Optimization of Lithium ion 3D microbatteries: electrochemical modelling using finite element methodology

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The increasing demand for the high performance on-board power supplies for a variety of small scale portable devices pushes the battery development in to the next level. In order to fabricate smaller batteries with higher power and energy density, the introducing of the three-dimentional (3D) architectures have been proposed. These are expected to increase electrode-electrolyte surface area, thus promoting the ion transport. The geometry of the 3D microbatteries (MB) depends on a number of parameters like the electrode layer thickness at the sides and at the tip of the current collector pillar, current collector height and electrolyte layer thickness in different areas of the battery *etc*. Therefore, to optimize the geometry configurations the electrochemical modelling in the means of the Finite Element Method (FEM) and optimization algorithms has been found very useful tools. Previous work with the concentric Li-ion MB architecture focused on simulating of different possible geometries to find the optimal electrode configuration by maximizing the homogeneity of the electrochemical activity in the electrodes and the cell capacity [1]. Additionally, fully coupled thermal-electrochemical model was created by introducing the temperature dependence in order to achieve more realistic material behavior. Therefore three different 3D-MB architectures were simulated and benchmarked at various discharge rates to highlight critical regions which most likely could lead to the performance bottlenecks and safety hazards. Although these studies demonstrate that the 3D-MB battery performance is determined by the volume of the electrode material and the balance of the electrode energy density, the results also indicate strong dependence on the structure of the composite electrode and the ionic and electronic conductivities of the used materials.

References

[1] P. Priimägi, D. Brandell, S. Srivastav, A. Aabloo, H. Kasemägi, V. Zadin, Optimizing the design of 3D-pillar microbatteries using finite element modelling, Electrochim. Acta. 209 (2016) 138–148.

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