Mass Spectrometry & Advanced Vibrational Spectroscopy Workshop

Artem Filipenko, Ph.D., National Applied Markets Manager, Bruker Daltonics
Sergey Shilov, Ph.D., Product Manager, Bruker Optics

Friday, September 30th 12:00 PM-4:15 PM

Address:
Cullen College of Engineering 1
Engineering Building 1, Room 102D
4226 Martin Luther King Blvd,
Houston, TX 77204

12:00PM – 1:30PM
Characterization of Polymers using MALDI & TIMS

Mass Spectrometry (MS) has become an indispensable tool for polymer analysis and has been widely used to study polymer structure and composition, end-groups and additives, molecular weight distribution, degree of polymerization, and so on. MS analysis is extremely sensitive, allowing the detection and identification of minor polymer components and synthesis by-products, as well as low-level impurities and products of decomposition. Matrix Assisted Laser Desorption Ionization (MALDI) MS is a well-established method of polymer characterization that continues to be developed and improved with new generations of MS instruments, bringing new analytical capabilities and enhanced performance. Modern MALDI-MS instruments generate rich chemical information highly specific for polymer structural analysis, copolymer composition and complex polymer mixtures characterization, and can even be used for imaging of synthetic polymer surfaces. Because of its unique capabilities, this technology has been widely used in a great variety of polymer analysis applications in both academic and industrial settings. In some cases, MALDI-MS is the only technique that can provide the information required to solve a practical problem. It allows for rapid MS analysis where no prior sample treatment or extensive separation is needed, including characterization of challenging insoluble polymers.

TIMS technology has redefined the capabilities of Ion Mobility separation by providing an unmatched combination of resolution, speed, robustness and sensitivity. In polymer analysis applications, the timsTOF instruments expand the analytical boundaries by combining the TIMS technology with ultra-high-performance MS and providing an additional dimension for separation of complex polymer mixtures and structural analysis of challenging polymer compositions. Compatible with HPLS-ESI, GC-APCI and MALDI workflows, Bruker timsTOF fleX is a go-to multitool for a modern polymer lab.

1:30 PM – 2:30 PM
Fast identification and characterization of polymers by FT-IR spectroscopy

Thousands of polymeric compounds and materials have been developed over the years to optimize the properties and performance of products spanning nearly every industry. Vibrational spectroscopy is a widely used technique for the characterization of polymers because in most cases it does not require sample preparation or expensive consumables. Recent developments in instrumentation allow spectra to be collected under challenging conditions such as low sample transmission, low sample concentration, and rapid chemical changes.

The following topics will be discussed in detail:

- Polymers identification and classification
- Additives and contaminations
- Thermal properties by TG-FTIR technique
- Orientation of polymer segments

- Monitoring of crosslinking reactions

3:00 PM – 4:15 PM

Failure analysis and reverse engineering using vibrational spectroscopy

Failure analysis is a critical part of new product development and the troubleshooting of existing products. Product performance can be compromised due to incorrect formulations, insufficient homogeneity, degradation, contaminations, and many other factors. A physical examination from the macro to microscopic scale combined with the chemical analysis can many times reveal the reason for failure. Molecular spectroscopy is among the most powerful tools for this application. Each molecule has a unique infrared and Raman signature providing great specificity in the identification process.

This presentation will be focused on the process of utilizing IR and Raman spectroscopy to characterize contaminations of various industrial and pharmaceutical products down to a scale of a few microns:

- Sample preparation and standard routines of failure analysis
- Distribution of chemicals in inhomogeneous samples
- Analysis of multilayer films
- Search through spectroscopy libraries

Real-world examples of product troubleshooting such as contamination in liquids, polymers, and circuit boards will be presented.