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Vibrational studies using neutrons

Several neutron spectrometers are available for use at the Bragg Institute. In particular a low energy band pass neutron spectrometer that operates in the range of ~ 50 - 1200 cm^{-1} has very recently been commissioned and first experiments run on TAIPAN. The so-called Beryllium-filter spectrometer is predominantly used to obtain vibrational density of states spectra from those materials that contain hydrogen, thus making this instrument especially important in the chemical, biological, geological and environmental sciences. In many aspects a neutron spectrum obtained using the Beryllium-filter spectrometer is very similar to spectra obtained in the far-infrared or terahertz regime making neutron spectroscopy a complementary technique to other spectroscopies such as photon (electromagnetic radiation)-based techniques. The neutron's properties are unique amongst other fundamental probes like light, such as outstanding materials penetrability, isotopic sensitivity, magnetic sensitivity and lack of vibrational selection rules. Furthermore because hydrogen possesses a large incoherent scattering cross-section much of the observed vibrational modes are molecular in origin.

Calculation using DFT-codes and/or molecular dynamics approaches are an integral part of a complete study investigating any material with neutron spectroscopy. A number of interesting examples are presented that highlight the capabilities of the Be-filter spectrometer along with a description of the spectrometer itself, how it works and the analysis involved.

Primary author(s) : Dr STAMPFL, Anton (Australian Nuclear Science and Technology Organisation)

Presenter(s) : Dr STAMPFL, Anton (Australian Nuclear Science and Technology Organisation)