QUASIELASTIC NEUTRON SCATTERING pdf

1: Quasielastic scattering - Wikipedia

Quasielastic neutron scattering (QENS) designates a limiting case of inelastic neutron scattering, characterized by energy transfers being small compared to the incident energy of the scattered particles.

Article Synopsis Neutron scattering is a severely underused technique for studies of catalysts. In this review we describe how and why neutrons are useful to catalysis. We illustrate the range of systems that have been studied by both elastic and inelastic neutron scattering. These range from structural studies of adsorbates in zeolites to determination of the structure of surface adsorbates, characterisation of nanoparticles, the measurement and mechanism of diffusion and spectroscopic characterisation of adsorbed species. We conclude with how to access neutron facilities and some future prospects for the application of these techniques to industrially useful materials. Neutron scattering is undoubtedly a severely underutilised capability in catalysis research. This is probably for two main reasons: These perceptions are not correct: There are a small number of centres for neutron scattering worldwide, since the production of sufficient neutrons for useful science requires highly specialised facilities. The aim of this review is to show that even within the constraint of a limited number of facilities, neutron scattering can usefully contribute to many areas of catalysis that range across structure determination at the micro- to the nanoscale and atomic and molecular dynamics from the femtosecond vibrational spectroscopy to the sub-microsecond diffusion timescale. Neutron Properties and their Applications The usefulness of neutron scattering arises from the properties of the neutron, which is an uncharged particle of mass 1. Hence neutrons only interact weakly with matter and as a result are highly penetrating; for example the attenuation at 1. For neutron diffraction studies it is straightforward to study light elements in the presence of heavy ones. The scattering cross section is both atom and isotope dependent, Figure 1 , and is not a monotonic function of atomic number as it is for X-ray scattering. Hydrogen-in-metal systems are perhaps the most important example of systems which are ideal for study using neutron techniques, but it is also a valuable way to determine the precise location of oxygen in heavy metal oxides in fields ranging from high-temperature superconductors to oxide ion conductors in fuel cells. Neutron scattering cross section as a function of atomic number Bond distances are generally more accurate from neutron scattering data than from X-ray techniques, particularly for bonds involving hydrogen, since the maximum electron density is not located at the atomic position but is displaced towards the heavier atom. These elements have identical scattering power for X-rays since they have the same number of electrons but different neutron cross sections, 1. The atomic nucleus acts as a point-like scatterer, unlike the electron cloud, which is of finite size compared to the wavelengths used. Thus the smaller d spacing information is relatively better determined in a neutron experiment compared to a similar X-ray experiment. This results in more precise atomic thermal parameters being determined from powder neutron data than from the powder X-ray data. The most striking difference in cross section occurs for 1H and 2H, hydrogen and deuterium: Hence hydrogen is overwhelmingly an incoherent scatterer while deuterium is primarily a coherent scatterer. Coherent scattering gives information on long range properties such as structure while incoherent scattering is a local probe. The neutron may be scattered without a change in energy elastic scattering as in diffraction, or there may be exchange of energy between the sample and the neutron inelastic scattering. The latter may be coherent or incoherent, but for any material containing hydrogen, the incoherent scattering dominates. Since much of catalysis involves the transfer of hydrogen from reactant to product, the sensitivity to hydrogen is a major advantage of the technique. However, for structural studies it may be necessary to use deuterated materials, since the incoherent scattering from hydrogen results in a significant background that complicates the data analysis. In short, neutron scattering can be summarised as: This ranges from the atomic scale for structure determination to typical sizes of colloids. The investigation of structure is the major use of neutrons in this area, particularly by powder diffraction. The location of n-heptane in silicalite-1 1 provides an example of what can be achieved. This system shows an inflection in the adsorption isotherm at a loading near four molecules per unit cell that has been ascribed to a commensurate freezing of n-heptane in the sinusoidal channels of silicalite To investigate the unusual behaviour, the adsorption of C7D16 was followed in situ by

