polymers

MDPI

Predicted studies of branched and cross-linked polyurethanes based on polyhydroxybutyrate with polycaprolactone triol in soft segments

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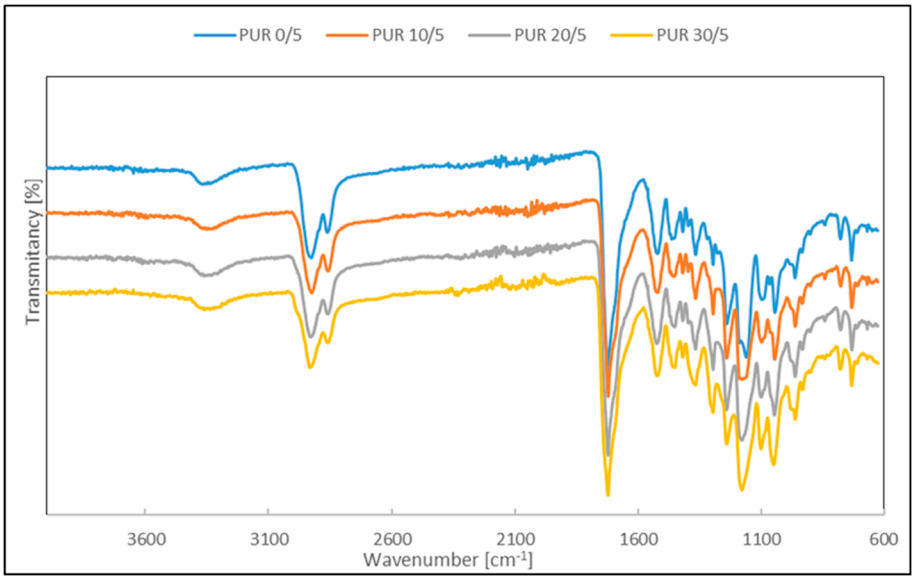

