

Oxidation Behavior of P3HT Layers on Bare and TiO₂-covered ZnO Ripple Structures Evaluated by Photoelectron Spectroscopy

Dae Han Kim, Myung-Geun Jeong, Hyun Ook Seo and Young Dok Kim*

Department of Chemistry, Sungkyunkwan University, Suwon, 440-746, Korea

Procedure of XPS Spectrum Fitting

Each core-level XPS spectrum was fitted with linear combination of Gaussian and Lorentzian functions with a ratio of 7:3 after Shirley-background subtraction using CASA-XPS software. Each spectrum was fitted by varying only its intensity with fixed full-width of the half-maximum (FWHM) position for each component.

1. S 2p core-level

For S 2p XPS spectrum, it was fitted with four different components, which are non-oxidized S 2p_{3/2} at 164.7 eV, sulfoxide S 2p_{3/2} at 165.2 eV, sulfone S 2p_{3/2} at 166.7 eV and total-oxidized S 2p_{3/2} at ~ 170.0 eV. Spin-orbit splitting (S 2p_{3/2} and 2p_{1/2}) was considered with a fixed peak area ratio of 2:1 and the relative position of S 2p_{3/2} was always lower than that of S 2p_{1/2} with a binding energy of 1.2 eV.

2. C 1s core-level

For C 1s XPS spectrum fitting, six different components were used; three for non-oxidized C species (C=C-C, C-C and C=C-S at 285.3, 285.9 and 286.1 eV, respectively with a relative intensity of 1:3:1) and three for oxidized C species (C-OH, C=O and COOH at 286.9, 288.3 and 289.8 eV, respectively).