Study on Electrochemical Processes of NiO Model Electrode during the First Lithiation/delithiation Cycle via Electrochemical Impedance Spectroscopy

Lei Wang, Haixia Wu^{*} and Shouwu Guo^{*}

Department of Electronic Engineering, School of Electronic Information and Electrical Engineering, Shanghai Jiao Tong University, Shanghai 200240, P. R. China

^{*}E-mail: haixiawu@sjtu.edu.cn, swguo@sjtu.edu.cn

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Transition metal oxides (TMOs) have been researched as active electrode materials for Li-ion batteries for over 20 years owing to their large specific capacity based on conversion reactions rather than intercalation/deintercalation mechanism. Here, NiO was chosen not only as a representative among those TMOs but also as a model electrode material to fundamentally study its electrochemical processes during the first lithiation/delithiation cycle via electrochemical impedance spectroscopy (EIS). The NiO model electrode was constructed by electrodepositing a pure NiO film on the surface of the copper foil and directly served as a working electrode in Li-ion half cells without any other additives. These cells were stopped at certain states in the first lithiation/delithiation cycle and ready for the EIS test. Interestingly, other two semicircles were found in Nyquist plots, which were ascribed to NiO and structure transformation besides the normal two semicircles related to solid electrolyte interphase (SEI) and the interface between NiO and electrolyte. Furthermore, bounded diffusion was more suitable than semi-infinite diffusion to explain Li⁺ diffusion process in conversion-type electrodes. Thus, a new fitting circuit was proposed and the electrochemical processes of the NiO model electrode were studied quantitatively according to fitted data.

Keywords: NiO, EIS, Li-ion battery, fitting circuit

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