Hydrogen-Absorbing Material Could Find Use in Fuel Cells

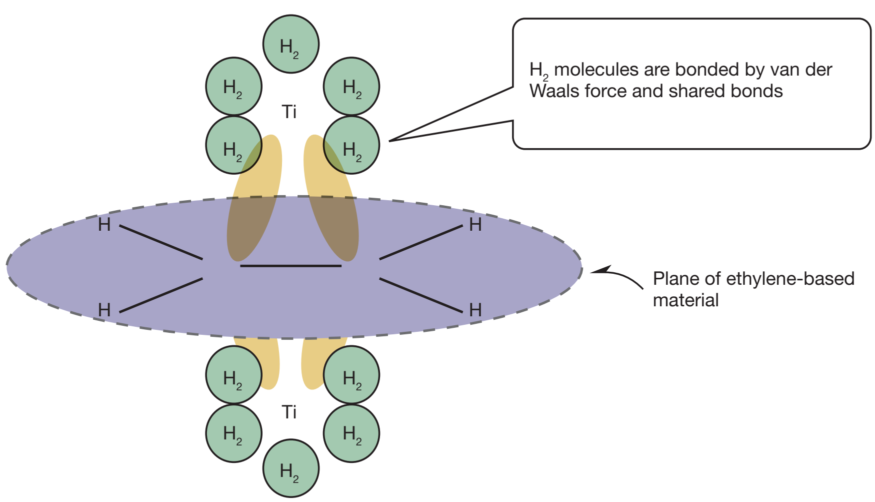
On November 9, 2007, researchers at the University of Virginia (UVa) in the US announced the development of a material capable of high-efficiency absorption (14mass%) of hydrogen at room temperature of 300K (27°C). Hydrogen-absorbing material is used in the hydrogen (H_2) storage tanks of fuel-cell vehicles, among other things. According to Toyota Motor Corp and other sources, H_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_2H_4) and titanium (Ti), probably as C_2H_4-Ti_2 with two titanium stops bonded to a single ethylene group (see Fig). It was developed by Prof Bellave S Shivaram 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_2 absorption at 300K showed 14mass% performance, they report.



Structure of H_2 Storage Material Achieving 14mass% Theoretical prediction of the structure of a material capable of 14mass% H_2 storage. Ti atoms are bonded above and below the plane (defined by C and H atoms). Up to five H_2 atoms can bond to a single Ti atom. The C atoms appear to have five bonds, but because sp3 mixed orbits spread symmetrically above and below the plane, both Ti atoms are bonded.

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_2) absorption, however, commenting, "The fact that D_2 absorption is double the mass% of H_2 is solid evidence that the material is indeed absorbing H_2, not oxygen."

Another issue is the high temperature needed to extract the H_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_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_2 will be released by 800K, if not at lower temperatures, based on an analysis of the bonding energy of the H_2 and the material. In that case, the C_2H_4-Ti_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