[III-16]

Characterization of the Atomic and Molecular Oxygen Species on V(110) using HREELS and NEXAFS

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The interaction of oxygen with a V(110) surface has been investigated using High-Resolution Electron Energy Loss Spectroscopy (HREELS) and Near-Edge X-ray Absorption Fine Structure (NEXAFS) techniques.

Oxygen was adsorbed on V(110) both dissociatively and molecularly at 80 K. The dissociative adsorption of oxygen was identified by the observation of a ν(V-O) vibrational feature at 615 cm^{-1}, which is most likely related to atomic oxygen residing on the quasi three-fold sites. The molecularly adsorbed oxygen was characterized by a ν(O-O) mode at 1025 cm^{-1}. The presence of atomic oxygen was also identified by a NEXAFS σ^*-resonance at 539.5 eV. Upon heating, the molecularly adsorbed oxygen dissociates on the surface at temperates below 400 K. Oxygen atoms start to diffuse into the bulk at higher temperatures, as indicated by the observation of subsurface oxygen species in the temperature range of 500 - 1000 K. The onset of subsurface oxygen species is characterized by a ν(V-O) mode at 1050 cm^{-1}. This 1050 cm^{-1} feature is differentiated from the 1025 cm^{-1} ν(O-O) mode by a different angular-dependency in the off-specular HREELS measurements and by the differences in the NEXAFS spectra. Finally, a vanadium oxide layer can be produced by repeated cycles of oxygen dosing 400 K followed by annealing to 600 K. The stoichiometry of the oxide layer is estimated to be VO, based on the comparison of the NEXAFS spectrum of O/V(110) with those of V_2O_3, V_2O_4 and V_2O_5 model compounds.