Mechanism of Site-Specific Ion Desorption from Core-Excited PMMA Thin Film

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Core-excitation takes place within quite local area, so a specific atom in a molecule can be excited resonantly. Using tunable synchrotron radiation, site-selective core excitation can be achieved and site-selective bond braking is expected in the vicinity of the atom where the primary core excitation takes place. This suggests the possibility that the resonant excitation by soft x-ray can control chemical bond scission selectively. Recently, the mechanism of site-specific photon stimulated ion desorption (PSID) of PMMA has been studied in detail by using an Auger electron - photoion coincidence spectroscopy and ab initio MO calculations[1,2]. In the case of C 1s excitation, CH_n^+ (n=1-3) ions are desorbed efficiently in the excitation to the O-CH_3 anti-bonding orbital. Moreover, in this excitation, it was revealed that desorbed CH_3^+ and CH_2^+ ions are mainly produced via a Auger final states with hole(s) in O-CH_3 bonding orbitals. It was found that site-specific PSID by core-excitation is promoted by the decline of bonding due to attachment of electron to anti-bonding orbital and the Coulomb repulsion due to removal of electrons from bonding orbitals, and the possibility of controlling the scission of chemical bonds is discussed.

This work was supported by a Grant-in-Aid on Research for the Future "Photoscience" (JSPS-RFTF-98P-01202) from Japan Society for the promotion Science.

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