3D Microstructure-Resolved Modeling Of Zinc-Air Batteries: Impact On Rechargeability And Performance

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Abstract

The performance and rechargeability of zinc-air batteries are found to be significantly influenced by the microstructure of the zinc anode [1]. It is evident that features such as porosity, connectivity, and spatial distribution of solid phases exert a considerable influence on ionic transport, current density, and local reaction kinetics. In order to systematically investigate the effects described above, a multiphysics model of a zinc-air cell was developed using COMSOL Multiphysics.

The model was developed in two stages. Firstly, a one-dimensional electrochemical model was constructed in order to capture the fundamental processes, including zinc dissolution and deposition, oxygen reduction/evolution reactions, and hydroxide ion transport. The model was validated using experimental discharge data from commercial zinc-air coin cells (Figure 1). The framework was then extended to a three-dimensional domain, using tomography images to generate realistic anode geometries. Two distinct microstructures, namely lamellar and cellular, were segmented and directly meshed for the purpose of simulation, thus enabling a detailed comparison of their impact on battery behaviour. This 3D microstructure-resolved approach facilitates simulations on realistic electrode geometries, thus offering a robust framework for quantitatively connecting structural characteristics to electrochemical performance and aiding in the design of optimised electrode architectures.

The Tertiary Current Distribution (Nernst-Planck) interface was utilised to simulate the transport of ions and electrochemical reactions within the electrolyte. The present study employed a stepwise study sequence, initiated with an initial current distribution step, followed by a time-dependent simulation to evaluate the full dynamic response. The modelling of ionic transport was conducted through the mechanisms of diffusion and migration, in response to concentration gradients and electric fields, respectively. To simplify the analysis, the effects of convection were neglected. Electrochemical reactions, including zinc dissolution/precipitation at the anode and oxygen reduction/evolution at the cathode, were implemented using concentration-dependent Butler-Volmer kinetics at the relevant interfaces.

The results obtained demonstrated that the anode microstructure significantly influences the discharge curve (Figure 2), local current density (Figure 3), ion transport pathways, and zinc oxide (ZnO) accumulation. The lamellar structure was found to result in more uniform current distribution and slower ZnO clogging during discharge, while the cellular structure showed localized current hotspots and earlier transport limitations due to pore blockage. The observed disparities in recharge efficiency and spatial utilisation of active material can be attributed to these differences.

The study demonstrates that 3D microstructure-resolved simulation, informed by tomography, provides critical insight into the interplay between structure and electrochemical behaviour. This modeling approach links local morphology to macroscopic performance, thus enabling a predictive assessment of electrode designs and offering a computational path to optimizing microstructure to enhance rechargeability. The present work demonstrates the capabilities of COMSOL Multiphysics in integrating experimental imaging data with multiphysics simulation for advanced battery modelling. The integration of realistic geometries, electrochemical kinetics, and transport physics enables the targeted evaluation of design strategies. It lays the groundwork for future studies involving microstructure evolution, degradation mechanisms, and electrode optimization.

Reference

[1] Franke-Lang, Robert, et al., Enhanced Zinc–Air Batteries through the Fabrication of Structured Zinc Electrodes Using Freeze-Casting, Advanced Engineering Materials, 26, 14 (2024).

