

Project HC-9: Hydrogen in hydrides, carbon and zeolites

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IEA HIA 2003 AR

The following summarises the project results of the Salford group during 2003:

1. We have continued our measurements of hydrogen on SWNT (Carbolux: Selected grade) and on highly oriented graphene surfaces, using microgravimetry measurements of hydrogen absorption isotherms and neutron scattering. IINS measurements of the H₂ molecular rotational level (para to ortho, J=0 to J=1) show characteristic splitting due to the perturbed potential energy surface at the adsorbing sites which splits the J=1 level. By remeasuring the spectrum at various stages of hydrogen dosing (measured in terms of BET surface areas and at fixed temperatures around 20K), we have shown that there are at least two distinct sites being occupied. One of these has tetragonal symmetry, splitting in the ratio 2:1 in intensity while the other has a more or less unperturbed site (14.7 meV). A fourth peak appearing at 14.3meV is a little uncertain, as we would not expect to see a shift associated with an unsplit level. It seems unlikely to be due to a molecular vibration as this would have an intensity associated with the para-para cross section which is comparatively small. Further useful information is extracted from the "free recoil" part of the cross-section. This is effectively fitted with an H-H distance and an effective temperature. The fitted temperatures are higher than the physical temperatures due probably to lateral interactions between hydrogen molecules on the surface at higher coverages.
2. We have also carried out diffraction measurements of the diffraction from the nanotube bundles as deuterium is added. The fundamental peak from the bundle moves distinctly to lower Q, implying that the tube separation increases but recent measurements at the ILL (Role et al) using the isotopes of argon as adsorbates have suggested that the split is actually due to the enhanced scattering intensity on the surface of the bundle.
3. We have also been making IINS measurements on well ordered graphitic surfaces. Analysis of this data is not complete but suggest that the sites are unperturbed at lower coverage but show signs of molecule-molecule interactions at higher coverages.
4. We have also been using neutron scattering to understand the binding state of hydrogen in a variety of activated carbons (with Peter Albers). This work demonstrates the value of inelastic neutron scattering techniques in understanding the behaviour of residual hydrogen in activated carbons.
5. Recent metal hydride investigations have been concerned with understanding the influence of hydrogen on the magnetic properties of YCo₃/H. As hydrogen is added, the structure goes from ferro- (or ferri-) magnetic to para-magnetic and then to ferri-magnetic and finally to anti-ferromagnetic. The hydrogen positions in the 4 phases have been determined by neutron diffraction. Ab initio calculations have shown that the magnetic structure of each phase and the meta-magnetic behaviour of the system at high field can be explained by changes in the coupling of cobalt spins on different crystallographic sites in the lattice.