

Stochastic Models of Carbon Fibre-Based Electrode Materials

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Carbon fibre-based materials often play key roles at the electrodes of batteries and fuel cells. These materials are manufactured to be highly porous, mechanically strong, and highly electrically and thermally conductive. Manufacturers have some control over the anisotropy, porosity, and porosity distribution. To inform the design process of next-generation material, we should physically model these materials with similar parameters being adjustable. Recent efforts to create three dimensional stochastic reconstructions of these materials have demonstrated the feasibility of creating digital models of these materials in domains of up to 1-2 mm length scales [1]. This work will provide simple instructions to create reproducible fibre-scale models of porous carbon-fibre materials. Furthermore, a method is introduced to extract the topology and pore-scale information in the form of a pore network, capable of simulating two-phase drainage, diffusion, and permeation. Existing materials are reconstructed from porosity distribution data [2]. Drainage experiments (e.g., mercury intrusion porosimetry) are simulated, with results compared to experimental data available in literature [3,4] for validation.

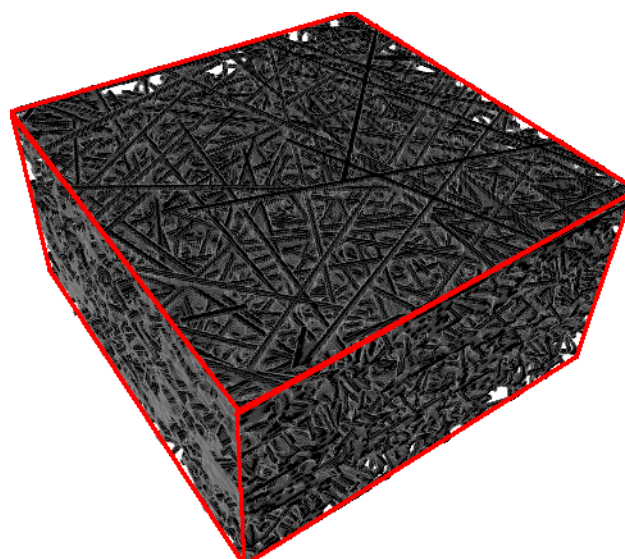


Figure 1: Simulated carbon fibre material with dimensions $650 \mu\text{m} \times 650 \mu\text{m} \times 380 \mu\text{m}$. Grey areas represent simulated deposits of binder material at fibre intersections.

References:

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