Simulation of Thin Film All-Solid-State Lithium Ion Batteries

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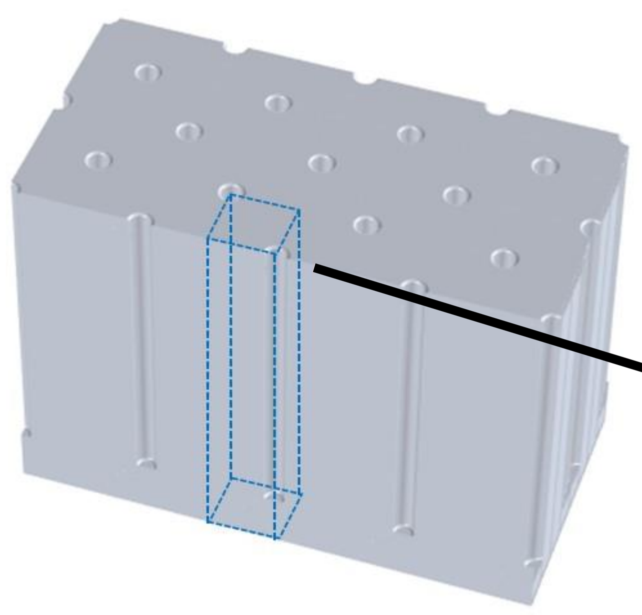
Abstract

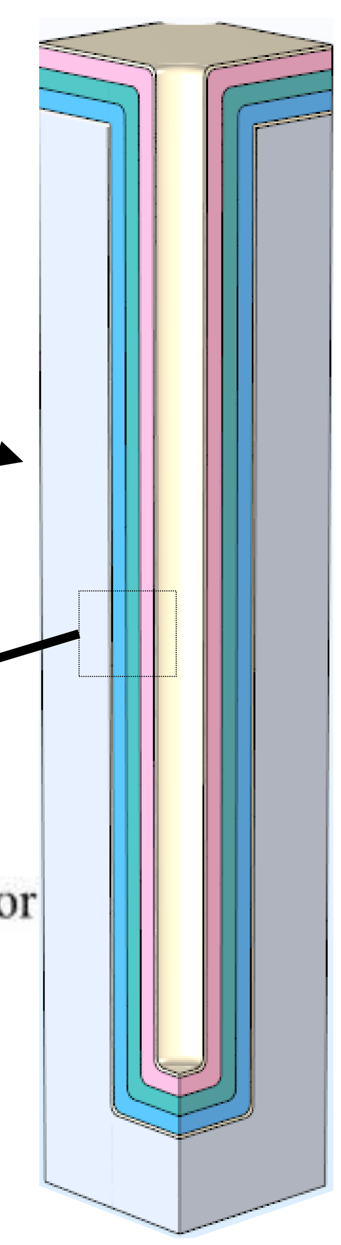
Three-dimensional all-solid-state lithium-ion batteries molded by nano-scale thin film are attractive, because they would allow the improvement of their conductivity dramatically. In this work, we present a simulation research based on a three dimensional model of thin film all-solid-state lithium-ion batteries using COMSOL Multiphysics@. The concentrations of lithium-ion and lithium and the current density are obtained in charge/discharge process. Also, the charge/discharge curves (cell voltage *vs.* time) for various charge/ discharge rates are analyzed.

