Li-ion battery design through microstructural optimization using generative AI

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In this work, we demonstrate how recent advances in generative artificial intelligence (AI) can accelerate the design of lithium-ion battery electrodes by directly relating manufacturing parameters to microstructure and, ultimately, to full-cell performance [1]. Our approach addresses a fundamental challenge in electrode design: varying just a few common parameters, such as active material fraction and calendering pressure, can lead to a vast range of achievable microstructures, each with different transport properties and electrochemical behavior. Traditionally, bridging this “manufacturing-to-performance” gap would require expensive or time-consuming physics-based simulations and/or extensive experimental campaigns.

We overcome these challenges by training a data-driven, conditionalized generative model on a small dataset of electrode cross-sectional images. These images capture microstructural data varying three key parameters: active material weight percentage, porosity, and a binder adhesion metric. Crucially, after seeing only 21 training samples, our generative model accurately reproduces unseen microstructures while also predicting effective transport and interfacial properties. The fidelity of these generated microstructures is verified by comparing microstructural metrics (e.g., tortuosity factor, surface area) with those from samples withheld from training. The average relative errors are below a few percent, indicating reliable interpolation across the parameter space.

Once trained, the generative model is able to generate accurate microstructural data five orders of magnitude faster than a state-of-the-art physics-based manufacturing simulation. As such, it can be embedded in a Bayesian optimization loop. Each iteration begins by selecting a set of manufacturing parameters. The model generates corresponding microstructures, from which we extract effective properties (e.g., active material volume fraction, pore tortuosity factor, as shown in Figure 1). We used our own GPU accelerated solver, *TauFactor2* [2], to extract the transport metrics. These properties parameterize a pseudo-two-dimensional (P2D) full-cell model, enabling rapid electrochemical performance evaluation (implemented in *PyBaMM* [3]). An acquisition function balances exploration and exploitation, seeking manufacturing parameters that maximize application-specific objectives such as energy density or power density.

We demonstrate the efficacy of this approach with multiple case studies, including both half- and full-cell optimizations in a 4680 cylindrical battery format. Our findings reveal that design choices are highly sensitive to how performance is measured (e.g., specific energy versus cell-level energy density), underscoring the importance of industrially relevant normalization. By capturing the complex interplay among manufacturing steps, microstructural features, and large-scale performance, our framework (see Figure 2) offers a promising and scalable AI-based solution for rapidly optimizing electrodes and other advanced materials.

This approach has recently formed the basis of a spin-out company from Imperial College London called Polaron (www.polaron.ai). Polaron can perform various microstructural analysis tasks, including dimensionality expansion (i.e. 2D to 3D) [4] and accelerated human-in-the-loop segmentation

References

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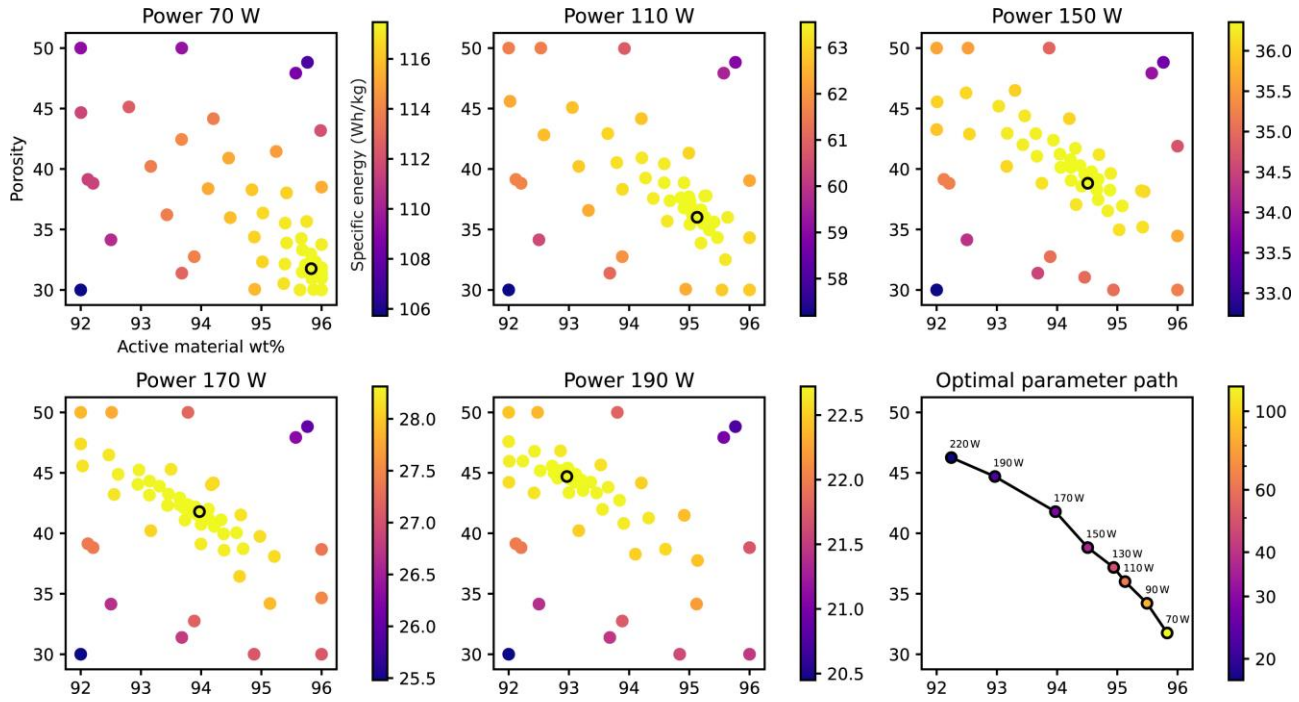

