Relaxor-ferroelectrics

Relaxor-ferroelectric materials such as lead magnesium niobate–lead titanate (PMN–PT) with large electrostrictive strain near the Curie temperature are used in actuators having advantages such as low hysteresis and a return to zero displacement when voltage is removed. At C-MET, Hyderabad actuators based on multilayer relaxor materials are being made.

Other projects include integrating ferroelectric thin films on MEMS structures, for the development of RF MEMS, useful in microwave applications at the University of Hyderabad; and nano porous materials such as nano-titania integrated onto MEMS for use as chemical sensors at IIT, Kharagpur. Work is being done on multilayer-stacked ferroelectric-relaxor-based actuators at NAL, Bangalore.

Finally, smart technology has been identified as an important tool for development in India. The national programme aims to coordinate a national effort for optimally using limited resources for critical segments contributing to technological growth and self-reliance.

Fabricating MEMS devices is a field of research with huge potential and is all set to develop rapidly with the arrival of more sophisticated micromachines. The only limiting factor would be the level of smart thinking of humans to stretch the extent of creativity for developing smart MEMS devices. Being multidisciplinary and the products permeating our lives so inextricably, it is apparent that India needs a lot more 'hands' working in areas of both strategic and civilian interest. An exciting field indeed to enthuse young scientific minds!

ACKNOWLEDGEMENTS. I thank all those who contributed insights into recent Indian developments in this area and especially V. K. Aatre, who loaned books on this subject from his personal collection that made background reading for this article both pleasurable and informative.

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RESEARCH NEWS

Neutron scattering, quantum entanglement and chemical formula of water*

K. R. Rao

Even after nearly 50 years since neutron scattering came up as a bouquet of powerful techniques to unravel structure, magnetism and excitations of solids and liquids, new findings continue to be announced making the neutron a very unique and useful probe. As the flux of neutrons on the samples moved up by nearly four/five orders of magnitude during this period, techniques became powerful to elicit new information. One such technique is Neutron Compton Scattering (NCS), often referred to as 'deep inelastic neutron scattering'.

Compton effect, first observed in 1923 by A. H. Compton, relates to reduction in energy of high-energy X-ray or γ-ray photons when they are scattered by free electrons in solids or liquids. When a photon of energy E_o and momentum p_o collides with an electron, the electron of initial energy E and momentum p recoils with energy E_e and momentum p_e. By conservation of energy and momentum, one can show that there will be a shift in the wavelength of the photon after scattering with the electron. The shift in wavelength is given by, $\lambda - \lambda_o = (\hbar/mc)(1 - \cos\theta)$, where θ is the scattering angle of the photon. One can derive from detailed measurements the momentum distribution of the electrons as it was before scattering. Hence X-rays/γ-rays (and so also high energy electrons) are used to derive momentum distribution of electrons in atoms and molecules in solids.

NCS from atomic nuclei is analogous to X-ray or γ-ray scattering from electrons of atoms. During the scattering process, at large momentum transfer, the neutron effectively interacts with the nucleus of a single atom. The scattering process is subject to usual conservation laws of momentum and energy transfers. Hence from measurement of scattered neutron intensity as a function of momentum transfer $\hbar\mathbf{Q}$ and energy transfer $\hbar\omega$ during the scattering process, the momentum distribution of the nuclei before scattering can be derived. NCS and high-energy electron Compton scattering (ECS) are being used as complementary techniques for study of momentum distributions of nuclei/atoms in a variety of solids and liquids.

The electron-volt spectrometer (eVS) based on time-of-flight (TOF) technique at ISIS spallation neutron source in UK is being extensively used for these studies. In this instrument one makes use of epithermal neutrons for scattering experiments. The eVS at ISIS has undergone significant modifications, resulting in better resolution during 2001 and is re-christened as VESOVIO.

