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Nanoscale Advances

COMMUNICATION - ESI

Electronic Supplementary Information (ESI)

PU Nanocomposites from Bifunctional Nanoparticles: Impact of Liquid Interphase on Mechanical Properties

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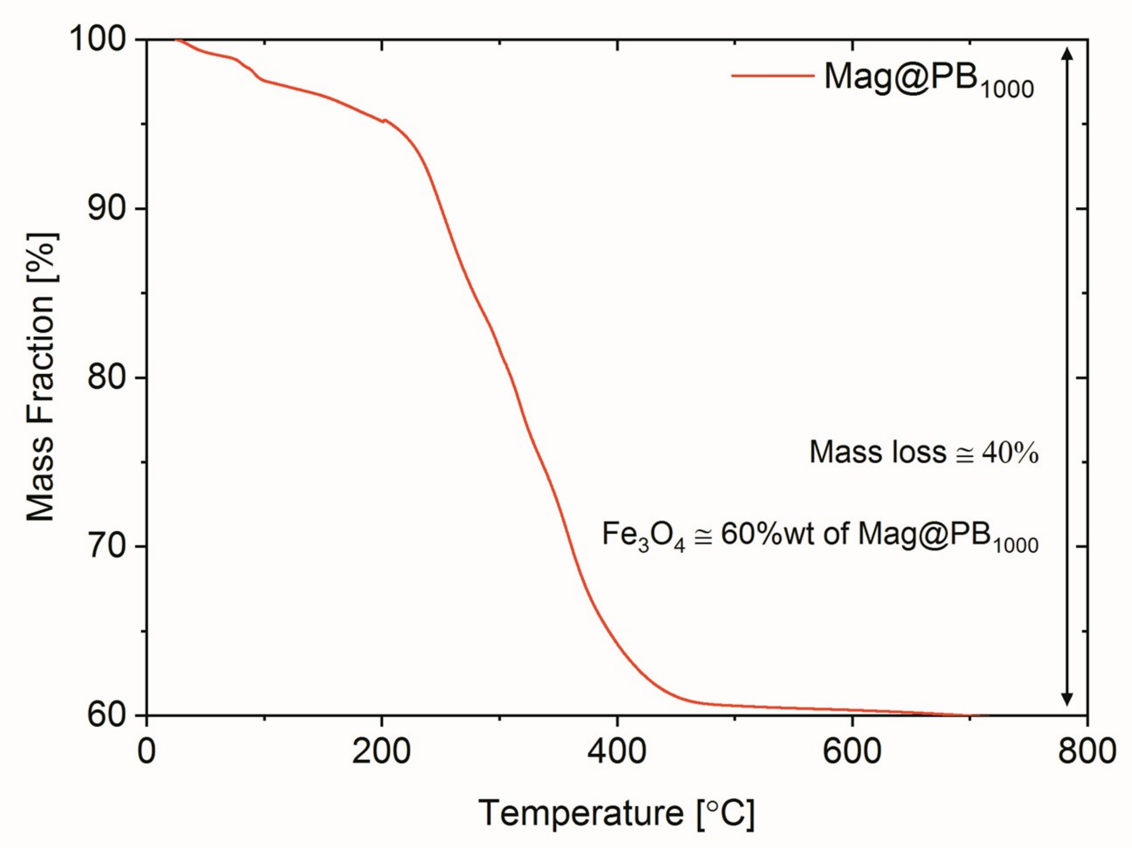

Fig. S1 Thermogravimetric analysis of the hybrid nanoparticle Mag@PB_{1000}. Analysis performed at heating rate of 10 °C min^{-1} and under N_2 atmosphere.