powder neutron diffraction. Deuterated heptane was used to reduce the incoherent background. The results show that the straight channels are first filled, then near four molecules per unit cell, the molecules also fill the sinusoidal channels, Figure 2. Thus the diffraction data show that the inflection point in the isotherm is due to self-blocking of the channels at junctions. Locations of C7D16 molecules within silicalite-1 obtained from Rietveld refinement of neutron diffraction patterns. At low loading, 4 molecules per unit cell both the straight and the sinusoidal channels are occupied black and green molecules respectively. Reprinted with permission from 1. Copyright American Chemical Society Diffraction methods are well-suited to operando measurements and this is already utilised for neutron diffraction studies of batteries 2 and proton conductors 3. The activation process is shown in Figure 3 following the reduction of CuO and the growth of Cu. In situ neutron diffraction was able to show that the nanostructured Cu generated by reduction of the CuO precursor has a high concentration of stacking faults and also that they were stable under industrial methanol synthesis conditions 5. Normalised integrated intensities of the CuO 11â€"1 and Cu peaks correlated with: The missing ionâ€"current between and min is an experimental artefact. Reproduced from 4 with permission of Elsevier Pair distribution function PDF analysis or total scattering analysis 6 is a well-established technique for the structural characterisation of poorly- or non-crystalline materials including nanoparticles. The alternative formulation as Pd OH 2 is clearly untenable and the simulation shows that the material has a core of poorly crystalline PdO. The neutron diffraction differential correlation function, DN r , for as received hydrous palladium oxide red. Reprinted with permission from 7. Copyright American Chemical Society The PDF approach has been extended to enable the local structure of adsorbed species in zeolites 8 and on surfaces 9 to be determined. The advantage of the method is that it does not require long range order and that bond distances can be obtained by inspection of the radial distribution function. However, the method greatly benefits from input by ab initio methods as was done for acetylene on nickel ion exchanged zeolite NaY 8 and hydrogen on Raney nickel 9. Figure 5 shows a comparison of the experimental data for hydrogen on Raney Ni and the radial distribution function generated from a periodic density functional theory calculation of hydrogen on Ni for an fcc metal, the face is the lowest energy surface so is expected to predominate on nanoparticles. It can be seen that the agreement is excellent. The extension of the method to more complicated systems involving chemisorbed organic species is an active area of investigation. This is the Fourier transform of the normalised difference of the catalyst before and after addition of hydrogen. The spectrum is abscissa scaled so that the large peaks at 2. No ordinate scaling has been applied, all the distances come directly from the ab initio calculation 9. Reproduced by permission of the Royal Society of Chemistry Inelastic Scattering â€" How Atoms Move As shown in Figure 6 , inelastic scattering covers a vast range of length and time scales. For catalysis, the most relevant are quasielastic neutron scattering QENS which probes whole-body motions such as diffusion on and within materials and neutron vibrational spectroscopy or inelastic neutron scattering INS , which probes the motion of atoms and molecules within a material. The time and energy ranges spanned by inelastic neutron scattering Quasielastic scattering 10 is a very low energy inelastic process which usually manifests itself as a broadening of the elastic line and is most commonly the result of diffusional translational or rotational motion of atoms. Translational and rotational diffusion occur simultaneously but on different timescales. Thus resolution and timescale are inversely related and the slower the motion, the higher the required resolution. No single spectrometer can access all of this range and typically three are needed: Understanding the diffusion behaviour of molecules in microporous materials is important for the design of membranes for separations and for catalysts, particularly for applications in the petrochemical industry. QENS is ideally suited for the measurement of diffusion constants in technologically relevant materials The QENS timescales also match those accessible by classical molecular dynamics MD simulations which can provide insight into the diffusion mechanism. However, until very recently 12 , the agreement between observed and calculated diffusion constants could differ by as much as two-to-three orders of magnitude, Figure 7. The improvement is the result of using fully atomistic models for both adsorbate and framework, adsorbate loadings that match those used experimentally and a flexible framework that deforms as the molecule moves through the channel. Diffusion coefficients of n-alkanes in silicalite: However, an understanding of the diffusion of branched alkanes is crucial to understand the effect of molecular shape on

