ries, but the negative CdOOH electrode has been replaced by a hydrogen electrode (the economic advantage is a higher charge capacity, the environmental advantage a Cd-free battery).

Neutron vibrational spectroscopy

One of the hydrogen storage materials which is used is $ZrV_{2-x}Ni_x$, where Ni as an indispensable catalyst replaces part of V in the parent cubic Laves phase ZrV_2. All interstitial sites in ZrV_2 are tetrahedral sites, but there are three kinds: Zr_2V_2, ZrV_3 and V_4 sites. A fundamental question concerns the location of the hydrogen in the storage material. Literature reports were contradictory before we started our combined neutron vibrational spectroscopy and muon spin rotation investigation.

The neutron results for three selected H concentrations show that the neutron vibrational spectrum for $ZrV_2H_{0.5}$, consisting of a comparatively narrow maximum at 145 MeV with two district shoulders, does not change much with temperature. We attribute this to the presence of hydrogen on the (energetically most favourable) Zr_2V_2 site, which owing to its low point-symmetry, gives rise to three non-degenerate vibrational modes.

The spectrum for $ZrV_2H_{3.0}$ exhibits additional scattering intensity on the low energy side of the main maximum which we attribute to an additional occupation of ZrV_3 sites. For $ZrV_2H_{4.5}$ we detect additional scattering on the high energy side of the main maximum which is assumed to be due to hydrogen atoms on V_4 sites. A quantitative comparison with the predictions of a simple dynamical model for the H vibrations confirmed this qualitative analysis.

μSR

A fortunate feature of the ZrVNi system in a μSR investigation is that the V nuclei possess a large nuclear magnetic moment and the Zr nuclei essentially none. The three types of sites mentioned above are therefore magnetically quite different, and easily distinguished using the second moment of the local magnetic field distribution, mirrored in the low temperature static muon spin depolarization rate σ_o (frozen-in muon).

In order to scan the available hydrogen sites with the positive muon, we charged ZrV_2 with hydrogen. At *low temperatures*, the H atoms occupy the lowest energy sites: the implanted muon will initially occupy one of the available sites at random. The low temperature plateau of the measured depolarization rate, *i.e.* the static muon spin depolarization rate σ_o, increased with increasing H content so we conclude that more and more of the sites with the lowest σ, namely the Zr_2V_2 sites, become inaccessible to the muon. These are obviously the lowest energy sites. In $ZrV_2H_{3.25}H_{3.6}$, the measured values of the depolarization rate are close to the theoretical value for the ZrV_3 site, *i.e.*, at this H concentration the 12 Zr_2V_2 sites per formula unit are essentially blocked. This is a multiple site blocking, since an H atom blocks besides its own site about three other Zr_2V_2 sites, and resembles the situation in binary bcc metal hydrides, where blocking extending into the third coordination sphere has been observed.

Eventually, at the highest H concentrations ($ZrV_2H_{4.0}$ and $ZrV_2H_{4.8}$), the experimental depolarization rates are greater than theoretical values for the ZrV_3 sites: the majority of the ZrV_3 sites seems to be blocked and a large fraction of the muons is initially thermalized at a third type of site with a large σ, *i.e.*, a site surrounded by more than three vanadium atoms. This is the V_4 site.

Now consider the σ plateau at *intermediate temperatures*. At around 60 K, the thermal energy is apparently sufficient to release those muons which were initially thermalized at energetically unfavourable sites. They perform some diffusional jumps and very quickly find a vacancy in the sublattice of the energetically lower sites. The muons are trapped and — between 90 and 160 K — do not escape from these sites during their lifetime. Thus, in $ZrV_2H_{3.25}$, $ZrV_2H_{3.60}$ and $ZrV_2H_{4.0}$ the muons find empty Zr_2V_2 sites, whereas at the highest H concentration the number of vacancies in the Zr_2V_2 sublattice is obviously too small and the muons have to be content with ZrV_3 sites.

Conclusions

There exists an increasing number of cases where either neutron vibrational spectroscopy or muon spin resonance was used to determine hydrogen sites in metal alloys, but to our knowledge, the only example of where both neutrons and muons have been applied as microscopic probes of local atomic topology is the ZrV_2/H system.

For disordered metal/hydrogen systems, both approaches offer advantages over the standard diffraction technique owing to the lack of translational symmetry. We anticipate that the future will bring many more interesting and informative investigations using neutrons and muons. They are promising and prospering tools, not only in the vast field of disordered materials (ranging from a simple random solid solution of hydrogen in metals to the almost total disorder of hydrogen in metallic glasses), but also in more general research on metal/hydrogen systems.

FURTHER READING

[1] Springer T. and Richter D., "Neutron Scattering", *Methods of Experimental Physics* **23B**, p. 131; Eds. D.L. Price and K. Sköld (Academic Press, London) 1987.

[2] Richter D., "Neutron Scattering and Muon Spin Rotation", *Springer Tracts in Modern Physics* **101** (Springer, Berlin) 1983.

[3] Kondo J. in "Fermi Surface Effects", Eds. J. Kondo and A. Yoshimo, *Springer Series in Solid State Sciences* **77** (1988).

[4] Kehr K.W. *et al.*, *Phys. Rev. B* **26** (1982) 567; Hartman O. *et al.*, *Phys. Rev. B* **37** (1988) 4425.

[5] Steinbinder D. *et al.*, *Europhys. Lett.* **6** (1988) 535.

[6] Richter D. *et al.*, *Z. Phys. Chem. NF* **164** (1989) 907.

[7] Hempelmann R. *et al.*, *J. Less-Common Metals* (1991) in print.

[8] Hempelmann R. *et al.*, *J. Phys. Chem.* **90** (1989) 1935.

Mobility Information Now Available by Email

Information on the European Mobility Scheme for Physics Students (see *Europhysics New* **22** (1991) 82) can now be obtained by electronic mail.

For a listing of documents describing the scheme and its arrangements, simply send a one line message "INDEX" to MAILSERV @ UNIGE.CH or to MAILSERV @ CGEUGE53.BITNET (depending on the network you have available).

To receive by electronic mail one of the documents stored on the server send the one line message "SEND [EPS_MOBILITY] document" to either of the two email adresses, where "document" is one of the documents now available, namely PROPOSAL.MAR91 and QUESTIONNAIRE.MAR91. A draft of the convention and a list of interested universities will be added shortly, followed by other documents as they are introduced.

E. Heer, Chairman, EMSPS