The NCS technique has been used by a number of scientists at ISIS for momentum distribution studies in a variety of materials. Amongst them Chatzidimitriou-Dreismann from Technical University of Berlin and his collaborators have studied protonic motions in various systems like water, liquid H_2O–D_2O mixtures, metallic hydrides, all at room temperature. The experimental results from H_2O–D_2O mixtures[1] are believed to show an anomalous effect, namely the scattering cross-section from hydrogen nuclei was less than expected values.

*Dedicated to Prof. S. Ramaseshan on his 80th birthday.

Can one understand this 'anomalous effect'? Study of low dimensional magnetic systems such as linear chain antiferromagnets and cold atoms at very low temperatures is undertaken to study what is referred to as 'quantum entanglement'[2]. The NCS experimental results are also analysed on the basis of theories that involve quantum entanglement[3]. The anomalous effect observed in NCS experiments is attributed to the hydrogen atoms being quantum entangled for very short times of the order of attosec (attosec = 10^{-18} s).

Recently, Roger A. Cowley has made critical comments on the NCS experimental results[4]. He has noted that 'scattering experiments can probe whether states are entangled and that a characteristic signature of entanglement is that the elastic scattering is absent at lowest temperature and at higher temperature is smaller than would be obtained if the systems are not entangled . . .' and that 'the conditions (separating elastic scattering and scattering from excitations in the system) are not satisfied in recent deep inelastic scattering experiments from hydrogen-containing system that have been interpreted as showing the existence of quantum entanglement for short times, for example, water at room temperature'. The following are some of the salient points made in ref. 4: First of all, Cowley notes that 'most experiments that investigate quantum entanglement require very low temperature and relatively isolated systems. It is therefore surprising that quantum effects are observed in liquid water at room temperature'. Apart from criticizing Karlsson and Lovesey's theoretical model[3], which dealt with NCS results from protons and quantum entanglement and its unsatisfactory implications *vis-à-vis* liquid ^{4}He results and first moment sum rule, etc., Cowley comments on several data analyses aspects as a function of TOF. Large corrections due to variation of incident neutron flux as a function of neutron energy and the Jacobian for conversion of TOF spectrum to a constant-Q spectrum have to be taken into account for proper comparison with theoretical predictions. In conclusion, Cowley notes that 'it is difficult to identify whether the experiments are flawed . . . (however) it is unlikely that evidence for quantum entanglement has been observed by neutron deep inelastic scattering technique in systems containing hydrogen at room temperature'.

I remember that nearly 40 years ago, Roger Cowley had published an AECL report[5] on excitations in liquids, which had questioned the results of TOF measurements. The abstract of that report noted: 'Calculations are made of the neutron scattering from a liquid. The model for the liquid is to assume the scattering function, $S(Q, \omega)$, is for each wave vector **Q**, a Gaussian function of frequency, ω, centred around $\omega = 0$, with a height and width chosen so that $S(Q, \omega)$ is consistent with the measured structure factor, $S(Q)$, and the known second moment of a classical liquid. The results for the calculation of the neutron time-of-flight technique give peaks *at finite energy transfers* (emphasis added). When the location of these peaks is plotted as a dispersion curve in (ω, Q) space, the results are in agreement with those reported from experiments on liquids. It is concluded that the earlier interpretation of these peaks in terms of phonon-like excitations in liquids may not be correct.'

A recent paper by Chatzidimitriou-Dreismann *et al.*[6] contains new experimental results that seem to counter the observations of Cowley. It deals with comparison of ECS (electron–nucleus scattering) data obtained at the Australian National University, Canberra and its comparison with the NCS data, both from a solid polymer, formvar ($C_8H_{14}O_2$) at 295 K. Figure 1 shows typical NCS–TOF spectrum measured using VESUVIO (formerly eVS) from formvar at a scattering angle of nearly 50°. The ratio of the peak due to hydrogen with reference to that of C and O is nearly 40% less than conventional estimates (for details see ref. 6). Once again this effect corroborates the earlier results from NCS experiments in materials like liquid H_2O–D_2O mixtures[1], metallic hydrides, etc.

