Contribution ID: **47**  Type: **Poster**

# Enhancing battery recharge performance by combined Machine Learning and PDE modelling

*Thursday, 30 July 2020 13:00 (1 hour)*

My PhD research concerns mathematical modelling, numerical simulations and applications to electrochemical energy storage devices, in particular Zn-air batteries (ZAB).
Zn-air battery (ZAB) concepts exhibit storage potentialities ranging from low-power portable consumer electronics, to automotive and home applications (see [2]). During recharge, the regeneration of Zn is however daunted by severe morphological changes leading to low cycle life. These morphological changes are related to metal growth instabilities.
The main goal of the project is to set up a research framework aimed at attacking such battery electrode problems with a Machine Learning (ML) approach based on a Training Set of data resulting from numerical solutions of a reaction-diffusion PDE model, that is able to capture the essential features of unstable material growth in electrochemical systems by means of the so-called Turing patterns (see [1,2,3] and reference therein).
In this mesoscopic model, referred to as the "DIB model", the recharge instability is controlled by the interaction between material "shape" and material "chemistry"; the source terms include the physics describing the growth process and the parameters involved account for the battery operating conditions (chiefly electrolyte chemistry and charge rate). One of the key results of the analysis of the model [3,4,5] is the correlation of the values of the model parameters with the occurrence and type of growth instabilities. In particular, in [3] a segmentation of the parameter space in morphological classes has been proposed (see [6]).

The first application I am planning is to train the ML algorithm with a computed set of morphological maps, and to use it to classify a set of experimental maps, obtained by optical microscopy observations of electrodeposited alloys.

REFERENCES
[1] Lacitignola D, Bozzini B, Sgura I- Spatio-temporal organization in a morphochemical electrodeposition model: Hopf and Turing instabilities and their interplay, European Journal of Applied Mathematics (2015) 26(2) 143-173, dx.doi.org/10.1017/S0956792514000370
[2] Bozzini B, Mele C, D'Autilia MC, Sgura I. - Dynamics of zinc-air battery anodes: An electrochemical and optical study complemented by mathematical modelling, Metallurgia Italiana (2019) 111(7-8), 33-40
[3] Lacitignola D, Bozzini B, Frittelli M, Sgura I- Turing pattern formation on the sphere for a morphochemical reaction-diffusion model for electrodeposition, Communications in Nonlinear Science and Numerical Simulation (2017) 48, 484-508, dx.doi.org/10.1016/j.cnsns.2017.01.008
[4] Sgura I, Lawless A, Bozzini B - Parameter estimation for a morphochemical reaction-diffusion model of electrochemical pattern formation, Inverse Problems in Science and Engineering (2019) 27(5), 618-647 doi.org/10.1080/17415977.2018.1490278
[5] Sgura I, Bozzini B - XRF map identification problems based on a PDE electrodeposition model, Journal of Physics D: Applied Physics (2017) 50(15), dx.doi.org/10.1088/1361-6463/aa5a1f
[6] https://www.researchgate.net/figure/Segmentation-of-the-Turing-region-six-subregions-R-0-R-1-R-5-from-top-to-bottom_fig4_326338358

**Primary author:** Mrs MONTI, Angela (University of Salento)

**Co-authors:** BOZZINI, Benedetto (Politecnico di Milano); SQURA, Ivonne (University of Salento)

**Presenter:** Mrs MONTI, Angela (University of Salento)

**Session Classification:** Posters 3