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Hierarchical Numerical Modeling of Tortuosity Modifications in Laser-Engineered Carbon-based Supercapacitor Electrodes

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Fast and efficient charging in electrochemical energy storage devices relies heavily on the design of highly porous nanocarbon-based electrodes. Their hierarchical pore structure should facilitate rapid ion transport while maximizing the accessible surface area for charge storage. The microporous structure of supercapacitor electrodes plays a crucial role in their performance, affecting electronic and ionic transport properties, as well as mechanical stability, due to the non-uniform distribution of phases. Optimizing the microporous structure is essential for enabling high-rate charging, while maintaining high energy density, which is key for developing next-generation electrodes capable of overcoming transport limitations [1]. A strategy based on laser-assisted processing of the electrode/electrolyte interphase aims to create a 3D morphology by opening channels that facilitate faster electrolyte diffusion, hence enhancing charge/discharge rates. While such studies have primarily focused on battery electrodes, these improvements are critical for the development of high-performance supercapacitors designed for energy storage applications that require rapid energy delivery and long operational lifetimes [2].
This work explores how laser-assisted microstructure modification influences the performance of electrodes. Various laser fluences have been utilized to modify the structure and morphology of slurry-based activated carbon electrodes prepared using the conventional doctor-blade coating method. A 3D imaging technique in Photoshop, based on creating channels to detect subtle variations in morphology and perform measurements of the area of interest, has been developed to characterize the porosity of modified electrodes in comparison to untreated electrodes. This technique appears more favorable as it reduces human intervention in calculations compared to the thresholding approach [3]. The surface area is determined using the Brunauer–Emmett–Teller (BET) method.
Tortuosity factor is obtained through numerical modeling of diffusion transport inside microporous structure. A combination of X-ray Computed Tomography (XCT), a non-destructive method capable of analyzing larger structures, and Focused Ion Beam Scanning Electron Microscopy (FIB-SEM), which offers higher resolution, provides comprehensive insight into electrode morphology [4]. The 3D reconstructions obtained from these techniques are used to develop numerical models for steady state diffusion inside a free space control volume and comparing it with diffusion transport through pores (in the actual structure). Additionally, a "zoom-in" approach (a window within another window) is adopted to bridge the different length scales investigated by XCT and FIB-SEM. This hierarchical modeling method provides a more accurate representation of the complex pathways for ion and electron transport, aiding to identify bottlenecks and heterogeneities within the porous medium that affect performance.
By correlating structural parameters with transport properties, the study aims to provide design guidelines for optimizing electrode architecture. The integration of imaging and modeling techniques contributes to the development of next-generation supercapacitor electrodes with improved efficiency, higher power density, and enhanced long-term stability.

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