Electronic Supplementary Material (ESI) for Polymer Chemistry.

Electronic Supplementary Information (ESI)

Synthesis, Structure and Properties of Copolymers of Syndiotactic Polypropylene with 1-Hexene and 1-Octene.

Miriam Scoti,* Rocco Di Girolamo, Fabio De Stefano, Angelo Giordano, Anna Malafronte, Giovanni Talarico, Roberta Cipullo, Claudio De Rosa*

Dipartimento di Scienze Chimiche, Università di Napoli Federico II, Complesso Monte S.Angelo, Via Cintia, I-80126 Napoli, Italy.

Experimental

X-ray diffraction patterns have been obtained with Ni-filtered Cu Kα radiation with an automatic Philips diffractometer. The degrees of crystallinity (x_c) were determined from the powder diffraction profiles of the as-synthesized and compression molded films by the ratio between the crystalline diffraction area (A_c) and the area of the whole diffraction profiles (A_t), $x_c = (A_c/A_t)\times100$. The area of the crystalline diffraction A_c was evaluated by subtracting the area of the amorphous halo from the area of the whole diffraction profiles A_t. The diffraction profiles of the amorphous phase were obtained from the X-ray diffraction profiles of the amorphous samples obtained by compression molding of samples with comonomer concentration higher than 5-6 mol%. In fact, these samples do not crystallize by cooling the melt to room temperature and amorphous films are obtained by compression molding. The amorphous samples then slowly crystallize by aging at room temperature.

Compression-molded samples have been prepared by melting as-prepared samples under a press at low pressure and slow cooling to room temperature (about 10 °C/min). Samples with comonomer concentrations lower than 5-6 mol% crystallize upon cooling from the melt, whereas samples with higher hexene or octene concentrations are amorphous soon after the cooling but

they crystallize if they are kept at room temperature for an aging time that depends on the comonomer concentration. Therefore, the compression-molded films were kept at room temperature for different aging times to complete the crystallization.

Mechanical tests have been performed at room temperature on compression-molded films with a miniature mechanical tester apparatus (Minimat, by Rheometrics Scientific) following the standard test method for tensile properties of thin plastic sheeting ASTM D882-83. Rectangular specimens 3 mm long, 2 mm wide and 0.3 mm thick have been stretched up to the break or up to a given deformation $\varepsilon = [(L_f - L_0)/L_0] \times 100$, where L_0 and L_f are the initial and final lengths of the specimen, respectively. Two benchmarks have been placed on the test specimens and used to measure elongation.

Values of tension set and elastic recovery have been measured after breaking. Ten minutes after breaking, the two pieces of the sample have been fit carefully together so that they are in contact over the full area of the break and the final total length L_r of the specimen has been obtained by measuring the distance between the two benchmarks. The tension set after breaking has been calculated as $t_b = [(L_r - L_0)/L_0]\times100$, whereas the elastic recovery has been calculated as $r_b = [(L_f - L_r)/L_r]\times100$ and the percentage of the total strain ($L_f - L_0$) that is recovered after breaking is calculated as $R_b = 100\times(L_f - L_r)/(L_f - L_0) = 100\times(\varepsilon_b - t_b)/\varepsilon_b$.

In the mechanical tests, the ratio between the drawing rate and the initial length was fixed equal to 0.1 mm/(mm×min) for the measurement of Young's modulus and 10 mm/(mm×min) for the measurement of stress−strain curves and the determination of the other mechanical properties (stress and strain at break and tension set). The reported values of the mechanical parameters are averaged over at least five-eight independent experiments. The values of the mechanical parameters are reported in Table S1 for four selected samples. The values of Young's modulus, stress at yield and deformation at break of all samples are reported in Figure S1 as a function of the comonomer concentration.

