Application 2018

Effects of Zirconium and Polytetrafluoroethylene on the hydrogen sensing properties of Yttrium-Palladium based hydrogen indicator

Peter Ngene

Delft University of Technology, Delft

We have developed a low-cost hydrogen detector based on Yttrium-palladium thin films deposited on quartz substrate. The device indicates the presence of hydrogen merely by a reversible and tunable color change. We discovered that the addition of Zr to the Y sensing layer has a tremendous effect on the thermodynamics of the hydrogen sorption in the Y, while the optical contrast is not compromised. Thermodynamically, Y and Zr are immiscible, but with magnetron sputtering we manage to make some kind of alloy. However with XRD we see that there is no Vegard type of behavior. We observe the Y hcp phase, but from the d-spacing we find that only a fraction of the Zr goes into the Yttrium structure. We conclude that there must be some amorphous or nanocrystalline ZrHx-phase. From Hydrogenography, we deduce the formation of both a Y(Zr)H2 phase and a Y(Zr)H3 phase on hydrogenation, but we have no idea what the nature of these phases is.

Furthermore we discovered that alloying of the Pd catalyst with Au and the used of a sputtered Polytetrafluoroethylene (PTFE) as a protective coating strongly influenced the hydrogen sorption kinetics and selectivity of the hydrogen indicator. At the moment, these effects are not well understood and we would like to carry out further investigations to study the mechanisms behind these effects.

Therefore, for these systems we would like to do in-situ measurements where we can follow the Raman and Infrared (IR) signals of the YHx , ZrHx , PdHx , PdAu and PTFE as a function of Hydrogen pressure, typically from vacuum to 2000 mbar (2 bar) H2 at room temperature. The Raman signals will also be recorded during unloading or dehydrogenation of the detector in a 20% O2/Ar gas mixture. Additionally the composition of the evolving gases will be monitored to study the effect of PTFE and Au on the surface chemistry of the detector in the presence of both oxygen and hydrogen. From these experiments we expect to get some insight about the structural and chemical changes occurring in the YHx, ZHx Pd, PdAu and PTFE during hydrogenation and dehydrogenation.

Specifically for the Y/Zr system the measurements can reveal if Y-Zr alloys are indeed formed after sputtering, and how the composition of Zr in the composites affect the formation of such alloys. We would like to know if during hydrogenation, a new hydride phase such as YZrHx is formed or separate phases of YHx and/or ZrHx are formed, and how how the phase formation evolves as a function of the hydrogen pressure.

For the Au and PTFE, we would like to understand how the presence of PTFE influence the surface chemistry of H2 and O2 adsorption and reaction on a Pd (or Pd-Au alloy) surface. Are there chemical interaction or bonding between the Pd (or Pd-Au alloy) and the PTFE?

How does such bonding/interactions change the structure and the adsorption strengths of H_2 and O_2 on the Pd and PdAu surfaces. Finally using an in-situ mass spectrometer, we would be able to determine if the composition of the evolving gases depends on the nature of the catalyst surface.