Modelling Lithium Transport in Intercalation-type Active Materials Suitable for Transportation Applications

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Lithium-ion batteries are important for the future of transportation sustainability. With the depletion and rejection of fossil fuels, it is clear that mobility will depend ever increasingly on electric vehicles. However concurrent with this increase, is the need to properly evaluate and optimize lithium-ion battery electrode materials, electrolyte composition operating conditions, which include the C-rate and operating temperature, and the cell design in general. This is especially with regard to improving energy density, durability, recharge time and safety. Active materials are used in the electrodes and it is necessary to understand the lithium transport within such materials.

Providing that the discharge of the lithium-ion battery is long and the C-rate is low, then using Fick's Law gives reasonable results. For high-power current pulses however, commonly found in transportation applications, which require short discharge and a high C-rate, using Fick's Law without modification is not appropriate as the assumption has to be made that lithium propagates with an infinite velocity. Also the causality or inertia effect is not taken into account at short-time scales which means the lithium flux develops instantaneously with lithium concentration gradient.

In this work Fick's Law is used to calculate lithium transport within intercalation-type active materials but use is also made of the Maxwell-Cattaneo-Vernotte (MCV)[1] theory which captures the impact of lithium transport inertia on the electrochemical response of materials. The theory should take into account finite speeds. For the concentration gradient of a chemical species, a similar MCV equation is used here, which is hyperbolic, and does not have infinite speed propagation, hence keeping the transients finite.

References

[1] M.C. Cattaneo Comptes Rendus Hebd. Seances Acad. Sci., 247 (1958) 431-433.

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