Figure 1. Optimization results showing the specific energy for tested parameters. The color of each dot represents the specific energy at the cell level for a microstructure generated with a given parameter set. In the five plots showing individual optimizations at a given cell-level power, the black circled dot indicates the optimal parameter set that gives the highest specific energy. In the final subplot, these black circled points are plotted together to show the path of optimality through the parameter space.

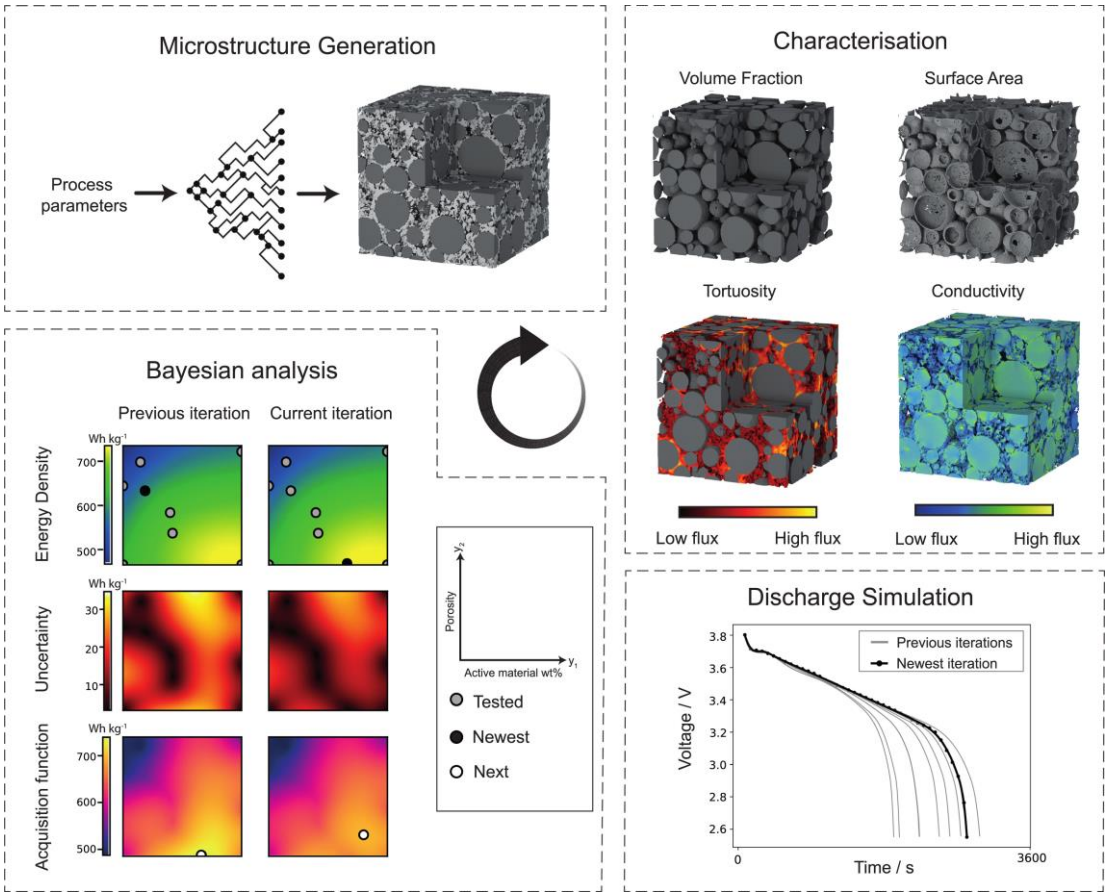

Figure 2. Bayesian optimization loop. Microstructure generation involves the prediction of a representative 2563 voxel cube microstructure based on a manufacturing label vector, y, using a trained generative model. Characterization of this dataset using TauFactor 2 allows key microstructural properties to be extracted. A discharge simulation then uses these properties to parameterize a P2D model, which returns performance at the cell-level. Finally, an acquisition function determines the best next label to test. In the example shown here, active material wt % and porosity are optimized.