

Application News

MALDI-TOF Mass Spectrometry

No.B08

Structural Analysis of Industrial Materials by MALDI-MS/MS 01 - Analysis of the Organic Light-Emitting Diode (OLED) Polymers -

MALDI-TOF MS is a widely used analytical technique for the structural analysis of various industrial materials. Although information is easily obtained from MALDI-TOF MS analysis on the masses of monomer repeat units and terminal end groups, it has been more challenging to obtain structural information. Using the high-energy collision-induced dissociation (high-energy CID) feature of the MALDI-TOF MS, MS/MS analysis was applied to a polymer used for OLED (organic light-emitting diode), and structural analysis was conducted using the mass spectra of product ions of a specific ion. This Application News article introduces such an analysis example.

There are 2 types of emissive electroluminescent layers that can be used in OLED displays, a low-

molecular weight type and a polymer type, the latter of which is receiving attention for future development because it can be produced in large sizes and made flexible (Fig.1). A uniquely structured polymer with a long conjugated system is often used as the polymer, and although NMR analysis and pyrolysis GC/MS analysis are often used, complete structural determination is difficult. For this reason, MS/MS analysis by MALDI-TOF MS is often used in conjunction with these other analysis techniques. Fig. 2 shows the mass spectrum of a polymer used for the light-emitting layer.

(Analysis example kindly provided by: Nobuyuki Sato and Yoshihiko Taguchi of Toray Research Center, Inc.)

