Supplementary Information

Innovative enhancement on gas barrier property of biodegradable poly(butylene succinate) nanocomposite films by introducing confined crystals

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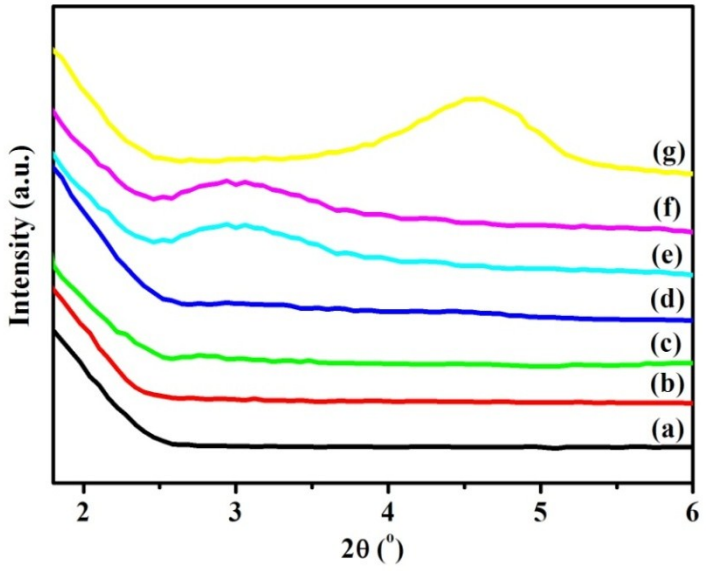

Fig. S1 1D-WAXD curves of (a) neat PBS, (g) neat clay, PBS nanocomposites with clay contents of (b) 0.67 vol. %, (c) 3.4 vol. %, (d) 6.9 vol. %, (e) 14 vol. %, and (f) 31 vol. %.

The WAXD patterns at small diffraction angles are used to evaluate the exfoliation level of clays within PBS, which was carried out at the beamline BC16B of Shanghai Synchrotron Radiation Facility (SSRF, Shanghai, China) with an X-ray detector (Model Mar165). The wavelength of the X-ray is 0.1542 nm. Linear 1D-WAXD profiles were obtained from circularly integrated intensities of the 2D-WAXD patterns. The characteristic diffraction peak of clay (001) plane of neat clays in Figure S1 is observed at $2\theta = 4.65°$, corresponding to a layer-to-layer distance of 1.85 nm. But, in the nanocomposites, it shifts to much lower $2\theta = 2.8^{o}$, corresponding to a layer-to-layer distance of 2.24 nm, especially in the nanocomposites containing clay loading of 0.67 vol. % where the peak of clays is not detected. Combination of WAXD and TEM results suggests that clays are well intercalated or exfoliated individual platelets, and uniformly dispersed in the PBS matrix. Meanwhile, when the content of clay is achieved to 14 vol% and 31 vol%, the peak of clay shifts to higher values of $2\theta = 3.2^{o}$ corresponding to a layer-to-layer distance of 1.96 nm, indicating the poorer exfoliation or dispersion.

Table S1 T_{m1}, T_{m2} and X_c of PBS/clay nanocomposites obtained from DSC melting curves.

Sample	T_{m1} (°C)	T_{m2} (°C)	X_c (%)
Neat PBS	102.2	112.3	47.6
0.67 vol. % clay/PBS nanocomposite	102.9	112.3	47.5
3.4 vol. % clay/PBS nanocomposite	102.3	112.3	45.6
6.9 vol. % clay/PBS nanocomposite	100.7	111.9	41.1
14 vol. % clay/PBS nanocomposite	-----	111.8	37.8
31 vol. % clay/PBS nanocomposite	-----	112.2	31.2

We have calculated the degree of crystallinity of PBAT according to DSC:

$$X_c = \frac{\Delta H_{m1} + \Delta H_{m2} - \Delta H_{cc}}{(1-w)\Delta H_0}$$

where ΔH_0 is the enthalpy of pure PBS crystal (200 J/g). [1] ΔH_{m1} and ΔH_{m2} are the melting enthalpy of imperfect crystal and perfect crystal of PBS respectively. ΔH_{cc} is the re-crystallization enthalpy of PBS. w is the weight content of clays. The result is exhibited in Table S1. Through the results of crystallinity acquired from DSC, we found that the variation tendency with clay content between DSC and 1D-WAXD is very similar. The slight difference is that the crystallinity calculated from DSC is bigger than by 1D-WAXD in every contents of clay.

Notes and references

1. Miyata, T.; Masuko, T. *Polymer,* **1998,** *39*, 1399-1404.