Supplemental Information

Poly(butylene 2,5-furan dicarboxylate), a biobased alternative to PBT: synthesis, physical properties and crystal structure

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Table S1. Bond lengths (Å) in PBF structure as shown in Fig. 8.

C2-O1	1.425	C1-C2	1.534
C3-O1	1.359	C1-C10	1.518
C3-O2	1.230	C4-C5	1.350
C4-O3	1.359	C5-C6	1.417
		C3-C4	1.495

Table S2. Comparison between cell parameters of PBF and α- and β-PBT.

	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
α-PBT	4.83	5.94	11.59	99.7	115.2	110.8
β-PBT	4.95	5.67	12.95	101.7	121.8	99.9
PBF	4.78	6.03	12.31	110.1	121.1	100.6

Table S3. Young's modulus, elongation to break and stress at break for PBF sample 6 differing in crystallinity.

Sample No.	Melting enthalpy contribution to initial crystallinity, J/g	Crystallinity, % from X-ray	Young's Modulus (MPa)	Elongation at break, %	Stress at break (MPa)
6-1*	6.3	8.1	959±58	1055±56	31.8±2.9
6-2	9.2	24.9	1054±60	445±32	27.5±0.4
6-3	39.5	37.7	1091±45	284±93	35.5±1.9
6-4	47.2	44.0	1112±53	7.4±2	43.2±8.5
PBT	48.0		950±70	272±71	37.6±2.5

[a] The true stress at break calculated after correction for the cross-sectional area.

*Different thermal processing on sample 6 , the details were described in experimental section.

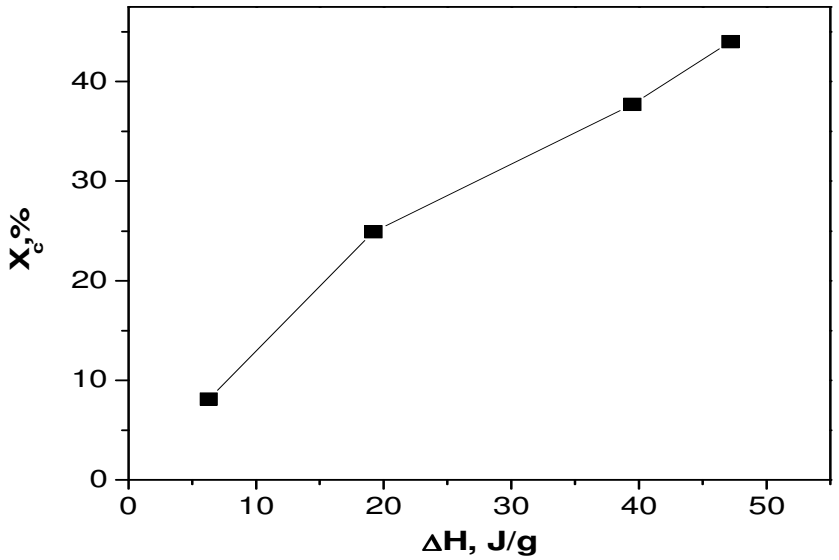

Figure S1a Relationship of %-crystallinity, determined by X-ray diffraction, and DSC determined values of enthalpy difference (ΔH = difference between the melting enthalpy and the cold crystallization enthalpy) for PBF sample 6 annealed under different conditions.