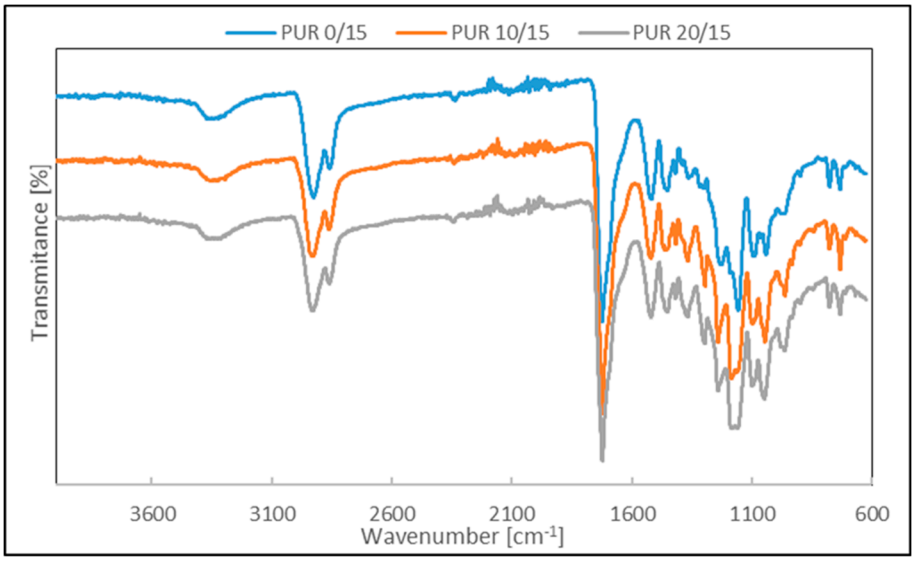

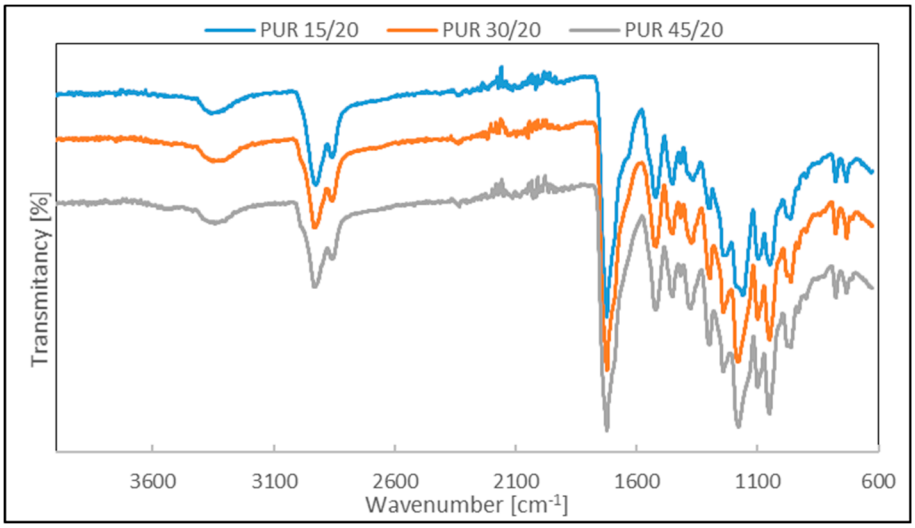

Figure S1. ATR-FTIR spectra of PURs

Table S1. ATR-FTIR bands of polyurethanes in the range of 4000 cm^{-1} to 1200 cm^{-1}.

Sample	–N-H stretching vibration [cm^{-1}]	–C=O stretching vibration [cm^{-1}]	N–H bending vibr. and C–N stretching vibr. (amide II band) [cm^{-1}]	C–N stretching vibr. (amide III band) [cm^{-1}]
PUR 0/5	3366.9	1721.7	1520.8	1238.7
PUR 10/5	3351.4	1720.7	1518.6	1239.2
PUR 20/5	3363.0	1720.9	1522.1	1239.5
PUR 30/5	3360.6	1721.2	1521.8	1239.3
PUR 0/15	3359.2	1723.7	1520.7	1227.9 (overlept)
PUR 10/15	3354.3	1721.5	1519.8	1240.9
PUR 20/15	3360.4	1722.8	1520.0	1241.0
PUR 15/20	3359.7	1720.4	1520.3	1239.6
PUR 30/20	3316.3	1721.6	1519.2	1241.4
PUR 45/20	3342.6	1722.4	1519.0	1242.5

Table S2. ATR-FTIR bands of polyurethanes in the range of 1300 cm^{-1} to 1000 cm^{-1}.

Sample	Multiplet band of C–O bonds in soft segments [cm^{-1}]			
PUR 0/5	1238.7	1158.5 (+ small 1185,0)	1095.8	1043.4 (+ small 1063.50)
PUR 10/5	1239.2	1176.2	1096.8	1044.3 (+ small 1058.7)
PUR 20/5	1239.5	1177.7	1099.3	1045.3
PUR 30/5	1239.3	1177.3	1099.8	1048.0
PUR 0/15	1227.3	1156.9 (+ small 1184.6)	1088.5	1041.3 (+ small 1060.7)
PUR 10/15	1240.9	1187.0 (+ small 1161.4)	1097.5	1045.9 (+ small 1056.3)
PUR 20/15	1241.0	1181.6 (+ small 1157.1)	1098.1	1048.0
PUR 15/20	1239.6	1161.0 (+ small 1196.0)	1097.8	1048.6
PUR 30/20	1241.4	1179.3	1099.0	1050.0
PUR 45/20	1242.5	1177.9	1099.4	1050.9

Table S3. Degradation temperature (T_{degr}) at three stages of degradation from DTG curves

Sample	T_{degr1} [°C]	T_{degr2} [°C]	T_{degr3} [°C]
PUR 0/5	-	356.2	-
PUR 10/5	256.8	339.6	430.9
PUR 20/5	258.1	337.0	429.2
PUR 30/5	255.5	325.6	429.0
PUR 0/15	-	361.8	-
PUR 10/15	260.0	350.8	422.2
PUR 20/15	260.0	350.8	433.4
PUR 15/20	247.0	339.5	429.4
PUR 30/20	257.8	335.2	429.2
PUR 45/20	260.0	333.9	429.0

