Formation and Stability of Defects on Gas Exposed CeO_2(111)

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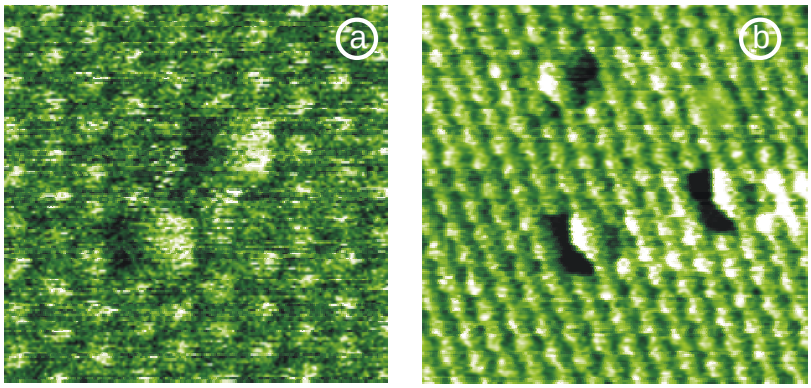
Cerium dioxide (ceria) is a catalytically active material and plays a major role as a catalyst in automotive exhaust gas treatment systems. The (111) surface of CeO_2 in various oxidation states is important for catalytic activity and some of its details relating to surface oxygen atoms have already been studied with dynamic scanning force microscopy [1]. Defects play a crucial role for the adsorption of small molecules on this surface and facilitate surface reactions [2].This surface offers the opportunity to observe stable defects by dynamic SFM and to study their configurational changes and detailed structures [3]. Here, we address the question whether dosing an oxygen deficient surface with molecular oxygen will lead to dissociation of the O_2-molecule and subsequently heal the surface.
We show that there are two main defect structures on the non-stoichiometric ceria surface. A protrusion type (a) and a vacancy type (b) defect. Upon oxygen exposure, the differences but also a certain relationship between the two structures becomes apparent. The protruding defect does not react at all with oxygen, while the pit like structure changes its appearance to a protruding type. We do not observe healing of vacancies. This behaviour points to an interpretation, that the protruding type, which is very prominent at the surface, is hydrogen adsorbed at the surface forming a hydroxyl group. Dosing oxygen seems to have no direct effect as vacancies cannot be healed. However, as residual gas spectra show, oxygen can remove water from the UHV chamber walls and dissociated water may strongly react with the defective surface.



[1] Fukui K-I, Namai Y, Iwasawa Y (2002) *Appl. Surf. Sci.* **188** 252
[2] Namai Y, Fukui K-I, Iwasawa Y (2004) *Nanotechnology* **15** S49
[3] Gritschneder S, Namai Y, Iwasawa Y, Reichling M (2005) *Nanotechnology* **16** S41