Further, the momentum distributions of H and other atoms are also derived from the ECS and NCS data. Figure 2 shows intercomparison of the momentum distributions. Without going into details, it may be noted that there is remarkable agreement between NCS and ECS results. This is the first time that a direct comparison between results from the two different techniques is made. Chatzidimitriou-Dreismann *et al.* conclude that these 'results provide further direct evidence for this striking effect (anomalous deep inelastic neutron scattering effects observed over the past decade), which has been ascribed to attosecond quantum entanglement of the protons'.

It is indeed intriguing how the experimental results can be cast in terms that can catch headlines in news briefs. In two write-ups released immediately after publication of the paper[6], one finds the following eye-catching notes:

- In an article entitled 'The chemical formula H_2O—a misnomer'[7], the author has noted: 'Is the chemical formula H_2O a misnomer? From the perspective of neutrons and electrons interacting with protons of water molecules for less than 10^{-15} s, the ratio of hydrogen to oxygen is about 1.5 : 1, not the familiar 2 : 1 . . . . About one-quarter of the water protons were 'invisible' to the bombarding neutrons.'
- In another article entitled 'A water molecule's chemical formula is really not H_2O (ref. 8), it is stated: 'A water molecule's chemical formula is really not H_2O, at least from the perspective of neutrons and electrons interacting with the molecule for only attoseconds. According to new and recent experiments, neutrons and electrons colliding with water for just attosecond will see a ratio of hydrogen to oxygen of roughly 1.5 to 1, so a more accurate formula for water under these circumstances would be $H_{1.5}O$ . . . . Such effects may revise conventional textbook notions of water and other everyday molecules.'

In my opinion, these can mislead non-specialists as the write-ups do not highlight

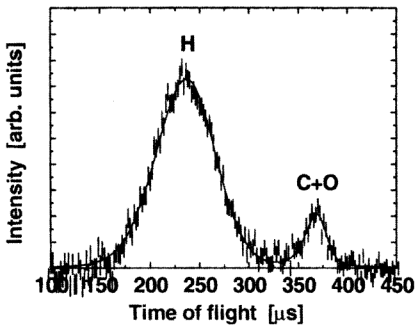

Figure 1. Typical TOF spectrum by NCS of formvar at $\theta = 51.27°$. The ratio of the hydrogen peak area: combined C + O peak area is 40% lower than expected ratio (Reproduced with permission from ref. 6).

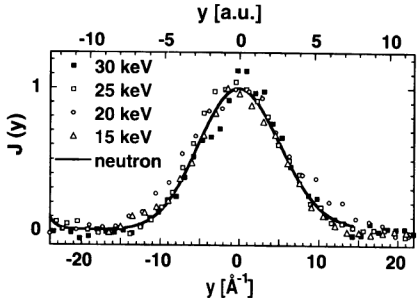

Figure 2. Compton profiles $J(y)$ derived from ECS and NCS data. $\hbar y$ is the hydrogen momentum componenet (before collision) along direction of momentum transfer $\hbar\mathbf{Q}$ (Reproduced with permission from ref. 6).

the basic concept of scattering cross-section from an entity, as new concepts are invoked.

It seems that interesting debates are underway involving experimenters, instrument scientists and theoreticians about epi-thermal neutron spectroscopic data and their interpretation currently.