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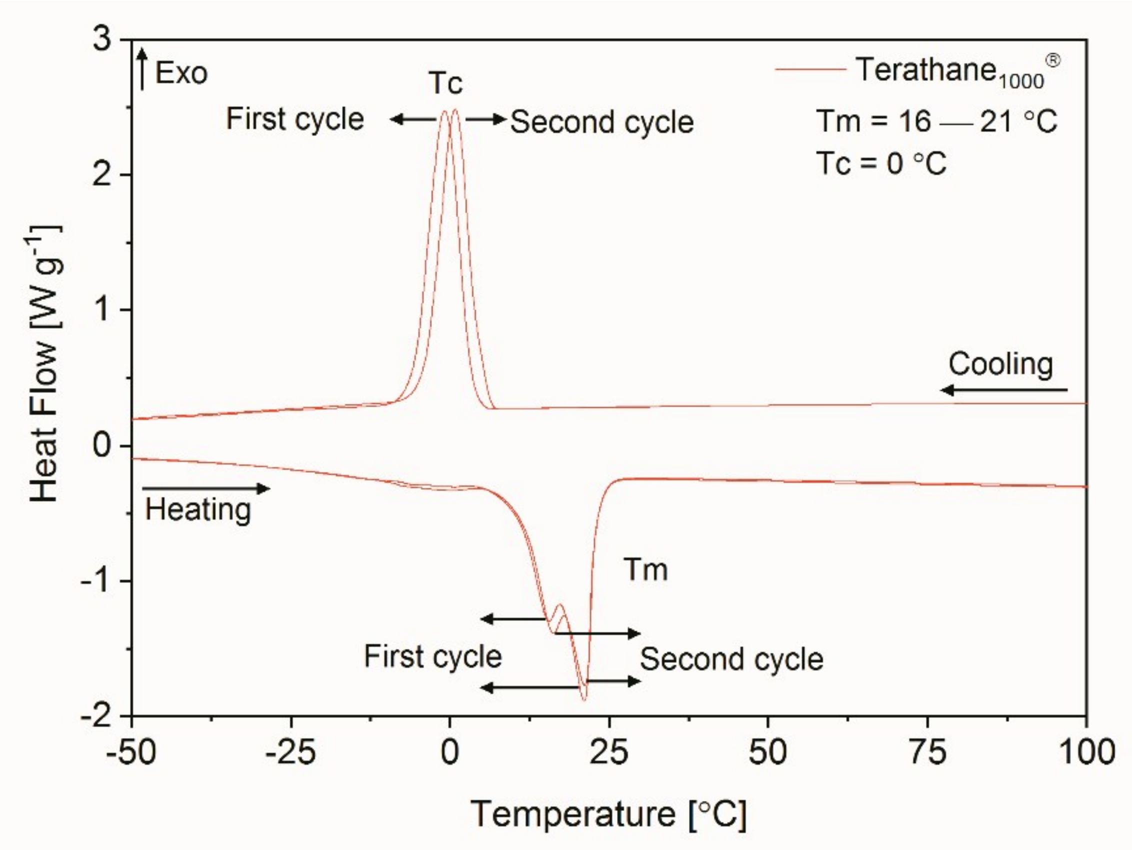

Fig. S2 Differential scanning calorimetry heat flow curve of commercial $Terathane_{1000}$®. Analysis performed at heating rate of 10 °C min^{-1} and N_2 atmosphere.

