Phase-field simulation and discrete element modeling of the interaction of diffusion and mechanics in electrode particles and electrodes of lithium ion batteries

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ABSTRACT

In active electrode materials of litium ion batteries, there exists a coupling beween the field of lithium concentration on the one hand and mechanical strain on the other. When lithium ions are inserted in the electrode particles, this may cause significant stresses, which may lead to particle failure. For individual particles, we study the interaction of diffusion and mechanical stresses in cathode particles by means of a phase-field model employing the Cahn–Hilliard equation. Although the porous structure of electrodes allows for the improvement of cell power due to shortened diffusion paths in the solid phase for lithium ions, it constitutes issues with respect to the transport of electrons. In the second part of this discussion, the effective conductivity of the porous electrode is described by a resistor network method, coupled to DEM to account for the interaction with mechanical loadings.