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Generating 3D Battery Cathode Microstructures using Gaussian Mixture Models and Pix2Pix

Authors : Wesley Teskey, Vedran Glavas, Julian Wegener

Abstract : Generating battery cathode microstructures is an important area of research, given the proliferation of the use of automotive batteries. Currently, finite element analysis (FEA) is often used for simulations of battery cathode microstructures before physical batteries can be manufactured and tested to verify the simulation results. Unfortunately, a key drawback of using FEA is that this method of simulation is very slow in terms of computational runtime. Generative AI offers the key advantage of speed when compared to FEA, and because of this, generative AI is capable of evaluating very large numbers of candidate microstructures. Given AI generated candidate microstructures, a subset of the promising microstructures can be selected for further validation using FEA. Leveraging the speed advantage of AI allows for a better final microstructural selection because high speed allows for the evaluation of many more candidate microstructures. For the approach presented, battery cathode 3D candidate microstructures are generated using Gaussian Mixture Models (GMMs) and pix2pix. This approach first uses GMMs to generate a population of spheres (representing the "active material" of the cathode). Once spheres have been sampled from the GMM, they are placed within a microstructure. Subsequently, the pix2pix sweeps over the 3D microstructure (iteratively) slice by slice and adds details to the microstructure to determine what portions of the microstructure will become electrolyte and what part of the microstructure will become binder. In this manner, each subsequent slice of the microstructure is evaluated using pix2pix, where the inputs into pix2pix are the previously processed layers of the microstructure. By feeding into pix2pix previously fully processed layers of the microstructure, pix2pix can be used to ensure candidate microstructures represent a realistic physical reality. More specifically, in order for the microstructure to represent a realistic physical reality, the locations of electrolyte and binder in each layer of the microstructure must reasonably match the locations of electrolyte and binder in previous layers to ensure geometric continuity. Using the above outlined approach, a 10x to 100x speed increase was possible when generating candidate microstructures using AI when compared to using a FEA only approach for this task. A key metric for evaluating microstructures was the battery specific power value that the microstructures would be able to produce. The best generative AI result obtained was a 12% increase in specific power for a candidate microstructure when compared to what a FEA only approach was capable of producing. This 12% increase in specific power was verified by FEA simulation.

Keywords : finite element analysis, gaussian mixture models, generative design, Pix2Pix, structural design
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