Multiscale model to Interpret kinetic behavior of CO2RR system on Ag foil catalyst

김경수, 한동구, 나종걸[1], Stefan Ringe[2], 이웅†
한국과학기술연구원; [1]이화여자대학교; [2]경북대학교
(ulee@kist.re.kr†)

Electrochemical CO_2 reduction is a potential route to producing renewable fuels and chemicals. A precise model that can describe kinetics of the electrochemical CO2 reduction reaction (CO2RR) allows of understanding the mechanism underneath the associated experimental results, which can not fully understandable via thermodynamic interpretion alone. Here in, we have developed a multiscale model based on kinetic Monte Carlo (KMC) with its free energy calculated by density functional theory (DFT) and mass transport simulated by computational fluid dynamics (CFD). The developed multiscale model was fitted to experimental results of CO producing CO2RR on Ag electrode. The current densities depending on electrode potentials were fitted to the model and the resulted model showed high accuracy for predicting both CO and H2 partial current densities. As a result of model based sensitivity analysis, the rate limiting steps vary depending on the range of applied potential.