

Polyethylene glycol (PEG) Analysis with Argon Cluster Ion Beam connected with Q-ToF Mass Analyzer

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ToF-SIMS (Time-of-Flight Secondary Ion Mass Spectrometry) is a powerful tool for surface analysis that is potentiality both spectral analysis and chemical state imaging [1]. However, the challenge of ToF-SIMS is to analyze organic materials and polymers samples in the high-mass region (more than 500 u) because of the low sensitivity. In this work, the PEG sample with the chemical formula of $C_{2n}H_{4n+2}O_{n+1}$ was used in the analysis and investigation of mass spectra. The PEG (3,000 Da)-mixed trifluoroacetic acid sodium salt (NaTFA) sample at a molar ratio of 1:11.65 was prepared by the spin-coating technique.

For mass analysis, an Argon-gas cluster ion beam (Ar-GCIB) was used (with a primary energy of 10 keV and about 1 nA beam current) with a quadrupole ToF (Q-ToF) mass analyzer. The accumulation time was 100 s and the primary ion dose was about 2.5×10^{14} ions/cm². In the MS mode only the ToF analyzer was used; in the MS/MS mode the TOF and quadrupole mass analyzers were used simultaneously. From the experiment, the MS mass spectra could be measured to 3,500 Da. The MS mass spectrum and secondary ion distribution are shown in Fig. 1. $[M+Na]^+$ is the dominant peak in the regions of m/z 1,000 and 3,000, and the B and C series [2] are outstanding peaks around the region of m/z 1,000. Each series presents the m/z difference at 44. Surprisingly, a doubly charged ion could be observed because of the appearance of peaks at half the interval and the m/z difference at 22 (see inset in Fig. 1(a)). The doubly charged ion is dominant in the region around m/z 1,500. Peaks of the PEG spectrum were separated in four groups, $[M+Na]^+$, B, C and doubly charged ions (Fig. 1 (b)).

The doubly charged ion series was verified by the MS/MS technique as the precursor mass at $n=68$ and $n=69$ $[M+2Na]^{++}$. The mechanism of cationization in the polymer sample will be presented and discussed.

Keywords: PEG, ToF-SIMS, NaTFA, Ar-GCIB, Cationization

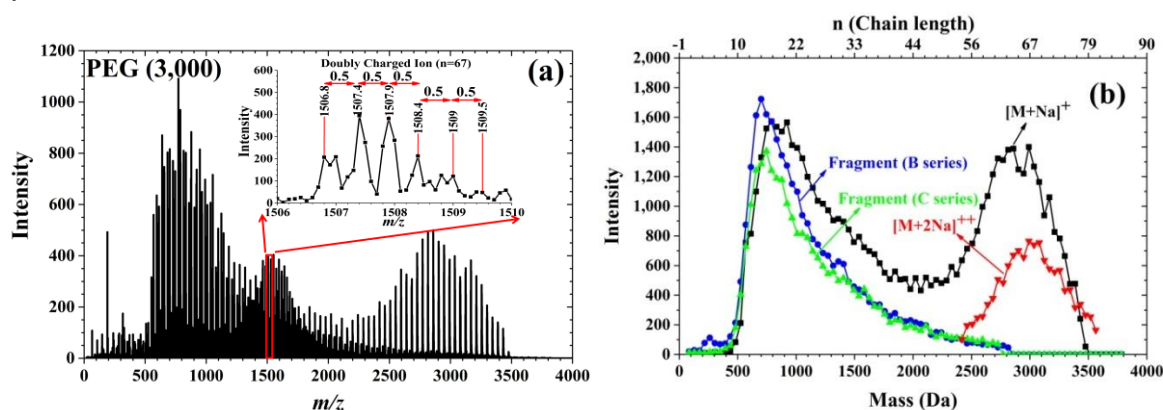


Fig.1 The MS mass spectrum (a) and integrated peak area (b) of the PEG sample, the $[M+Na]^+$ presents the molecular distribution. Inset in (a): Discrete spectrum around $m/z=1500$ showing doubly charged ions.

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