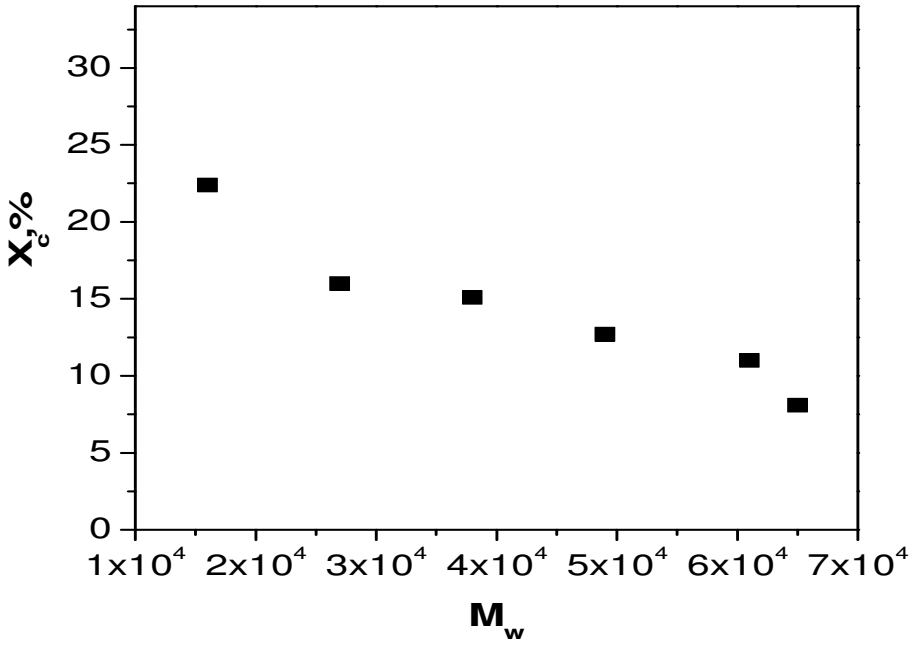

Figure S1b. Percent crystallinity of PBF sample bars for tensile testing as a function of molecular weight. Values of χ_c were determined from experimental ΔH values. That is, the plot shown in Figure S1a was used to correlate experimental ΔH and χ_c.

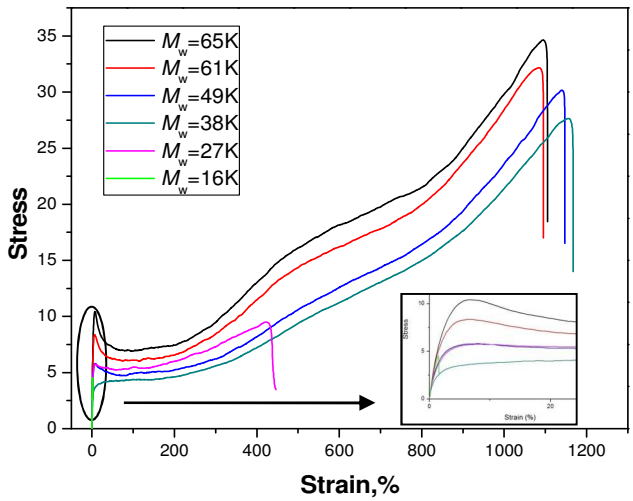

Figure S2. Stress-strain curves for the series of PBF Samples 1-6 with different M_w.

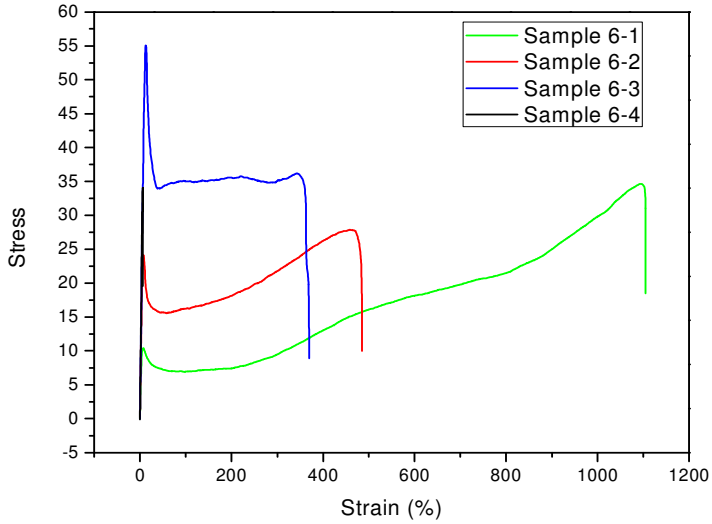

Figure S3. Stress-strain curves for the series of PBF Sample 6 with different crystallinity.