Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Mechanistic Study of Hydrogen Gas Sensing by PdO Nanoflake Thin Films at Temperatures below 250°C

Yu-Ju Chiang, Kuang-Chung Li, Yi-Chieh Lin and Fu-Ming Pan*

Department of Materials Science and Engineering, National Chiao Tung University,

Hsinchu, Taiwan 30010, R.O.C.

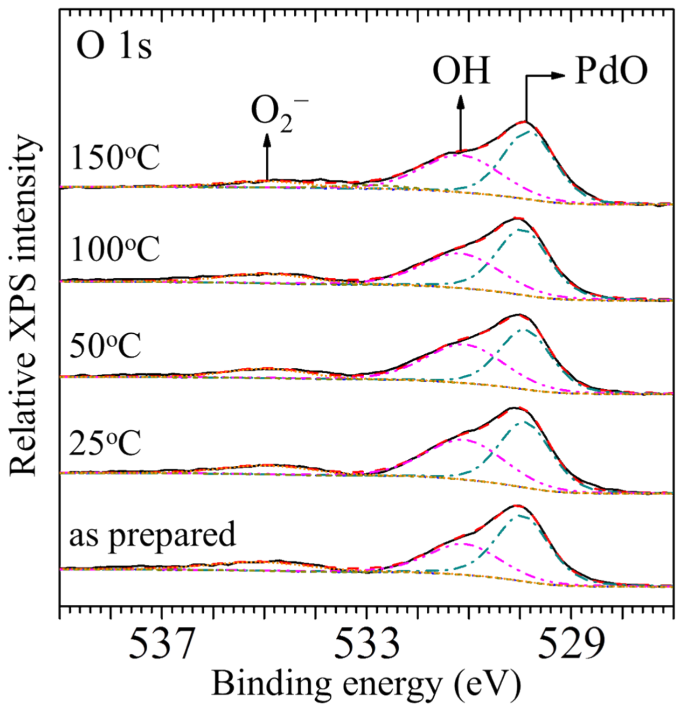

Fig. S1 O 1s XPS spectra for the PdO sensor after the 4000 ppm H_2 sensing test at temperatures from 25°C to 150°C. To remove the contribution of the Pd $3p_{3/2}$ signal from the O 1s spectra, we determined important peak parameters of the Pd $3p_{3/2}$ peak, such as the peak binding energy, peak width and peak area, by referring to the Pd $3p_{1/2}$ peak at 561.5 eV, which was calibrated by the binding energy of the Pt $4f_{7/2}$ electron. The peak width are chosen the same for the two peaks, and the peak area of the Pd $3p_{3/2}$ signal is two times that of the Pd $3p_{1/2}$ signal. The binding energy difference between the Pd $3p_{3/2}$ and Pd $3p_{1/2}$ peaks was determined by the energy difference between the two peaks of a Pd thin film sputter-deposited on the SiO_2 substrate. At temperatures below 100°C, the curve fitting requires three O 1s component peaks for the best fit. However, at temperatures above 100°C, one more component peak (532.9 eV), which is associated with the SiO_2 substrate, is needed for the best fit although its intensity contribution to the spectra is very small. The observation of the XPS signal emitted from the substrate is likely due to that morphology of the PdO sensor is significantly modified by the cyclic H_2 sensing test, which induces repetitive PdO reduction and Pd reoxidation on the PdO nanoflake thin film, resulting in thinning or cracking at some area of the thin film.