

Cluster-Induced Desorption/Ionization of Polystyrene – Detailed Information on Material Properties Based on a Soft Desorption Process

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Polymer materials are of growing importance for a variety of applications in the field of optical electronics, including organic light emitting diodes and solar cells. As the detailed molecular properties of the polymer molecules determine the electrical and optical properties of these devices, sample characterization is a crucial step for both research and production purposes, thus making a powerful analytical tool mandatory. Secondary-ion mass spectrometry (SIMS) is a widespread method for the characterization of solid samples of polymers and organic materials in general, however, it typically comes with significant fragmentation induced by the primary ions [1]. While this can be of advantage, e.g., for identification of larger molecules or for depth profiling of polymer samples, characterization of sample properties like the mass distribution of the smaller molecules requires a non-destructive approach.

Desorption/Ionization induced by Neutral SO₂ Clusters (DINeC) is such a soft desorption method [2,3]. In this contribution, we investigate in detail cluster-induced desorption of non-polar polystyrene oligomers. Clear peak progressions corresponding to intact polystyrene molecules are observed in the mass spectra and no fragmentation was detected (Fig. 1, left and center); efficient desorption was deduced from quartz crystal microbalance measurements. Molecular dynamics simulations further show that desorption proceeds via dissolution in the polar cluster fragments even in the case of the non-polar polystyrene molecules (Fig. 1, right). Experimentally, a reduced desorption efficiency for samples composed of molecules with higher chain length is observed. This is in contrast to the results of the molecular dynamics simulations, which indicate that, in a simple model, the desorption efficiency is largely independent of the chain length of the molecules. Backed by additional experiments with samples containing different distributions of chain length, the reduced desorption efficiency for longer molecules is attributed to an increasing entanglement of the polystyrene molecules with increasing chain length [4].

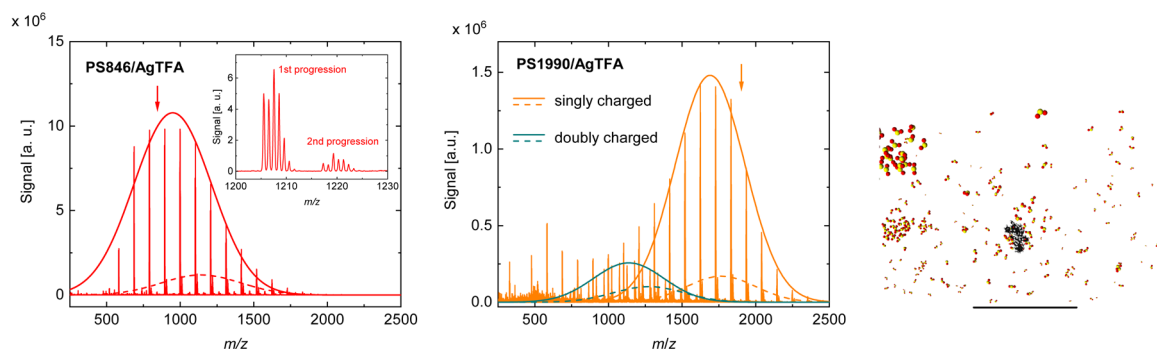


Figure 1 – DINeC mass spectrum of short (PS846, left) and long polystyrene (PS1990, center) with AgTFA as cationizing agent. Multiple peak progressions are observed, the envelopes of the first and second peak progression are highlighted by solid and dashed lines, respectively. Within each progression, peaks are separated by $\Delta(m/z) = 104$, equivalent to the mass of one styrene unit. Different progressions are shifted by a constant value relative to each other. The number average of the substance specified by the supplier is indicated by an arrow. Intensity of PS1990 is reduced when compared to PS846. Right: Snapshot of the cluster-induced desorption process as described by means of MD simulations. About 50 ps after cluster-surface collision, the polystyrene molecule is ultimately desorbed via dissolution in one of the cluster fragments.

References:

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