Unfolding the Reversible Phase Transition for Insertion Mechanism of Surface Modified-Anatase TiO_2 through Impedance Analysis

Winda Devina[a], Jaehoon Kim [a,b,c]

[a] Sungkyun Advanced Institute of Nano Technology (SAINT), Sungkyunkwan University, 2066, Seobu-ro, Jangan-Gu, Suwon, Gyeonggi-Do 16419, Republic of Korea

[b] School of Chemical Engineering, Sungkyunkwan University, 2066, Seobu-ro, Jangan-gu, Suwon, Gyeonggi-do 16419, Republic of Korea

[c] School of Mechanical Engineering, Sungkyunkwan University, 2066, Seobu-Ro, Jangan-Gu, Suwon, Gyeonggi-Do 16419, Republic of Korea

E-mail: windadevinaa@gmail.com

A noteworthy material, TiO_2, has been received a considerable attention as a potential anode material for rechargeable batteries because of its outstanding stability. In this work, mesoporous TiO_2 particles were prepared by one-pot synthesis in supercritical fluid. To enhance its electrochemical performance, *in-situ* surface modification of TiO_2 in the supercritical fluid and subsequent carbon-coating was performed. As a surface modifier and carbon precursor, the mixture of citric acid and PEG-methyl ether (CA/PEG-ME) was added. The as-prepared polymeric coated-TiO_2 nanocomposite exhibited an excellent Li^+/Na^+-ion insertion, leading to high reversible discharge capacity of 250 mAh g^{-1} for LIBs and 280 mAh g^{-1} for SIBs at 0.1 C-rate, respectively. To reveal the kinetic process during the Li^+/Na^+ insertion/extraction, electrochemical impedance spectroscopy (EIS) was employed for CA/PEG-ME@TiO_2 electrode at different state-of-charge according to the galvanotactic profiles. The impedance analysis displays the contribution of both surface resistance (R_e) and charge transfer resistance in the bulk phase (R_{ct}) during Li/Na^+ insertion. The surface process is dominated by a passivation solid electrolyte layer (SEI) formation, which formed during the ion insertion and underwent decomposition during the ion extraction confirming the cells withstand a reversible phase transition during Li^+/Na^+ insertion/extraction process.

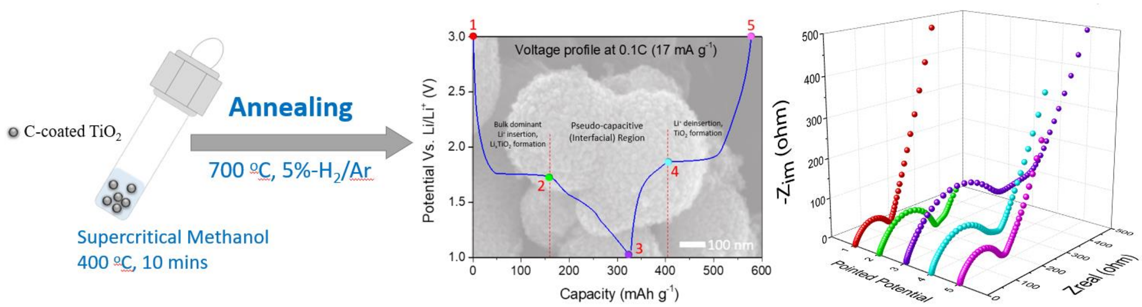

Figure 1. Schematic illustration of the fabrication process and electrochemical performance.

References:

[1] S.S. Zhang, K. Xu, T.R. Jow, Electrochimica Acta 51 (2006) 1636-1640.

[2] Ji-Yong Shin, Dominik Samuelis, Joachim Maier, Adv. Funct. Mat. 21 (2011) 3464-3472.

[3] A.D.C. Permana, et al., *Chemical Engineering Journal* **241** (2014) 216-227.

[4] Liming Wu, et al., Adv. Energy Mat. 5 (2015) 1401142