sigma_1(t)$ is not enough to ensure a minimization process that takes into account the full structure of the original data images



Time behavior of $\sigma_i^\theta(t)$, for $i = 1, .., p$.

- Open problem: Identification Problem: MIP + PIP (optimization in time and parameters)

Thanks
for your attention