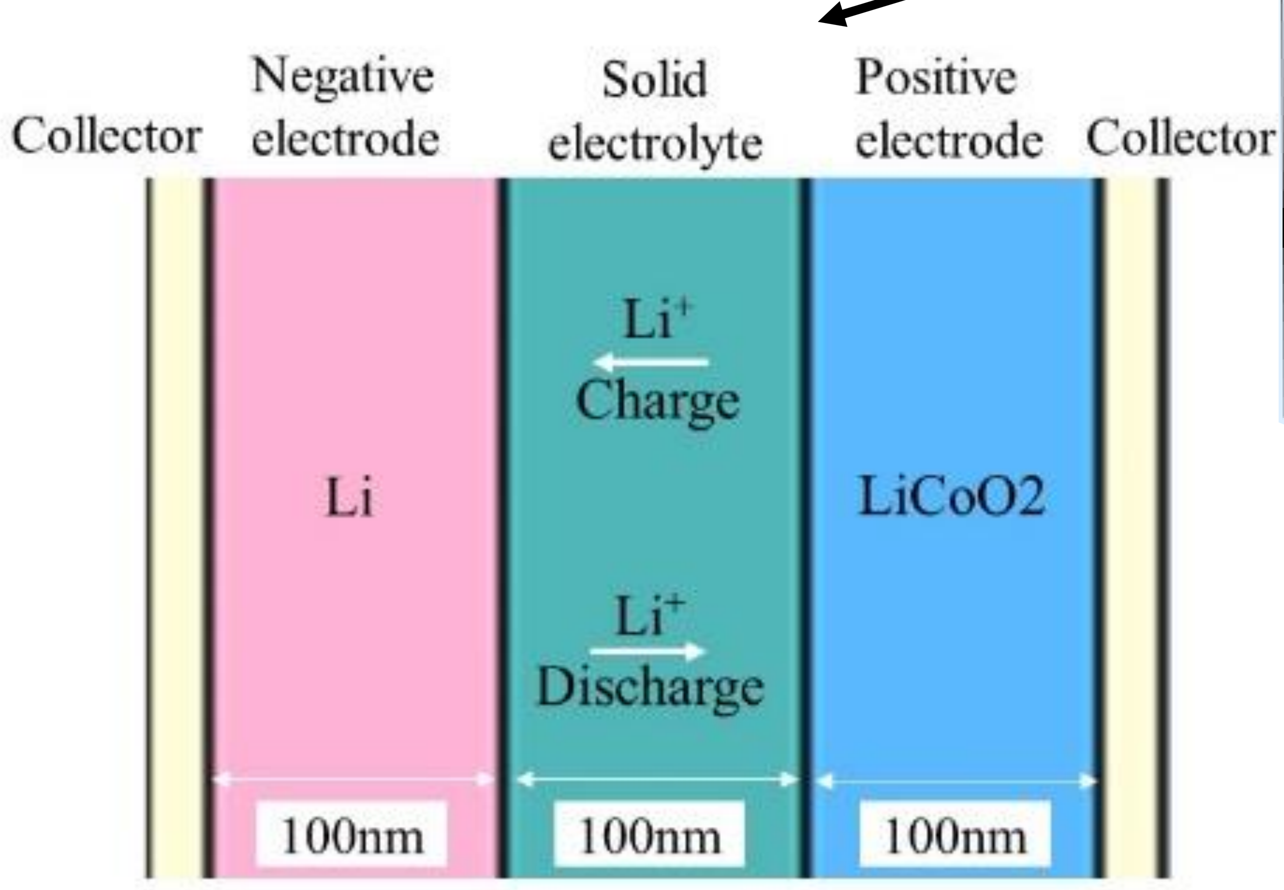
Numerical model



(a) Schematic of full cell

(b) Schematic of unit structure of cell





(c) Enlarged view of cross section of the cell and transport of Li+ in the electrolyte.

Figure 1. Schematic of 3D thin film all-solid-state lithium-ion battery.

