

Supplementary Data

Optimising Crystallisation during Rapid Prototyping of Fe₃O₄-PA6 Polymer Nanocomposite Component

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Section S1:

Table S1. Calculation of glass transition temperature, melting temperature, and degree of crystallinity from DSC plot for EtMgBr variation samples.

EtMgBr Variation	Glass Transition Temperature (°C)	Crystallizing Temperature (°C)	Melt Peak Temperature (°C)	Enthalpy (J/g)	Degree of Crystallinity (%)
10%	57 ± 2	201 ± 2.5	216 ± 3	58 ± 1.5	30 ± 1.5
30%	56 ± 3	197 ± 4.5	215 ± 1	65 ± 2	34 ± 2
50%	56 ± 3	190 ± 5	213 ± 1.5	91 ± 1.5	48 ± 1.5
70%	55 ± 2.5	174 ± 8	215 ± 1	87 ± 2.5	45 ± 2.5
100%	52 ± 1	172 ± 10	212 ± 4	79 ± 3	41 ± 3

Table S2. Calculation of glass transition temperature, melting temperature, and degree of crystallinity from DSC plot for NACL variation samples.

NACL Variations	Glass Transition Temperature (°C)	Crystallizing Temperature (°C)	Melt Peak Temperature (°C)	Enthalpy (J/g)	Degree of Crystallinity (%)
10%	53 ± 1	180 ± 4	217 ± 2	75 ± 8	39 ± 8
30%	54 ± 2	175 ± 0.5	216 ± 1	92 ± 1.5	48 ± 1.5
50%	52 ± 1.5	173 ± 6	215 ± 1	91 ± 4	48 ± 4
70%	53 ± 1.5	186 ± 1.5	214 ± 0.5	78 ± 2	41 ± 2
100%	53 ± 1	181 ± 8	212 ± 0.5	73 ± 1	31 ± 1

Table S3. Calculation of glass transition temperature, melting temperature, and degree of crystallinity from DSC plot for samples with variation of both the catalyst (EtMgBr) and activator (NACL).

EtMgBr & NACL Variations	Glass Transition Temperature (°C)	Crystallising Temperature (°C)	Melt Peak Temperature (°C)	Enthalpy (J/g)	Degree of Crystallinity (%)
10%	53 ± 1	109 ± 9	172 ± 12	38 ± 9	20 ± 9
30%	51 ± 1.5	182 ± 4	211 ± 2	65 ± 5	34 ± 5
50%	52 ± 2	172 ± 8	214 ± 2.5	91 ± 1.5	48 ± 1.5
70%	54 ± 2	167 ± 4.5	208 ± 2.5	81 ± 1.5	42 ± 1.5
100%	54 ± 3	171 ± 11	206 ± 3	64 ± 3.5	34 ± 3.5

Section S2:

The sample with 10% EtMgBr having very high content of unreacted monomer was dissolved in boiling water for a short duration and then the collected samples were run on DSC. The results of the first and the second sample run is as shown in the Figure S1 below.

