

Applications of Neutron Scattering Techniques to Hydrogen Storage Materials

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INTRODUCTION

Hydrogen is considered as a fuel for future vehicles because it may be generated from renewable energy sources, and envisioned to be environmentally friendly. However, it is extremely difficult to store hydrogen efficiently, presenting an obstacle to a future hydrogen economy. Although different approaches, such as metal hydrides, chemical H₂ storage, and H₂ storage based on physisorption, are being intensively investigated, none of them meets the system targets required by the US Department of Energy. Fundamental studies of hydrogen adsorption properties in different storage materials are one of the keys to help direct material synthesis.

Neutron scattering techniques are powerful tools with which to study hydrogen adsorption interactions. Small angle neutron scattering (SANS) has been used to understand the porous structure on the nano-scale. [1] Neutron powder diffraction can identify hydrogen adsorption sites accurately in many metal-organic frameworks (MOFs). [2] Inelastic neutron scattering (INS) has been applied to understand the adsorption sites and binding strength of adsorptions in carbon nanotubes and MOFs. [3]

In this paper, we present neutron scattering studies of hydrogen adsorption properties for one type of amorphous carbon, carbon aero-gels (AG). [4,5] Two different AG samples with the surface area of ?? (sample 1) and ?? (sample 2) were studied using NG7 and BT4 at the NIST Center for Neutron Research.

EXPERIMENTS AND DISCUSSIONS

SANS is used to probe the morphological difference between these two samples, as shown in Figure 1, where Q is the wavevector. The intensity difference between these two samples is due to the different packing density of the powder in the experiment cells. Despite the BET surface area difference, the local structures from both samples are almost identical since these two curves can collapse to one master curve by simply scaling them. Clearly, there are two different length scales. One is on the micrometer scale being due to either small particles or small domains of μm size. The Q^{-4} decay from $\sim 0.07 \text{ \AA}^{-1}$ to $\sim 0.02 \text{ \AA}^{-1}$ indicates the existence of sharp surface scattering. When $Q > 0.2 \text{ \AA}^{-1}$, the intensity, $I(Q)$,

decays more as Q^{-2} indicating some planar structures in the samples on the nm length-scale.

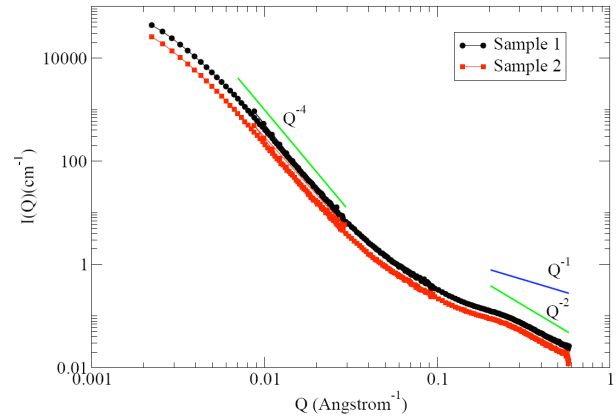


Fig. 1. SANS spectra of AG samples.

To understand the local potential where hydrogen molecules are adsorbed, INS spectra of H₂ in sample 1 was measured at 4 K as a function of loaded hydrogen (calculated as the ratio between the mass of adsorbed H₂ and that of the sample). H₂ is very light and is a very good quantum rotor showing a rotational transition at about 14.7 meV. The peak splitting is a good indication of the local potential barrier due to neighboring atoms, which can indirectly indicate differences of the adsorption sites.

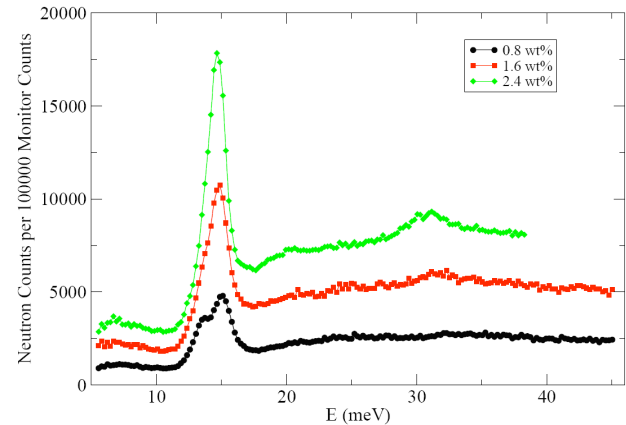


Fig. 2. INS spectra of H₂ in sample 1.

At a H₂ loading of 0.8 mass %, the peak at around 14.7 meV splits into two obvious peaks similar to what were observed in some single wall carbon nanotubes samples.

This seems to support the statement that the obvious splitting in some single wall carbon nanotubes is not likely due to the properties of the pristine carbon nanotube. [3] The peak become sharper with increasing H₂ loadings, indicating that H₂ experiences much less of a barrier to rotation consistent with a lower binding strength at higher coverages.

CONCLUSIONS

SANS and INS are used to study the morphology of the local structures and H₂ adsorption sites in AG samples. For the two samples studied here, the local structure is very similar with possible planar structure in nanometer scale. The INS spectra indicate the change of adsorption sites at different loadings.

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