The electrochemical reactions at the negative and positive electrodes can be represented by

$$\mathrm{Li} \leftrightarrow \mathrm{Li}^{+} + e^{-}\,, \tag{1}$$

$$\mathrm{LiCoO_2} \leftrightarrow \mathrm{Li}_{1-x}\mathrm{CoO_2} + x\mathrm{Li}^{+} + xe^{-} \tag{2}$$

The transport of Li^{+} and n^{-} is solved by the Nernst-Plank equation

$$\mathbf{N}_i = -D_i \nabla c_i + \frac{z_i F}{RT} D_i c_i \nabla \phi_l \tag{3}$$

where c_i and D_i are the concentration and diffusion coefficient of species, respectively, z_i is the charge of species, and ϕ_l is the electrolyte potential. The transport of lithium species in the positive electrode is described by the Fick's law

$$\mathbf{N}_{\mathrm{Li}} = -D_{\mathrm{Li}} \nabla c_{\mathrm{Li}}. \tag{4}$$

where c_{Li} and D_{Li} are the concentration and diffusion coefficient of lithium species in the positive electrode, respectively.

Results and discussions

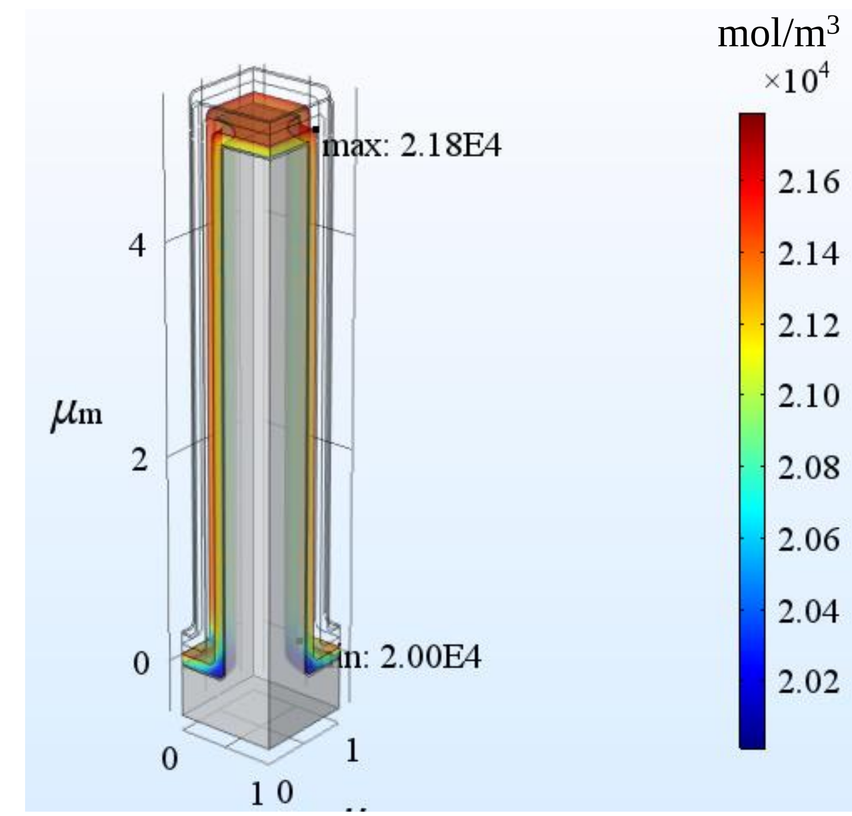


Figure 2. Concentration of lithium in the positive electrode at 50 s of discharge.