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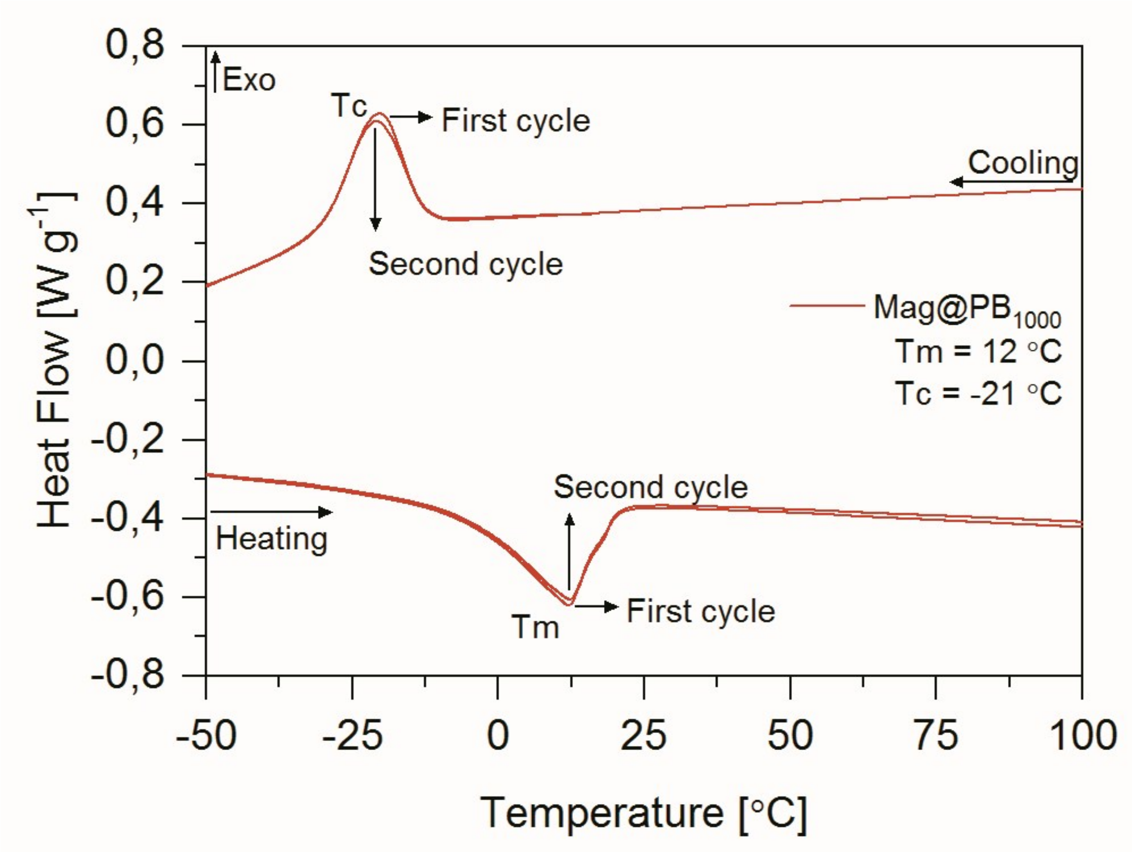

Fig. S3 Differential scanning calorimetry heat flow curve of Mag@PB_{1000} nanoparticles. Analysis performed at heating rate of 20 °C min^{-1} and N_2 atmosphere.

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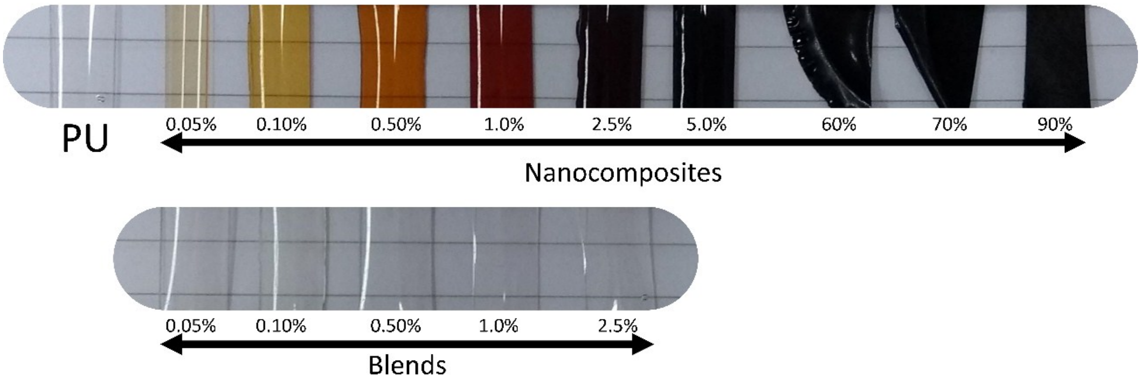

Fig. S4 Nanocomposites and non-filled formulations samples. The addition of nanoparticles changed the material's color and texture, that shifts from translucid and glossy to opaque and matte with very high nanoparticle loadings.

