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ELECTRO-CHEMO-MECHANICAL SIMULATION OF 3D-MICROSTRUCTURES FOR LITHIUM-ION BATTERIES

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A micromodel coupling lithium-ion diffusion and electric potentials[1] to a linear elasto-plastic model is applied and discretized with finite volumes. The numerical algorithm does not require the assembly of a Jacobian and applies the immersed interface method for the electro-chemical problem[2]. An established elastic solver optimized for non-linear heterogeneous structures is applied to describe mechanical strains resulting from lithium-ion intercalation. Numerical examples on several structures are given, including academic structures, and microstructures given by computer tomography compared with microstructures drawn from stochastic models[3]. Figure 1 shows the lithium-ion concentration and stress invariants in a 3D-microstructure of anode material charged with C-rate 1 at 40% state of charge.

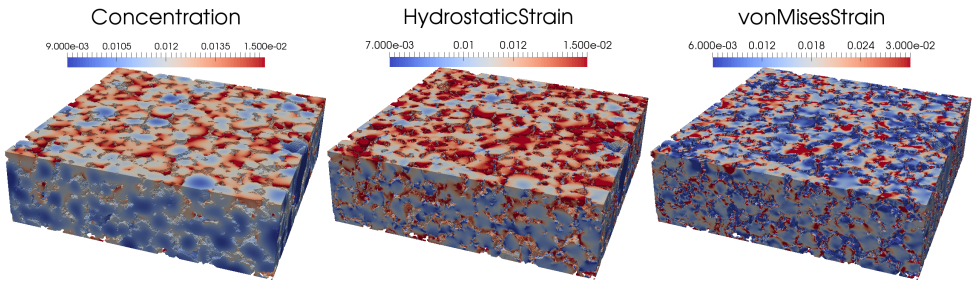

Figure 1: Concentration, hydrostatic and von-Mises strain on simulated 3D microstructures.

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