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Vibrational spectroscopy using the BeF spectrometer on TAIPAN

Vibrational spectroscopy using neutrons as a probe, as opposed to electromagnetic radiation, is a relatively new capability in Australia. A number of instruments at the Australian Centre for Neutron Scattering are capable of measuring vibrational density of states. In particular, the so-called Beryllium Filter Spectrometer, BeF, located on TAIPAN, is devoted to the measurement of vibrational density of states. Even though most scientists are familiar with techniques such as IR, Raman, NMR etc, vibrational spectroscopy using neutrons poses somewhat of a mystery as the equipment, technique, and analysis, are very different to those techniques using well-known electromagnetic probes.

Unlike light that strongly interacts through the electromagnetic force with the electronic structure, neutron radiation interacts through that part of the residual strong force directly with the atomic nucleus. As a consequence, thermal neutrons probe directly vibrational motion: all excitations are observable because of the lack of selection rules, and scattering cross sections are isotopically sensitive. In particular, scattering from hydrogen allows molecular-like, or localised, modes to be probed. A weighted density of vibrational states is directly measured that can be compared to calculation. In this way the dynamics and mechanical interaction of molecular units may be directly investigated.

For this presentation an overview of the BeF instrument is given, as well as the theory explaining how measured spectra are in fact the weighted density of vibrational states of the system under investigation. Analysis steps are given that take the raw spectra and turn them into spectra suitable for comparison to calculation.

Topic

Neutron Instruments & Techniques

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