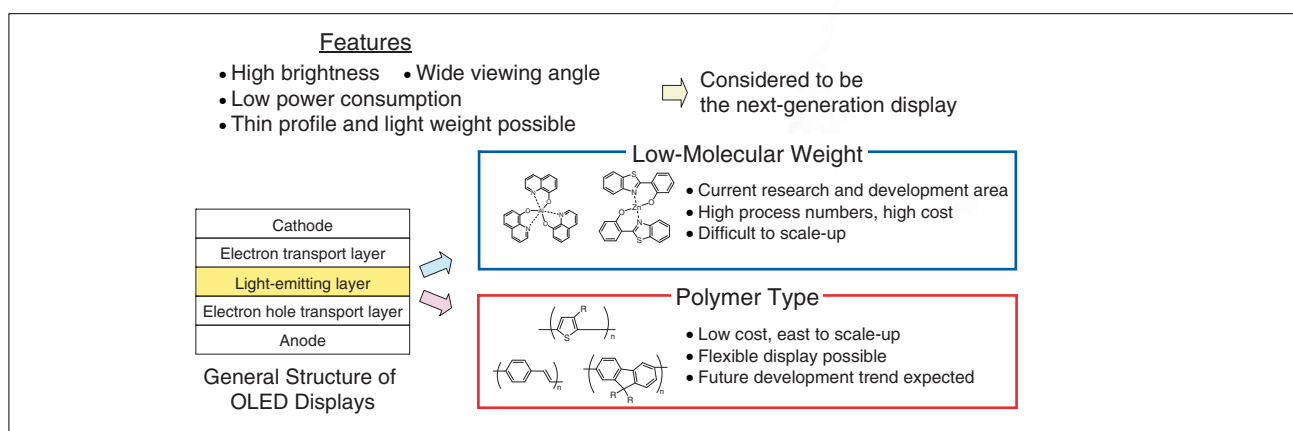


Fig. 1 Overview of OLED Displays

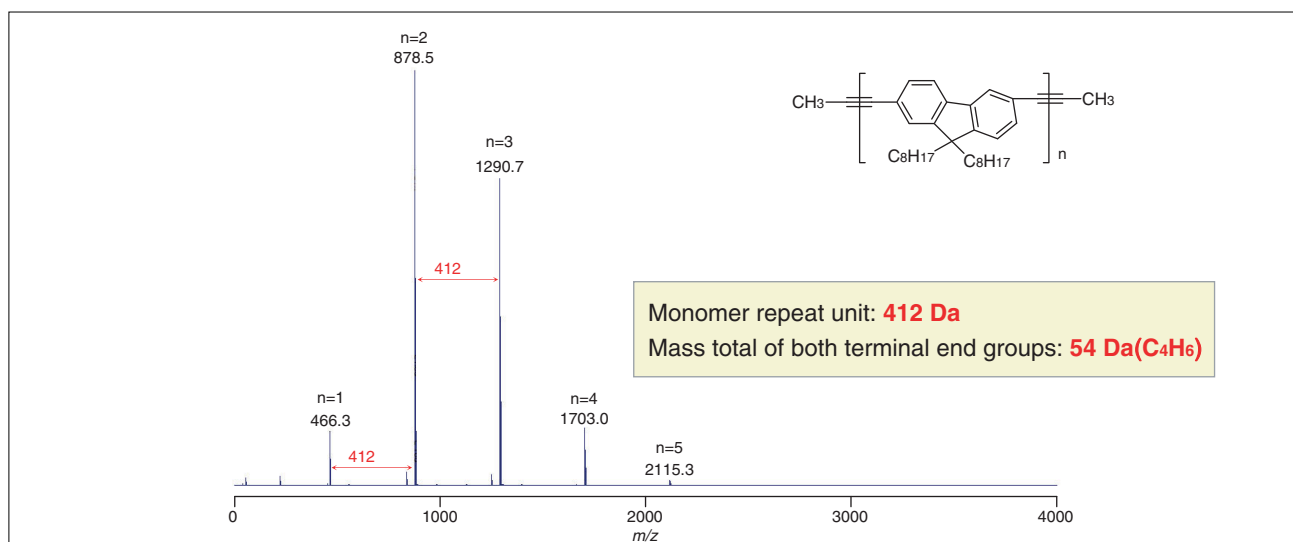


Fig. 2 Mass Spectrum of Polymer for OLED

It is clear from the results that the mass of the monomer repeat unit of the polymer comprising the light-emitting layer corresponds to 412 Da, and that the total mass of both terminal end groups is 54 Da. Fig. 3 shows the MS/MS spectrum obtained from analysis using the m/z 1291 (trimer) molecular ion as a precursor. Six peaks were observed at 112 and 113 intervals, which correspond to dissociation of octyl group. Similarly, when MS/MS analysis was conducted using the m/z 1704 (tetramer) molecular ion as a

precursor, as shown in Fig. 4, eight octyl radicals are detached, and it is clear that two octyl radicals were included in the monomer repeat unit.

MALDI-MS/MS analysis using the high-energy CID technique is a simple analytical technique that provides abundant information due to the many product ions formed that reflect partial structures, as compared with the conventional PSD technique. This enabled examination of the side-chain structure in a polymer used for OLED displays.

