

Engineering of B-metal exsolution on double layered PBMO for Superior Catalytic Activity of Anode Materials in Solid Oxide Fuel Cells

김경환, 한정우[†]

포항공과대학교

(jwhan@postech.ac.kr[†])

B-metal exsolution has been widely reported under reducing atmosphere at anode materials in solid oxide fuel cells (SOFCs), and the exsolved nanoparticles (NPs) showed higher catalytic activity and stability for various fuels. As a support material for B-metal exsolution, double layered PrBaMn₂O_{5+δ} (L-PBMO) has been received a lot of attentions due to its excellent redox stability as well as high tolerance of both coking and sulphur poisoning from hydrocarbon fuels as a anode material in SOFCs.

In previous works, we found the different exsolution tendency of different kinds of transition metals on L-PBMO. By engineering that concept, we have explored the possibility and detailed mechanism for various kinds of B-metal exsolution on L-PBMO. Based on our density functional theory (DFT) results, we will introduce (1) a possible driving force for B-metal NPs exsolution, (2) thermodynamically favorable mechanism for alloy NPs exsolution, and (3) how to boost B-metal exsolution to further improve cell performance SOFCs with the experimental verifications.