Defect Generation in TiO$_2$ Nanotube Anodes via Heat Treatment in Various Atmospheres for Lithium-Ion Batteries

Titania (TiO$_2$) is a promising anode material in lithium-ion batteries due to its environmental friendliness, abundance, and safety. It has been previously reported that the generation of point defects, such as oxygen and cation vacancies, in TiO$_2$ has resulted in enhanced electrochemical performance$^{1,2}$. In this study, we aim to induce point defects in TiO$_2$ nanotube electrodes through heat treatments in various atmospheres. Mott-Schottky analysis indicates that charge carrier density has increased due to oxygen-deficient atmospheres, suggesting oxygen vacancy formation. Crystallographic changes and defect production are also evident through decreases in peak intensity and peak shifts in the respective Raman spectra. The introduction of defects into the nanotube crystal structure results in changes in the charge storage behavior of the TiO$_2$ electrode observed via electrochemical characterization. The defects created through atmospheric treatments at elevated temperatures may then lead to enhanced battery functionalities of TiO$_2$ nanotube electrodes.

First-Principles Surface Interaction Studies of Aluminum-Copper and Aluminum-Copper-Magnesium Secondary Phases in Aluminum Alloys

First-principles density functional theory-based calculations are powerful tools to investigate a plethora of aspects in the atomic scale, from structural (for example, relaxation and reconstruction of a surface) to properties property changes (for example, change in the electronic and topological charge distribution after chemisorption). In this work, first-principles density functional theory-based calculations were performed to study 0-phase Al$_2$Cu, S-phase Al$_2$CuMg surface stability, as well as their interactions with water molecules and chloride (Cl$^-$) ions. These secondary phases are commonly found in aluminum-based alloys and are initiation points for localized corrosion. For both phases studied, Cl$^-$ ions cause atomic distortions on the surface layers. Electronic structure calculations revealed not only electron charge transfer from Cl$^-$ ions to alloy surface but also electron sharing, suggesting ionic and covalent bonding features, respectively. We also found a higher tendency of formation of new species, such as Al$^{3+}$, Al(OH)$^{2+}$, HCl, AlCl$^{3+}$, Al(OH)Cl$^{+}$, and Cl$_2$ on the S-phase Al$_2$CuMg surface. Surface chemical reactions and resultant species present contribute to establishment of local surface chemistry that influences the corrosion behavior of aluminum alloys.