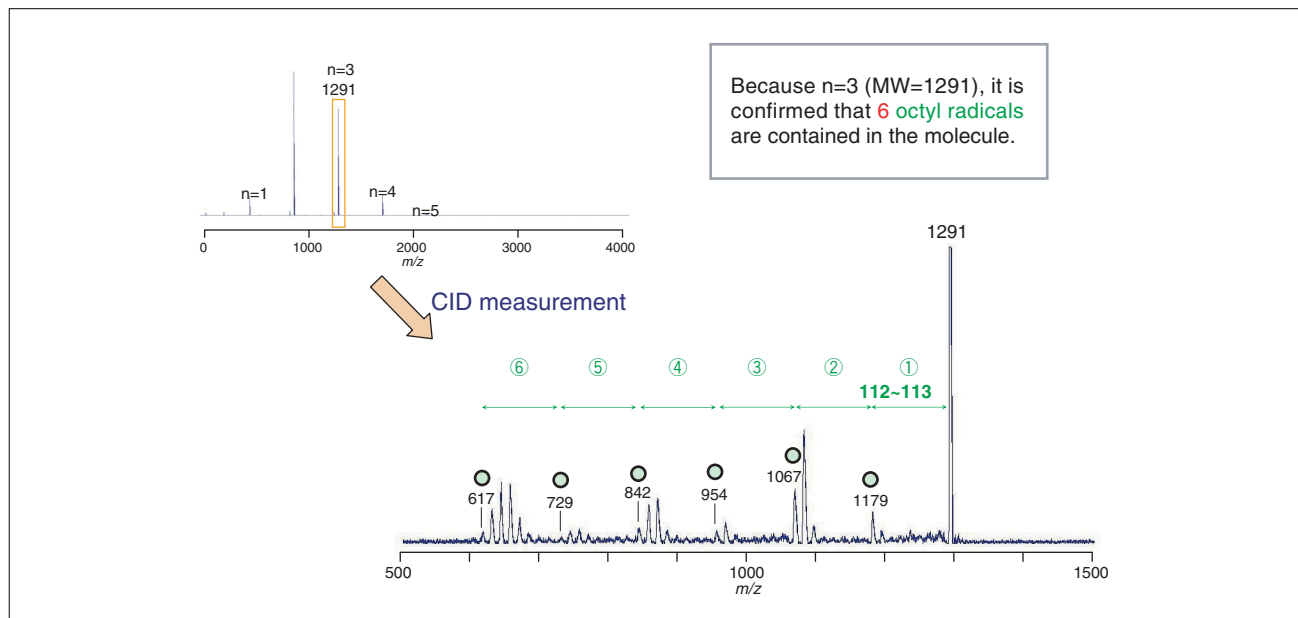


Fig. 3 MS/MS Spectrum of m/z 1291 ($n=3$) as a Precursor Ion

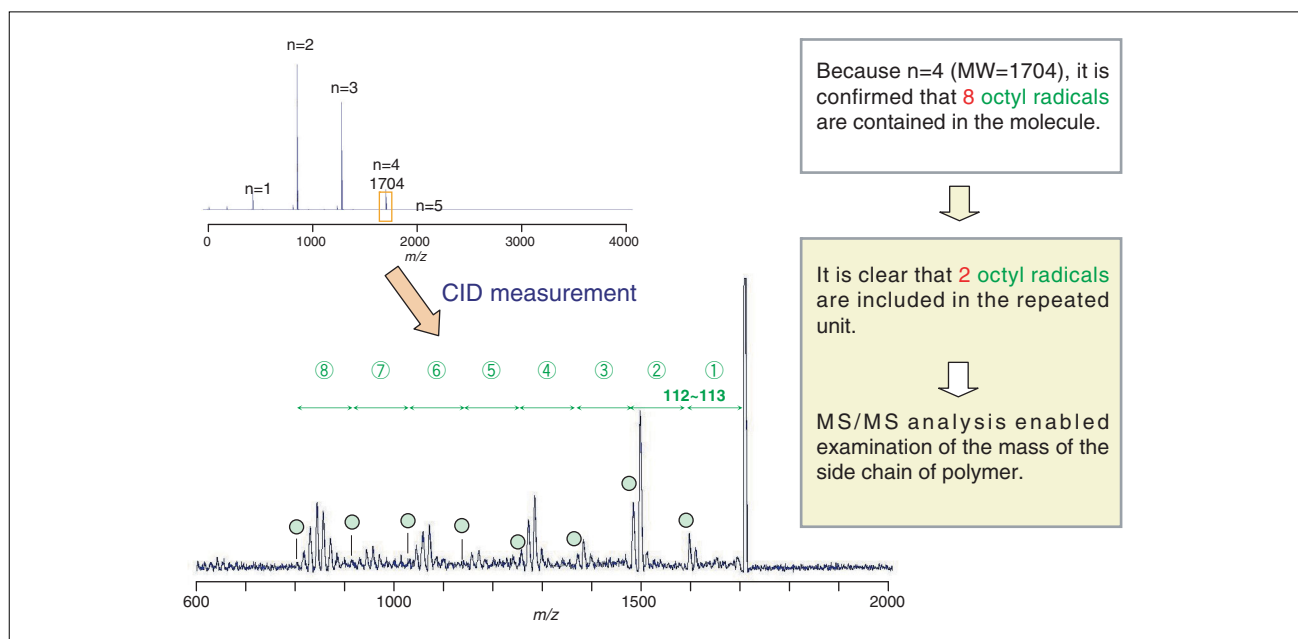


Fig. 4 MS/MS Spectrum of m/z 1704 ($n=4$) as a Precursor Ion

[References]

Yoshihiko Taguchi, Akiko Otsuki, Nobuyuki Sato: 10th Polymer Analysis Symposium Summary, p95 (2005)

NOTES:

*This Application News has been produced and edited using information that was available when the data was acquired for each article. This Application News is subject to revision without prior notice.



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