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The role of Oxygen States in NiO for Oxygen Evolution Reactions

Content

In recent years NiO has come into focus as a low-cost, efficient material in the Oxygen Evolution Reaction (OER) via electrochemical water splitting. However, the detailed mechanism of the electrochemically induced reaction is not yet fully understood.[1] Hence, two types of experiments were performed. Firstly, as a model catalyst, NiOx thin films were put in contact with oxygen and subsequently water vapor at 0.5 mbar and elevated temperatures and characterized by in situ NAP-XPS, NAP-XAS and ex-situ SEM. Heating and cooling in oxygen reveal the creation and replenishing of oxygen vacancies. Such vacancies manifest themselves mainly as distinct features on the low and high binding energy sides of the NiO main peak in the O1s region. The former can be directly related to vacancies while the latter represents OH chemisorbed at the vacancy site. Subsequent heating and cooling in water vapor suggests that these vacancies, in conjunction with a re-structuring of the NiOx surface, not only instigate H2O dissociation but, by way of OH chemisorption, act as precursors to the formation of stable OH-bonds. Secondly, in operando electrochemical experiments were performed on sputtered thin NiOx films. Initial cyclic voltammetry up 0.8 V reveals an oxidation peak at ~ 0.45 V (vs Ag/AgCl) as well as a reduction peak at ~ 0.25 V (vs Ag/AgCl) and leads to a transformation of NiOx into mainly NiOOH and Ni(OH)2. Above the oxidation peak, a pre-peak of oxygen appears in the OK-edge spectra at about 529 eV while its intensity is increased by increasing the potential. This peak is due to the delocalized holes in the O and Ni sites which produce new states in the gap and change the electronic structure of NiO to charge transfer gap. This both, experimental and theoretical results reveal that in the reactions oxygen vacancies are formed and seemingly play a crucial role acting as intermediate states in OER.

[1] L.J. Falling, J.J. Velasco-Vélez, R.V. Mom, A. Knop-Gericke, R. Schlögl, D. Teschner, T.E. Jones, Curr. Opin. Electrochem., 2021, 30, 100842.

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