both catalytic cracking and molecular sieving in zeolites. The diffusion is sufficiently slow that the neutron spin echo technique and long MD runs are required. Figure 8 a shows the neutron spin echo results 13 compared with fits for 3D and 1D diffusion models. This immediately shows that 2-methylpropane is able to explore both the straight and sinusoidal channels, in contrast to previous results that indicated the molecule was confined to the straight channels. The MD results support this conclusion and show that from an initial configuration where the 2-methylpropane molecules were placed in the large cages at the intersections of the straight and sinusoidal channels, the system evolves to have both types of channel populated, Figure 8 b. Diffusion of 2-methylpropane in silicalite: The solid lines are calculated with a 3D red and blue and a 1D green and gold diffusion model. Reprinted with permission from Copyright American Chemical Society The conversion of methanol to hydrocarbons over acid zeotype catalysts is an attractive route to increased value products. The mechanism of the process is still debated but an early step is the formation of methoxy by reaction of methanol with an acid site. The mobility of methanol in the catalyst is clearly important and was the focus of a QENS study that compared the mobility of methanol in the industrial catalyst, H-ZSM-5, and zeolite HY which has the same Si: Figure 9 compares the results of the two systems obtained with a backscattering spectrometer crystal analyser. It can be seen that the two systems behave completely differently. Zeolite HY shows a significant broadening at room temperature, consistent with simple Fickian diffusion through the material. In contrast, in H-ZSM-5 methanol is immobile on the timescale of the spectrometer. Reproduced from 14 with permission from The Royal Society of Chemistry To attempt to understand the striking difference in behaviour, INS spectra of the same samples that were used for the QENS measurements were recorded. INS spectroscopy has no selection rules, hence all modes are allowed. However, the intensity of a mode depends on the incoherent cross section and the amplitude of motion of the atoms in the mode. Both of these are large for normal hydrogen 1H , see Figure 1 , thus the spectrum is dominated by modes that involve hydrogen displacement. This has a corollary that most elements that occur in catalysis such as transition metals, metal oxides or carbon are largely invisible, so the spectra do not exhibit cut-offs due to lattice absorption as occurs with many supports with infrared spectroscopy and the entire 0â€" cmâ€"1 range is available. For HY, Figure 10 a and 10 b , it can be seen that the characteristic spectral features of methanol: This indicates that reaction between methanol and the H-ZSM-5 hydroxyls has occurred to generate bound methoxy, Equation i: INS spectra of solid methanol green line , the empty dehydrated zeolite blue line and methanol loaded into the zeolite purple line at incident energies of: The arrow in a shows the downshift of the framework hydroxyls on hydrogen-bonding to methanol. The spectrometer is described in 15 , On almost any working catalyst that involves reaction of hydrocarbons, over time there is a build-up of a hydrocarbonaceous overlayer, which may be detrimental to the catalyst activity by blocking access to the active sites or may be integral to its operation by controlling the flow of reactants to the surface. As part of the work, a method to quantify and speciate hydrogen on the surface of the catalyst was developed An even more challenging system for conventional spectroscopies is the Fischer-Tropsch synthesis of alkanes from synthesis gas. Historically, this has used an iron-based catalyst, although supported cobalt catalysts are becoming widely used. Cobalt is in limited supply, so iron catalysts are still of interest.

2: Dynamical Behavior of Human α-Synuclein Studied by Quasielastic Neutron Scattering

scattering lengths of atoms in your sample - can arise from the presence of different isotopes or from isotopes with non-zero nuclear spin combined with variation in the relative orientation of the neutron spin with the nuclear spin of.