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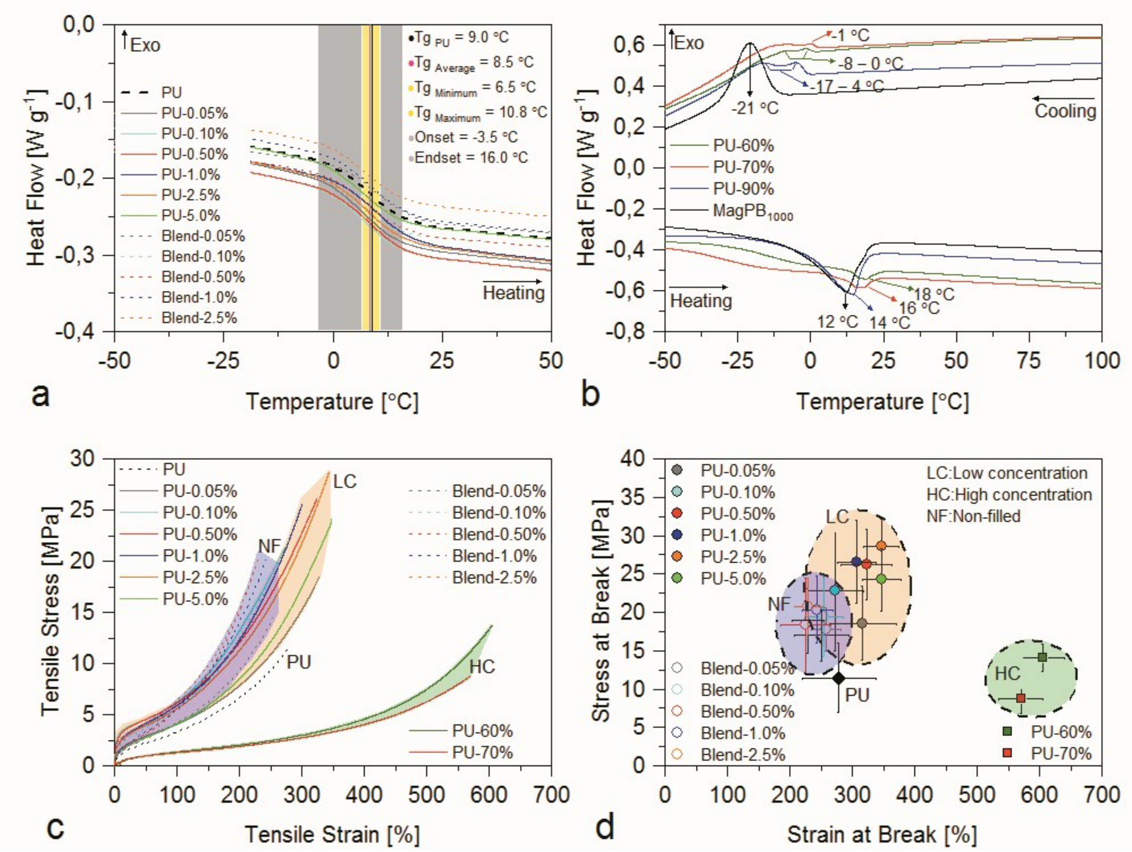

Fig. S5 Differential scanning calorimetry analysi s of (a) low concentration nanocomposites and non-filled compositions (analysis performed at heating rate of 10 °C min^{-1} and N_2 atmosphere) and (b) highly concentrated compositions and Mag@PB$_{1000}$ nanoparticles (analysis performed at heating rate of 20 °C min^{-1} and N_2 atmosphere); (c) Tensile stress-strain curves and (d) break points of Mag@PB$_{1000}$/PU nanocomposites and non-filled compositions (the highlighted regions represent the samples groups: non-filled compositions, low concentration nanocomposites and highly concentrated nanocomposites).

