Analysis of the Influence of Microstructures on the Impedance Response in Lithium-Ion Battery Electrodes

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The analysis of impedance response in the Lithium-ion battery (LIB) electrode can be useful for predicting cell performance and degradation. In this study, virtual 3-D microstructures of Li-ion battery with intercalation particles are designed to describe the influence of microstructure on effective electrical conductivity and the electrochemical impedance response. The technique of digital stochastic modeling has been employed for the generation of electrode microstructures consisting of active material, binder, conductive additive and electrolyte. Physicochemical properties for each of the constituent phases have been duly accounted for. Mathematical models have been developed to characterize the electrochemical impedance of LIB electrode [1-3]. In this work, we demonstrate the coupling of electrode microstructures to the solid state diffusion impedance response in LIB electrodes.

This model considers the effect of heterogeneity in active particle size on the local bounded diffusion impedance response. It also captures the effect of electrical conductivity on overall impedance response as shown in Figure 1. In addition, the impact of morphology of the active materials on the diffusion impedance response by using the characteristic diffusion length of active particles and an effective mean particle size have been demonstrated in Figure 2.

This approach is envisioned to offer a virtual impedance response probing framework to elucidate the influence of electrode microstructural variability and underlying electrochemical and transport interactions.

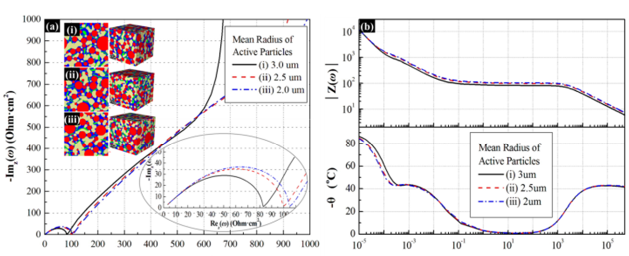

Figure 1. Dependence of the local bounded impedance response on the mean particle radius effect of virtual porous electrodes. The specific surface area of the particles is approximately 2735 cm^{-1} . The volume fraction of the particles is about 35.4% and the ratio of additive to PVDF in the 3D microstructure electrodes is 0.3:1. The electrical conductivity of electrolyte is 0.01 S/cm. The effective conductivities of solid-phase materials of (i), (ii), and (iii) are 2.41274E-6 S/cm, 1.67566E-6 S/cm, and 1.50049E-6 S/cm, respectively (a) Nyquist image of impedance response. (b) Bode plots of impedance response

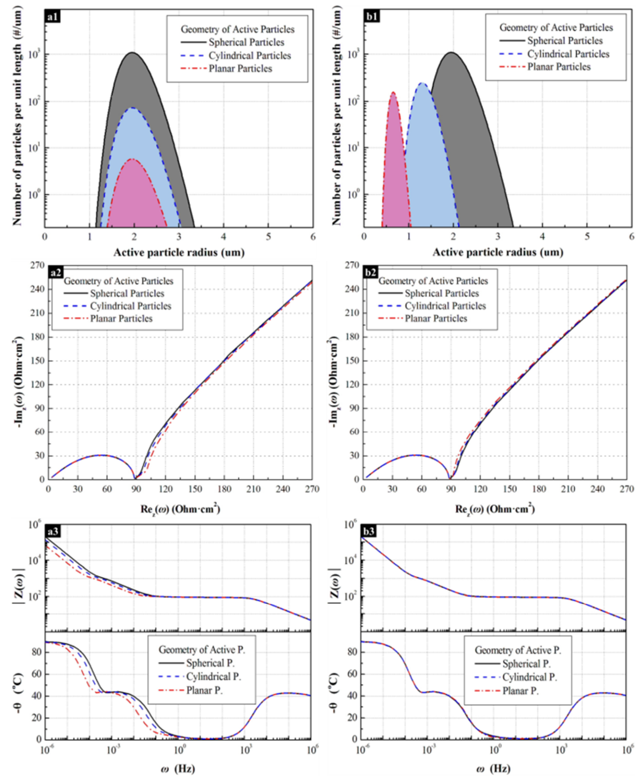

Figure 2. The morphology effect of the active material on the impedance response of the imaginary electrodes. The aspect ratios of cylindrical particles(1:γ) and planar particles(1:α:β) are 1:10 and 1:10:10,respectively. The specific surface area of active particles is 2900 cm^{-1} and the effective conductivity of solid-phase materials is 2E-6 S/cm. The electrolyte conductivity is 0.01 S/cm. (a) The characteristic mean diameter is 4um. The volume fractions of spherical, cylindrical, and planar active particles are 20%, 30%, and 60%, respectively. (a1) Active particle size distribution function. (a2) Nyquist image of impedance response. (a3) Bode plots of impedance response. (b) The Sauter mean diameter is 4um, and the volume fraction of active particles is 20%. (b1) Active particle size distribution function. (b2) Nyquist image of impedance response. (b3) Bode plots of impedance response.

References:

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