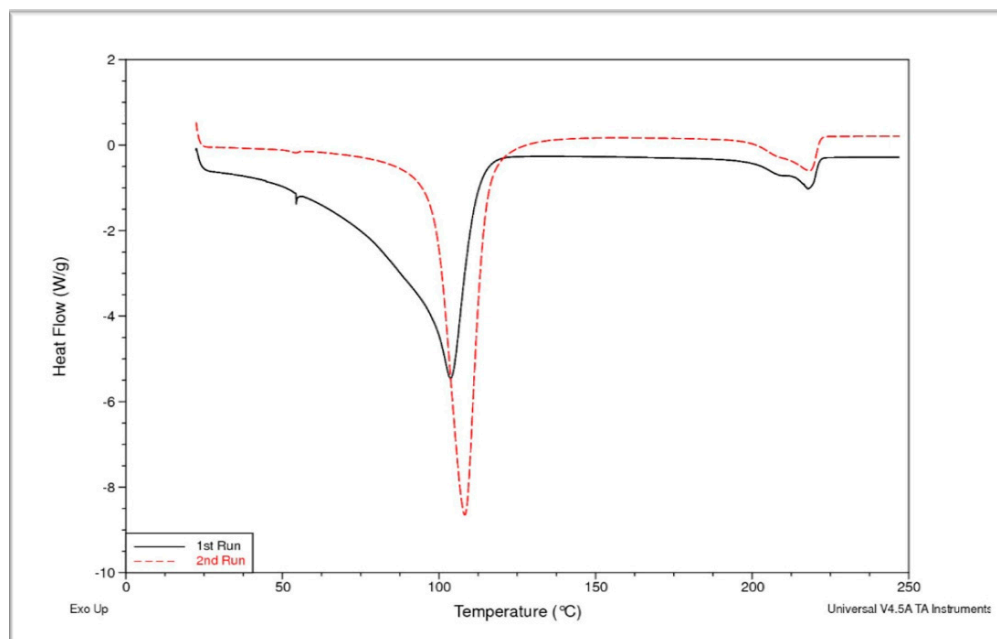


Figure S1. DSC plot for the initiator (EtMgBr) – 10% concentration - Boiled water sample (to remove unreacted monomer).

The discussion on the trend and captured multiple endothermic peaks in the DSC run are discussed in detail in the main text with comparison to the other DSC results.

Section S3:

Calculated crystallite sizes of all the variation samples –

The crystallite sizes are calculated utilising the FWHM from the XRD plot pertaining to the PA6 peaks. The following Scherrer formula (1) was used to calculate the crystallite sizes from FWHM of the most intense peaks. The Scherrer equation gives the relation between the peak width (B) and the crystallite size (L). It states that peak width is inversely proportional to crystallite size.

$$B(2\theta) = \frac{K\lambda}{L \cos \theta} \quad (1)$$

The crystallite sizes for all the sample variations are summarised here in following Table S4.

Table S4. Calculated crystallite sizes for all the samples prepared with variations of EtMgBr, NACL and EtMgBr+NACL concentration.

Sample	Peak Position (2 θ)	FWHM (@ 2 θ)	Crystallite Size (nm)
10% EtMgBr Conc.	23.58413	2.61943	3.24
30% EtMgBr Conc.	23.24327	2.83181	2.98
50% EtMgBr Conc.	23.33219	3.79462	2.23
70% EtMgBr Conc.	23.40629	3.17525	2.67
100% EtMgBr Conc.	23.40629	3.11595	2.72
10% NACL Conc.	23.49521	2.91618	2.91
30% NACL Conc.	23.40629	3.21587	2.64
50% NACL Conc.	23.33219	3.24035	2.62
70% NACL Conc.	23.40629	2.78499	3.04
100% NACL Conc.	23.33219	2.71504	3.12
10% EtMGBr-NACL Conc.	23.92499	2.96514	2.86
30% EtMGBr-NACL Conc.	23.67305	2.6002	3.26
50% EtMGBr-NACL Conc.	23.49521	2.73445	3.10
70% EtMGBr-NACL Conc.	23.49521	3.51723	2.41
100% EtMGBr-NACL Conc.	23.40629	3.05066	2.78

Section S4:**DSC analysis of Composite Dog-bone Part prepared by Rapid Prototyping setup**

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The DSC analysis done on the samples collected from the two marked regions of the dog-bone sample were analysed for their degree of crystallinity. The achieved data from the sample runs of the distinctive regions are included in Table S5.

Table S5. DSC result of the final polymer nanocomposite sample formed.

Region	T _m (°C)	Enthalpy (J/g)	Degree of Crystallinity (%)
1	216 ± 2	84.16 ± 3	44.29 ± 3
2	211 ± 4	76.31 ± 4	40.16 ± 5