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.

References: