Simulation of Intercalation Processes in Poorly Conductive Materials

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Currently, the search for new electrode materials for metal-ion batteries, based on the identification of crystal structures with ionic mobility and the ability for reversible intercalation process, often leads to materials with low conductivity, especially electronic. In fact, these are dielectric materials, a striking example of which are many polyanionic compounds. At the same time, these materials are often characterized by potentially attractive characteristics, such as low volume change during cycling, ease of synthesis, moderate values of specific capacity, and others.

However, the implementation of the intercalation process and especially its kinetics represent a significant difficulty for dielectric materials, despite their thermodynamic attractiveness. Even nanosized materials at low currents in the electrodes show low specific capacitance for this reason. The physical model includes a description of mass transfer and charge transfer in the phases of the electrode material and electrolyte, connected by the condition of transformation at the interface between them. A single-particle model using COMSOL Multiphysics was modeled to calculate the process of intercalation and accumulation of intercalation phase in the bulk of the initial active material phase. A distinctive feature of the model is considering the distribution of the intercalation process over the surface, in contrast to the dominant approach based on the use of the idea of particle surface equipotentiality. The influence of the number of electron contacts to the particle on the kinetics of the process is also considered.

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