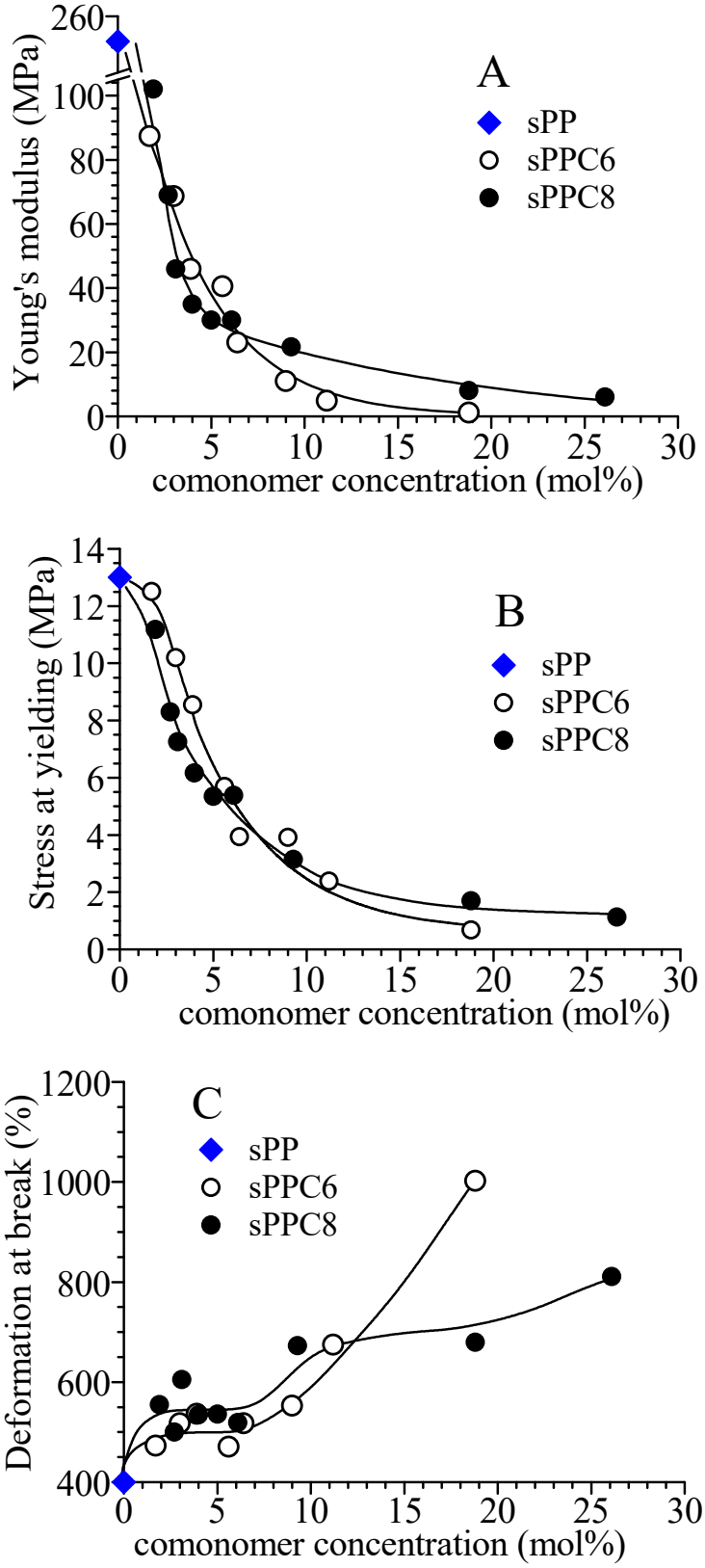

Figure S1. Values of Young's modulus (A), stress at yield (B) and deformation at break (C) of compression-molded films of sPP homopolymer (◆) and sPPC6 (○) and sPPC8 (●) copolymers as a function the comonomer concentration.

Table S1. Young Modulus (E), Strain (ε_y) and Stress (σ_y) at Yield, Strain (ε_b) and Stress (σ_b) at Break, Tension Set at Break (t_b), Percentage of the Strain that is Recovered after Breaking (R_b) and Crystallinity (x_c) of Compression-Molded Films of the four Selected Samples of sPPC6 and sPPC8 Copolymers of Figure 13.

Samples	Comonomer	Hexene or 1-octene (mol%)	*E* (MPa)	ε_y (%)	σ_y (MPa)	ε_b (%)	σ_b (MPa)	t_b (%)	R_b (%)	x_c (%)
sPPC6-3	1-Hexene	3.9	46±4	44 ±3	8.6±0.7	543±32	24±1	47±17	91	36
sPPC6-8	1-Hexene	18.8	1.2±0.1	60±10	0.7±0.1	1003±27	6±1	0	100	15
sPPC8-4	1-Octene	4.0	35±5	32±6	6.2±0.4	535±38	25±2	29±10	95	26
sPPC8-7	1-Octene	9.3	22±1	55±4	3.3±0.2	673±58	7.9±0.8	18±5	97	18