Figures used in the abstract

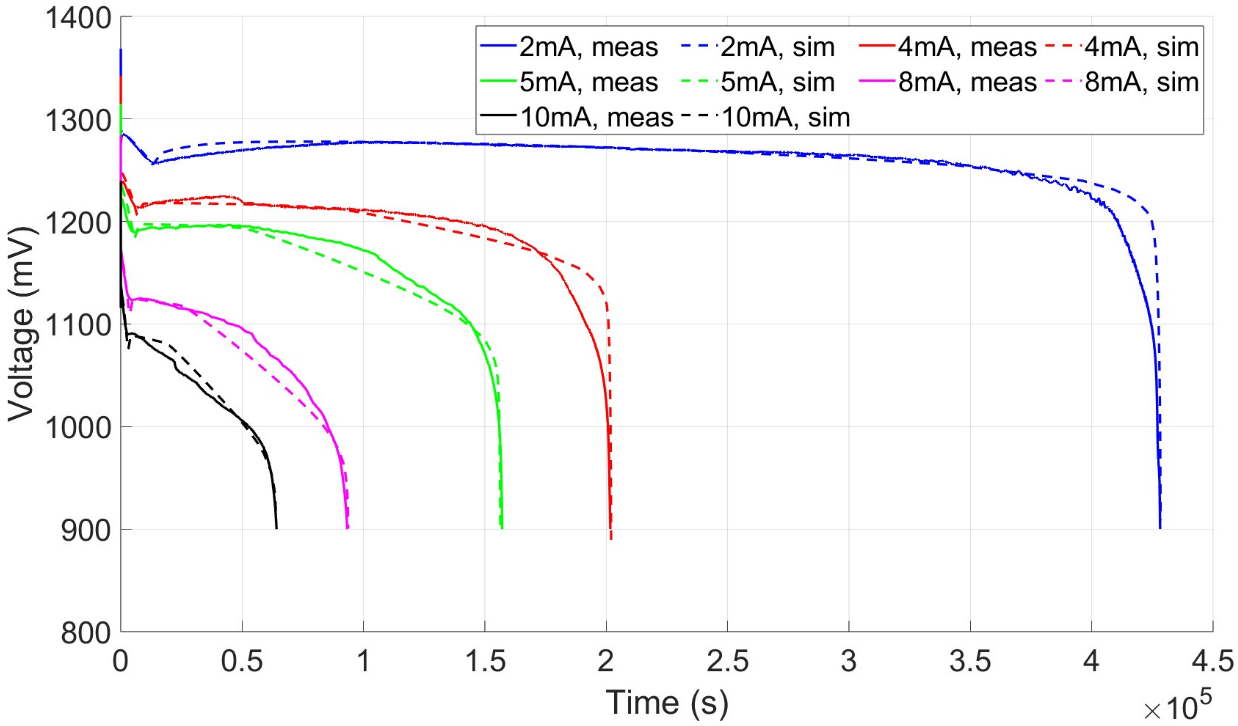

Figure 1 : Validation of the 1D model against experimental data for commercial zinc-air cells at discharge currents of 2mA, 4mA, 5mA, 8mA, and 10mA.

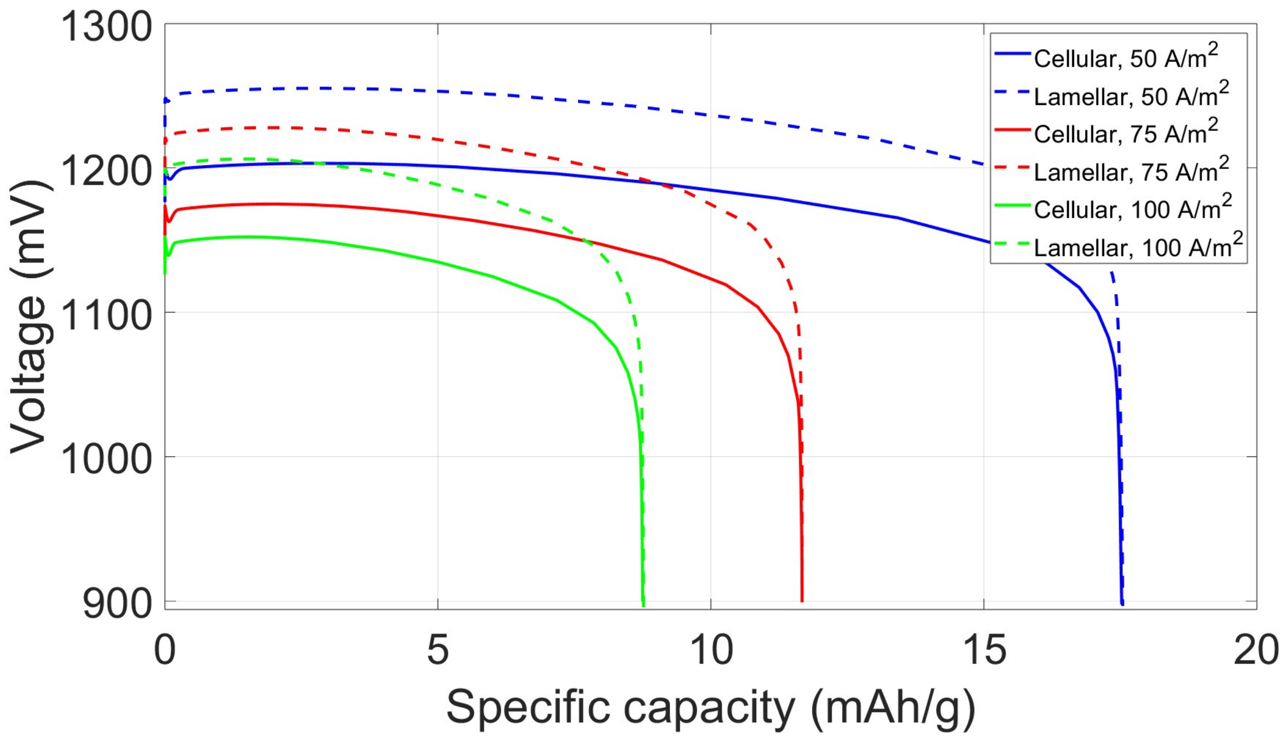

Figure 2 : Simulated voltage profiles of cellular and lamellar microstructures under discharge current densities of 50, 75, and 100 A/m² with the same specific capacity to isolate and compare the impact of microstructure on electrochemical performance.