All relevant data are within the paper and its Supporting Information files. We prepared the solution sample of 9. Analysis of the QENS spectra obtained shows that diffusive global motions are observed in the monomeric state but largely suppressed in the fibril state. However, the amplitude of the side chain motion is shown to be larger in the fibril state than in the monomeric state. The larger amplitude of the side chain motion in the fibril state than in the monomeric state implies that the fibril state is entropically favorable. This diverse group of diseases is referred to as synucleinopathies. This recombinant protein forms amyloid fibrils, depending on the solution conditions under which the proteins are dispersed. Formation of amyloid fibrils in general involves partial unfolding of the proteins and the subsequent growth of the protofilaments and the mature fibrils, the latter possibly being formed by lateral association of the protofilaments [5]. Involvement of the partial unfolding implies that the dynamics of the proteins plays an important role in the process of amyloid fibril formation. Elucidating the role of the proteins dynamics requires a thorough understanding how the underlying fluctuations at the ps-to-ns scale are related to slower conformational changes. Inhibiting the dynamics at the ps-to-ns scale suppresses the activity of the protein [8]. Investigating the dynamics of these proteins during fibril formation is therefore important for elucidating the mechanism of this process. Incoherent quasielastic neutron scattering QENS provides information on the correlation times and the amplitudes of diffusive motions of atoms. Because about half of the atoms in the proteins are hydrogen atoms and because they are pseudo-homogeneously distributed in the protein, QENS provides information on the average motion of the hydrogen atoms within the whole protein. Many studies have been conducted using the QENS approach to obtain insights into how the protein dynamics at ps-to-ns time scales is related to functionally relevant structural changes, including, for example, studies related to protein folding [12 â€" 20], the photosynthesis systems [21 â€" 23], hemoglobin [24], and bacteriorhodopsin during its photocycle [25]. Furthermore, the studies combining QENS with other techniques such as NMR [26] and molecular dynamics simulation [21 , 27] show that the consistent results can be obtained with these techniques. These studies demonstrate usefulness of QENS as well as other incoherent techniques of neutron scattering including elastic incoherent neutron scattering and inelastic neutron scattering [11 , 28]. This solution sample is thus considered to be monomeric. The final concentration of this solution was 9. About 2 ml of this sample solution was put into a double-cylindrical aluminum cell with the sample thickness of 1. The thickness of the sample in this cell was 0. For the CD measurements, the solutions in both states were diluted to about 0. Excess sample solution was removed by blotting with filter-paper and air drying. The results of these measurements are shown in S1 Fig. The exposure time was about 6 hours for a single measurement. The spectra of the empty cell were subtracted from the spectra of the samples and the buffers, with the transmission values as the scaling factors. The spectra obtained were then normalized to those of the vanadium standard. The spectra of the PBS buffer in D2O were then subtracted from those of the samples with appropriate scaling factors. Details of how the scaling factors were estimated are described in S1 Text. The data reduction was done separately for the data of the samples in the cylindrical cells and those in the flat cells. Analysis of the spectra in the Q-region between 0. Note that we examined various possible systematic errors that could distort the resulting spectra, and verified that these possible errors were negligible see S2 Text. The results of the fits are shown in Fig 1 c and 1 d.

3: Neutron diffraction | Applications of Neutron Scattering in Catalysis

Neutron scattering and NMR spectroscopy both provide insight into protein dynamics, albeit with differing dynamic resolution; whereas neutron scattering provides information on global flexibility of a protein, solution NMR has the potential of measuring dynamics at an atomic level on a timescale ranging from picoseconds to seconds.

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4: Quasielastic neutron scattering - Wikipedia

Double differential cross-section Differential cross-section Total cross-section The cross-section is measured in the non-SI unit of area the barn (m2) Inelastic neutron scattering.

5: Quasielastic Neutron Scattering and Solid State Diffusion - Oxford Scholarship

1 Chapter 8 - ELASTIC AND QUASIELASTIC/ INELASTIC NEUTRON SCATTERING Structures are investigated using elastic scattering instruments whereas dynamics are probed using quasielastic/inelastic scattering instruments.

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