Neutrons and Numbers: The VISION challenge. The world's first high throughput Inelastic Neutron Scattering Spectrometer

Anibal J. (Timmy) Ramirez-Cuesta

Chemical Spectroscopy Group, Chemical and Engineering Materials Division, NScD, Oak Ridge National Laboratory, Oak Ridge TN 37831-6473
E-mail: ramirezcueaj@ornl.gov

Molecular spectroscopy is a very powerful tool to study the dynamical properties of solid, liquid and gases. Inelastic Neutron scattering is a very powerful tool to study hydrogen-containing materials. With the development of neutron spallation sources, and the use of epithermal neutrons, inelastic neutron scattering can measure the vibrational spectra of materials on the whole range of vibrational motions (0-4400 cm^{-1}) and effectively opening up the field of neutron spectroscopy.[1] INS is a technique that was mostly used to study hydrogen-containing materials due to the high cross section of hydrogen.[2]

The recently commissioned VISION spectrometer at the SNS in Oak Ridge Tennessee has an increased overall flux at low energy transfers up to 4000 times over its predecessors and it has unprecedented sensitivity. I will examine the limits of what is now possible in INS thanks to VISION. From the determination of INS spectra of publishable quality in minutes (for samples in the gram quantity range),[3] measuring the signal of samples in the milligram range to the direct determination of the signal of 2 mmol of CO_2 adsorbed on functionalized catalysts.[4]

Sample environment developments are a crucial part of an effective neutron scattering program, at VISION we have developed the world's largest single crystal diamond anvil cell and measured the INS spectra of 1 mm^3 of a HMB sample. Gas handling experiments are trivial to perform. A sample changer designed for VISION is being built, it is a whole new concept that will allow continuous operation for large number of samples (hundreds at a time) that will enhance the mail-in program for sample measurement. Recently, a simultaneous Raman and INS center-stick has been developed and tested in VISION measuring simultaneously the rotational spectra of hydrogen in the gas, liquid and in the solid state as function of the relative para-ortho hydrogen concentrations. We also have in-situ dielectric spectroscopy capabilities. There is a catalysis cell and gas handling equipment that is currently being built to perform in-situ chemical reactions.

Finally, the major challenges that we are facing will be discussed, in particular methods to automate data analysis and interpretation through computer modelling.[5] We have recently commissioned VirtuES (VIRTUal Experiments in Spectroscopy), March 2016, a computer cluster dedicated to analyse VISION data. We are developing the software to maximize the potential of the technique by generation of automated VDoS, generation of thermodynamic data, creation of databases etc.

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