Mathematical modelling and simulation of the effect of adhesive strength on the cycling performance of silicon electrodes for lithium ion batteries

Williams Agyei Appiah[1], Joonam Park[1], Seoungwoo Byun[1], Jihun Song[1], Myung-Hyun Ryou[2] and Yong Min Lee[1]*

[1]*Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science and Technology (DGIST), 333 Techno Jungang-daero, Hyeonpung-myeon, Dalseong-gun, Daegu, 42988, Republic of Korea*

[2]*Department of Chemical and Biological Engineering, Hanbat National University, 125 Dongseo-daero, Yuseong-gu, Daejeon, 34158, Republic of Korea*

Email: yongmin.lee@dgist.ac.kr

ABSTRACT

A coupled chemo-mechanical model which considers the contact resistance as well as the influence of the attractive forces inside the contact area between the electrode and current collector is developed to demonstrate the effect of the adhesive strength of binding materials on the cycle performance of silicon based lithium ion batteries. The developed model is incorporated into the Newman's Porous Composite Electrode (PCE) framework and implemented in the COMSOL Multiphysics battery module to simulate the cycle performance of Li/Si half-cell. The proposed model is used to investigate the correlation between the adhesive strength, contact resistance, solid electrolyte interphase (SEI) and formation of dead particles due to isolation on the cycle performance.