Effect of Mechanical Strain on Lattice Cation Segregation at Solid Oxide Fuel Cell Cathodes (SOFCs)

권형욱, 구본재[1], 서한길[1], 정우철[1], 한정우†
서울시립대학교; [1]한국과학기술원
(jwhan@uos.ac.kr†)

Cation segregation, which transmutes physical structure and chemical properties of surface, directly affects the overall performance of various devices in positive or negative ways. Especially, A-site cation segregation on perovskite-type oxide (ABO_3) surfaces often deteriorates the reactivity and stability of solid oxide fuel cell (SOFC) cathodes. However, underlying origin of the segregation behavior has not been thoroughly elucidated because it arises from the complex factors. In particular, compared to dopant segregation on surface of A-site doped $LaBO_3$-type perovskites, not as much is known about lattice cation (Sr) segregation on surface of $SrTi_{1-x}Fe_xO_{3-\delta}$ (STF). Using density functional theory (DFT) calculations, we aim to demonstrate the main driving force of Sr segregation depending on mechanical biaxial strain, which was observed by our experimental collaborators. According to our theoretical results, the degree of lattice strain is a clear factor for controlling Sr segregation. We believe that our results will provide useful information for understanding the lattice segregation in detail.