Hydrogen-Absorbing Material Could Find Use in Fuel Cells

On November 9, 2007, researchers at the University of Virginia (UVa) in the US announced the development of a material capable of high-efficiency absorption (14mass%) of hydrogen at room temperature of 300K (27°C). Hydrogen-absorbing material is used in the hydrogen (H\textsubscript{2}) storage tanks of fuel-cell vehicles, among other things. According to Toyota Motor Corp and other sources, H\textsubscript{2}-storage materials capable of handling the repetitive use that fuel-cell vehicles require have only been about 2mass%. Even if it is still in the laboratory stage, a practical material with 14mass% performance would represent an enormous step forward for fuel cells.

**Ethylene, Titanium Base**

The new material is based on ethylene (C\textsubscript{2}H\textsubscript{4}) and titanium (Ti), probably as C\textsubscript{2}H\textsubscript{4}-Ti\textsubscript{2} with two titanium stops bonded to a single ethylene group (see Fig). It was developed by Prof Bellave SShivaram of the UVa Dept of Physics and UVa post-doctoral student Adam B Phillips. The developers explained, “We began experiments to confirm theoretical research by Professor Yildirim.”

Prof Tanar Yildirim works at the Center for Neutron Research, National Institute of Standards & Technology (NIST) of the US. Together with Prof Salim Ciraci of Bilkent University, Turkey, he published a theoretical paper computationally predicting the material, at the end of 2006.

Shivaram and Phillips first vaporized Ti in ethylene gas, then deposited the resulting material on a substrate to form a thinfilm. H\textsubscript{2} absorption at 300K showed 14mass% performance, they report.

**Key Issues**

Yildirim himself expressed astonishment that the theoretical maximum should be reached on the first attempt, and clarified that he has been unable to reproduce the experiment under different conditions: “We have tried to reproduce it using several hundred mg of material in bulk, but have not succeeded yet.” He praised the results of the experiment performed by Shivaram on deuterium (D\textsubscript{2}) absorption, however, commenting, “The fact that D\textsubscript{2} absorption is double the mass% of H\textsubscript{2} is solid evidence that the material is indeed absorbing H\textsubscript{2}, not oxygen.”

Another issue is the high temperature needed to extract the H\textsubscript{2}. If the temperature is too high it would make commercial use more difficult. Experiments by Shivaram and Phillips indicate that a portion of the H\textsubscript{2} remains even after extraction at temperature over 1,000K. Theoretically, however, there is still hope for commercial application. Yildirim explained: “It is likely that most of the H\textsubscript{2} will be released by 800K, if not at lower temperatures, based on an analysis of the bonding energy of the H\textsubscript{2} and the material. In that case, the C\textsubscript{2}H\textsubscript{4}-Ti\textsubscript{2} would remain stable.” Shivaram and Phillips added, “We are still investigating the discrepancies between experimental results and theory, and will make further announcements.”

---

by Tetsuo Nozawa