Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Water dissociate on faceted NiO(111)[1] LIXIA LIU, Institute of Physics,Chinese Academy of Sciences (CAS), SHUAI WANG, School of Physical Sciences, University of Chinese Academy of Sciences,, SHUMING LIU, QINLIN GUO, JIANDONG GUO, Institute of Physics,Chinese Academy of Sciences (CAS)
— The interaction of water with metal oxide surface is important in heterogeneous catalysis, geochemistry, electrochemistry and corrosion science. It has been reported that water molecules physically absorb on NiO(100) surface while they dissociate as OH on NiO(111) surface. As a typical polar surface, NiO(111) is instable, and the polar compensation may lead to surface reconstruction, segregation of oxygen vacancies, or formation of facets. Faceted NiO(111) surface, consisting of Ni(100) or NiO(110) facets, introduces new surface states and provides complex chemical environment for water adsorption and dissociation. We prepare faceted NiO(111) films with different thickness and observe water dissociation on the surface. The dissociated OH can be detected at high temperature up to 700K on the thin film surface, while on the surface of relative thick film, the OH amount is significantly reduced and the thermo stability lowered. The morphology characterization of the film shows that the size and number density of the facets are thickness dependent – the thinner the films is, the smaller the facets are, and the higher the density of facets is. We conclude that the boundary sites on NiO(111) facilitate the dissociative adsorption of water. This work is supported by Chinese NSFC (11474334 & 11274237).

[1]Chinese NSFC (11474334 11274237).

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Date submitted: 09 Nov 2016 Electronic form version 1.4