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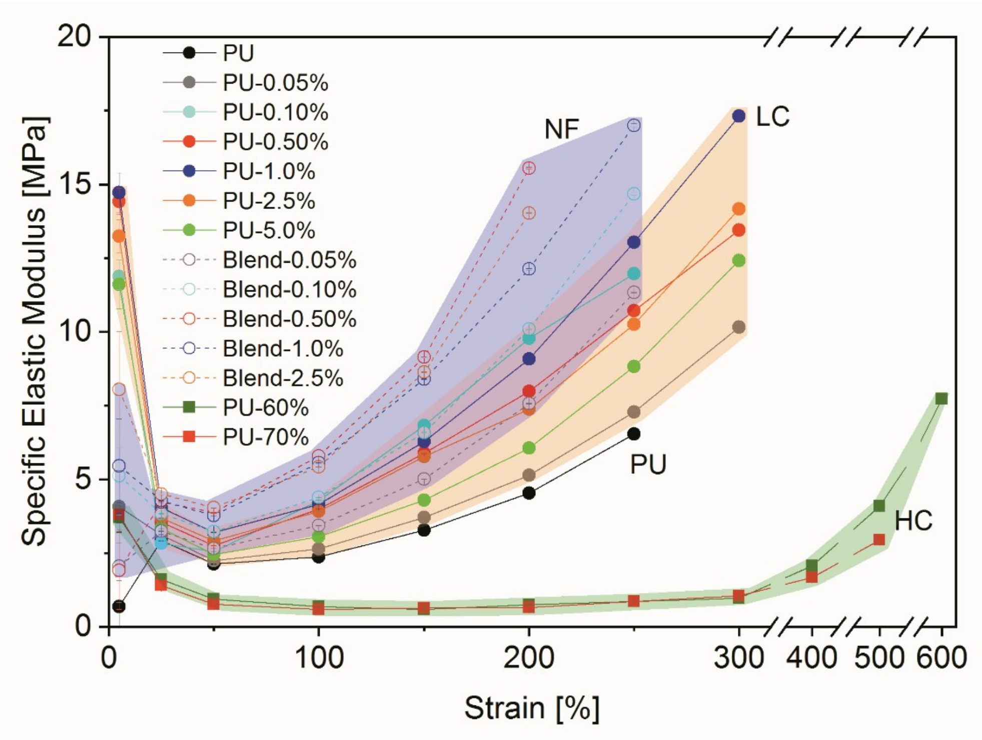

Fig. S6 Higher-strain modulus at different points of strain, calculated from the stress-strain curve for all formulations. The highlighted regions represent the samples groups: non-filled compositions, low concentration nanocomposites and highly concentrated nanocomposites.

Observation on calculation method of elastic and higher-strain moduli:

The elastic modulus calculation was performed in accordance with the EN10002 and ASTM E8 standards using the BlueHill3 software. The automatic calculation determines the material's elastic modulus using a standard linear regression technique, with an offset of 0.2%.

The higher-strain moduli were calculated from the slope of a fitting curve of the stress-strain curves at each strain value of interest. The limit points for the fitting curves were ± 1% strain for modulus at 5% strain and ± 10% strain for moduli at strain values above and including 25% strain.

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Table S1 Composition of the all formulations in percentage in weight.

NCs Formulations	Blends Formulations	Mag@PB_{1000} in Composite [wt%]	60%wt of NP Fe_3O_4 in Composite [%wt]	40%wt of NP PB_{1000} in Composite and in Blend [%wt]
PU-0.05%	Blend-0.05%	0.05	0.03	0.02
PU-0.10%	Blend-0.10%	0.10	0.06	0.04
PU-0.50%	Blend-0.50%	0.50	0.30	0.20
PU-1.0%	Blend-1.0%	1.0	0.60	0.40
PU-2.5%	Blend-2.5%	2.5	1.5	1.00
PU-5.0%	---	5.0	3.0	2.0
PU-60%	---	60	36	24
PU-70%	---	70	42	28
PU-90%	---	90	54	36

Table S2. Glass transition values of the nanocomposites and non-filled compositions.

Formulations	Tg [°C]
Polyurethane Reference Formulation	
PU	8.9
Low Concentration Nanocomposite Formulations	
PU-0.05%	7.8
PU-0.10%	5.7
PU-0.50%	8.7
PU-1.00%	10.7
PU-2.50%	7.4
PU-5.00%	7.3
Blend Formulations	
Blend-0.05%	11.2
Blend-0.10%	6.6
Blend-0.50%	8.5
Blend-1.0%	8.5
Blend-2.5%	7.8

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