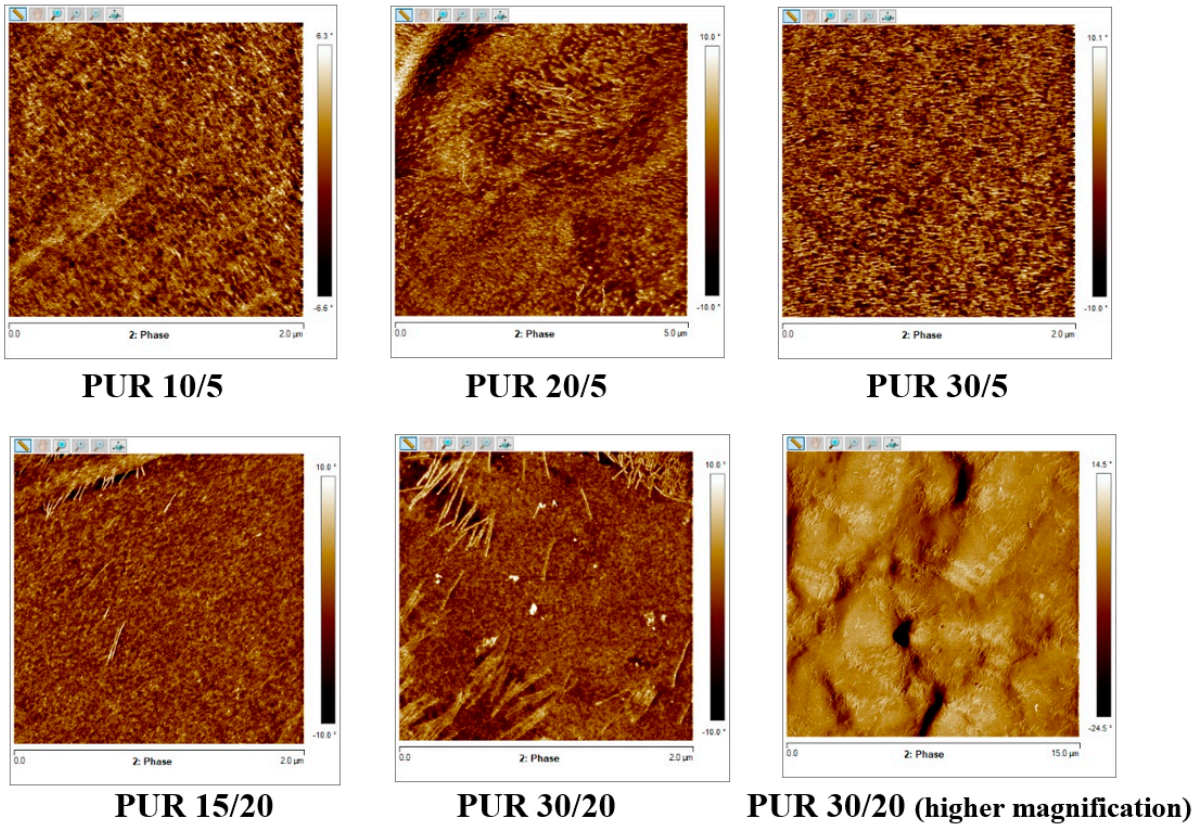

Figure S2. AFM cross-section images of PURs

Table S4. Root mean square roughness (Rq) and average roughness (Ra) of AFM and contact angle of PURs

Sample	Contact angle [°]			Root mean square roughness (R_q) [nm]	Average roughness (R_a) [nm]
	0 min	1 min	3 min		
PUR 0/5	84.5±0.9	79.9±1.5	75.5±0.8	85	67
PUR 10/5	78.2±6.3	72.4±7.3	67.5±3.0	28	19
PUR 20/5	78.2±4.1	70.5±3.8	67.9±0.2	20	16
PUR 30/5	80.9±1.6	69.1±2.1	65.7±2.6	14	11
PUR 0/15	89.1±3.3	83.1±3.3	79.1±3.6	10	8
PUR 10/15	84.5±0.9	76.5±3.0	72.5±3.0	16	7
PUR 20/15	89.8±1.8	82.8±2.6	77.8±2.5	20	17
PUR 15/20	79.9±2.0	71.1±2.3	65.3±3.1	21	16
PUR 30/20	78.6±1.6	71.1±2.3	65.3±3.1	20	14
PUR 45/20	78.6±2.5	71.4±4.6	67.3±4.9	18	14

Table S5. Hardness of the obtained polyurethanes

Sample	**Hardness [°Shore A] ± SD**
PUR 0/5	91.7 ± 1.3
PUR 10/5	89.5 ± 0.1
PUR 20/5	90.4 ± 1.0
PUR 30/5	89.5 ± 2.6
PUR 0/15	93.7 ± 0.7
PUR 10/15	92.4 ± 1.0
PUR 20/15	90.4 ± 5.8
PUR 15/20	94.1 ± 3.0
PUR 30/20	93.3 ± 1.8
PUR 45/20	93.4 ± 0.6