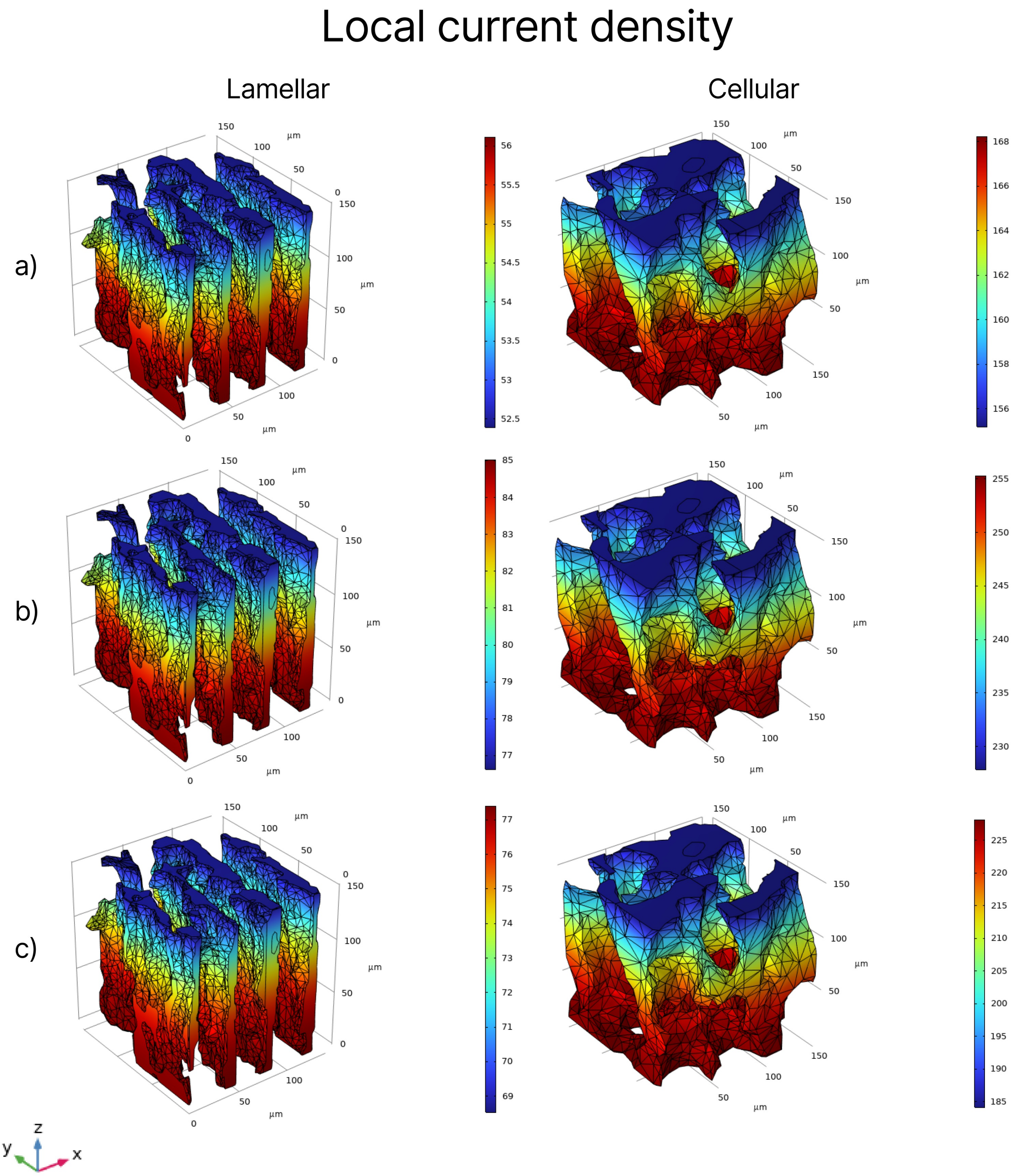

Figure 3 : Local current densities of cellular and lamellar microstructures under discharge current densities of a) 50, b) 75, and c) 100 A/m².