1. Chatzidimitriou-Dreismann, C. A. *et al.*, *Phys. Rev. Lett.*, 1997, **79**, 2839–2842.
2. Quantum entanglement is an effect of quantum mechanics that blurs the distinction between individual particles such that it is impossible to describe the particles separately no matter how far apart they are moved. There is a link between two or more particles in which some of the quantum properties of those particles become 'shared'. In the entangled state correlations between the particles are much stronger than any classical correlations.
3. Karlsson, E. B. and Lovesey, S. W., *Phys. Rev.*, 2000, **A61**, 062714; Karlsson, E. B. and Lovesey, S. W., *Phys. Scr.*, 2002, **65**, 112; Karlsson, E. B., *Phys. Rev. Lett.*, 2003, **90**, 095301.
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7. http://www.chemweb.com/alchem/articles/156984211785.html
8. Schewe, P., Riordon, J. and Stein, B., *Physics news update*, 31 July 2003 number 648 #1, in http://www.aip.org/enews/physnews/ 2003/split/648-1.html

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A molecular voltmeter: Solution to a fifty-year-old puzzle?*

M. K. Mathew

These are the best of times for membrane biologists with a surge of interest in membrane proteins and processes, and an ever-increasing number of techniques coming to bear on all matters membranous. These are the worst of times for membrane biologists with the disparity between the number of structures of soluble and membrane proteins solved growing to three orders of magnitude and counting. The voltage-gated K^+ channel is now perhaps the best studied membrane protein, with a variety of techniques mapping aspects of function onto specific portions of the sequence. However, an understanding of how the protein senses transmembrane potential and transduces changes in potential into channel opening requires a three-dimensional structure. This has now been provided by the recent structures of the archaebacterial channel KvAP reported by Rod MacKinnon's group[1,2].

Electrical signalling in the nervous system is digital in nature, nerve cells generating an 'all-or-none' action potential that propagates down the nerve axon. The electrical events underlying the action potential were elucidated fifty years ago by Hodgkin and Huxley. The nerve cell, which is initially slightly permeable to potassium, becomes massively permeable first to sodium and then to potassium, before returning to its initial low conductance state. These changes in permeability have since been shown to be brought about by ion-channel proteins which mediate phenomenal fluxes of ions – up to 10^8 ions/second through a single channel – but are exquisitely selective for the ions they pass. Moreover, they are closed at resting membrane potentials but open in response to changes in membrane potential, i.e. they are gated by transmembrane voltage. The 'holy grail' of channel biophysicists over the past 50 years has been to explain the manner in which these apparently contradictory design requirements are met.

The very high flux through a single channel can only be explained by the protein enclosing a column of water traversing the membrane, through which the ions diffuse. The column has to be wide enough to permit free diffusion of the ions, but also have a region narrow enough to allow for discrimination. At this point, the 'selectivity filter', the column diameter would be comparable to that of the unsolvated ion to permit interaction with the protein. An hour-glass shaped aqueous column was imagined (Figure 1). High selectivity normally implies strong binding, which is incompatible with fluxes as high as 10^8 per second. Moreover, the issue of gating the channel had to be resolved.

The first major breakthrough in getting at the architecture of these proteins was the cloning of cDNAs encoding voltage-gated ion channels. Numa's group cloned a rat brain Na^+ channel in 1984 (ref. 3), but the molecule was huge – with a predicted amino acid sequence close to 2000

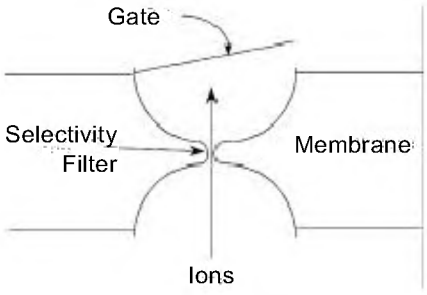

Figure 1. Schematic of an ion channel. The protein was presumed to stabilize a column of water spanning the membrane. The column was wide enough to allow free diffusion of the ion, but at its narrowest point was comparable in diameter to the unsolvated ion to facilitate interactions with the protein, ensuring selectivity. This cartoon presents an exaggerated view of the pore, the selectivity filter and a structure which physically 'gates' the channel.

*Dedicated to Prof. S. Ramaseshan on his 80th birthday.