A comparative study of surface kinetics in carbon anodes of Li-ion battery

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To accomplish the ever-increasing demand for higher energy densities, it is necessary to develop next generation Li-ion batteries that requires micro-scale modelling based on fundamental governing equations of migration, diffusion processes as well as kinetics of intercalation. However, such a physico-chemical model will also require precisely evaluated model parameters for the material under consideration. Commercially, graphite is the choice of negative electrode in Li-ion battery due to its low cost, low operating potential vs. Li/Li^+, high capacity, good reversibility and higher structural stability [1]. MCMB is a popular spherical form of graphite due to its higher edge surface area which is effective in rapid charge transfer. Moreover, conducting additives and nano-fillers such as carbon black (CB) and carbon nanotubes (CNT) play a significant role in influencing charge transfer kinetics on the surface of carbon anode in Li-ion batteries [2]. In this work, we address the aspect related to the change in kinetic processes in the presence of different aspect ratio nano-fillers through controlled experiments in Li-ion half-cells. We accomplish this by measurement of various kinetic parameters for different weight fractions nano-fillers in MCMB electrode. The relationship between discharge current and kinetic overpotential can be demarcated into different zones of dependencies using the Butler-Volmer equation under charge transfer controlled process of deintercalation [3]. Shown in Figure 1 is a plot of current density i as a function of overpotential η_k. The kinetic parameters such as exchange current density (i_0) and transfer coefficient (α) for different nano-fillers have been measured in the irreversible kinetic zone. In this work, exchange current density for MCMB electrode with traditional CB additives (4% of total electrode weight) is measured to be 0.255 $mAcm^{-2}$ which increases to 0.302 $mAcm^{-2}$ when CB was replaced by the same weight fraction of CNT. Interestingly, this value is even higher, i.e., 0.406 $mAcm^{-2}$ for a mixture of conducting nano-fillers (1%CB+3%CNT) as shown in Table 1. In addition, the transfer coefficient α with these additives shows negligible variation as shown in Table 1. We anticipate that evaluation of effective kinetic parameters will lead to future development of a physico-chemical model that could be used to develop a fundamental understanding of charge-transfer kinetics and transport mechanisms in carbon electrodes composed of hybrid nano-fillers.

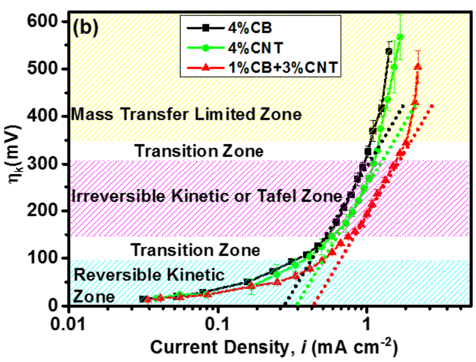

Table 1: Values of exchange current density, i_0 and transference coefficient, α for Li deintercalation

Composition	Exchange Current Density, i_0 ($mAcm^{-2}$)	Transfererence Coefficient, α
4%CB	0.255±0.020	0.230±0.035
4%CNT	0.302±0.007	0.224±0.036
1%CB+3%CNT	0.406±0.021	0.212±0.010

Figure 1: Tafel-like plot for MCMB carbon with different conducting additives.

References:
[1] W.A. Van Schalkwijk, B. Scrosati, Advances in Lithium Ion Batteries, Springer, New York, 2002.
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[3] A.J. Bard, L.R. Faulkner, Electrochemical methods, Fundamentals and applications, John Wily & Sons, New York, 1980.