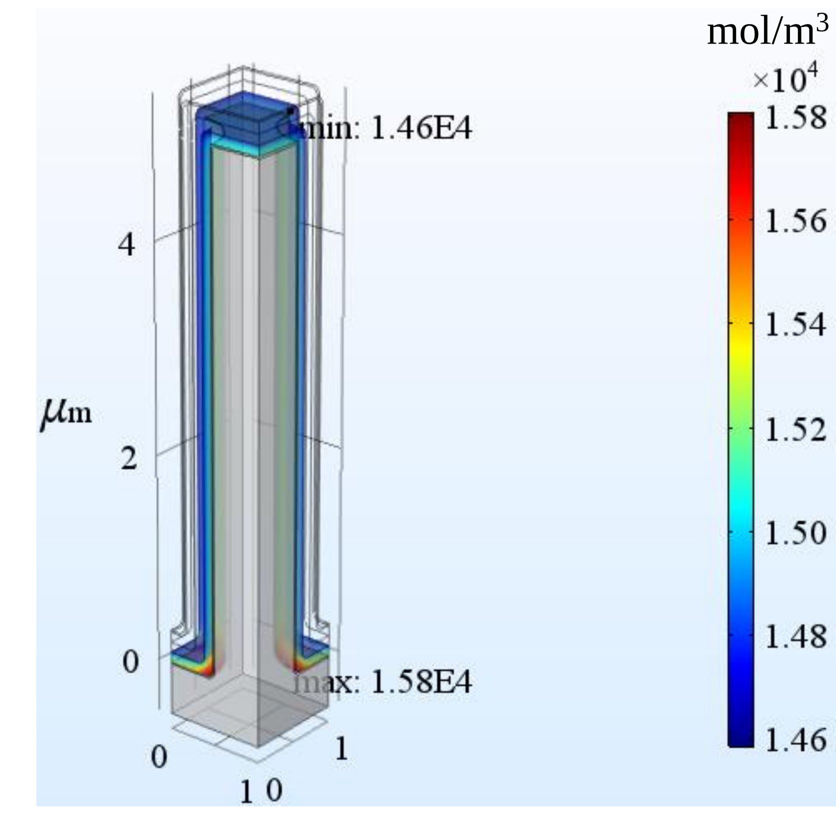


Figure 3. Concentration of lithium in the positive electrode at 50 s of charge.

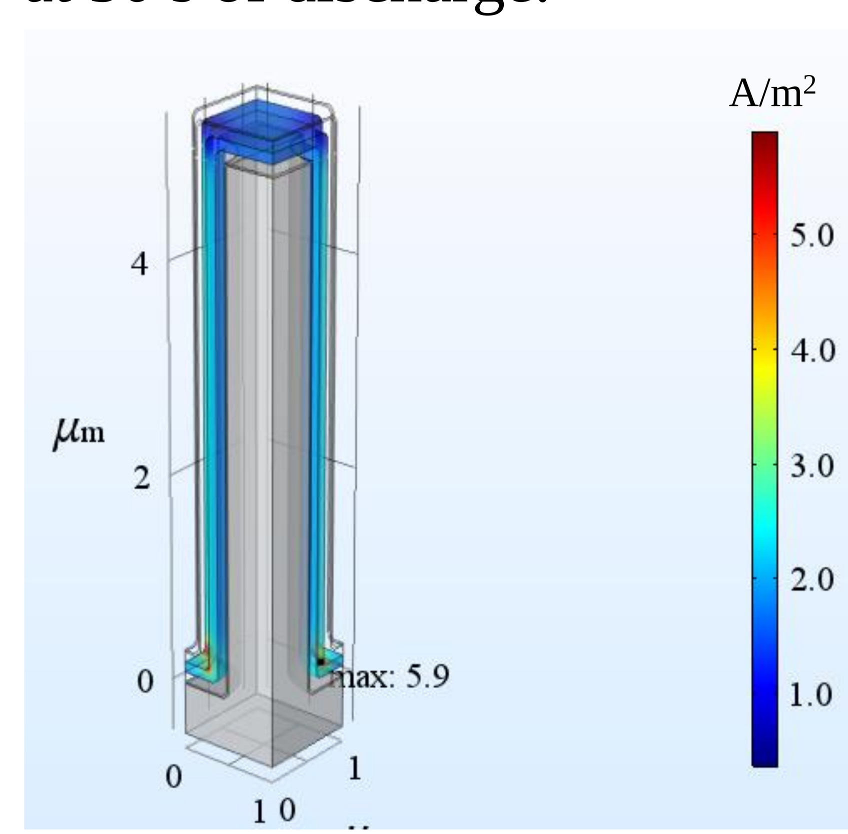


Figure 4. Current density in the electrolyte at 50 s of discharge.

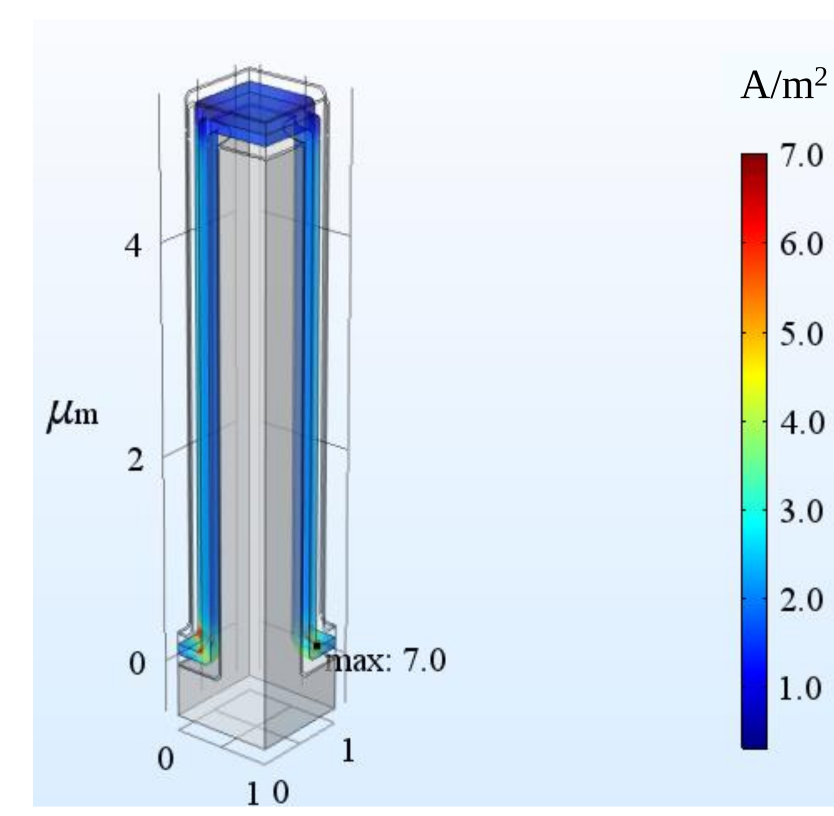


Figure 5. Current density in the electrolyte at the 50 s of charge.

