Electronic structure and electrochemical properties of Lithium and Sodium intercalated V_2O_5 thin films

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The intercalation of sodium into V_2O_5 thin films grown by physical vapor deposition (PVD) on highly ordered pyrolytic graphite (HOPG) substrates is studied by X-ray- and UV-induced photoelectron spectroscopy (XPS and UPS). The vanadium ions in the as-prepared V_2O_5 are mostly in a pentavalent V^{5+} state. The intercalated sodium strongly affects the electronic structure and causes a Fermi level shift of about 0.9 eV. The core level spectra show that the vanadium gets partially reduced to the V^{4+} oxidation state. About 0.83 electrons per intercalated sodium atom are transfered from the Na3s-orbitals into V3d-like states. For a completely sodium-intercalated V_2O_5 film with a composition of $Na_xV_2O_5$ ($x \approx 1$) a further increase in deposition time leads to sodium adsorption on the V_2O_5 surface and thus to the formation of surface oxides and metallic sodium. Partially the vanadium gets reduced even further to V^{3+}, V^{2+} and V^{1+} states indicating a decomposition reaction. The work function decreases with increasing sodium deposition time due to sodium intercalation into the V_2O_5, as well as to the sodium adsorption accompanied by the formation of surface dipoles.

The electronic structure of pure and sodium intercalated V_2O_5 thin films has also been studied by resonant photoemission using synchrotron radiation at BESSY II (Berlin). Thus, the partial valence band densities of states (PVBDOS) could be obtained.

The changes in the electronic structure can clearly be correlated to battery voltages derived from cyclic electrochemical charging and discharging measurements of the thin film devices.

Furthermore the structural changes due to sodium intercalation have been recorded using x-ray diffraction (XRD).

The lithium intercalated vanadium pentoxide has also been studied by XPS, UPS, XRD and electrochemical experiments qualitatively showing the same results.