Gradient composition distribution in poly(2,6-dimethylphenylene oxide)/ polystyrene blend nanorods

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Supplementary Information

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Determination of PPO content in PPO/PS blends by FTIR. To obtain a calibration for FTIR data of PPO/PS blends, PPO and PS powder blends with PPO content of 8.7%, 15.7%, 30.0%, 40.2%, 49.4%, 59.9%, and 69.5% respectively were each mixed with potassium bromide (KBr) powder in the agate mortar and pressed into a transparent disk for FTIR measurement. The PPO and PS are dispersed uniformly within KBr matrix. Each FTIR spectrum was collected at 2 cm\(^{-1}\) resolution with 128 scans. We are interested in the bands at 990 and 880 cm\(^{-1}\) (Figure S1) because the peak at 959 cm\(^{-1}\) is caused by the in-plane CH wagging of PPO\(^1\) and the peak at 906 cm\(^{-1}\) is the characteristic of out-of-plane vibration of benzene ring of PS\(^2\).
Fig. S1  (A) Infrared spectra of PPO/PS blends with known PPO content of: (a) 8.7%; (b) 15.7%; (c) 30.0%; (d) 40.2%; (e) 49.4%; (f) 59.9%; and (g) 69.5%.

According to Beer’s law, the intensities of absorption bands are linearly proportional to the concentration of each component in a homogeneous mixture. Thus, the intensity ratio of peak at 959 cm$^{-1}$ (PPO) to peak at 906 cm$^{-1}$ (PS) is related to the concentration (mass) ratio because of the identical path length of source beam in the same mixed disk samples. Therefore, the intensity ratio of 959 to 906 cm$^{-1}$ band and the PPO content in PPO/PS blend films can be written by

$$\frac{A_{PPO}}{A_{PS}} = \frac{a_{PPO}b_{PPO}c_{PPO}}{a_{PS}b_{PS}c_{PS}} = \frac{a_{PPO}}{a_{PS}}, \quad m_{PPO} = k \frac{m_{PPO}}{m_{PS}}$$

(1)

$$C_{PPO} = \frac{m_{PPO}}{m_{PPO} + m_{PS}} = \frac{A_{PPO}}{A_{PPO} + kA_{PS}}$$

(2)
where $A_{PPO}$ and $A_{PS}$ are the intensity (band area) of PPO at 959 cm$^{-1}$ and PS at 906 cm$^{-1}$ (Looks for the highest intensity in the wavenumber range and for the minima left and right from this maximum. The baseline in this region is then defined by the local minima to obtain the band area under the FTIR curve.), $m_{PPO}$ and $m_{PS}$ are the mass of PPO and PS in the blends, $k$ is the ratio of absorptive coefficients of $a_{PPO}/a_{PS}$, $C_{PPO}$ is the content of PPO components in the PPO/PS blends.

Fig. S2  Calibration curve of the ratio of the absorbances of peak at 959 cm$^{-1}$ to peak at 906 cm$^{-1}$ in PPO/PS blends.

On the basis of various known compositions of the PPO/PS blends, the calibration curve can be obtained by the specified frequency at 959 and 906 cm$^{-1}$. The calibration curves of PPO/PS blends in Figure S2 which was fitted using linear regression, yields the $k$ value of 3.69±0.07.
Therefore, using the absorbance measurements of 959 and 906 cm\(^{-1}\) in the FTIR spectra, the following relationship is obtained to calculate the absolute PPO content in PPO/PS blend nanorods/film

\[
C_{\text{PPO}} = \frac{A_{959}}{A_{959} + 3.69A_{906}}
\]

(3)

\[
C_{\text{PS}} = 100\% - C_{\text{PPO}}
\]

(4)

where \(C_{\text{PPO}}\) and \(C_{\text{PS}}\) represent the content of PPO and PS in the PPO/PS blends, \(A_{959}\) and \(A_{906}\) are the respective band area for peaks at 959 and 906 cm\(^{-1}\), 3.69 is the ratio of absorptive coefficients of the peak at 959 cm\(^{-1}\) to the peak at 906 cm\(^{-1}\).

References
