

The problem

One of the key requirements of hydrogen storage materials is good cycling performance. Ti-V-Cr-Mo alloys have been suggested as potential hydrogen storage systems, as they have the highest reversible storage capacity of materials of their type. Unfortunately, this capacity decreases with cycling. The key to understanding capacity loss is to identify the exact location of hydrogen during cycling.



Figure 1. An example of a hydrogen storage tank (Toyota, © Nikkei Technology)

The solution

Neutrons scatter very strongly from hydrogen atoms, and almost not at all from the Ti-Cr-V-Mo alloy developed by Toyota. This means that neutron diffraction experiments can pinpoint the location of the hydrogen atoms within the solid.

Dynamic experiments, performed under high pressure to fill the alloy with hydrogen, and then under vacuum to remove the hydrogen, have clearly identified the cause of capacity loss.

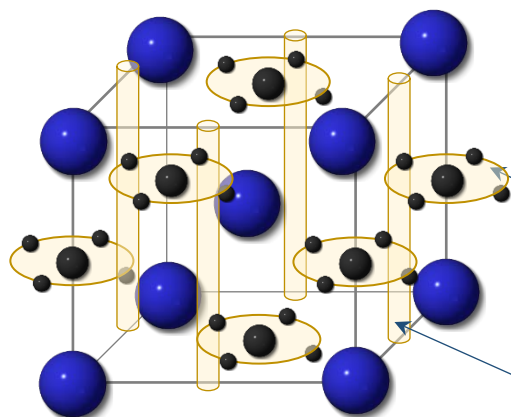


Figure 2. A view of the atomic structure of the material under study. Neutron diffraction techniques pinpoint sites of hydrogen occupancy.

Disc = high probability of H₂ occupancy

Tube = low probability of H₂ occupancy

The result

Neutron investigations provide new opportunities for improving the hydrogen storage materials to be used in hydrogen-fuelled vehicles.

[Sources. Kamazawa et al., *Advanced Energy Materials* (2013) and ISIS website]

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