

The Filter Difference Spectrometer (FDS) is used for molecular vibrational spectroscopy by inelastic neutron scattering. The instrument is designed for high count rates by use of large solid-angle detectors. FDS is therefore most useful for measurements requiring high sensitivity; for example, very dilute systems or molecules adsorbed on surfaces such as in catalysts. Other applications of this instrument include hydrogen-bonded molecular crystals, biomolecular model systems, and high explosives. While most experiments are done on hydrogen-containing molecules, it is also possible to study molecular vibrations involving other atoms; for example, O in CMR (colossal magnetoresistance) materials.

FOR MORE INFORMATION,
CONTACT:

Raja Chellappa
raja@lanl.gov
(505) 664-0217

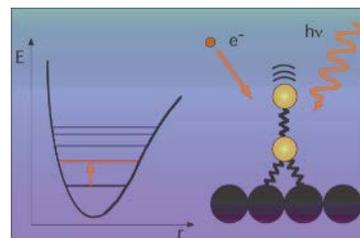
Vibrational spectra are obtained by neutron energy loss. During scattering from the sample, incoming neutrons excite molecular vibrations by giving up energy. FDS determines the change in energy by the use of low-energy band-pass filters (Be) between the sample and detector. These filters will only allow neutrons of a certain energy to reach the detector. The scattered neutrons are sorted by their total time of flight as they journey from the sample to the detector. From this information, their incident energies can then be determined. Data reduction is accomplished by either variable numerical deconvolution of the spectrometer response function or maximum-entropy methods. The instrument's energy resolution can thereby be varied as needed, and ranges from 2% - 5% of the energy transfer.

Molecular Vibrational Spectroscopy

- Vibrational spectra in the mid- to far-infrared are fingerprints for molecular species identification.
- Surface molecular vibrational spectra, in conjunction with modern computation tools, provide information of adsorption sites, orientations, surface bonding, and local chemical environments of adsorbed species on surfaces.
- Raman, FTIR, and HREELS are typical vibrational spectroscopy techniques.

It is also possible to do vibrational spectroscopy with neutrons. In conjunction with numerical modeling, inelastic neutron spectroscopy is a powerful technique that has several advantages over optical techniques including the following:

- High sensitivity to H (large incoherent neutron scattering cross-section).
- No selection rules.
- No complicated electron/photon interactions.
- Enhanced contrast from the large difference in H and D cross-section.
- "Real" surfaces (no need for ultraclean, single-crystal surfaces).



Specifications	
Energy-transfer range	50 - 5000 cm^{-1} (6 - 620 meV)
Q range	1.5 - 17 \AA^{-1}
Energy-transfer resolution	2% - 5%, depending on data treatment
Beam size at sample	10-cm high x 2.5-cm wide
Detectors	60 ^3He (1.3 cm in diameter)
Filter analyzers	10 Be each subtending a scattering angle of 18° refrigerated
Moderators	Chilled water at 283 K
Sample environment	10 - 325 K, closed-cycle refrigerator, in situ gas absorption cell; Be-Cu pressure cell to 20 kbar; 20 - 800 K, hot stage closed-cycle refrigerator
Sample size	0.5 - 100 g
Experiment duration	2 hours to 2 days

