thermoscientific



Analytical solutions for improved battery and energy storage products



FTIR

Fourier-transform Infrared Spectroscopy (FTIR) is a commonly used vibrational spectroscopy that reveals molecular information about

the sample. FTIR spectrometers accommodate an array of sampling accessories. Several third-party companies also offer a number of specialized FTIR sampling accessories useful in battery research.

The Thermo Scientific[™] Nicolet[™] iS50 FTIR spectrometer accommodates technique modules for FT-Raman, IR-TGA, IR-GC and a dedicated NIR unit. All or our spectrometers use our award-winning Thermo Scientific[™] OMNIC[™] software that provides fast and easy materials identification, and features designed for time-resolved experiments, kinetics and advanced spectroscopic studies such as phase modulation infrared reflection-absorption (PM-IRRAS) spectroscopy.

Enabling maximum sample ease-of-use on all Thermo Scientific FTIR spectrometers are attenuated total reflectance (ATR) sampling. Simply place the sample over the reflectance crystal (diamond, germanium), clamp down the material and acquire data. The use of Raman and IR spectroscopy as complementary techniques means that Raman can be used to examine structural changes in the electrode material and IR to probe the interface between the lithium and the organic electrolyte.

In developing research for battery materials FTIR has been shown to be useful in providing specific information about chemical bonds and functional groups used to identify transient lithium species. FTIR is nondestructive and supported by a comprehensive library of IR spectra for common lithium species. FTIR supports researchers actively exploring batteries alternatives like Li–S, Li–O2, Na-ion, Mg batteries and different metal–organic batteries.

Due to its versatile sample handling capabilities and large accessory chamber, FTIR is now found in several *in operando* experiments to investigate the decomposition process of the electrolyte solutions. *In situ* FTIR can provide real-time information about the chemical nature of adsorbates and solution species as well as intermediate/product species involved in the electrochemical reactions.

FTIR at a glance

- Acquires infrared spectra of solids, liquids and gases
- Provides information about chemical bonds and functional groups
- Spectral fingerprinting enables rapid identification of unknowns
- ATR sampling provides quick and easy data collection
- Multiple sampling capabilities for specialized studies

FTIR

- Monitors time-based and dynamic events
- In operando and in situ sampling capabilities

Thermo Scientific Nicolet iS50 FTIR spectrometer

Thermo

Raman microscopy

Raman spectroscopy provides a structural fingerprint by which molecules in a sample can be identified. The Raman technique measures the energy shift in light scattered photons that yields molecular and structural information. Combining small spot microscopy with precision stage movement enables chemical mapping across a sample area. Raman spectroscopy is an important technique in analyzing various forms of carbon such as graphene and graphite, and diamond-like materials.

Raman is a useful technique in developing alternatives to lithium cobalt oxide cathodes, such as manganese spinel material. Raman is useful in looking at lithium cobalt doping with transition metals to synthesize materials with different morphologies.

In developing anode materials, Raman has been useful in studying carbon allotropes besides graphite. Raman spectral data can be used to determine the number of sheets of graphene in a stack, provide information on defects and disorder in the structure of graphene, and determine diameters of single wall carbon nanotubes.

Raman spectroscopy can be used to study the degree of association of electrolyte ions in solutions and in polymer materials. The association of ions has a direct effect on the ion mobility and ion conductivity and thus affects battery performance. Raman can measure the effects of additives used to suppress the crystallinity of the polymer matrix and to improve the mechanical and electrochemical properties of the resulting composite polymer electrolytes.



- Visualize chemical compositional distribution on component surfaces
- Profile chemical changes during battery cycling
- Evaluate the spatial distribution of phases in a sample
- Ideal for studying allotropes of carbon and transition metals



A Raman map showing the distribution of the two different spinel phases in a sample. The red-yellow locations (such as location 2) indicate areas of the P4332 phase whereas the blue-green areas (such as location 1) represent areas of the Fd3m phase. Mapping data collected using a DXR2 Raman microscope with a motorized stage and Atlµs software.*

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