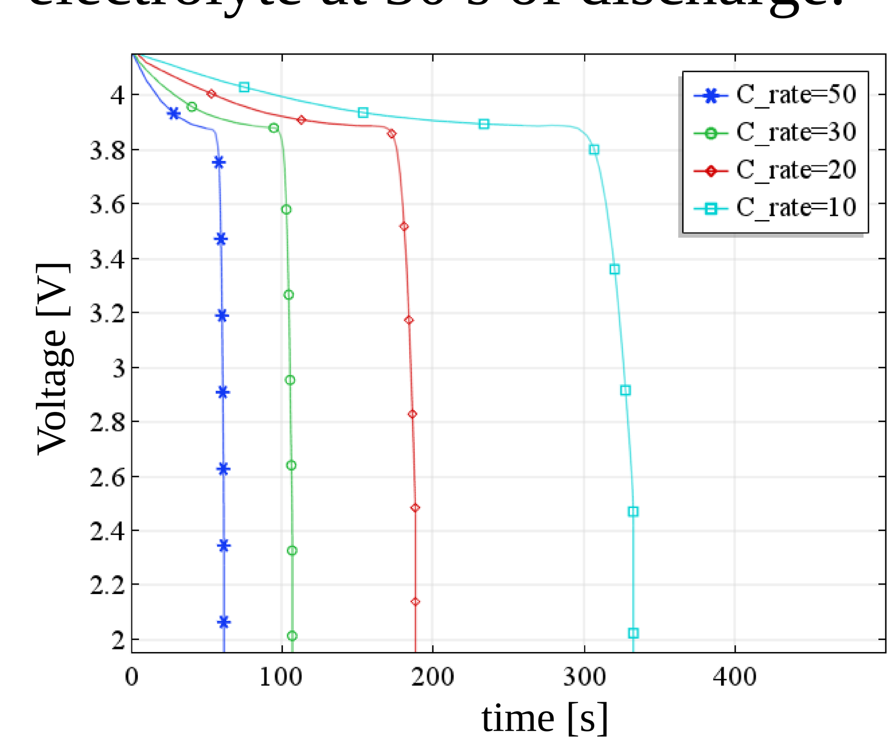


Figure 6. Discharge for various discharge rates.

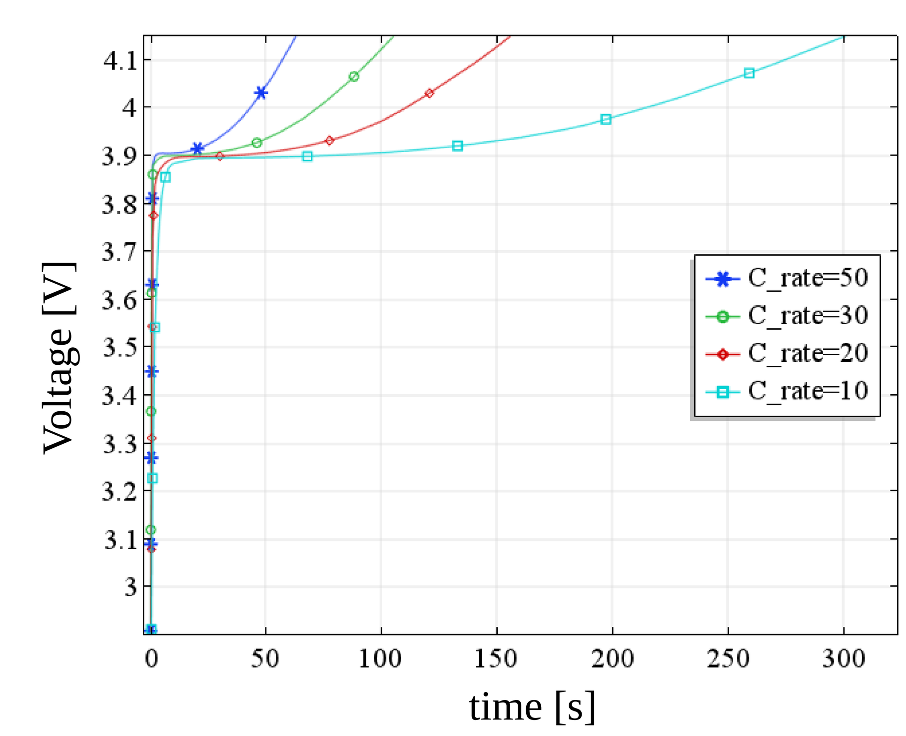


Figure 7. Charge curves for various charge rates.

The results shows that the maximum current density occurs on the corner of bottom in both charge/discharge processes. It is obvious that the shape of the thin film cell greatly affects performance of the battery.

Concluding remarks

This paper reports the simulation results of three-dimensional model of thin film all-solid-state lithium-ion batteries using COMSOL Multi-physics@. It is found that the battery can be quickly charged at the initial stage of charge process, and it has a smooth discharge before depletion for the different charge/ discharge rates. Also, the results shows that the maximum current density occurs on the corner of bottom in both charge/discharge processes. The present results would be beneficial to the improvement of all-solid-state lithium ion batteries molded by nano-scale thin film.

References

1. A. Pearse, T. Schmitt and K. E. Gregorczyk, "Three-dimensional solid-state lithium-ion batteries fabricated by conformal vapor-phase chemistry", *ACS. Nano* **10**, 1021 (2018).