# Phase-field modeling of dendritic zinc deposition in Zinc-Nickel flow batteries

Divyaraj Desai, Andrea Lamorgese, Yasumasa Ito, Dhiraj Patil, Sanjoy Banerjee, Dan Steingart
Department of Chemical Engineering
City College of New York, New York, USA

**Abstract**
Flow-assisted zinc-nickel batteries offer an inexpensive and safe solution to grid-scale energy storage [1]. However, they remain prone to dendrite formation on charging, limiting battery cycling. Dendritic zinc deposition occurs under a mass-transfer limitation and convection improves cycle life but the phenomenon is not well understood. Naybour [2] qualitatively studied the effect of convection on dendritic growth of zinc. However, the flow modeled was not laminar and significantly higher than required for feasible operation of a flow-assisted battery. Gallaway et al [3] reported a strong dependence of zinc deposition on electrolyte flow and current density, which highlights the need for theoretical model to predict the growth and form of zinc dendrites.

Existing numerical models are unable to predict the wide range of structures of electrodeposited zinc. A phase-field model of electrochemistry, proposed by Shibuta [4] was modified to simulate the deposit morphology. The Shibuta model in its original form did not explicitly track the motion of the electrons. The proposed phase field model correctly represents electrons as charge carriers in the electrode and ions as charge carriers in the electrolyte.

Interfacial reaction kinetics was added to the model in the form of a linearized Butler-Volmer expression [5], and two-dimensional simulations were performed using the electrochemical parameters for zinc deposition in an alkaline solution. The effect of flow was added using the form given by Tong et al [6].

Lattice Boltzmann methods were used to solve for the concentration and momentum equation, and a hybrid phase field-lattice Boltzmann scheme is incorporated in performing the simulations.

Preliminary results of zinc growth report the dependence of zinc morphology on current density and concentration.

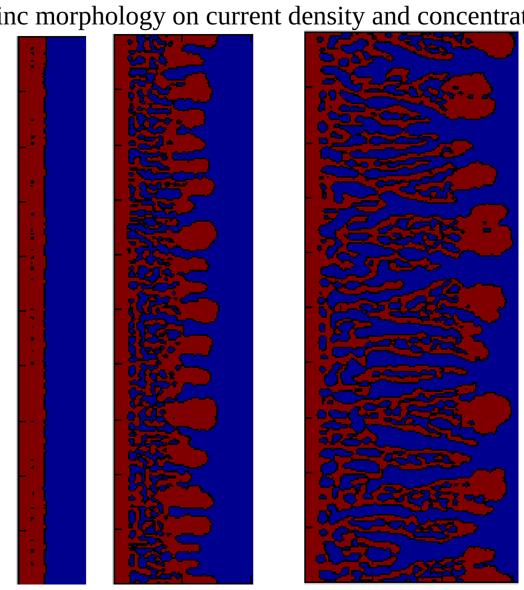

**Figure 1 Dendritic zinc in Mass-Transfer limitation**

The simulation morphologies were validated by comparing to zinc electrodeposited in Zinc-Nickel flow batteries, obtained through carefully conducted experiments.

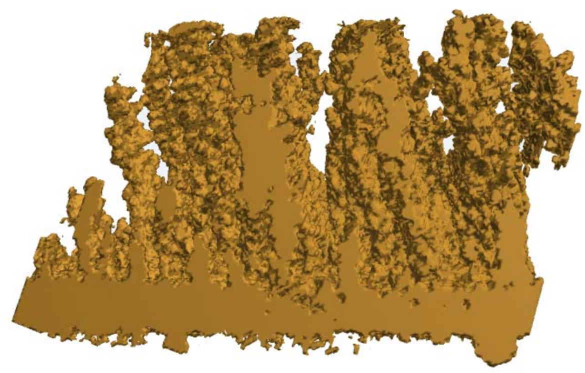

**Figure 2 Reconstructed 3-D zinc dendrites**

Micro X-ray computed tomography was used to reconstruct the three dimensional structure of zinc, and the fractal dimensions were compared with simulation. The results are in good agreement, indicating the future use of phase field models to predict morphologies of electrodeposited materials.

**References:**

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