Photochemical Modification of Polyethylene Terephthalate Surface

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Abstract

The prospect of obtaining desired surface-mediated characteristics while retaining bulk-mediated physical properties and avoiding potential environmental issues with wet chemical technology lends considerable appeal to photochemical approaches to surface modification.

We undertook a combined experimental and computational approach to investigate the effect of deep UV irradiation on the polyethylene terephthalate (PET) surface. Its response to 172 nm UV from a xenon excimer lamp in the absence of oxygen was characterized with X-ray Photoelectron Spectroscopy (XPS), Time of Flight/Secondary Ion Mass Spectrometry (ToF/SIMS), transmission infrared spectroscopy (IR), and Atomic Force Microscopy (AFM). The surface chemistry details suggested that the primary photochemical reactions involved a Norrish type I based decarbonylation and a Norrish type II process yielding terminal carboxylic acid groups, consistent with the possible photochemistry from $n\text{-}\pi^*$ type lowest singlet excited states of PET according to the computational modeling results. By directly populating $n\text{-}\pi^*$ type excited states, 172 nm UV promoted effective surface photochemistry of PET with further helps from the high UV absorptivity and the high surface mobility of the molecules.

Utilizing this active surface radical chemistry, a new grafting strategy was developed to impart desirable functional properties to the surface. A broad range of grafting chemicals can be employed in their vapor forms, demonstrated with an alkene or an alkane. Surface analysis with XPS, ToF/SIMS, AFM, and water contact angle measurements confirmed the effectiveness of the approach, supporting the notion of the surface radical initiated processes.

A potentially useful anti-stain/soil coating was developed by grafting with a fluorocarbon species. Surface analysis suggested that the grafted fluorocarbon formed a nano-scale self-assembled monolayer. The coating had a similar water contact angle as that of a pure fluoropolymer but a better oil repellency due to the special molecular orientation in the graft layer.

A potential antimicrobial application was demonstrated with amine chemicals. Structure characterization and computational modeling results suggested that the photochemistry of the UV active grafting chemicals also played an important role in the grafting process. A double bond structure in the amine species protected the amine functional groups and the resulting coating demonstrated antimicrobial activity against *E. Coli.*