High-Precision Molecular Orientation Analysis for Organic Thin Films

We are looking to out-license the technology for its commercialization.

Enables high-precision measurement and analysis of molecular orientation of amorphous materials such as organic semiconductors and biomembranes

◆Background

p-Polarized Multiple-Angle Incidence Resolution Spectrometry (pMAIRS) is a spectroscopic technique that enables functional-group-level analysis of molecular orientation in thin films, even in amorphous materials. It plays a crucial role in elucidating interfacial chemical reaction mechanisms and in the development of functional materials. By combining Fourier-Transform Infrared Spectroscopy (FT-IR) with the pMAIRS method, it has become possible to simultaneously obtain both in-plane (IP) and out-of-plane (OP) spectra—traditionally acquired separately via transmission and reflection-absorption methods—on a unified vertical scale. This advancement enables quantitative analysis of molecular orientation in thin films [JP4340814].

However, conventional IR spectroscopic methods including pMAIRS have faced issues such as the inability to eliminate optical fringes (interference patterns) and water vapor peaks (noise) arising from samples or substrates. Additionally, changes in the incident angle cause variations in the irradiated area, which introduces instability in measurements..

◆Description

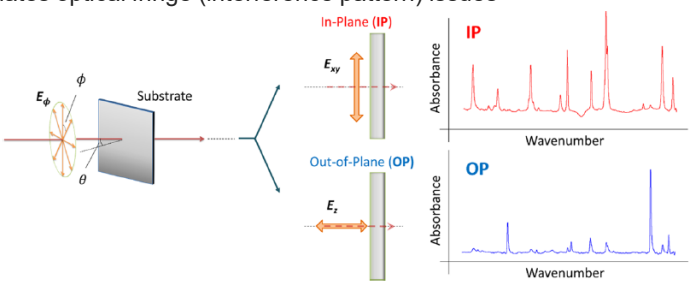
To overcome these issues, the inventors developed an improved method called MAIRS2 [JP 6861351][Fig. 1], which analyzes IP and OP spectra by varying the polarization angle (φ) of linearly polarized light, instead of changing the incidence angle (θ). This new approach significantly reduces interference from water vapor and allows even small absorption peaks to be clearly detected. It also enables the removal of optical fringes originating from the sample or substrate [Fig.2].

➢ **Key Strengths of pMAIRS and the Enhanced MAIRS2 Method**

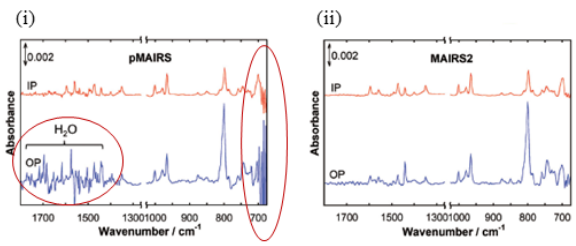
- Enables simultaneous acquisition of two types of spectra—equivalent to transmission and reflection-absorption methods—from a single sample
- Allows quantitative analysis of molecular orientation in thin films at the level of individual functional groups by combining with FT-IR
- Capable of analyzing molecular orientation in amorphous regions that are difficult to measure using X-ray diffraction (XRD)
- Enables analysis of molecular orientation in low-smoothness thin films where polarization analysis methods such as ellipsometry are ineffective

➢ **Fundamental Solution to the Common Challenges of Conventional Thin-Film IR Spectroscopy, Including pMAIRS** [Fig.2]

- Avoids the issue of residual water vapor peaks characteristic of FT-IR
- Eliminates optical fringe (interference pattern) issues



【Fig.1】Schematic of MAIRS2 Spectra Analysis



【Fig.2】The pMAIRS(i) and MAIRS2(ii) spectra of a tetraphenylporphyrin thin film on Si

◆ Development Stage

- Inventor's prior invention [JP4340814] and current invention [JP6861351] licensed to spectroscopic instrument manufacturers by respective licensors; currently available as commercial products.
- Licensing available to multiple sectors.

◆Application Fields

- Molecular structure analysis of thin films and surfaces
- Organic materials/biological

◆Reference

- MAIRS: Innovation of Molecular Orientation Analysis in a Thin Film
- Second Generation of Multiple-Angle Incidence Resolution

◆Intellectual Property

JP6861351
Registered in the US, UK, Germany, and France
Applicant: Kyoto University

◆Offers

- Non-exclusive licensing agreements
- Option agreements
- Joint research collaborations

◆Contact

TLO-KYOTO Co., Ltd.
Mail: event@tlo-kyoto.co.jp
Phone: +81-75-753-9150
Yoshidahonmachi, Sakyo-ku, Kyoto, 606-8501, Japan
Within the Institutional Advancement and Communications Headquarters, Kyoto University

Institutional Advancement and Communications

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