



XAS study on PEDOT:PSS thin films

(NSU – Aichi Pref. Joint Research Program)

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keywords : PEDOT:PSS, XAS, conductivity, thermoelectric properties

1. Introduction

Poly(3,4-ethylenedioxythiophene):polystyrene-sulfonate (PEDOT:PSS) becomes the most successful intrinsically conductive polymers in terms of the practical application. Because PEDOT:PSS can be dispersed in water and some polar organic solvents, it can be processed into thin films by solution processing techniques like coating and printing. Its conductivity can enhanced from 10^{-1} S/cm to >3000 S/cm through a treatment with H_2SO_4 .^[1] A further treatment of a H_2SO_4 -treated PEDOT:PSS film with NaOH solution can enhance its thermoelectric properties.^[2] The Seebeck coefficient can enhanced from 15-18 $\mu V/k$ to ~ 39 $\mu V/K$. However, there are arguments on the structure change of PEDOT:PSS during the treatment with H_2SO_4 or NaOH. We try to understand the structural changes during these treatments by X-ray absorption spectroscopy.

2. Experiment

The pristine, H_2SO_4 -treated and H_2SO_4 -then-NaOH-treated PEDOT:PSS films was measured at the Aichi Synchrotron Radiation Center. Both CEY (sensitive to surface) and PFY (sensitive to bulk) XANES spectra were collected for each sample. The S K-edge XANES were analyzed with with the *Athena* program.

3. Results and Discussions

There are two types of S atoms in PEDOT:PSS (Fig. 1). The one appearing at the energy below 2475 eV arises from PEDOT, and the other at higher energy is due to the S atoms of PSS. The CEY and PFY XANES spectra of the pristine PEDOT:PSS suggest the presence of PSS⁻ and PSSH. The difference in the XANES spectra between H_2SO_4 -treated PEDOT:PSS and pristine PEDOT:PSS suggest some SO_4^{2-} anions enter PEDOT:PSS and become the counter anions of PEDOT:PSS during the H_2SO_4 treatment. In addition, the H_2SO_4 treatment may not further oxidize PEDOT. The XANES of PEDOT:PSS sequentially treated with H_2SO_4 and NaOH indicate that ion exchange between the NaOH solution and PEDOT:PSS may occur only in the surface and not in bulk. The NaOH treatment dedope the protonic acid doping of PEDOT:PSS.

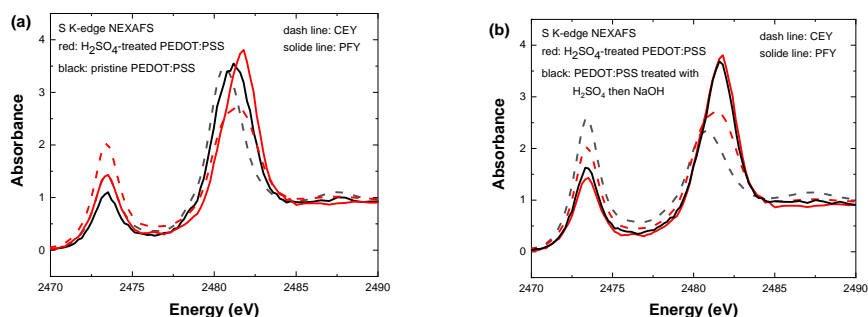


Fig. 1 NEXAFS spectra of psritine PEDOT:PSS, H_2SO_4 -treated PEDOT:PSS and PEDOT:PSS sequentially treated with H_2SO_4 and NaOH.

4. References

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2. Z. Fan, P. Li, D. Du, and J. Ouyang, *Advanced Energy Materials* (2017), 7, 1602116.