Geophysical Research Abstracts, Vol. 7, 01580, 2005
SRef-ID: 1607-7962/gra/EGU05-A-01580

Hydrogen and Hydrogen-storage materials

Marco Zoppi
CNR - Istituto Sistemi Complessi, Via Madonna del Piano, Sesto Fiorentino, Italy

An effective transition towards a *Hydrogen Economy* calls for the solution of a number of open problems, in many fields, that range from physical and chemical science, to engineering and technological activity, up to investing political and sociological aspects. Even from a merely scientific point of view, there are various problems that should be faced and solved in order to govern an effective transition from the present, fossil fuels economy, to a future, renewable energy sources economy, where hydrogen should play the essential role of leading energy vector.

Of the various processes entering into a hydrogen-based energy scenario, i.e. production, storage, and utilization of the fuel, the second one appears the weakest point, which might represent the bottleneck for an effective transition. As a matter of fact, at present, the production and utilization stages appear scientifically well established and ***only*** technological developments seem to be needed, aiming to obtain more cost-effective processes. On the other hand, problems concerning efficient hydrogen storage are still fighting with basic laws of chemistry and thermodynamics and need more insight at the level of the fundamental scientific research.

As is well known, hydrogen is a gas, at room temperature, and should be compressed (at the expenses of some energy) for an efficient storage and transportation system. This represents, more or less, the present situation, where hydrogen is stored in steel cylinders at $p \approx 200$ bar. Hydrogen can also be liquefied (at the expenses of some 30% of its energy content) at $T \approx 20$ K, but the huge temperature gradient, with respect to the ambient conditions, make the evaporation losses unbearable, especially for long time periods.

However, there is a third possible way of storing hydrogen, i.e. adsorbed in a solid matrix. Simple metal hydrides represent one possibility, where hydrogen is chemically absorbed, in atomic form, and the pressure mainly controls the intake and release of the gas. Palladium represents the most familiar material, but more effective hydrides do exist and are currently synthesized. Another possibility contemplates the physical adsorption of molecular hydrogen on the huge specific surface of nanoporous materials like, for example, carbon-based nanomaterials, zeolites, metal organic frameworks, and so on.

Thus, the basic problem one has to face is to learn as much as possible about the fundamental interaction processes of hydrogen, both at the atomic or the molecular level, with the various substances that are proposed as efficient storage materials. In this respect neutrons can play a role of paramount importance. On one side, the neutron cross-section of the proton for neutron scattering is almost two orders of magnitude larger than the average neutron cross section of a generic nucleus. Which implies that hydrogen can be detected, and his dynamics can be effectively probed, using neutron spectroscopy. On the other hand, one could counterbalance the small coherent cross section of the proton, which is important for microscopic structure determinations, using his heavier isotope, deuterium, for which the coherent/incoherent ratio of the cross sections is more favourable.

It will be shown how, in spite of the apparent simplicity of hydrogen, its microscopic structural and dynamic properties were successfully dealt with, in recent times, and how neutrons have shown to be precious in this research activity. Then the scenario will be enlarged, describing how neutrons can give their important contribution in the investigation of novel materials that are considered promising for an efficient and safe storage of hydrogen.

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